

ON EXPLICIT L^2 -CONVERGENCE RATE ESTIMATE FOR PIECEWISE DETERMINISTIC MARKOV PROCESSES IN MCMC ALGORITHMS

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We establish L^2 -exponential convergence rate for three popular piecewise deterministic Markov processes for sampling: the randomized Hamiltonian Monte Carlo method, the zigzag process and the bouncy particle sampler. Our analysis is based on a variational framework for hypocoercivity, which combines a Poincaré-type inequality in time-augmented state space and a standard L^2 energy estimate. Our analysis provides explicit convergence rate estimates, which are more quantitative than existing results.

1. Introduction. Sampling approaches based on piecewise deterministic Markov processes (PDMPs) [16], which involve random jumps and deterministic trajectories in between, have recently attracted a lot of attention: several classes of Markov chain Monte Carlo (MCMC) algorithms have been developed based on PDMPs, including the randomized Hamiltonian Monte Carlo (RHMC) [12, 21], the zigzag process [7] and the bouncy particle sampler [14, 35]. Compared with MCMC algorithms based on diffusion, such as overdamped and underdamped Langevin Monte Carlo, the methods based on PDMPs do not need time discretization for the random part and the deterministic dynamics can either be explicitly integrated (for zigzag and bouncy particle) or be dealt with high order numerical integration (for RHMC), which make them promising to have better numerical performance [5, 6, 12, 13, 24, 38]. The zigzag and bouncy particle samplers are also suitable for the big data situation, as they can be unbiased even if a stochastic gradient is used [7, 14].

Typical PDMPs for sampling purpose introduce an auxiliary “velocity” variable $v \in \mathbb{R}^d$ that facilitates simulation, which is often chosen from a fixed distribution. For this paper, we will only consider the case that the velocity variable is drawn from the standard Gaussian distribution $d\kappa(v) = (2\pi)^{-\frac{d}{2}} e^{-\frac{|v|^2}{2}} dv$. In the PDMPs, the velocity variable is redrawn independently from the Gaussian distribution at a certain rate, and between two redraws the trajectory of state variable (x, v) consists of deterministic routes and random bounces so that the spatial variable x will explore the state space in all different directions with the help of v . The PDMPs are designed so that the x samples the desired target distribution.

We now present the general mathematical formulation of PDMPs. Let $f = f(t, x, v) : \mathbb{R}_+ \times \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ be the expectation of some observable function $f_0(x, v)$ at time t , and therefore satisfies the backward Kolmogorov equation

$$(1) \quad \partial_t f = \mathcal{L}f, \quad f(t = 0, x, v) = f_0(x, v),$$

where the infinitesimal generator \mathcal{L} associated with PDMPs is given by

$$(2) \quad \mathcal{L} = v \cdot \nabla_x - F_0(x) \cdot \nabla_v + \sum_{k=1}^K (v \cdot F_k(x))_+ (\mathcal{B}_k - \mathcal{I}) + \gamma(\Pi_v - \mathcal{I}).$$

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Here \mathcal{I} denotes the identity operator, and $(s)_+ := \max\{s, 0\}$. The vector fields $F_k : \mathbb{R}^d \rightarrow \mathbb{R}^d$, $k = 0, 1, \dots, K$ depend only on the position variable x (examples will be discussed below). The jump operators \mathcal{B}_k correspond to reflections of the velocity variable through the hyperplanes orthogonal to F_k , defined as

$$(3) \quad \mathcal{B}_k f(t, x, v) := f(t, x, v - 2(v \cdot n_k(x))n_k(x)),$$

where

$$(4) \quad n_k(x) = \begin{cases} F_k(x)/|F_k(x)| & \text{if } F_k(x) \neq 0, \\ 0 & \text{otherwise,} \end{cases}$$

and Π_v is the projection operator on Gaussian with respect to v variable

$$(5) \quad (\Pi_v f)(t, x) := \int_{\mathbb{R}^d} f(t, x, v) d\kappa(v).$$

In (2), $\gamma > 0$ is the refreshment rate of the velocity variable, whose choice will impact the convergence rate of the dynamics. Our analysis will provide optimal choices of γ .

Different PDMPs correspond to different choices of the vector fields F_k . While our framework can be generalized to various situations, for definiteness, we will only focus on the three most prominent examples:

- The randomized Hamiltonian Monte Carlo (RHMC) [12, 21] corresponds to the choice $K = 0$ and $F_0 = \nabla_x U$, where U is some potential function. The corresponding equation (1) can be seen as a particular linear Boltzmann equation [4] with the collision operator given by $\gamma(\Pi_v - \mathcal{I})$;
- The zigzag process (ZZ) [7] corresponds to $K = d$, $F_0 = 0$ and $F_k = \partial_{x_k} U e_k$ where $(e_k)_{k \in \{1, \dots, d\}}$ is the canonical basis of \mathbb{R}^d ;
- The bouncy particle sampler (BPS) corresponds to the choice $K = 1$, $F_0 = 0$ and $F_1 = \nabla_x U$. The BPS was first proposed in [35] and extended in [14].

All these PDMP processes above satisfy $\sum_{k=0}^K F_k = \nabla_x U$, and thus are designed so that they admit a unique stationary distribution [11, 12, 32] given by

$$(6) \quad d\rho_\infty(x, v) = d\mu_U(x) d\kappa(v),$$

where

$$d\mu_U(x) = \frac{1}{Z_U} e^{-U(x)} dx, \quad Z_U = \int_{\mathbb{R}^d} e^{-U(x)} dx.$$

Other PDMPs have been proposed for sampling purposes, including Hamiltonian BPS [39], the Coordinate Sampler [42], the Gibbs zigzag sampler [37], the Boomerang sampler [8], and more general bounces involving randomization [30, 39, 41]. While our framework can be generalized to these algorithms, we will not consider these variants in this work.

Our goal is to derive explicit decay rate estimates in L^2 for PDMPs, based on the variational framework developed in [2] and our previous work for the underdamped Langevin dynamics [15], the idea of which originates from the pioneering work [29]. More precisely, we will obtain explicit estimates for some $\nu > 0$ and a universal constant $C > 1$ independent of U , γ and d such that for $f = f(t, x, v)$ solving (2) and $\int f_0 d\rho_\infty = 0$, we have

$$(7) \quad \|f(t, \cdot, \cdot)\|_{L^2_{\rho_\infty}} \leq C e^{-\nu t} \|f_0\|_{L^2_{\rho_\infty}}.$$

Geometric convergence for ZZ has been established in [11] and for BPS in [17, 22, 32], however the expressions of the convergence rates are either implicit or complicated. The work [1] established explicit convergence rates for these processes, however only in terms of the

dimension d ; the comparison of their result with ours will be further elaborated below after we present our main results.

Other theoretical studies of the PDMPs include scaling limits and spectral analysis: The work [18] established the scaling limit of first coordinate for BPS, and [9] proved scaling limits of ZZ and BPS for several statistical observables. Spectral analysis of PDMP were considered in [10, 31] in one-dimension and [26] for the metastable regime.

More generally, convergence result of type (7) for hypocoercive equations was established in $H^1(\rho_\infty)$ in [33, 40] for a class of kinetic equations. Hypocoercivity estimate in terms of a modified L^2 space was developed in [19, 20, 27] and a series of works based on this framework [3, 25, 36].

Notation. Throughout the paper we assume I to be the time interval $(0, T)$, and we use $d\lambda(t) = \chi_{(0,T)}(t) dt$ to denote the Lebesgue measure on I . Define C_b^k to be the set of functions f such that they are k -times differentiable with bounded derivatives up to order k . We define the Sobolev space

$$H^1(\mu_U) := \{f : f(x) \in L^2(\mu_U) \text{ and } \partial_{x_k} f \in L^2(\mu_U), \forall k = 1, \dots, d\}.$$

We also define

$$L^2(\lambda \times \mu_U) := \left\{ f = f(t, x) : \int_{I \times \mathbb{R}^d} f^2 dt d\mu_U(x) < \infty \right\},$$

and its corresponding norm

$$\|f\|_{L^2(\lambda \times \mu_U)} := \left(\int_{I \times \mathbb{R}^d} f^2 dt d\mu_U(x) \right)^{\frac{1}{2}}.$$

The space $L^2(\lambda \times \rho_\infty)$ for functions on $I \times \mathbb{R}^d \times \mathbb{R}^d$ and its corresponding norm are defined similarly. We define the average of $f : I \times \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ over $\lambda \times \rho_\infty$ as

$$(f)_{\lambda \times \rho_\infty} := \frac{1}{T} \int_{I \times \mathbb{R}^{2d}} f(t, x, v) dt d\rho_\infty(x, v),$$

and for $g : I \times \mathbb{R}^d \rightarrow \mathbb{R}$ we define its average over $\lambda \times \mu_U$ as

$$(g)_{\lambda \times \mu_U} := \frac{1}{T} \int_{I \times \mathbb{R}^d} g(t, x) dt d\mu_U(x).$$

We use

$$\nabla_x^* F := -\nabla_x \cdot F + F \cdot \nabla_x U$$

to denote the $L^2(\mu_U)$ -adjoint operator of ∇_x . For time-augmented state space $I \times \mathbb{R}^d$ equipped with measure $\lambda \times \mu_U$, we use the convention $\partial_{x_0} := \partial_t$, the shorthand notation $\bar{\nabla} := (\partial_t, \nabla_x)^\top$, and the notation $\Delta_{t,x} := -\partial_{tt} + \nabla_x^* \nabla_x$ to denote the ‘‘Laplace’’ operator on $L^2(\lambda \times \mu_U)$.

1.1. *Assumptions and main results.* Below are three fundamental assumptions that $U(x)$ must satisfy in our framework. The convergence rates get better if we have stronger assumptions on U .

ASSUMPTION 1 (Poincaré inequality for μ_U). The measure $d\mu_U$ corresponding to $U(x)$ satisfies a Poincaré inequality with constant $m > 0$:

$$(8) \quad \int_{\mathbb{R}^d} \left(f - \int_{\mathbb{R}^d} f d\mu_U \right)^2 d\mu_U \leq \frac{1}{m} \int_{\mathbb{R}^d} |\nabla f|^2 d\mu_U \quad \forall f \in H^1(\mu_U).$$

ASSUMPTION 2. The potential $U \in C^2(\mathbb{R}^d)$, and the Hessian of U , $\nabla^2 U$ satisfies

$$(9) \quad \|\nabla^2 U(x)\| \leq M(1 + |\nabla U(x)|) \quad \forall x \in \mathbb{R}^d$$

for some constant $M \geq 1$, where $\|\cdot\|$ denotes the matrix operator norm

$$\|A\| := \sup_{\xi \in \mathbb{R}^d \setminus \{0\}} \frac{|A\xi|}{|\xi|}.$$

ASSUMPTION 3. The embedding $H^1(\mu_U) \hookrightarrow L^2(\mu_U)$ is compact.

The Assumption 2 is commonly used in the literature, see, for example, the books [34, 40] for underdamped Langevin dynamics, and is satisfied when U grows at most exponentially fast as $x \rightarrow \infty$. Assumption 3 is satisfied as long as

$$\lim_{|x| \rightarrow \infty} \frac{U(x)}{|x|^\alpha} = \infty$$

for some $\alpha > 1$ (see [28] for a proof). While previous works on hypocoercivity [20] and works following its framework [1, 3, 36] use the elliptic regularity estimate in x for which Assumption 1 suffices, our proof, in particular the construction of test functions in Lemma 2.2, relies on spectral decomposition of the operator $\nabla_x^* \nabla_x$, which is only guaranteed through the slightly stronger Assumption 3.

It is established in [23] that BPS and ZZ are well-defined Markov processes whose generators admit $C_b^2(\mathbb{R}^d \times \mathbb{R}^d)$ as a core, and similar arguments can be used to establish that the RHMC generator has the same core. It is standard that $C_b^2(\mathbb{R}^d \times \mathbb{R}^d)$ is dense in $L^2(\rho_\infty)$. Moreover, the operator \mathcal{L} is closed in $L^2(\rho_\infty)$, and generates a strongly continuous contraction semigroup $(P_t)_{t \geq 0}$ on $L^2(\rho_\infty)$. These set up the basic regularity assumptions needed in this work.

Below we present the main result of this work.

THEOREM 1.1. Under Assumptions 1, 2 and 3, there exist a constant $\nu > 0$ and universal constants C_0, c_0 independent of all parameters such that, for any f satisfying $f_0 \in L^2(\rho_\infty)$ and

$$(10) \quad \int_{\mathbb{R}^{2d}} f_0 \, d\rho_\infty(x, \nu) = 0,$$

and solving the PDMP equation (1), we have for every $t > 0$,

$$(11) \quad \|f(t, \cdot)\|_{L^2(\rho_\infty)} \leq C_0 \exp(-\nu t) \|f_0\|_{L^2(\rho_\infty)}.$$

Moreover, let R be the parameter that describes the ‘‘convexity barrier’’ of U , defined as

$$(12) \quad R = R(U) := \begin{cases} 0 & \text{if } U \text{ is convex;} \\ \sqrt{L} & \text{if } \nabla_x^2 U(x) \geq -L I, \forall x; \\ M\sqrt{d} & \text{if only (9) is assumed.} \end{cases}$$

Then, there exists a universal constant C , independent of all parameters, such that the convergence rate ν can be explicitly estimated for the three PDMPs as

$$(13) \quad \nu \geq C \begin{cases} \frac{m\gamma}{(\sqrt{m} + R + \gamma)^2} & \text{for RHMC;} \\ \frac{m\gamma}{(\sqrt{m} + R_{ZZ} + \gamma)^2} & \text{for ZZ;} \\ \frac{m\gamma}{(\sqrt{dm} + R\sqrt{d} + \gamma)^2} & \text{for BPS.} \end{cases}$$

Here $R_{ZZ} = \sqrt{L}$ if $\|\nabla_x^2 U\| \leq L, \forall x$ and $R_{ZZ} = M\sqrt{d}$ otherwise.

TABLE 1
 Summary of lower bound on the convergence rate ν and optimal choice of γ depending on d, m, L under the assumption $m\mathcal{I} \leq \nabla_x^2 U \leq L\mathcal{I}$ for the regime $m \ll 1 \ll L$

	Convergence rate ν	Optimal γ
RHMC	$O(\sqrt{m})$	\sqrt{m}
ZZ	$O(\frac{m}{\sqrt{L}})$	\sqrt{L}
BPS	$O(\sqrt{\frac{m}{d}})$	\sqrt{dm}

We will prove this theorem in Section 2.

Given the expression of (13), we can choose the optimal γ to maximize the rate ν for the three PDMPs:

$$(14) \quad \gamma = \begin{cases} \sqrt{m} + R & \text{for RHMC;} \\ \sqrt{m} + R_{ZZ} & \text{for ZZ;} \\ \sqrt{dm} + R\sqrt{d} & \text{for BPS.} \end{cases}$$

Therefore the optimal convergence rate is given by

$$(15) \quad \nu \geq C \begin{cases} \frac{m}{\sqrt{m} + R} & \text{for RHMC;} \\ \frac{m}{\sqrt{m} + R_{ZZ}} & \text{for ZZ;} \\ \frac{m}{\sqrt{dm} + R\sqrt{d}} & \text{for BPS.} \end{cases}$$

Table 1 summarizes the result under the assumption $m\mathcal{I} \leq \nabla_x^2 U \leq L\mathcal{I}$ (and hence guarantee Assumptions 1–3) in the most interesting regime $m \ll 1 \ll L$, with optimal choice of γ .

Compared to [1], we are able to derive an explicit scaling of ν not only on d , but also explicitly on γ, m, L as well. For RHMC, we obtain the optimal convergence rate $O(\sqrt{m})$, which is the same as for the underdamped Langevin dynamics [15]. The $O(\sqrt{m})$ rate is optimal as can be checked for the Gaussian case $U(x) = \frac{m|x|^2}{2}$. For the zigzag process, we are able to derive dimension independent convergence rate with the smoothness assumption $\|\nabla_x^2 U\| \leq L$, which is more quantitative than the result in [1]. Finally, although we are unable to obtain a dimension independent rate for BPS, our rate $O(d^{-1/2})$ under the assumption $\nabla_x^2 U \geq -L\mathcal{I}$ is still an improvement from the rate in [1], whose estimate provides a rate of $O(d^{-(1+\omega)/2})$ under the assumption $\Delta_x U(x) \leq cd^{1+\omega} + |\nabla_x U(x)|^2/2$. It is unclear whether a dimension independent convergence rate is possible for BPS.

Before we move on to the proof of Theorem 1.1, let us give a brief introduction on the strategy of the proof. A naive energy estimate yields

$$\begin{aligned} \frac{d}{dt} \|f(t, \cdot)\|_{L^2(\rho_\infty)}^2 &= -\frac{1}{2} \sum_{k=1}^K \int_{(s,t) \times \mathbb{R}^{2d}} |v \cdot F_k| (f - \mathcal{B}_k f)^2 dt d\rho_\infty \\ &\quad - 2\gamma \int_{(s,t) \times \mathbb{R}^{2d}} (f - \Pi_v f)^2 dt d\rho_\infty. \end{aligned}$$

While the above establishes the L^2 energy decay, it does not directly yield exponential decay rate. In particular, the energy dissipation is only present in the velocity variable. However, instead of looking at single time layers, we should look at time intervals, since after time propagation, the dissipation in v together with the transport and bouncing terms in x will lead to

dissipation in x . With the help a Poincaré-type inequality in the augmented state space established in Theorem 2.1, we can prove exponential convergence still using the standard energy estimate, with $\gamma(\Pi_v - \mathcal{I})$ playing the role of “dissipation,” in line with the moral “hypocoercivity is simply coercivity with respect to the correct norm,” quoted from [2], page 4.

2. Proofs. We first state the following modified Poincaré-type inequality that generalizes [2], Theorem 1.2, and [15], Theorem 2, to the PDMP dynamics under consideration.

THEOREM 2.1. *There exists a constant C independent of all parameters such that for all functions $f(t, x, v) \in C_b^1(I \times \mathbb{R}^{2d})$,*

$$\begin{aligned}
 & \|f - (f)_{\lambda \times \rho_\infty}\|_{L^2(\lambda \times \rho_\infty)} \\
 (16) \quad & \leq (1 + C_{\mathcal{J}}) \|f - \Pi_v f\|_{L^2(\lambda \times \rho_\infty)} + C \left(\frac{1}{\sqrt{m}} + T \right) \\
 & \quad \times \left\| \partial_t f - v \cdot \nabla_x f - \sum_{k=1}^K (v \cdot F_k)_+ (\mathcal{B}_k - I) f + F_0 \cdot \nabla_v f \right\|_{L^2(\lambda \times \rho_\infty)}.
 \end{aligned}$$

Here $C_{\mathcal{J}}$ is a constant defined as

$$(17) \quad C_{\mathcal{J}} = \begin{cases} C \left(1 + \frac{1}{\sqrt{m}T} + \frac{R}{\sqrt{m}} + RT \right) & \text{for RHMC;} \\ C \left(1 + \frac{1}{\sqrt{m}T} + \frac{R_{ZZ}}{\sqrt{m}} + R_{ZZ}T \right) & \text{for ZZ;} \\ C\sqrt{d} \left(1 + \frac{1}{\sqrt{m}T} + \frac{R}{\sqrt{m}} + RT \right) & \text{for BPS,} \end{cases}$$

where R and R_{ZZ} are the same quantities as defined in Theorem 1.1.

REMARK 2.1. We remark that Theorem 2.1 also applies to any $f(t, x, v)$ which is the solution to (1) with initial condition $f_0 \in L^2(\rho_\infty)$. Since \mathcal{L} generates a contraction semigroup, for $f(t, \cdot, \cdot) = P_t f_0$ we have $P_t f_0 \in L^2(\rho_\infty)$, and therefore for any fixed t ,

$$\partial_t f - v \cdot \nabla_x f - \sum_{k=1}^K (v \cdot F_k)_+ (\mathcal{B}_k - I) f + F_0 \cdot \nabla_v f = \gamma(\Pi_v f - f) \in L^2(\rho_\infty).$$

Hence the right-hand side of (16) is finite for any f being the solution to (1), and therefore Theorem 2.1 holds for f by density argument.

To prove Theorem 2.1, we need the following lemma, established in our previous work [15], which provides crucial test functions that satisfy a divergence equation with Dirichlet boundary conditions. To make the paper self-contained, we include the proof in the Appendix.

LEMMA 2.2 ([15], Lemma 2.6). *For any function $f = f(t, x) \in L^2(\lambda \times \mu_U)$ with $(f)_{\lambda \times \mu_U} = 0$, there exist $\bar{\phi} = (\phi_0, \phi_1, \dots, \phi_d)^\top \in H^1(\lambda \times \mu_U)^{d+1}$ solving*

$$(18) \quad -\partial_t \phi_0 + \sum_{i=1}^d \partial_{x_i}^* \phi_i = f, \quad \phi(t = 0, \cdot) = \phi(t = T, \cdot) = 0,$$

with estimates

$$(19) \quad \|\bar{\phi}\|_{L^2(\lambda \times \mu_U)} \leq C \max \left\{ \frac{1}{\sqrt{m}}, T \right\} \|f\|_{L^2(\lambda \times \mu_U)},$$

$$(20) \quad \left(\sum_{i,j=0}^d \|\partial_{x_i} \phi_j\|_{L^2(\lambda \times \mu_U)}^2 \right)^{1/2} \leq C \left(1 + \frac{1}{\sqrt{mT}} + \frac{R}{\sqrt{m}} + RT \right) \|f\|_{L^2(\lambda \times \mu_U)}.$$

Here C is some universal constant, and R is the ‘‘convexity barrier’’ parameter for potential U defined in Theorem 1.1.

Before proceeding to the proof of Theorem 2.1, we present two elementary but useful lemmas: one regarding the properties of reflections \mathcal{B}_k , and the other on intergrating the v variable with $(v \cdot n)_+$.

LEMMA 2.3. *The operators \mathcal{B}_k defined in (3) satisfy the following properties:*

1. for any functions f, g ,

$$\mathcal{B}_k(fg) = \mathcal{B}_k f \mathcal{B}_k g;$$

2. $\mathcal{B}_k^2 = \mathcal{I}$;

3. \mathcal{B}_k is symmetric in $L^2(\kappa)$: For any two functions f, g ,

$$(21) \quad \int_{\mathbb{R}^d} \mathcal{B}_k f g \, d\kappa(v) = \int_{\mathbb{R}^d} f \mathcal{B}_k g \, d\kappa(v);$$

as a direct consequence, letting $g = 1$, we have for any function f ,

$$\int_{\mathbb{R}^d} \mathcal{B}_k f \, d\kappa(v) = \int_{\mathbb{R}^d} f \, d\kappa(v);$$

4. for any function f ,

$$(22) \quad \int_{\mathbb{R}^d} (v \cdot F_k)_+ \mathcal{B}_k f \, d\kappa(v) = \int_{\mathbb{R}^d} (-v \cdot F_k)_+ f \, d\kappa(v).$$

PROOF. The first and second properties can be verified directly using definition (3). The third property follows from a change of variable $\tilde{v} := v - 2(v \cdot n_k)n_k$ in v , so that $v = \tilde{v} - 2(\tilde{v} \cdot n_k)n_k$, and $\kappa(\tilde{v}) = \kappa(v)$:

$$\begin{aligned} \int_{\mathbb{R}^d} \mathcal{B}_k f g \, d\kappa(v) &= \int_{\mathbb{R}^d} f(v - 2(v \cdot n_k)n_k) g(v) \, d\kappa(v) \\ &= \int_{\mathbb{R}^d} f(\tilde{v}) g(\tilde{v} - 2(\tilde{v} \cdot n_k)n_k) \, d\kappa(\tilde{v}) = \int_{\mathbb{R}^d} f \mathcal{B}_k g \, d\kappa(v). \end{aligned}$$

Finally for the fourth property, we change the variables in the same way as the proof of the third one, so that $v \cdot F_k = -\tilde{v} \cdot F_k$:

$$\begin{aligned} \int_{\mathbb{R}^d} (v \cdot F_k)_+ \mathcal{B}_k f \, d\kappa(v) &= \int_{v \cdot F_k \geq 0} (v \cdot F_k) f(v - 2(v \cdot n_k)n_k) \, d\kappa(v) \\ &= \int_{\tilde{v} \cdot F_k \leq 0} -(\tilde{v} \cdot F_k) f(\tilde{v}) \, d\kappa(\tilde{v}) \\ &= \int_{\mathbb{R}^d} (-v \cdot F_k)_+ f \, d\kappa(v). \end{aligned} \quad \square$$

LEMMA 2.4. *For any vector $q \in \mathbb{R}^d$ and any two functions $\varphi(v \cdot q)$ and $\psi(v)$ such that $\varphi(v \cdot q)\psi(v)$ is even in v and $\varphi(0) = 0$, it holds*

$$(23) \quad \int_{\mathbb{R}^d} \varphi((v \cdot q)_+) \psi(v) \, d\kappa(v) = \frac{1}{2} \int_{\mathbb{R}^d} \varphi(v \cdot q) \psi(v) \, d\kappa(v).$$

PROOF. The identity is obtained as follows, in which we use a change of variables $v \mapsto -v$ in the second equality, the symmetry of Gaussian $\kappa(v)$ in the sense that $\kappa(v) = \kappa(-v)$ in the third equality, and $\varphi(0) = 0$ in the last equality:

$$\begin{aligned} \int_{\mathbb{R}^d} \varphi(v \cdot q) \psi(v) \, d\kappa(v) &= \int_{v \cdot q \geq 0} \varphi(v \cdot q) \psi(v) \, d\kappa(v) + \int_{v \cdot q \leq 0} \varphi(v \cdot q) \psi(v) \, d\kappa(v) \\ &= \int_{v \cdot q \geq 0} \varphi(v \cdot q) \psi(v) \, d\kappa(v) + \int_{v \cdot q \geq 0} \varphi(-v \cdot q) \psi(-v) \, d\kappa(-v) \\ &= 2 \int_{v \cdot q \geq 0} \varphi(v \cdot q) \psi(v) \, d\kappa(v) = 2 \int_{\mathbb{R}^d} \varphi((v \cdot q)_+) \psi(v) \, d\kappa(v). \quad \square \end{aligned}$$

We are now ready to prove Theorem 2.1.

PROOF OF THEOREM 2.1. Without loss of generality we assume

$$(f)_{\lambda \times \rho_\infty} = 0.$$

We now take $\bar{\phi} = (\phi_0, \phi_1, \dots, \phi_d)^\top$ to be the test functions given by Lemma 2.2 with $\Pi_v f$ playing the role of f .

Define (for simplicity of notation, we denote $\phi = (\phi_1, \dots, \phi_d)^\top$ and treat ϕ as a d -vector)

$$(24) \quad \mathcal{J} := -\partial_t \phi_0 + v \cdot \nabla_x \phi_0 + v \cdot \partial_t \phi - \sum_{i=1}^d v_i v \cdot \partial_{x_i} \phi + F_0 \cdot \phi - 2 \sum_{k=1}^K (-v \cdot F_k)_+ (v \cdot n_k) (\phi \cdot n_k).$$

We claim the following estimate, the proof of which will be deferred.

LEMMA 2.5. *The quantity \mathcal{J} can be controlled by $\Pi_v f$ in the sense of*

$$(25) \quad \|\mathcal{J}\|_{L^2(\lambda \times \rho_\infty)} \leq C_{\mathcal{J}} \|\Pi_v f\|_{L^2(\lambda \times \mu_U)}.$$

Here $C_{\mathcal{J}}$ is the constant defined in Theorem 2.1.

Before proceeding with the proof of Theorem 2.1, let us provide a heuristic justification for Lemma 2.5: if we calculate $\|\mathcal{J}\|_{L^2(\lambda \times \rho_\infty)}^2$, then its expression consists of terms that are up to the fourth moment of v multiplied with ϕ_k , $\partial_{x_i} \phi_j$ or $\phi_k \nabla_x U$. Therefore, integrating out the v component against Gaussian, and by Lemma 2.2 all terms can be controlled by $\|\Pi_v f\|_{L^2(\lambda \times \mu_U)}^2$. The actual constants will be estimated separately for each PDMP in a later part of the paper.

Now let us return to the proof of Theorem 2.1 assuming Lemma 2.5. To simplify notation, we define the operator

$$(26) \quad Af := \partial_t f - v \cdot \nabla_x f - \sum_{k=1}^K (v \cdot F_k)_+ (\mathcal{B}_k - I) f + F_0 \cdot \nabla_v f.$$

We now estimate the L^2 norm of $\Pi_v f$. Using Lemma 2.4 for $q = -F_k$, $\varphi(v \cdot q) = v \cdot q$ and $\psi(v) = (v \cdot n_k) (\phi \cdot n_k)$ and integrating out v , we have

$$\begin{aligned} (27) \quad 2 \int_{I \times \mathbb{R}^{2d}} (-v \cdot F_k)_+ (v \cdot n_k) (\phi \cdot n_k) \, dt \, d\rho_\infty &= - \int_{I \times \mathbb{R}^{2d}} (v \cdot F_k) (v \cdot n_k) (\phi \cdot n_k) \, dt \, d\rho_\infty \\ &= - \int_{I \times \mathbb{R}^d} \phi \cdot F_k \, dt \, d\mu_U(x). \end{aligned}$$

Therefore, by the construction of the test functions $\bar{\phi}$, and noticing $\nabla_x U = \sum_{k=0}^K F_k$, we have

$$\begin{aligned}
 \|\Pi_v f\|_{L^2(\lambda \times \mu_U)}^2 &= \int_{I \times \mathbb{R}^d} \Pi_v f \left(-\partial_t \phi_0 - \nabla_x \cdot \phi + \phi \cdot \sum_{k=0}^K F_k \right) dt \, d\mu_U(x) \\
 &\stackrel{(27)}{=} \int_{I \times \mathbb{R}^{2d}} \Pi_v f \left(-\partial_t \phi_0 - \nabla_x \cdot \phi + \phi \cdot F_0 \right. \\
 &\quad \left. - 2 \sum_{k=1}^K (-v \cdot F_k)_+ (v \cdot n_k) (\phi \cdot n_k) \right) dt \, d\rho_\infty \\
 (28) \quad &= \int_{I \times \mathbb{R}^{2d}} \Pi_v f \left(-\partial_t \phi_0 + v \cdot \nabla_x \phi_0 + v \cdot \partial_t \phi - \sum_i v_i v \cdot \partial_{x_i} \phi + \phi \cdot F_0 \right. \\
 &\quad \left. - 2 \sum_{k=1}^K (-v \cdot F_k)_+ (v \cdot n_k) (\phi \cdot n_k) \right) dt \, d\rho_\infty \\
 &\stackrel{(24)}{=} \int_{I \times \mathbb{R}^{2d}} f \mathcal{J} \, dt \, d\rho_\infty - \int_{I \times \mathbb{R}^{2d}} (f - \Pi_v f) \mathcal{J} \, dt \, d\rho_\infty \\
 &\stackrel{(25)}{\leq} \int_{I \times \mathbb{R}^{2d}} f \mathcal{J} \, dt \, d\rho_\infty + C_{\mathcal{J}} \|\Pi_v f\|_{L^2(\lambda \times \mu_U)} \|f - \Pi_v f\|_{L^2(\lambda \times \rho_\infty)},
 \end{aligned}$$

where the third equality follows from introducing a dummy v variable and noting that by the basic properties of Gaussian measure κ , $\int_{\mathbb{R}^d} v_i \, d\kappa(v) = 0$, and $\int_{\mathbb{R}^d} v_i v_j \, d\kappa(v) = \delta_{ij}$.

To estimate the first term on the RHS of (28) we use integration by parts. For time derivatives, we crucially use that $\bar{\phi}$ vanish at both boundaries $t = 0$ and $t = T$; for derivatives in space and velocity, we use $\int_{\mathbb{R}^d} \nabla_x f \cdot g \, d\mu_U(x) = \int_{\mathbb{R}^d} f (-\nabla_x g + g \cdot \nabla_x U) \, d\mu_U(x)$ and $\int_{\mathbb{R}^d} \nabla_v f \cdot g \, d\kappa(v) = \int_{\mathbb{R}^d} f (-\nabla_v g + g \cdot v) \, d\kappa(v)$:

$$\begin{aligned}
 &\int_{I \times \mathbb{R}^{2d}} f \mathcal{J} \, dt \, d\rho_\infty \\
 &\stackrel{(24)}{=} \int_{I \times \mathbb{R}^{2d}} f \left(-\partial_t \phi_0 + v \cdot \nabla_x \phi_0 + v \cdot \partial_t \phi - \sum_{i=1}^d v_i v \cdot \partial_{x_i} \phi + F_0 \cdot \phi \right. \\
 &\quad \left. - 2 \sum_{k=1}^K (-v \cdot F_k)_+ (v \cdot n_k) (\phi \cdot n_k) \right) dt \, d\rho_\infty \\
 &= \int_{I \times \mathbb{R}^{2d}} \left(\partial_t f \phi_0 - v \cdot \nabla_x f \phi_0 + f \phi_0 v \cdot \sum_{k=0}^K F_k - \partial_t f v \cdot \phi + (v \cdot \nabla_x f) (v \cdot \phi) \right. \\
 &\quad \left. - (v \cdot \nabla_x U) (v \cdot \phi) f + f \phi \cdot F_0 - 2 \sum_{k=1}^K (-v \cdot F_k)_+ (v \cdot n_k) (\phi \cdot n_k) f \right) dt \, d\rho_\infty \\
 &= \int_{I \times \mathbb{R}^{2d}} \left((\partial_t f - v \cdot \nabla_x f) (\phi_0 - v \cdot \phi) + f \phi_0 v \cdot F_0 + f \phi \cdot F_0 - (v \cdot F_0) (v \cdot \phi) f \right. \\
 &\quad \left. + \left(v \cdot \sum_{k=1}^K F_k \right) (\phi_0 - v \cdot \phi) f - 2 \sum_{k=1}^K (-v \cdot F_k)_+ (v \cdot n_k) (\phi \cdot n_k) f \right) dt \, d\rho_\infty
 \end{aligned}$$

$$\begin{aligned}
 &= \int_{I \times \mathbb{R}^{2d}} \left(\left(\partial_t f - v \cdot \nabla_x f + \sum_{k=1}^K (v \cdot F_k)_+ f \right) (\phi_0 - v \cdot \phi) - \sum_{k=1}^K (-v \cdot F_k)_+ (\phi_0 - v \cdot \phi) f \right. \\
 &\quad \left. + \phi_0 F_0 \cdot \nabla_v f - (F_0 \cdot \nabla_v f)(v \cdot \phi) - 2 \sum_{k=1}^K (-v \cdot F_k)_+ (v \cdot n_k) (\phi \cdot n_k) f \right) dt d\rho_\infty \\
 &= \int_{I \times \mathbb{R}^{2d}} \left(\left(\partial_t f - v \cdot \nabla_x f + \sum_{k=1}^K (v \cdot F_k)_+ f + F_0 \cdot \nabla_v f \right) (\phi_0 - v \cdot \phi) \right. \\
 &\quad \left. - \sum_{k=1}^K (-v \cdot F_k)_+ \mathcal{B}_k (\phi_0 - v \cdot \phi) \mathcal{B}_k^2 f \right) dt d\rho_\infty \\
 &\stackrel{(21),(22)}{=} \int_{I \times \mathbb{R}^{2d}} \left(\left(\partial_t f - v \cdot \nabla_x f - \sum_{k=1}^K (v \cdot F_k)_+ (\mathcal{B}_k - I) f + F_0 \cdot \nabla_v f \right) \right. \\
 &\quad \left. \times (\phi_0 - v \cdot \phi) \right) dt d\rho_\infty \\
 &\stackrel{(26)}{\leq} \|\phi_0 - v \cdot \phi\|_{L^2(\lambda \times \rho_\infty)} \|\mathcal{A}f\|_{L^2(\lambda \times \rho_\infty)}.
 \end{aligned}$$

Since $\bar{\phi}$ is independent of v , expanding and integrating out v with respect to κ , we obtain

$$\|\phi_0 - v \cdot \phi\|_{L^2(\lambda \times \rho_\infty)}^2 = \|\bar{\phi}\|_{L^2(\lambda \times \mu_U)}^2 \stackrel{(19)}{\leq} C \left(\frac{1}{\sqrt{m}} + T \right)^2 \|\Pi_v f\|_{L^2(\lambda \times \mu_U)}^2.$$

Thus

$$(29) \quad \int_{I \times \mathbb{R}^{2d}} f \mathcal{J} dt d\rho_\infty \leq C \left(\frac{1}{\sqrt{m}} + T \right) \|\Pi_v f\|_{L^2(\lambda \times \mu_U)} \|\mathcal{A}f\|_{L^2(\lambda \times \rho_\infty)}.$$

Combining (28) and (29) we arrive at

$$\|\Pi_v f\|_{L^2(\lambda \times \mu_U)} \leq C \left(\frac{1}{\sqrt{m}} + T \right) \|\mathcal{A}f\|_{L^2(\lambda \times \rho_\infty)} + C_{\mathcal{J}} \|f - \Pi_v f\|_{L^2(\lambda \times \rho_\infty)},$$

and therefore by the triangle inequality

$$\begin{aligned}
 \|f\|_{L^2(\lambda \times \rho_\infty)} &\leq \|f - \Pi_v f\|_{L^2(\lambda \times \rho_\infty)} + \|\Pi_v f\|_{L^2(\lambda \times \mu_U)} \\
 &\leq C \left(\frac{1}{\sqrt{m}} + T \right) \|\mathcal{A}f\|_{L^2(\lambda \times \rho_\infty)} + (1 + C_{\mathcal{J}}) \|f - \Pi_v f\|_{L^2(\lambda \times \rho_\infty)}. \quad \square
 \end{aligned}$$

PROOF OF THEOREM 1.1. We first notice that

$$\int_{\mathbb{R}^{2d}} f(t, x, v) d\rho_\infty(x, v) = 0$$

for all $t > 0$. In view of (10), it suffices to prove

$$\frac{d}{dt} \int_{\mathbb{R}^{2d}} f(t, x, v) d\rho_\infty(x, v) \stackrel{(1)}{=} \int_{\mathbb{R}^{2d}} \mathcal{L}f(t, x, v) d\rho_\infty(x, v) = 0.$$

Notice

$$\mathcal{L} = v \cdot \nabla_x - \nabla_x U \cdot \nabla_v + \sum_{k=1}^K \mathcal{L}_k + \gamma(\Pi_v - \mathcal{I}),$$

where $\mathcal{L}_k = (v \cdot F_k)_+(\mathcal{B}_k - \mathcal{I}) + F_k \cdot \nabla_v$. Therefore, as it is clear that both operators $v \cdot \nabla_x - \nabla_x U \cdot \nabla_v$ and $\Pi_v - \mathcal{I}$ preserve ρ_∞ , it suffices to show that \mathcal{L}_k preserves ρ_∞ as well. Indeed,

$$\begin{aligned} \int_{\mathbb{R}^{2d}} \mathcal{L}_k f \, d\rho_\infty(x, v) &= \int_{\mathbb{R}^{2d}} ((v \cdot F_k)_+ \mathcal{B}_k f - (v \cdot F_k)_+ f + F_k \cdot \nabla_v f) \, d\rho_\infty \\ &\stackrel{(22)}{=} \int_{\mathbb{R}^{2d}} ((-v \cdot F_k)_+ f - (v \cdot F_k)_+ f + f v \cdot F_k) \, d\rho_\infty = 0. \end{aligned}$$

Next we establish the energy decay properties of f . Take any two positive numbers $0 < s < t$. Following [1], Proposition 8, we denote the symmetric part of \mathcal{L} by

$$(30) \quad \mathcal{S} = \frac{1}{2} \sum_{k=1}^K |v \cdot F_k| (\mathcal{B}_k - \mathcal{I}) + \gamma (\Pi_v - \mathcal{I}).$$

Using the properties of \mathcal{B}_k in Lemma 2.3,

$$\begin{aligned} \int_{(s,t) \times \mathbb{R}^d \times \mathbb{R}^d} |v \cdot F_k| (\mathcal{B}_k f)^2 \, dt \, d\rho_\infty &= \int_{(s,t) \times \mathbb{R}^d \times \mathbb{R}^d} |v \cdot F_k| \mathcal{B}_k f^2 \, dt \, d\rho_\infty \\ &\stackrel{(21)}{=} \int_{(s,t) \times \mathbb{R}^d \times \mathbb{R}^d} \mathcal{B}_k |v \cdot F_k| f^2 \, dt \, d\rho_\infty \\ &= \int_{(s,t) \times \mathbb{R}^d \times \mathbb{R}^d} |v \cdot F_k| f^2 \, dt \, d\rho_\infty. \end{aligned}$$

Therefore

$$(31) \quad \int_{(s,t) \times \mathbb{R}^d \times \mathbb{R}^d} |v \cdot F_k| (f - \mathcal{B}_k f)^2 \, dt \, d\rho_\infty = 2 \int_{(s,t) \times \mathbb{R}^d \times \mathbb{R}^d} |v \cdot F_k| f (\mathcal{I} - \mathcal{B}_k) f \, dt \, d\rho_\infty.$$

On the other hand, since

$$\int_{(s,t) \times \mathbb{R}^d \times \mathbb{R}^d} f \Pi_v f \, dt \, d\rho_\infty = \int_{(s,t) \times \mathbb{R}^d \times \mathbb{R}^d} (\Pi_v f)^2 \, dt \, d\rho_\infty = \int_{(s,t) \times \mathbb{R}^d} (\Pi_v f)^2 \, dt \, d\mu_U(x),$$

we have

$$\int_{(s,t) \times \mathbb{R}^d \times \mathbb{R}^d} (f - \Pi_v f)^2 \, dt \, d\rho_\infty = \int_{(s,t) \times \mathbb{R}^d \times \mathbb{R}^d} f (\mathcal{I} - \Pi_v) f \, dt \, d\rho_\infty.$$

Therefore we have an elementary energy estimate, noticing the anti-symmetric part of \mathcal{L} does not contribute to the integral $\int_{(s,t) \times \mathbb{R}^d \times \mathbb{R}^d} f \mathcal{L} f \, dt \, d\rho_\infty$:

$$\begin{aligned} &\|f(t, \cdot)\|_{L^2(\rho_\infty)}^2 - \|f(s, \cdot)\|_{L^2(\rho_\infty)}^2 \\ &= 2 \int_{(s,t) \times \mathbb{R}^d \times \mathbb{R}^d} f \partial_t f \, dt \, d\rho_\infty \stackrel{(30)}{=} 2 \int_{(s,t) \times \mathbb{R}^d \times \mathbb{R}^d} f \mathcal{S} f \, dt \, d\rho_\infty \\ &= \sum_{k=1}^K \int_{(s,t) \times \mathbb{R}^d \times \mathbb{R}^d} |v \cdot F_k| f (\mathcal{B}_k - \mathcal{I}) f \, dt \, d\rho_\infty \\ (32) \quad &+ 2\gamma \int_{(s,t) \times \mathbb{R}^d \times \mathbb{R}^d} f (\Pi_v - \mathcal{I}) f \, dt \, d\rho_\infty \\ &\stackrel{(31)}{=} -\frac{1}{2} \sum_{k=1}^K \int_{(s,t) \times \mathbb{R}^d \times \mathbb{R}^d} |v \cdot F_k| (f - \mathcal{B}_k f)^2 \, dt \, d\rho_\infty \\ &\quad - 2\gamma \int_{(s,t) \times \mathbb{R}^d \times \mathbb{R}^d} (f - \Pi_v f)^2 \, dt \, d\rho_\infty \\ &\leq -2\gamma \|f - \Pi_v f\|_{L^2(\lambda_{(s,t)} \times \rho_\infty)}^2, \end{aligned}$$

where we use $\lambda_{(s,t)}$ to denote the Lebesgue measure on (s, t) . In particular,

$$(33) \quad \text{the mapping } t \mapsto \|f(t, \cdot)\|_{L^2(\rho_\infty)}^2 \text{ is nonincreasing.}$$

By equation (1) and definition of the operators (2) and (26),

$$(34) \quad \|\mathcal{A}f\|_{L^2(\lambda_{(s,t)} \times \rho_\infty)} = \gamma \|f - \Pi_v f\|_{L^2(\lambda_{(s,t)} \times \rho_\infty)}.$$

Therefore, for any $0 < s < t$ (note that Theorem 2.1 applies by Remark 2.1),

$$\begin{aligned} & \|f(t, \cdot)\|_{L^2(\rho_\infty)}^2 - \|f(s, \cdot)\|_{L^2(\rho_\infty)}^2 \\ & \stackrel{(32)}{\leq} -2\gamma \|f - \Pi_v f\|_{L^2((s,t) \times \rho_\infty)}^2 \\ & \stackrel{(34)}{=} -\frac{2\gamma}{(1 + C_{\mathcal{J}} + C\gamma(\frac{1}{\sqrt{m}} + t - s))^2} \left((1 + C_{\mathcal{J}}) \|f - \Pi_v f\|_{L^2(\lambda_{(s,t)} \times \rho_\infty)} \right. \\ & \quad \left. + C\left(\frac{1}{\sqrt{m}} + t - s\right) \|\mathcal{A}f\|_{L^2(\lambda_{(s,t)} \times \rho_\infty)} \right)^2 \\ & \stackrel{(16)}{\leq} -\frac{2\gamma}{(1 + C_{\mathcal{J}} + C\gamma(\frac{1}{\sqrt{m}} + t - s))^2} \|f\|_{L^2(\lambda_{(s,t)} \times \rho_\infty)}^2 \\ & \stackrel{(33)}{\leq} -\frac{2\gamma(t - s)}{(1 + C_{\mathcal{J}} + C\gamma(\frac{1}{\sqrt{m}} + t - s))^2} \|f(t, \cdot)\|_{L^2(\rho_\infty)}^2. \end{aligned}$$

Now fixing a $T > 0$ to be optimized later, for any $t > 0$, we pick the integer k satisfying $kT \leq t < (k + 1)T$. Applying above inequality iteratively and using the monoticity (33), we obtain

$$\begin{aligned} \|f(t, \cdot)\|_{L^2(\rho_\infty)}^2 & \leq \left(1 + \frac{2\gamma T}{(1 + C_{\mathcal{J}} + C\gamma(\frac{1}{\sqrt{m}} + T))^2} \right)^{-k} \|f_0\|_{L^2(\rho_\infty)}^2 \\ & \leq \left(1 + \frac{2\gamma T}{(1 + C_{\mathcal{J}} + C\gamma(\frac{1}{\sqrt{m}} + T))^2} \right)^{-\frac{t}{T} + 1} \|f_0\|_{L^2(\rho_\infty)}^2 \\ & \leq \left(1 + \frac{2\gamma T}{(1 + C_{\mathcal{J}} + C\gamma(\frac{1}{\sqrt{m}} + T))^2} \right) \\ & \quad \times \exp\left(-\frac{t}{T} \log\left(1 + \frac{2\gamma T}{(1 + C_{\mathcal{J}} + C\gamma(\frac{1}{\sqrt{m}} + T))^2}\right)\right) \|f_0\|_{L^2(\rho_\infty)}^2. \end{aligned}$$

The prefactor

$$1 + \frac{2\gamma T}{(1 + C_{\mathcal{J}} + C\gamma(\frac{1}{\sqrt{m}} + T))^2} \leq 1 + \frac{2\gamma T}{(1 + C\gamma T)^2} \leq 1 + \frac{1}{C}$$

is bounded above by a universal constant. Therefore, using $\log(1 + x) \geq \frac{1}{C}x$ for $x \in [0, 1 + \frac{1}{C}]$ for some universal constant C , this yields (11) with the exponential decay rate

$$(35) \quad \begin{aligned} v & = \sup_{T>0} \frac{1}{2T} \log\left(1 + \frac{2\gamma T}{(1 + C_{\mathcal{J}} + C\gamma(\frac{1}{\sqrt{m}} + T))^2}\right) \\ & \geq C \sup_{T>0} \frac{\gamma}{(1 + C_{\mathcal{J}} + \gamma(\frac{1}{\sqrt{m}} + T))^2}. \end{aligned}$$

Substituting (17) into (35), we get

$$(36) \quad v \geq C \begin{cases} \frac{\gamma}{(1 + \frac{1}{\sqrt{m}T} + \frac{R}{\sqrt{m}} + RT + \frac{\gamma}{\sqrt{m}} + \gamma T)^2} & \text{for RHMC;} \\ \frac{\gamma}{(1 + \frac{1}{\sqrt{m}T} + \frac{R_{ZZ}}{\sqrt{m}} + R_{ZZ}T + \frac{\gamma}{\sqrt{m}} + \gamma T)^2} & \text{for ZZ;} \\ \frac{\gamma}{(\sqrt{d}(1 + \frac{1}{\sqrt{m}T} + \frac{R}{\sqrt{m}} + RT) + \gamma(\frac{1}{\sqrt{m}} + T))^2} & \text{for BPS.} \end{cases}$$

We arrive at the rates (13) by optimizing the choice of T for each case:

$$T = \begin{cases} m^{-\frac{1}{4}}(R + \gamma)^{-\frac{1}{2}} & \text{for RHMC;} \\ m^{-\frac{1}{4}}(R_{ZZ} + \gamma)^{-\frac{1}{2}} & \text{for ZZ;} \\ d^{\frac{1}{4}}m^{-\frac{1}{4}}(\sqrt{d}R + \gamma)^{-\frac{1}{2}} & \text{for BPS.} \end{cases} \quad \square$$

The remaining task is to prove Lemma 2.5. For RHMC,

$$\mathcal{J} = -\partial_t \phi_0 + v \cdot \nabla_x \phi_0 + v \cdot \partial_t \phi - \sum_{i=1}^d v_i v \cdot \partial_{x_i} \phi + \phi \cdot \nabla_x U.$$

The norm $\|\mathcal{J}\|_{L^2(\lambda \times \rho_\infty)}$ is already estimated in [15], Proof of Theorem 2, and the proof is thus omitted here. In the two subsequent subsections we will estimate $C_{\mathcal{J}}$ for ZZ and BPS respectively.

2.1. *The zigzag process.* In this case

$$\mathcal{J} = -\partial_t \phi_0 + v \cdot \nabla_x \phi_0 + v \cdot \partial_t \phi - \sum_{i=1}^d v_i v \cdot \partial_{x_i} \phi - 2 \sum_{k=1}^d (-v_k \partial_{x_k} U)_+ v_k \phi_k.$$

LEMMA 2.6. *Let $\phi_i, i = 0, \dots, d$ be test functions as in Lemma 2.2. Then*

$$(37) \quad \begin{aligned} & \sum_{k=1}^d \int_{I \times \mathbb{R}^d} (\phi_k \partial_{x_k} U)^2 dt d\mu_U(x) \\ & \leq C \left(1 + \frac{1}{\sqrt{m}T} + \frac{R_{ZZ}}{\sqrt{m}} + R_{ZZ}T \right)^2 \int_{I \times \mathbb{R}^d} (\Pi_v f)^2 dt d\mu_U(x). \end{aligned}$$

Here R_{ZZ} is defined as in Theorem 1.1.

PROOF. Using integration by parts,

$$\begin{aligned} \sum_{k=1}^d \int_{I \times \mathbb{R}^d} (\phi_k \partial_{x_k} U)^2 dt d\mu_U(x) &= \sum_{k=1}^d \int_{I \times \mathbb{R}^d} \partial_{x_k} (\phi_k^2 \partial_{x_k} U) dt d\mu_U(x) \\ &= 2 \sum_{k=1}^d \int_{I \times \mathbb{R}^d} \phi_k \partial_{x_k} \phi_k \partial_{x_k} U dt d\mu_U(x) \\ &\quad + \sum_{k=1}^d \int_{I \times \mathbb{R}^d} \phi_k^2 \partial_{x_k x_k} U dt d\mu_U(x) \end{aligned}$$

$$\begin{aligned} &\leq \sum_{k=1}^d \int_{I \times \mathbb{R}^d} \left(\frac{1}{2} (\phi_k \partial_{x_k} U)^2 + 2 |\partial_{x_k} \phi_k|^2 \right) dt d\mu_U(x) \\ &\quad + \sum_{k=1}^d \int_{I \times \mathbb{R}^d} \phi_k^2 \partial_{x_k x_k} U dt d\mu_U(x). \end{aligned}$$

After rearranging, we have

$$\begin{aligned} &\sum_{k=1}^d \int_{I \times \mathbb{R}^d} (\phi_k \partial_{x_k} U)^2 dt d\mu_U(x) \\ &\leq C \sum_{k=1}^d \int_{I \times \mathbb{R}^d} (|\partial_{x_k} \phi_k|^2 + \phi_k^2 \partial_{x_k x_k} U) dt d\mu_U(x) \\ (38) \quad &\stackrel{(20)}{\leq} C \left(1 + \frac{1}{\sqrt{mT}} + \frac{R}{\sqrt{m}} + RT \right)^2 \int_{I \times \mathbb{R}^d} (\Pi_v f)^2 dt d\mu_U(x) \\ &\quad + C \sum_{k=1}^d \int_{I \times \mathbb{R}^d} \phi_k^2 \partial_{x_k x_k} U dt d\mu_U(x). \end{aligned}$$

We first discuss the easier case where $\|\nabla_x^2 U\| \leq L$:

$$\begin{aligned} \sum_{k=1}^d \int_{I \times \mathbb{R}^d} \phi_k^2 \partial_{x_k x_k} U dt d\mu_U(x) &\leq L \sum_{k=1}^d \int_{I \times \mathbb{R}^d} \phi_k^2 dt d\mu_U(x) \\ &\stackrel{(19)}{\leq} CL \left(\frac{1}{\sqrt{m}} + T \right)^2 \int_{I \times \mathbb{R}^d} (\Pi_v f)^2 dt d\mu_U(x). \end{aligned}$$

In the general setting where only Assumption 2 is assumed, by [15], Lemma 2.2, we have

$$(39) \quad \|\phi_k |\nabla_x U|\|_{L^2(\lambda \times \mu_U)} \leq C (\|\nabla_x \phi_k\|_{L^2(\lambda \times \mu_U)} + Md \|\phi_k\|_{L^2(\lambda \times \mu_U)}).$$

Therefore, by the Cauchy–Schwarz inequality,

$$\begin{aligned} &\sum_{k=1}^d \int_{I \times \mathbb{R}^d} \phi_k^2 \partial_{x_k x_k} U dt d\mu_U(x) \\ &\stackrel{(9)}{\leq} CM \sum_{k=1}^d \int_{I \times \mathbb{R}^d} (1 + |\nabla_x U|) \phi_k^2 dt d\mu_U(x) \\ &\leq CM \|\phi\|_{L^2(\lambda \times \mu_U)}^2 + CM \sum_{k=1}^d \|\phi_k\|_{L^2(\lambda \times \mu_U)} \|\phi_k |\nabla_x U|\|_{L^2(\lambda \times \mu_U)} \\ &\stackrel{(39)}{\leq} CM \left(\|\phi\|_{L^2(\lambda \times \mu_U)}^2 + \sum_{k=1}^d \|\phi_k\|_{L^2(\lambda \times \mu_U)} (\|\nabla_x \phi_k\|_{L^2(\lambda \times \mu_U)} + Md \|\phi_k\|_{L^2(\lambda \times \mu_U)}) \right) \\ &\stackrel{(19)}{\leq} CM \left(\left(\sum_{k=1}^d \|\phi_k\|_{L^2(\lambda \times \mu_U)}^2 \right)^{\frac{1}{2}} \left(\sum_{k=1}^d \|\nabla_x \phi_k\|_{L^2(\lambda \times \mu_U)}^2 \right)^{\frac{1}{2}} + Md \|\phi\|_{L^2(\lambda \times \mu_U)}^2 \right) \\ &\stackrel{(19),(20)}{\leq} C \left(1 + \frac{1}{\sqrt{mT}} + \frac{M\sqrt{d}}{\sqrt{m}} + M\sqrt{dT} \right)^2 \|\Pi_v f\|_{L^2(\lambda \times \mu_U)}^2. \end{aligned}$$

This proves the lemma with $R_{ZZ} = M\sqrt{d}$. \square

PROOF OF LEMMA 2.5 FOR ZIGZAG PROCESS. To estimate $\|\mathcal{J}\|_{L^2(\lambda \times \rho_\infty)}^2$, we expand its terms, categorize them according to their powers on v and whether $(-v_k \partial_{x_k} U)_+$ is contained, and integrate out the v variable for each term.

We start with terms that do not contain $(-v_k \partial_{x_k} U)_+$, in which all terms with odd power of v vanish:

Terms with 0th power of v :

$$\int_{I \times \mathbb{R}^d} (\partial_t \phi_0)^2 dt d\mu_U(x).$$

Terms with 2nd power of v :

$$\begin{aligned} & \int_{I \times \mathbb{R}^{2d}} \left((v \cdot \nabla_x \phi_0)^2 + (v \cdot \partial_t \phi)^2 + 2(v \cdot \partial_t \phi)(v \cdot \nabla_x \phi_0) + 2 \sum_{i,j=1}^d v_i v_j \partial_t \phi_0 \partial_{x_i} \phi_j \right) dt d\rho_\infty \\ &= \int_{I \times \mathbb{R}^d} \left((\nabla_x \phi_0)^2 + (\partial_t \phi)^2 + 2(\partial_t \phi \cdot \nabla_x \phi_0) + 2\partial_t \phi_0 \sum_{i=1}^d \partial_{x_i} \phi_i \right) dt d\mu_U(x) \\ &\leq \int_{I \times \mathbb{R}^d} \left(2(\nabla_x \phi_0)^2 + 2(\partial_t \phi)^2 + 2\partial_t \phi_0 \sum_{i=1}^d \partial_{x_i} \phi_i \right) dt d\mu_U(x). \end{aligned}$$

Terms with 4th power on v :

$$\begin{aligned} & \int_{I \times \mathbb{R}^{2d}} \sum_{i,j,p,q=1}^d v_i v_j v_p v_q \partial_{x_i} \phi_j \partial_{x_p} \phi_q dt d\rho_\infty \\ &= \int_{I \times \mathbb{R}^d} \left(3 \sum_{i=1}^d (\partial_{x_i} \phi_i)^2 + \sum_{1 \leq i \neq j \leq d} (|\partial_{x_i} \phi_j|^2 + \partial_{x_i} \phi_i \partial_{x_j} \phi_j + \partial_{x_i} \phi_j \partial_{x_j} \phi_i) \right) dt d\mu_U(x) \\ &\leq \int_{I \times \mathbb{R}^d} \left(\left(\sum_{i=1}^d \partial_{x_i} \phi_i \right)^2 + 2 \sum_{i,j=1}^d |\partial_{x_i} \phi_j|^2 \right) dt d\mu_U(x). \end{aligned}$$

Now we look at the terms with “ $(-v_k \partial_{x_k} U)_+$ ”.

Terms where $(-v_k \partial_{x_k} U)_+$ are appearing twice, in which case the overall power of v is even and thus Lemma 2.4 is applicable:

$$\begin{aligned} & \int_{I \times \mathbb{R}^{2d}} 4 \sum_{k,p=1}^d (-v_k \partial_{x_k} U)_+ (-v_p \partial_{x_p} U)_+ v_k v_p \phi_k \phi_p dt d\rho_\infty \\ &= \int_{I \times \mathbb{R}^{2d}} \left(2 \sum_{k=1}^d (-v_k \partial_{x_k} U)^2 v_k^2 \phi_k^2 + \sum_{1 \leq k \neq p \leq d} v_k^2 v_p^2 \phi_k \partial_{x_k} U \phi_p \partial_{x_p} U \right) dt d\rho_\infty \\ &= \int_{I \times \mathbb{R}^d} \left(6 \sum_{k=1}^d \phi_k^2 (\partial_{x_k} U)^2 + \sum_{1 \leq k \neq p \leq d} \phi_k \partial_{x_k} U \phi_p \partial_{x_p} U \right) dt d\mu_U(x) \\ &= \int_{I \times \mathbb{R}^d} \left(\left(\sum_{k=1}^d \phi_k \partial_{x_k} U \right)^2 + 5 \sum_{k=1}^d \phi_k^2 (\partial_{x_k} U)^2 \right) dt d\mu_U(x). \end{aligned}$$

Cross terms with $(-v_k \partial_{x_k} U)_+$ where we could still use Lemma 2.4 due to an overall even power of v :

$$\begin{aligned} & \int_{I \times \mathbb{R}^{2d}} \left(4 \partial_t \phi_0 \sum_{k=1}^d (-v_k \partial_{x_k} U)_+ v_k \phi_k + 4 \sum_{i,j,k=1}^d v_i v_j \partial_{x_i} \phi_j (-v_k \partial_{x_k} U)_+ v_k \phi_k \right) dt d\rho_\infty \\ &= \int_{I \times \mathbb{R}^{2d}} \left(-2 \partial_t \phi_0 \sum_{k=1}^d v_k^2 \partial_{x_k} U \phi_k - 2 \sum_{i=1}^d v_i^4 \partial_{x_i} \phi_i \partial_{x_i} U \phi_i \right. \\ &\quad \left. - 2 \sum_{1 \leq i \neq j \leq d} v_i^2 v_j^2 \partial_{x_i} \phi_i \partial_{x_j} U \phi_j \right) dt d\rho_\infty \\ &= \int_{I \times \mathbb{R}^d} \left(-2 \partial_t \phi_0 \sum_{k=1}^d \partial_{x_k} U \phi_k - 6 \sum_{i=1}^d \partial_{x_i} \phi_i \partial_{x_i} U \phi_i - 2 \sum_{1 \leq i \neq j \leq d} \partial_{x_i} \phi_i \partial_{x_j} U \phi_j \right) dt d\mu_U(x) \\ &\leq \int_{I \times \mathbb{R}^d} \left(-2 \left(\partial_t \phi_0 + \sum_{i=1}^d \partial_{x_i} \phi_i \right) \left(\sum_{k=1}^d \phi_k \partial_{x_k} U \right) + 2 \sum_{i=1}^d (|\partial_{x_i} \phi_i|^2 + |\phi_i \partial_{x_i} U|^2) \right) dt d\mu_U(x). \end{aligned}$$

Finally cross terms with $(-v_k \partial_{x_k} U)_+$ where one cannot use Lemma 2.4 due to an overall odd power of v . In this case, instead of calculating an exact integral (which we actually can, but it does not yield a better bound), for simplicity we control these terms by what we have calculated above:

$$\begin{aligned} & -4 \int_{I \times \mathbb{R}^{2d}} v \cdot (\partial_t \phi + \nabla_x \phi_0) \sum_{k=1}^d (-v_k \partial_{x_k} U)_+ v_k \phi_k dt d\rho_\infty \\ &= -4 \int_{I \times \mathbb{R}^{2d}} \sum_{k=1}^d (\partial_t \phi_k + \partial_{x_k} \phi_0) (-v_k \partial_{x_k} U)_+ v_k^2 \phi_k dt d\rho_\infty \\ &\leq \int_{I \times \mathbb{R}^{2d}} \left(\sum_{k=1}^d v_k^4 (\partial_t \phi_k + \partial_{x_k} \phi_0)^2 + 4 \sum_{k=1}^d (-v_k \partial_{x_k} U)_+^2 \phi_k^2 \right) dt d\rho_\infty \\ &= \int_{I \times \mathbb{R}^{2d}} \left(3 \sum_{k=1}^d (\partial_t \phi_k + \partial_{x_k} \phi_0)^2 + 2 \sum_{k=1}^d (v_k \partial_{x_k} U)^2 \phi_k^2 \right) dt d\rho_\infty \\ &\leq \int_{I \times \mathbb{R}^d} \left(6 \sum_{k=1}^d ((\partial_t \phi_k)^2 + (\partial_{x_k} \phi_0)^2) + 2 \sum_{k=1}^d \phi_k^2 (\partial_{x_k} U)^2 \right) dt d\mu_U(x). \end{aligned}$$

Therefore, combining these calculations, we obtain finally

$$\begin{aligned} \|\mathcal{J}\|_{L^2(\lambda \times \rho_\infty)}^2 &\leq \int_{I \times \mathbb{R}^d} \left(\left| \partial_t \phi_0 + \sum_{i=1}^d \partial_{x_i} \phi_i - \sum_{i=1}^d \phi_i \partial_{x_i} U \right|^2 + 8 \sum_{i,j=0}^d |\partial_{x_i} \phi_j|^2 \right. \\ &\quad \left. + 9 \sum_{k=1}^d (\partial_{x_k} U)^2 \phi_k^2 \right) dt d\mu_U(x) \\ &\stackrel{(18),(20),(37)}{\leq} C \left(1 + \frac{1}{\sqrt{m}T} + \frac{R_{ZZ}}{\sqrt{m}} + R_{ZZ}T \right)^2 \|\Pi_v f\|_{L^2(\lambda \times \mu_U)}^2. \quad \square \end{aligned}$$

REMARK 2.7. Our bound in Lemma 2.6 can be improved for some specific cases. For example, if the potential has a separate form $U(x) = \sum_{k=1}^d U_k(x_k)$ with $U_k''(x) \geq -L$ for

all k , we claim the convergence rate ν is dimension independent, regardless of the growth condition of U , recovering the result in [1].

For the proof of this, we need to revisit the construction of the test functions ϕ_k in the proof of [15], Lemma 2.6, and make a more refined estimate than that in Lemma 2.6. We will follow the notation of the proof of [15], Lemma 2.6. Let us decompose

$$\Pi_\nu f = f^\perp + c_0 \left(t - \frac{T}{2} \right) + \sum_\alpha (c_\alpha^+ e^{\alpha t} + c_\alpha^- e^{\alpha(T-t)}) w_\alpha(x),$$

where c_0, c_α^\pm are numbers, f^\perp is perpendicular to all harmonic functions in $\lambda \times \mu_U$, in the sense that for any $g \in H^2(\lambda \times \mu_U)$,

$$\Delta_{t,x} g = -\partial_{tt} g + \nabla_x^* \nabla_x g = 0 \quad \Rightarrow \quad \int_{I \times \mathbb{R}^d} f^\perp g \, dt \, d\mu_U(x) = 0,$$

and α^2, w_α are corresponding eigenvalues and eigenfunctions of $\nabla_x^* \nabla_x$:

$$\nabla_x^* \nabla_x w_\alpha = \alpha^2 w_\alpha, \quad \|w_\alpha\|_{L^2(\mu_U)} = 1.$$

By linear combination, it suffices to prove in both cases $\Pi_\nu f = f^\perp$ and $\Pi_\nu f = e^{\alpha t} w_\alpha(x)$ (note in the case $\Pi_\nu f = t - \frac{T}{2}$ the corresponding $\phi_k = 0$ for $k \geq 1$, and thus (40) trivially holds), the corresponding functions ϕ_k satisfy

$$(40) \quad \sum_{k=1}^d \int_{I \times \mathbb{R}^d} \phi_k^2 \partial_{x_k x_k} U \, dt \, d\mu_U(x) \leq \|\Pi_\nu f\|_{L^2(\lambda \times \mu_U)}^2.$$

First consider the case $\Pi_\nu f = f^\perp, \phi_k = \partial_{x_k} u$ where u is the solution of the elliptic equation

$$(41) \quad \begin{cases} \Delta_{t,x} u = f^\perp & \text{in } I \times \mathbb{R}^d, \\ \partial_t u(t=0, \cdot) = \partial_t u(t=T, \cdot) = 0 & \text{in } \mathbb{R}^d. \end{cases}$$

By Bochner’s formula, using the fact that $U(x) = \sum_{k=1}^d U_k(x_k)$,

$$\begin{aligned} \sum_{i,j=0}^d \|\partial_{x_i x_j} u\|_{L^2(\lambda \times \mu_U)}^2 &= \|\Delta_{t,x} u\|_{L^2(\lambda \times \mu_U)}^2 - \int_{I \times \mathbb{R}^d} \nabla_x u^\top \nabla_x^2 U \nabla_x u \, dt \, d\mu_U(x) \\ &= \|f^\perp\|_{L^2(\lambda \times \mu_U)}^2 - \sum_{k=1}^d \int_{I \times \mathbb{R}^d} (\partial_{x_k} u)^2 U_k''(x_k) \, dt \, d\mu_U(x), \end{aligned}$$

this yields (40) since $\phi_k = \partial_{x_k} u$.

For the case $\Pi_\nu f = e^{\alpha t} w_\alpha$ for a particular $\alpha, \phi_k = \psi(t) \partial_{x_k} w_\alpha(x)$, where

$$\|\psi(t)\|_{L^2(I)} \leq \frac{1}{\alpha^2} \|\Pi_\nu f\|_{L^2(\lambda \times \mu_U)}.$$

Moreover, again by Bochner’s formula, using $\|\nabla_x^* \nabla_x w_\alpha\|_{L^2(\mu_U)} = \alpha^2 \|w_\alpha\|_{L^2(\mu_U)} = \alpha^2$,

$$\begin{aligned} \sum_{i,j=1}^d \|\partial_{x_i x_j} w_\alpha\|_{L^2(I \times \mu_U)}^2 &= \|\nabla_x^* \nabla_x w_\alpha\|_{L^2(\lambda \times \mu_U)}^2 - \int_{I \times \mathbb{R}^d} \nabla_x w_\alpha^\top \nabla_x^2 U \nabla_x w_\alpha \, d\mu_U(x) \\ &= \alpha^4 - \sum_{k=1}^d \int_{I \times \mathbb{R}^d} (\partial_{x_k} w_\alpha)^2 U_k''(x_k) \, d\mu_U(x). \end{aligned}$$

Therefore $\sum_{k=1}^d \int_{I \times \mathbb{R}^d} (\partial_{x_k} w_\alpha)^2 U_k''(x_k) \, d\mu_U(x) \leq \alpha^4$ and hence

$$\begin{aligned} \sum_{k=1}^d \int_{I \times \mathbb{R}^d} \phi_k^2 \partial_{x_k x_k} U \, dt \, d\mu_U(x) &= \|\psi(t)\|_{L^2(I)}^2 \sum_{k=1}^d \int_{I \times \mathbb{R}^d} (\partial_{x_k} w_\alpha)^2 U_k''(x_k) \, d\mu_U(x) \\ &\leq \|\Pi_v f\|_{L^2(\lambda \times \mu_U)}^2. \end{aligned}$$

The estimate (40) follows from linear combination. Substituting into (38) we obtain (37) with $R_{ZZ} = R$, so that we have a dimension-independent convergence rate assuming $U_k''(x_k) \geq -L$, even without an upper bound on $\nabla_x^2 U$ besides Assumption 2. Moreover, if we further assume $U_k''(x_k) \geq 0$ for all k , then we have convergence rate $O(\sqrt{m})$ after optimizing in γ .

2.2. *Bouncy particle sampler.* In this case $K = 1$, and $n_1 = \frac{\nabla_x U}{|\nabla_x U|}$. In order to avoid notation conflicts, in this section, we write $\mathbf{n} = n_1$ and use

$$n_i = \frac{\partial_{x_i} U}{|\nabla_x U|}$$

to denote the i th component of \mathbf{n} . As \mathbf{n} is normalized, $\sum_{i=1}^d n_i^2 = 1$.

Recall that we want to estimate \mathcal{J} , which for BPS is given by

$$\mathcal{J} = -\partial_t \phi_0 + v \cdot \nabla_x \phi_0 + v \cdot \partial_t \phi - \sum_{i=1}^d v_i v \cdot \partial_{x_i} \phi - 2(-v \cdot \mathbf{n})_+ (v \cdot \mathbf{n}) (\phi \cdot \nabla_x U).$$

LEMMA 2.8. *Let $\phi_i, i = 0, \dots, d$ be the test functions as in Lemma 2.2. Then*

$$(42) \quad \begin{aligned} &\int_{I \times \mathbb{R}^d} (\phi \cdot \nabla_x U)^2 \, dt \, d\mu_U(x) \\ &\leq Cd \left(1 + \frac{1}{\sqrt{m}T} + \frac{R}{\sqrt{m}} + RT \right)^2 \int_{I \times \mathbb{R}^d} (\Pi_v f)^2 \, dt \, d\mu_U(x). \end{aligned}$$

Here R is defined as in Theorem 1.1.

Let us remark that the factor d on the right-hand side of the above estimate is the reason that the convergence rate we obtain is degraded by a factor of \sqrt{d} for BPS.

PROOF. By construction of the test functions (18), we have

$$\phi \cdot \nabla_x U = \Pi_v f + \partial_t \phi_0 + \sum_{i=1}^d \partial_{x_i} \phi_i.$$

Thus

$$\begin{aligned} \int_{I \times \mathbb{R}^d} (\phi \cdot \nabla_x U)^2 \, dt \, d\mu_U(x) &= \int_{I \times \mathbb{R}^d} \left(\Pi_v f + \partial_t \phi_0 + \sum_{i=1}^d \partial_{x_i} \phi_i \right)^2 \, dt \, d\mu_U(x) \\ &\leq (d+2) \int_{I \times \mathbb{R}^d} \left((\Pi_v f)^2 + (\partial_t \phi_0)^2 + \sum_{i=1}^d (\partial_{x_i} \phi_i)^2 \right) \, dt \, d\mu_U(x) \\ &\stackrel{(20)}{\leq} Cd \left(1 + \frac{1}{\sqrt{m}T} + \frac{R}{\sqrt{m}} + RT \right)^2 \int_{I \times \mathbb{R}^d} (\Pi_v f)^2 \, dt \, d\mu_U(x), \end{aligned}$$

where the first inequality follows from Cauchy–Schwarz. \square

PROOF OF LEMMA 2.5 FOR BOUNCY PARTICLE SAMPLER. Similar to the proof for ZZ, we will expand $\|\mathcal{J}\|_{L^2(\lambda \times \rho_\infty)}^2$ and organize its terms according to their powers on v and whether $(-v \cdot \mathbf{n})_+$ appears in the expression. Terms that do not contain $(-v \cdot \mathbf{n})_+$ are identical to those for ZZ and thus calculations are omitted.

Next we look at terms where $(-v \cdot \mathbf{n})_+$ appears twice, in which the overall power of v is even so Lemma 2.4 can be applied:

$$\begin{aligned}
 & \int_{I \times \mathbb{R}^{2d}} 4(-v \cdot \mathbf{n})_+^2 (v \cdot \mathbf{n})^2 (\phi \cdot \nabla_x U)^2 dt d\rho_\infty(x, v) \\
 &= \int_{I \times \mathbb{R}^{2d}} 2(v \cdot \mathbf{n})^4 (\phi \cdot \nabla_x U)^2 dt d\rho_\infty(x, v) \\
 &= \int_{I \times \mathbb{R}^{2d}} 2 \sum_{i,j,k,p=1}^d v_i v_j v_k v_p n_i n_j n_k n_p (\phi \cdot \nabla_x U)^2 dt d\rho_\infty(x, v) \\
 (43) \quad &= \int_{I \times \mathbb{R}^{2d}} \left(2 \sum_{i=1}^d v_i^4 n_i^4 + 6 \sum_{1 \leq i \neq j \leq d} v_i^2 v_j^2 n_i^2 n_j^2 \right) (\phi \cdot \nabla_x U)^2 dt d\rho_\infty(x, v) \\
 &= \int_{I \times \mathbb{R}^d} \left(6 \sum_{i=1}^d n_i^4 + 6 \sum_{1 \leq i \neq j \leq d} n_i^2 n_j^2 \right) (\phi \cdot \nabla_x U)^2 dt d\mu_U(x) \\
 &= 6 \int_{I \times \mathbb{R}^d} \left(\sum_i n_i^2 \right)^2 (\phi \cdot \nabla_x U)^2 dt d\mu_U(x) \\
 &= 6 \int_{I \times \mathbb{R}^d} (\phi \cdot \nabla_x U)^2 dt d\mu_U(x).
 \end{aligned}$$

Cross terms with $(-v \cdot \mathbf{n})_+$ appearing once and the overall power of v is even:

$$\begin{aligned}
 & \int_{I \times \mathbb{R}^{2d}} \left(4\partial_t \phi_0 (-v \cdot \mathbf{n})_+ (v \cdot \mathbf{n}) (\phi \cdot \nabla_x U) \right. \\
 & \quad \left. + 4 \sum_{i,j=1}^d v_i v_j \partial_{x_i} \phi_j (-v \cdot \mathbf{n})_+ (v \cdot \mathbf{n}) (\phi \cdot \nabla_x U) \right) dt d\rho_\infty \\
 &= -2 \int_{I \times \mathbb{R}^{2d}} \left(\partial_t \phi_0 (v \cdot \mathbf{n})^2 + \sum_{i,j=1}^d v_i v_j \partial_{x_i} \phi_j (v \cdot \mathbf{n})^2 \right) (\phi \cdot \nabla_x U) dt d\rho_\infty \\
 &= -2 \int_{I \times \mathbb{R}^{2d}} \left(\partial_t \phi_0 \sum_{i=1}^d n_i^2 + \sum_{i,j,p,q=1}^d v_i v_j v_p v_q n_p n_q \partial_{x_i} \phi_j \right) (\phi \cdot \nabla_x U) dt d\rho_\infty \\
 &= -2 \int_{I \times \mathbb{R}^{2d}} \left(\partial_t \phi_0 + \sum_{i=1}^d v_i^4 n_i^2 \partial_{x_i} \phi_i + \sum_{1 \leq i \neq j \leq d} v_i^2 v_j^2 n_j^2 \partial_{x_i} \phi_i \right. \\
 & \quad \left. + 2 \sum_{1 \leq i \neq j \leq d} v_i^2 v_j^2 n_i n_j \partial_{x_i} \phi_j \right) (\phi \cdot \nabla_x U) dt d\rho_\infty \\
 &= -2 \int_{I \times \mathbb{R}^d} \left(\partial_t \phi_0 + 3 \sum_{i=1}^d n_i^2 \partial_{x_i} \phi_i + \sum_{1 \leq i \neq j \leq d} n_j^2 \partial_{x_i} \phi_i \right.
 \end{aligned}$$

$$\begin{aligned}
 &+ 2 \sum_{1 \leq i \neq j \leq d} \mathbf{n}_i \mathbf{n}_j \partial_{x_i} \phi_j \Big) (\phi \cdot \nabla_x U) \, dt \, d\mu_U(x) \\
 &= -2 \int_{I \times \mathbb{R}^d} \left(\partial_t \phi_0 + \sum_{i=1}^d \partial_{x_i} \phi_i + 2 \sum_{i,j=1}^d \mathbf{n}_i \mathbf{n}_j \partial_{x_i} \phi_j \right) (\phi \cdot \nabla_x U) \, dt \, d\mu_U(x) \\
 &\leq 2 \int_{I \times \mathbb{R}^d} \left(- \left(\partial_t \phi_0 + \sum_{i=1}^d \partial_{x_i} \phi_i \right) (\phi \cdot \nabla_x U) \right. \\
 &\quad \left. + \sum_{i,j=1}^d (\mathbf{n}_i^2 \mathbf{n}_j^2 (\phi \cdot \nabla_x U)^2 + (\partial_{x_i} \phi_j)^2) \right) dt \, d\mu_U(x) \\
 &= 2 \int_{I \times \mathbb{R}^d} \left(- \left(\partial_t \phi_0 + \sum_{i=1}^d \partial_{x_i} \phi_i \right) (\phi \cdot \nabla_x U) + (\phi \cdot \nabla_x U)^2 + \sum_{i,j=1}^d (\partial_{x_i} \phi_j)^2 \right) dt \, d\mu_U(x).
 \end{aligned}$$

Finally the cross terms with $(-v \cdot \mathbf{n})_+$ appearing once and an odd overall power on v , in which we again control by terms we have calculated above

$$\begin{aligned}
 &-4 \int_{I \times \mathbb{R}^{2d}} v \cdot (\partial_t \phi + \nabla_x \phi_0) (-v \cdot \mathbf{n})_+ (v \cdot \mathbf{n}) (\phi \cdot \nabla_x U) \, dt \, d\rho_\infty \\
 &\leq 2 \int_{I \times \mathbb{R}^{2d}} (|v \cdot (\partial_t \phi + \nabla_x \phi_0)|^2 + (-v \cdot \mathbf{n})_+^2 (v \cdot \mathbf{n})^2 (\phi \cdot \nabla_x U)^2) \, dt \, d\rho_\infty \\
 &\stackrel{(43)}{\leq} \int_{I \times \mathbb{R}^d} (4|\partial_t \phi|^2 + 4|\nabla_x \phi_0|^2 + 3(\phi \cdot \nabla_x U)^2) \, dt \, d\mu_U(x).
 \end{aligned}$$

Therefore, combining these calculations, we obtain

$$\begin{aligned}
 \|\mathcal{J}\|_{L^2(\lambda \times \rho_\infty)}^2 &\leq \int_{I \times \mathbb{R}^d} \left(\left(\partial_t \phi_0 + \sum_{i=1}^d \partial_{x_i} \phi_i - \phi \cdot \nabla_x U \right)^2 + 6 \sum_{i,j=0}^d |\partial_{x_i} \phi_j|^2 \right. \\
 &\quad \left. + 16(\phi \cdot \nabla_x U)^2 \right) dt \, d\mu_U(x) \\
 &\stackrel{(18),(20),(42)}{\leq} Cd \left(1 + \frac{1}{\sqrt{mT}} + \frac{R}{\sqrt{m}} + RT \right)^2 \|\Pi_v f\|_{L^2(\lambda \times \mu_U)}^2. \quad \square
 \end{aligned}$$

APPENDIX: PROOF OF LEMMA 2.2

In this appendix, we prove Lemma 2.2 to make the paper self-contained; the proof follows largely our previous work [15]. Let us first state an easy lemma on Poincaré inequality for the product space.

LEMMA A.1 (Poincaré inequality). For $f \in H^1(\lambda \times \mu_U)$,

$$(44) \quad \|f - (f)_{\lambda \times \mu_U}\|_{L^2(\lambda \times \mu_U)}^2 \leq \max \left\{ \frac{1}{m}, \frac{T^2}{\pi^2} \right\} (\|\partial_t f\|_{L^2(\lambda \times \mu_U)}^2 + \|\nabla_x f\|_{L^2(\lambda \times \mu_U)}^2).$$

PROOF. Define $(f)_x(t) = \int_{\mathbb{R}^d} f(x, t) \, d\mu_U(x)$. Then,

$$\begin{aligned}
 &\|f - (f)_{\lambda \times \mu_U}\|_{L^2(\lambda \times \mu_U)}^2 \\
 &= \|f - (f)_x\|_{L^2(\lambda \times \mu_U)}^2 + \|(f)_x - (f)_{\lambda \times \mu_U}\|_{L^2(\lambda \times \mu_U)}^2
 \end{aligned}$$

$$\begin{aligned}
 &\leq \int_0^T \|f(t, x) - (f)_x(t)\|_{L^2_{\mu_U}}^2 dt + \int_0^T \left(\int_{\mathbb{R}^d} \left(f(t, x) - \frac{1}{T} \int_0^T f(s, x) ds \right) d\mu_U(x) \right)^2 dt \\
 &\stackrel{(8)}{\leq} \frac{1}{m} \int_0^T \|\nabla_x f\|_{L^2_{\mu_U}}^2(t) dt + \int_{\mathbb{R}^d} \int_0^T \left(f(t, x) - \frac{1}{T} \int_0^T f(s, x) ds \right)^2 dt d\mu_U(x) \\
 &\leq \frac{1}{m} \|\nabla_x f\|_{L^2(\lambda \times \mu_U)}^2 + \frac{T^2}{\pi^2} \int_{\mathbb{R}^d} \|\partial_t f(x)\|_{L^2(0, T)}^2 d\mu_U(x) \\
 &= \max \left\{ \frac{1}{m}, \frac{T^2}{\pi^2} \right\} (\|\partial_t f\|_{L^2(\lambda \times \mu_U)}^2 + \|\nabla_x f\|_{L^2(\lambda \times \mu_U)}^2),
 \end{aligned}$$

where the last inequality follows the standard Poincaré inequality on $(0, T)$:

$$\left\| f - \frac{1}{T} \int_0^T f(s) ds \right\|_{L^2(0, T)} \leq \frac{T}{\pi} \|f'(t)\|_{L^2(0, T)}. \quad \square$$

LEMMA A.2 ([40], Lemma A.24). For any $\phi \in H^1(\lambda \times \mu_U)$, we have

$$(45) \quad \|\phi \nabla_x U\|_{L^2(\lambda \times \mu_U)}^2 \leq 8\|\nabla_x \phi\|_{L^2(\lambda \times \mu_U)}^2 + 2(M^2 d^2 + Md)\|\phi\|_{L^2(\lambda \times \mu_U)}^2,$$

where M is the constant in (9).

PROOF.

$$\begin{aligned}
 \|\phi \nabla_x U\|_{L^2(\lambda \times \mu_U)}^2 &= \int_{I \times \mathbb{R}^d} \phi^2 \nabla_x U \cdot \nabla_x U dt d\mu_U(x) \\
 &= \int_{I \times \mathbb{R}^d} \nabla_x \cdot (\phi^2 \nabla_x U) dt d\mu_U(x) \\
 &= 2 \int_{I \times \mathbb{R}^d} \phi \nabla_x \phi \cdot \nabla_x U dt d\mu_U(x) + \int_{I \times \mathbb{R}^d} \phi^2 \Delta_x U dt d\mu_U(x) \\
 &\stackrel{(9)}{\leq} \frac{1}{4} \|\phi \nabla_x U\|_{L^2(\lambda \times \mu_U)}^2 + 4\|\nabla_x \phi\|_{L^2(\lambda \times \mu_U)}^2 \\
 &\quad + Md\|\phi\|_{L^2(\lambda \times \mu_U)}^2 + Md \int_{I \times \mathbb{R}^d} \phi^2 |\nabla_x U| dt d\mu_U(x) \\
 &\leq \frac{1}{4} \|\phi \nabla_x U\|_{L^2(\lambda \times \mu_U)}^2 + 4\|\nabla_x \phi\|_{L^2(\lambda \times \mu_U)}^2 + Md\|\phi\|_{L^2(\lambda \times \mu_U)}^2 \\
 &\quad + M^2 d^2 \|\phi\|_{L^2(\lambda \times \mu_U)}^2 + \frac{1}{4} \|\phi \nabla_x U\|_{L^2(\lambda \times \mu_U)}^2.
 \end{aligned}$$

The estimate (45) is obtained after rearranging. \square

LEMMA A.3. For any $u \in H^2(\lambda \times \mu_U)$ such that $(\partial_t u, \nabla_x u)^\top \in H_0^1(\lambda \times \mu_U)^{d+1}$,

$$\begin{aligned}
 (46) \quad \|D^2 u\|_{L^2(\lambda \times \mu_U)}^2 &:= \sum_{i, j=0}^d \|\partial_{x_i} \partial_{x_j} u\|_{L^2(\lambda \times \mu_U)}^2 \\
 &\leq C_0 \left(\|\Delta_{t, x} u\|_{L^2(\lambda \times \mu_U)}^2 + R^2 \sum_{i=0}^d \|\partial_{x_i} u\|_{L^2(\lambda \times \mu_U)}^2 \right).
 \end{aligned}$$

Here C_0 is a universal constant, R is the same constant defined in (12).

PROOF. The starting point of the proof is Bochner’s formula

$$\sum_{i,j=0}^d |\partial_{x_i,x_j}u|^2 = \bar{\nabla}u \cdot \bar{\nabla}\Delta_{t,x}u - (\nabla_x u)^\top \nabla_x^2 U \nabla_x u - \Delta_{t,x} \frac{|\bar{\nabla}u|^2}{2}.$$

Integrate over $\lambda \times \mu_U$ and (noticing the last term above has integral zero) we get

$$(47) \quad \sum_{i,j=0}^d \|\partial_{x_i,x_j}u\|_{L^2(\lambda \times \mu_U)}^2 = \|\Delta_{t,x}u\|_{L^2(\lambda \times \mu_U)}^2 - \int_{I \times \mathbb{R}^d} (\nabla_x u)^\top \nabla_x^2 U \nabla_x u \, dt \, d\mu_U(x).$$

Let us first discuss the easier case when U satisfies $\nabla_x^2 U \geq -L\mathcal{I}$. We can estimate directly

$$(48) \quad \begin{aligned} \sum_{i,j=0}^d \|\partial_{x_i,x_j}u\|_{L^2(\lambda \times \mu_U)}^2 &= \|\Delta_{t,x}u\|_{L^2(\lambda \times \mu_U)}^2 - \int_{I \times \mathbb{R}^d} (\nabla_x u)^\top \nabla_x^2 U \nabla_x u \, dt \, d\mu_U(x) \\ &\leq \|\Delta_{t,x}u\|_{L^2(\lambda \times \mu_U)}^2 + L\|\nabla_x u\|_{L^2(\lambda \times \mu_U)}^2. \end{aligned}$$

This verifies the conclusion in cases U is convex (setting $L = 0$) and $\nabla_x^2 U \geq -L\mathcal{I}$.

We now deal with the more general case, without assuming $\nabla_x^2 U \geq -L\mathcal{I}$. For the rest of the proof, we let C_0 be a universal constant independent of all parameters, and may change line by line. Using (45) with $\phi = \partial_{x_i}u$, $i = 1, \dots, d$,

$$\begin{aligned} &\int_{I \times \mathbb{R}^d} |\nabla_x u|^2 |\nabla_x U|^2 \, dt \, d\mu_U(x) \\ &= \sum_{i=1}^d \int_{I \times \mathbb{R}^d} (\partial_{x_i}u)^2 |\nabla_x U|^2 \, dt \, d\mu_U(x) \\ &\stackrel{(45)}{\leq} C_0 \left(\|D^2u\|_{L^2(\lambda \times \mu_U)}^2 + M^2 d^2 \int_{I \times \mathbb{R}^d} |\nabla_x u|^2 \, dt \, d\mu_U(x) \right) \\ &\stackrel{(47)}{\leq} C_0 \left(\|\Delta_{t,x}u\|_{L^2(\lambda \times \mu_U)}^2 + M^2 d^2 \int_{I \times \mathbb{R}^d} |\nabla_x u|^2 \, dt \, d\mu_U(x) \right. \\ &\quad \left. - \int_{I \times \mathbb{R}^d} (\nabla_x u)^\top \nabla_x^2 U \nabla_x u \, dt \, d\mu_U(x) \right) \\ &\stackrel{(9)}{\leq} C_0 \left(\|\Delta_{t,x}u\|_{L^2(\lambda \times \mu_U)}^2 + M^2 d^2 \int_{I \times \mathbb{R}^d} |\nabla_x u|^2 \, dt \, d\mu_U(x) \right. \\ &\quad \left. + M \int_{I \times \mathbb{R}^d} |\nabla_x u|^2 (1 + |\nabla_x U|) \, dt \, d\mu_U(x) \right) \\ &\leq C_0 \left(\|\Delta_{t,x}u\|_{L^2(\lambda \times \mu_U)}^2 + M^2 d^2 \int_{I \times \mathbb{R}^d} |\nabla_x u|^2 \, dt \, d\mu_U(x) \right. \\ &\quad \left. + M^2 \int_{I \times \mathbb{R}^d} |\nabla_x u|^2 \, dt \, d\mu_U(x) \right) + \frac{1}{2} \int_{I \times \mathbb{R}^d} |\nabla_x u|^2 |\nabla_x U|^2 \, dt \, d\mu_U(x). \end{aligned}$$

Rearranging the terms, we arrive at

$$(49) \quad \begin{aligned} &\int_{I \times \mathbb{R}^d} |\nabla_x u|^2 |\nabla_x U|^2 \, dt \, d\mu_U(x) \\ &\leq C_0 \left(\|\Delta_{t,x}u\|_{L^2(\lambda \times \mu_U)}^2 + M^2 d^2 \int_{I \times \mathbb{R}^d} |\nabla_x u|^2 \, dt \, d\mu_U(x) \right). \end{aligned}$$

Therefore, by (49),

$$\begin{aligned}
 \|D^2u\|_{L^2(\lambda \times \mu_U)}^2 &\stackrel{(9),(47)}{\leq} C_0 \left(\|\Delta_{t,x}u\|_{L^2(\lambda \times \mu_U)}^2 + M \int_{I \times \mathbb{R}^d} |\nabla_x u|^2 (1 + |\nabla_x U|) dt d\mu_U(x) \right) \\
 &\leq C_0 (\|\Delta_{t,x}u\|_{L^2(\lambda \times \mu_U)}^2 + M \|\nabla_x u\|_{L^2(\lambda \times \mu_U)}^2 \\
 &\quad + M \|\nabla_x u\|_{L^2(\lambda \times \mu_U)} \|\nabla_x u\|_{\nabla_x U}\|_{L^2(\lambda \times \mu_U)}) \\
 &\stackrel{(49)}{\leq} C_0 (\|\Delta_{t,x}u\|_{L^2(\lambda \times \mu_U)}^2 + M \|\nabla_x u\|_{L^2(\lambda \times \mu_U)}^2 \\
 &\quad + M \|\nabla_x u\|_{L^2(\lambda \times \mu_U)} (\|\Delta_{t,x}u\|_{L^2(\lambda \times \mu_U)} + Md \|\nabla_x u\|_{L^2(\lambda \times \mu_U)})) \\
 &\leq C_0 (\|\Delta_{t,x}u\|_{L^2(\lambda \times \mu_U)}^2 + M^2 d \|\nabla_x u\|_{L^2(\lambda \times \mu_U)}^2). \quad \square
 \end{aligned}$$

LEMMA A.4. Consider the following elliptic equation:

$$(50) \quad \begin{cases} \Delta_{t,x}u = h & \text{in } I \times \mathbb{R}^d, \\ \partial_t u(t = 0, \cdot) = \partial_t u(t = T, \cdot) = 0 & \text{in } \mathbb{R}^d. \end{cases}$$

Assume $h \in H^{-1}(\lambda \times \mu_U)$, and $(h)_{\lambda \times \mu_U} = 0$. Define the function space

$$V = \left\{ u \in H^1(\lambda \times \mu_U) : \int_{I \times \mathbb{R}^d} u(t, x) dt d\mu_U(x) = 0 \right\}.$$

Then:

(i) There exists a unique $u \in V$ which is a weak solution to (50). More precisely, for any $v \in H^1(\lambda \times \mu_U)$, we have

$$\int_{I \times \mathbb{R}^d} (\partial_t u \partial_t v + \nabla_x u \cdot \nabla_x v) dt d\mu_U(x) = \int_{I \times \mathbb{R}^d} h v dt d\mu_U(x).$$

When $h \in L^2(\lambda \times \mu_U)$, we have the estimate

$$(51) \quad \|\partial_t u\|_{L^2(\lambda \times \mu_U)}^2 + \|\nabla_x u\|_{L^2(\lambda \times \mu_U)}^2 \leq \max \left\{ \frac{1}{m}, \frac{T^2}{\pi^2} \right\} \|h\|_{L^2(\lambda \times \mu_U)}^2.$$

(ii) If $h \in L^2(\lambda \times \mu_U)$, then the solution u to (50) satisfies $u \in H^2(\lambda \times \mu_U)$.

PROOF. (i) V is a linear Hilbert space and has nonzero elements (any function constant in t , and H^1 and mean zero in x is included in V). Moreover, V is a subspace of $H^1(\lambda \times \mu_U)$, and for the rest of the paper we equip it with the $H^1(\lambda \times \mu_U)$ norm. We also define the following inner-product:

$$B(u, v) := \int_{I \times \mathbb{R}^d} (\partial_t u \partial_t v + \nabla_x u \cdot \nabla_x v) dt d\mu_U(x).$$

One can easily verify $B(\cdot, \cdot)$ is an inner product on V . Notice that if $B(u, u) = 0$ then $\partial_t u = \nabla_x u = 0$, leaving u to be a constant, which has to be 0 since $\int_{I \times \mathbb{R}^d} u dt d\mu_U(x) = 0$. If u is a weak solution of (50), then for any $v \in V$, $B(u, v) = \int_{I \times \mathbb{R}^d} h v dt d\mu_U(x)$, and necessarily $\int_{I \times \mathbb{R}^d} h dt d\mu_U(x) = 0$ when we take $v = 1$.

Since $\int_{I \times \mathbb{R}^d} u(t, x) dt d\mu_U(x) = 0$, by Poincaré inequality (Lemma A.1) we can show B is coercive under $H^1(\lambda \times \mu_U)$ norm in the sense of

$$\begin{aligned}
 B[u, u] &= \|\partial_t u\|_{L^2(\lambda \times \mu_U)}^2 + \|\nabla_x u\|_{L^2(\lambda \times \mu_U)}^2 \\
 &\geq \frac{1}{C} (\|\partial_t u\|_{L^2(\lambda \times \mu_U)}^2 + \|\nabla_x u\|_{L^2(\lambda \times \mu_U)}^2 + \|u\|_{L^2(\lambda \times \mu_U)}^2) \\
 &= \frac{1}{C} \|u\|_{H^1(\lambda \times \mu_U)}^2.
 \end{aligned}$$

We can also show B is bounded above since it is an inner-product and $B[u, u] \leq \|u\|_{H^1(\lambda \times \mu_U)}^2$. Define a linear functional on V : $H(v) := \int_{I \times \mathbb{R}^d} hv \, dt \, d\mu_U(x)$. One can verify the boundedness of H :

$$|H(v)| \leq \|h\|_{H^{-1}(\lambda \times \mu_U)} \|v\|_{H^1(\lambda \times \mu_U)}.$$

Thus by Lax–Milgram’s theorem, the equation (50) has a unique weak solution $u \in V$. Finally when $h \in L^2(\lambda \times \mu_U)$

$$\begin{aligned} & (\|\partial_t u\|_{L^2(\lambda \times \mu_U)}^2 + \|\nabla_x u\|_{L^2(\lambda \times \mu_U)}^2)^2 \\ &= B[u, u]^2 = \left(\int_{I \times \mathbb{R}^d} hu \, dt \, d\mu_U(x) \right)^2 \leq \|h\|_{L^2(\lambda \times \mu_U)}^2 \|u\|_{L^2(\lambda \times \mu_U)}^2 \\ &\leq \max \left\{ \frac{1}{m}, \frac{T^2}{\pi^2} \right\} \|h\|_{L^2(\lambda \times \mu_U)}^2 (\|\partial_t u\|_{L^2(\lambda \times \mu_U)}^2 + \|\nabla_x u\|_{L^2(\lambda \times \mu_U)}^2), \end{aligned}$$

and the desired estimate follows.

(ii) For each $i = 1, 2, \dots, d$, consider the elliptic equation

$$(52) \quad \begin{cases} \Delta_{t,x} w_i = \partial_{x_i} h - \nabla_x u \cdot \nabla_x \partial_{x_i} U & \text{in } I \times \mathbb{R}^d, \\ \partial_t w_i(t = 0, \cdot) = \partial_t w_i(t = T, \cdot) = 0 & \text{in } \mathbb{R}^d. \end{cases}$$

We first verify the rhs has total integral zero. Indeed

$$\begin{aligned} & \int_{I \times \mathbb{R}^d} (\partial_{x_i} h - \nabla_x u \cdot \nabla_x \partial_{x_i} U) \, dt \, d\mu_U(x) \\ &= \int_{I \times \mathbb{R}^d} (h \partial_{x_i} U - \nabla_x u \cdot \nabla_x \partial_{x_i} U) \, dt \, d\mu_U(x) \\ &= \int_{I \times \mathbb{R}^d} ((-\partial_{tt} u + \nabla_x^* \nabla_x u) \partial_{x_i} U - \nabla_x u \cdot \nabla_x \partial_{x_i} U) \, dt \, d\mu_U(x) \\ &= \int_{I \times \mathbb{R}^d} (\partial_t u \partial_{t x_i} U + \nabla_x u \cdot \nabla_x \partial_{x_i} U - \nabla_x u \cdot \nabla_x \partial_{x_i} U) \, dt \, d\mu_U(x) = 0. \end{aligned}$$

The next step is to show rhs is in $H^{-1}(\lambda \times \mu_U)$. Pick a test function $\phi \in H^1(\lambda \times \mu_U)$ with $\|\phi\|_{H^1(\lambda \times \mu_U)} = 1$, and by Lemma A.2,

$$\begin{aligned} & \int_{I \times \mathbb{R}^d} (\partial_{x_i} h - \nabla_x u \cdot \nabla_x \partial_{x_i} U) \phi \, dt \, d\mu_U(x) \\ &\leq \int_{I \times \mathbb{R}^d} (-h \partial_{x_i} \phi + h \phi \partial_{x_i} U) \, dt \, d\mu_U(x) + \int_{I \times \mathbb{R}^d} |\phi \nabla_x u| |\nabla_x \partial_{x_i} U| \, dt \, d\mu(x) \\ &\stackrel{(9)}{\leq} \|h\|_{L^2(\lambda \times \mu_U)} (1 + \|\phi \partial_{x_i} U\|_{L^2(\lambda \times \mu_U)}) + M \int_{I \times \mathbb{R}^d} |\phi \nabla_x u| (1 + |\nabla_x U|) \, dt \, d\mu(x) \\ &\leq \|h\|_{L^2(\lambda \times \mu_U)} (1 + \|\phi \partial_{x_i} U\|_{L^2(\lambda \times \mu_U)}) + M \|\nabla_x u\|_{L^2(\lambda \times \mu_U)} (1 + \|\phi \nabla_x U\|_{L^2(\lambda \times \mu_U)}) \\ &\stackrel{(45),(51)}{\leq} C(M) \|h\|_{L^2(\lambda \times \mu_U)}, \end{aligned}$$

where $C(M) > 0$ is a constant depending on M . Therefore, by (i) we know there exists a $w_i \in V$ which is the weak solution of (52).

The next step is to verify $w_i = \partial_{x_i} u - \frac{1}{T} \int_{\lambda \times \mu_U} \partial_{x_i} u \, dt \, d\mu_U(x)$. We know both functions are in $L^2(\lambda \times \mu_U)$ with spatial integral zero. For derivations below, we use the shorthand notation

$(f, g) := \int_{I \times \mathbb{R}^d} fg \, dt \, d\mu_U(x)$, and we don't specify the regularities of f and g . Take any test function $\phi \in H^2(\lambda \times \mu_U)$. Using integration by parts it is easy to check

$$(-\partial_{tt} w_i + \nabla_x^* \nabla_x w_i, \phi) = (\partial_t w_i, \partial_t \phi) + (\nabla_x w_i, \nabla_x \phi).$$

Now we do the calculations using the equation

$$\begin{aligned} (-\partial_{tt} w_i + \nabla_x^* \nabla_x w_i, \phi) &= (\partial_{x_i} h - \nabla_x \partial_{x_i} U \cdot \nabla_x u, \phi) \\ &= (h, -\partial_{x_i} \phi + \phi \partial_{x_i} U) - (\nabla_x \partial_{x_i} U \cdot \nabla_x u, \phi) \\ &= (-\partial_{tt} u + \nabla_x^* \nabla_x u, -\partial_{x_i} \phi + \phi \partial_{x_i} U) - (\nabla_x \partial_{x_i} U \cdot \nabla_x u, \phi) \\ &= (\partial_t u, \partial_t (-\partial_{x_i} \phi + \phi \partial_{x_i} U)) + (\nabla_x u, \nabla_x (-\partial_{x_i} \phi + \phi \partial_{x_i} U)) \\ &\quad - (\nabla_x \partial_{x_i} U \cdot \nabla_x u, \phi) \\ &= (\partial_t u, \partial_t (-\partial_{x_i} \phi + \phi \partial_{x_i} U)) + (\nabla_x u, -\nabla_x \partial_{x_i} \phi + \partial_{x_i} U \nabla_x \phi) \\ &= (\partial_t \partial_{x_i} u, \partial_t \phi) + (\nabla_x \partial_{x_i} u, \nabla_x \phi). \end{aligned}$$

The equality holds when we replace $\partial_{x_i} u$ by $\partial_{x_i} u - \frac{1}{T} \int_{\lambda \times \mu_U} \partial_{x_i} u \, dt \, d\mu_U(x)$ as it is invariant under a constant shift. This shows that, as $L^2(\lambda \times \mu_U)$ functions, $w_i = \partial_{x_i} u - \frac{1}{T} \int_{I \times \mathbb{R}^d} \partial_{x_i} u \, dt \, d\mu_U(x)$. However we already have $w_i \in H^1(\lambda \times \mu_U)$, thus we have shown that $\partial_{x_i} u \in H^1(\lambda \times \mu_U)$ for each $i = 1, \dots, d$. Finally we use the equation $\partial_{tt} u = \nabla_x^* \nabla_x u - h$ to verify that $\partial_{tt} u \in L^2(\lambda \times \mu_U)$. This suffices to show $u \in H^2(\lambda \times \mu_U)$. \square

PROOF OF LEMMA 2.2. Let \mathbb{H} be the subspace of $L^2(\lambda \times \mu_U)$ that consists of ‘‘harmonic functions,’’ in other words, $f \in \mathbb{H}$ if and only if $\Delta_{t,x} f = 0$. We consider the decomposition $f = f^{(1)} + f^{(2)}$ where $f^{(1)} \in \mathbb{H}$ and $f^{(2)} \perp \mathbb{H}$. Since $1 \in \mathbb{H}$ we know $(f^{(2)})_{\lambda \times \mu_U} = 0$ and hence $(f^{(1)})_{\lambda \times \mu_U} = 0$. Therefore, by linearity it suffices to consider $f^{(1)}$ and $f^{(2)}$ separately. For $f^{(2)}$, the equation

$$(53) \quad \begin{cases} \Delta_{t,x} u = f^{(2)} & \text{in } I \times \mathbb{R}^d, \\ \partial_t u(t = 0, \cdot) = \partial_t u(t = T, \cdot) = 0 & \text{in } \mathbb{R}^d \end{cases}$$

has a unique solution $u \in V \cap H^2(\lambda \times \mu_U)$ by Lemma A.4. Moreover, for any $v \in \mathbb{H} \cap H^1(\lambda \times \mu_U)$, integration by parts yields

$$\begin{aligned} 0 &= \int_{I \times \mathbb{R}^d} f^{(2)} v \, dt \, d\mu(x) = B[u, v] \\ &= \int_{I \times \mathbb{R}^d} u \Delta_{t,x} v \, dt \, d\mu(x) + \int_{\mathbb{R}^d} (u(T) \partial_t v(T) - u(0) \partial_t v(0)) \, d\mu(x). \end{aligned}$$

Therefore, since v is arbitrary, we have $u(T) = u(0) = 0$, meaning $\nabla_x u \in H_0^1(\lambda \times \mu_U)^d$. We also have $\partial_t u \in H_0^1(\lambda \times \mu_U)$. Thus for the $f^{(2)}$ part, it suffices to take correspondingly $\phi_0^{(2)} = \partial_t u$, $\phi_i^{(2)} = \partial_{x_i} u$ with the estimates

$$(54) \quad \|\overline{\phi}^{(2)}\|_{L^2(\lambda \times \mu_U)}^2 = \|\overline{\nabla} u\|_{L^2(\lambda \times \mu_U)}^2 \stackrel{(51)}{\leq} \max\left\{\frac{1}{m}, \frac{T^2}{\pi^2}\right\} \|f^{(2)}\|_{L^2(\lambda \times \mu_U)}^2,$$

and

$$(55) \quad \|\overline{\nabla} \phi^{(2)}\|_{L^2(\lambda \times \mu_U)}^2 = \|D^2 u\|_{L^2(\lambda \times \mu_U)}^2 \stackrel{(46)}{\leq} C_0 \left(1 + \frac{R^2}{m} + R^2 T^2\right) \|f^{(2)}\|_{L^2(\lambda \times \mu_U)}^2.$$

We now consider the $f^{(1)}$ part. Since $\{1\} \cup \{w_\lambda\}$ forms an orthonormal basis in $L^2(\mu_U)$ and $(f^{(1)})_{\lambda \times \mu_U} = 0$, we have an orthogonal decomposition

$$f^{(1)}(t, x) = f_0(t) + \sum_{\lambda} f_\lambda(t)w_\lambda(x).$$

Since $f^{(1)}$ is harmonic,

$$0 = \Delta_{t,x} f^{(1)} = -f_0''(t) + \sum_{\lambda} (-f_\lambda''(t) + \lambda^2 f_\lambda(t))w_\lambda(x)$$

and therefore $f_0(t)$ is an affine function $f_0(t) = c(t - \frac{T}{2})$ for some constant c , as $f_0(t)$ has integral zero. Moreover, for every eigenvalue $\lambda > 0$ there exist constants c_{\pm}^λ such that

$$f_\lambda(t) = c_+^\lambda e^{\lambda t} + c_-^\lambda e^{\lambda(T-t)}.$$

The construction of $\bar{\phi}^{(0)}$ for $f_0(t)$ is easy: we can simply take $\phi_i^{(0)} = 0$ for $1 \leq i \leq d$ and $\phi_0^{(0)}(t, x) = \int_0^t f_0(\tau) d\tau$ (so that $\phi_0^{(0)}(T, x) = 0$ since f_0 integrates to 0), and thus

$$(56) \quad \|\bar{\phi}^{(0)}\|_{L^2(\lambda \times \mu_U)} \leq \frac{T}{\pi} \|f_0\|_{L^2(\lambda \times \mu_U)},$$

and

$$(57) \quad \|\bar{\nabla} \bar{\phi}^{(0)}\|_{L^2(\lambda \times \mu_U)} \leq \|f_0\|_{L^2(\lambda \times \mu_U)}.$$

Now without loss of generality, we assume $f^{(1)} = e^{\lambda t} w_\lambda(x)$ for a particular λ (the case $f^{(1)} = e^{\lambda(T-t)} w_\lambda(x)$ can be treated similarly by flipping time and the general case follows from a linear combination). Thus $\|f^{(1)}\|_{L^2(\lambda \times \mu_U)}^2 = \frac{e^{2\lambda T} - 1}{2\lambda}$. We need to find $\bar{\phi}^{(1)}$ such that

$$-\partial_t \phi_0^{(1)} + \sum_{i=1}^d \partial_{x_i}^* \phi_i^{(1)} = e^{\lambda t} w_\lambda(x).$$

Since $w_\lambda \in H^2(\lambda \times \mu_U)$, we can take the ansatz $\phi_0^{(1)} = \psi_1(t)w_\lambda(x)$ and for $i = 1, \dots, d$, $\phi_i^{(1)} = \psi_2(t)\partial_{x_i} w_\lambda(x)$, and the two functions $\psi_1(t), \psi_2(t)$ should satisfy $\psi_1(0) = \psi_1(T) = \psi_2(0) = \psi_2(T) = 0$ as well as the equation

$$(58) \quad -\psi_1'(t) + \lambda^2 \psi_2(t) = e^{\lambda t}.$$

Of course there exist infinitely many possible solutions, we will choose a particular one so that $\bar{\phi}^{(1)}$ satisfies the desired estimates. Let us introduce a shorthand notation $L = e^{\lambda T}$, so $\|f^{(1)}\|_{L^2(\lambda \times \mu_U)}^2 = \frac{L^2 - 1}{2\lambda}$. Let

$$h(x) = \begin{cases} \frac{4}{L-1}(x-1), & x \in \left[1, \frac{L+1}{2}\right]; \\ \frac{4}{L-1}(L-x), & x \in \left[\frac{L+1}{2}, L\right]. \end{cases}$$

Pick $g(s) = sh(s)$, then $g(1) = g(L) = 0$, and $\int_1^L \frac{g(s)}{s} ds = L - 1$. From the expression we can directly derive (using $\lambda \geq \sqrt{m}$)

$$0 \leq g(s) \leq 2s \quad \text{and} \quad |g'(s)| \leq \frac{L}{L-1} = 1 + \frac{1}{e^{\lambda T} - 1} \leq 1 + \frac{1}{\sqrt{mT}}.$$

Then pick $\psi_2(t) = \frac{1}{\lambda^2}g(e^{\lambda t})$. It is easy to compute

$$\begin{aligned} \|\psi_2\|_{L^2(I)}^2 &= \frac{1}{\lambda^4} \int_0^T g(e^{\lambda t})^2 dt = \frac{1}{\lambda^5} \int_1^L \frac{g(s)^2}{s} ds \leq \frac{2(L^2 - 1)}{\lambda^5} \quad \text{and} \\ \|\psi_2'\|_{L^2(I)}^2 &= \frac{1}{\lambda^2} \int_0^T g'(e^{\lambda t})^2 e^{2\lambda t} dt = \frac{1}{\lambda^3} \int_1^L g'(s)^2 s ds \leq \frac{L^2 - 1}{2\lambda^3} \left(1 + \frac{1}{mT^2}\right). \end{aligned}$$

Moreover, since $\psi_1'(t) = \lambda^2\psi_2(t) - e^{\lambda t}$ from (58),

$$\|\psi_1'\|_{L^2(I)}^2 \leq 2\lambda^4\|\psi_2\|_{L^2(I)}^2 + \frac{e^{2\lambda T} - 1}{\lambda} \leq \frac{5(L^2 - 1)}{\lambda}.$$

Finally since

$$|\psi_1(t)| = \left| \int_0^t (g(e^{\lambda s}) - e^{\lambda s}) ds \right| = \frac{1}{\lambda} \left| \int_1^{e^{\lambda t}} \left(\frac{g(\tau)}{\tau} - 1 \right) d\tau \right| \leq \frac{1}{\lambda} (e^{\lambda t} - 1),$$

we can estimate

$$\lambda^2\|\psi_1\|_{L^2(I)}^2 \leq \int_0^T (e^{\lambda t} - 1)^2 dt \leq \frac{L^2 - 1 + 2 \ln L}{\lambda} \leq 2 \frac{L^2 - 1}{\lambda}.$$

Now using $\|w_\lambda\|_{L^2(\lambda \times \mu_U)} = 1$ and $\|\nabla_x w_\lambda\|_{L^2(\lambda \times \mu_U)} = \lambda$, we estimate $\|\bar{\phi}^{(1)}\|_{L^2(\lambda \times \mu_U)}$:

$$\begin{aligned} \|\bar{\phi}^{(1)}\|_{L^2(\lambda \times \mu_U)}^2 &= \|\phi_0^{(1)}\|_{L^2(\lambda \times \mu_U)}^2 + \sum_{i=1}^d \|\phi_i^{(1)}\|_{L^2(\lambda \times \mu_U)}^2 \\ (59) \quad &= \|\psi_1 w_\lambda\|_{L^2(\lambda \times \mu_U)}^2 + \|\psi_2 \nabla_x w_\lambda\|_{L^2(\lambda \times \mu_U)}^2 \\ &= \|\psi_1\|_{L^2(I)}^2 + \lambda^2\|\psi_2\|_{L^2(I)}^2 \\ &\leq \frac{C}{\lambda^2} \|f^{(1)}\|_{L^2(\lambda \times \mu_U)}^2 \leq \frac{C}{m} \|f^{(1)}\|_{L^2(\lambda \times \mu_U)}^2. \end{aligned}$$

Combining (54), (56) and (59), we can derive (19).

We now shift our focus to $\|\bar{\nabla} \bar{\phi}^{(1)}\|_{L^2(\lambda \times \mu_U)}$. By (a slight tweak of) Lemma A.3 and $\nabla_x^* \nabla_x w_\lambda = \lambda^2 w_\lambda$,

$$\begin{aligned} \|\bar{\nabla} \bar{\phi}^{(1)}\|_{L^2(\lambda \times \mu_U)}^2 &= \|\bar{\nabla} \phi_0^{(1)}\|_{L^2(\lambda \times \mu_U)}^2 + \sum_{i=1}^d \|\bar{\nabla} \phi_i^{(1)}\|_{L^2(\lambda \times \mu_U)}^2 \\ &= \|\psi_1' w_\lambda\|_{L^2(\lambda \times \mu_U)}^2 + \|\psi_1 \nabla_x w_\lambda\|_{L^2(\lambda \times \mu_U)}^2 \\ &\quad + \|\psi_2' \nabla_x w_\lambda\|_{L^2(\lambda \times \mu_U)}^2 + \|\psi_2 D_x^2 w_\lambda\|_{L^2(\lambda \times \mu_U)}^2 \\ &= \|\psi_1'\|_{L^2(I)}^2 + \lambda^2\|\psi_1\|_{L^2(I)}^2 + \lambda^2\|\psi_2'\|_{L^2(I)}^2 + \|\psi_2\|_{L^2(I)}^2 (\lambda^4 + R^2 \lambda^2) \\ &\leq C_0 \left(1 + \frac{1}{mT^2} + \frac{R^2}{\lambda^2} \right) \|f^{(1)}\|_{L^2(\lambda \times \mu_U)}^2. \end{aligned}$$

Combining above with (55) and (57), and noticing $\frac{1}{\lambda^2} \leq \frac{1}{m}$, we finish the proof for (20). \square

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REFERENCES

- [1] ANDRIEU, C., DURMUS, A., NÜSKEN, N. and ROUSSEL, J. (2018). Hypocoercivity of piecewise deterministic Markov process-Monte Carlo. Preprint. Available at [arXiv:1808.08592](https://arxiv.org/abs/1808.08592).
- [2] ARMSTRONG, S. and MOURRAT, J.-C. (2019). Variational methods for the kinetic Fokker–Planck equation. Preprint. Available at [arXiv:1902.04037](https://arxiv.org/abs/1902.04037).
- [3] BERNARD, E., FATHI, M., LEVITT, A. and STOLTZ, G. (2020). Hypocoercivity with Schur complements. Preprint. Available at [arXiv:2003.00726](https://arxiv.org/abs/2003.00726).
- [4] BHATNAGAR, P. L., GROSS, E. P. and KROOK, M. (1954). A model for collision processes in gases. I. Small amplitude processes in charged and neutral one-component systems. *Phys. Rev.* **94** 511.
- [5] BIERKENS, J. (2016). Non-reversible Metropolis–Hastings. *Stat. Comput.* **26** 1213–1228. [MR3538633](https://doi.org/10.1007/s11222-015-9598-x) <https://doi.org/10.1007/s11222-015-9598-x>
- [6] BIERKENS, J., BOUCHARD-CÔTÉ, A., DOUCET, A., DUNCAN, A. B., FEARNHEAD, P., LIENART, T., ROBERTS, G. and VOLLMER, S. J. (2018). Piecewise deterministic Markov processes for scalable Monte Carlo on restricted domains. *Statist. Probab. Lett.* **136** 148–154. [MR3806858](https://doi.org/10.1016/j.spl.2018.02.021) <https://doi.org/10.1016/j.spl.2018.02.021>
- [7] BIERKENS, J., FEARNHEAD, P. and ROBERTS, G. (2019). The zig-zag process and super-efficient sampling for Bayesian analysis of big data. *Ann. Statist.* **47** 1288–1320. [MR3911113](https://doi.org/10.1214/18-AOS1715) <https://doi.org/10.1214/18-AOS1715>
- [8] BIERKENS, J., GRAZZI, S., KAMATANI, K. and ROBERTS, G. (2020). The boomerang sampler. In *International Conference on Machine Learning* 908–918. PMLR.
- [9] BIERKENS, J., KAMATANI, K. and ROBERTS, G. O. (2018). High-dimensional scaling limits of piecewise deterministic sampling algorithms. Preprint. Available at [arXiv:1807.11358](https://arxiv.org/abs/1807.11358).
- [10] BIERKENS, J. and LUNEL, S. M. V. (2019). Spectral analysis of the zigzag process. Preprint. Available at [arXiv:1905.01691](https://arxiv.org/abs/1905.01691).
- [11] BIERKENS, J., ROBERTS, G. O. and ZITT, P.-A. (2019). Ergodicity of the zigzag process. *Ann. Appl. Probab.* **29** 2266–2301. [MR3983339](https://doi.org/10.1214/18-AAP1453) <https://doi.org/10.1214/18-AAP1453>
- [12] BOU-RABEE, N. and SANZ-SERNA, J. M. (2017). Randomized Hamiltonian Monte Carlo. *Ann. Appl. Probab.* **27** 2159–2194. [MR3693523](https://doi.org/10.1214/16-AAP1255) <https://doi.org/10.1214/16-AAP1255>
- [13] BOU-RABEE, N. and SANZ-SERNA, J. M. (2018). Geometric integrators and the Hamiltonian Monte Carlo method. *Acta Numer.* **27** 113–206. [MR3826507](https://doi.org/10.1017/s0962492917000101) <https://doi.org/10.1017/s0962492917000101>
- [14] BOUCHARD-CÔTÉ, A., VOLLMER, S. J. and DOUCET, A. (2018). The bouncy particle sampler: A non-reversible rejection-free Markov chain Monte Carlo method. *J. Amer. Statist. Assoc.* **113** 855–867. [MR3832232](https://doi.org/10.1080/01621459.2017.1294075) <https://doi.org/10.1080/01621459.2017.1294075>
- [15] CAO, Y., LU, J. and WANG, L. (2019). On explicit L^2 -convergence rate estimate for underdamped Langevin dynamics. Preprint. Available at [arXiv:1908.04746](https://arxiv.org/abs/1908.04746).
- [16] DAVIS, M. H. A. (1984). Piecewise-deterministic Markov processes: A general class of nondiffusion stochastic models. *J. Roy. Statist. Soc. Ser. B* **46** 353–376. [MR0790622](https://doi.org/10.2307/2346222)
- [17] DELIGIANNIDIS, G., BOUCHARD-CÔTÉ, A. and DOUCET, A. (2019). Exponential ergodicity of the bouncy particle sampler. *Ann. Statist.* **47** 1268–1287. [MR3911112](https://doi.org/10.1214/18-AOS1714) <https://doi.org/10.1214/18-AOS1714>
- [18] DELIGIANNIDIS, G., PAULIN, D., BOUCHARD-CÔTÉ, A. and DOUCET, A. (2018). Randomized Hamiltonian Monte Carlo as scaling limit of the bouncy particle sampler and dimension-free convergence rates. Preprint. Available at [arXiv:1808.04299](https://arxiv.org/abs/1808.04299).
- [19] DOLBEAULT, J., MOUHOT, C. and SCHMEISER, C. (2009). Hypocoercivity for kinetic equations with linear relaxation terms. *C. R. Math. Acad. Sci. Paris* **347** 511–516. [MR2576899](https://doi.org/10.1016/j.crma.2009.02.025) <https://doi.org/10.1016/j.crma.2009.02.025>
- [20] DOLBEAULT, J., MOUHOT, C. and SCHMEISER, C. (2015). Hypocoercivity for linear kinetic equations conserving mass. *Trans. Amer. Math. Soc.* **367** 3807–3828. [MR3324910](https://doi.org/10.1090/S0002-9947-2015-06012-7) <https://doi.org/10.1090/S0002-9947-2015-06012-7>
- [21] DUANE, S., KENNEDY, A. D., PENDLETON, B. J. and ROWETH, D. (1987). Hybrid Monte Carlo. *Phys. Lett. B* **195** 216–222. [MR3960671](https://doi.org/10.1016/0370-2693(87)91197-x) [https://doi.org/10.1016/0370-2693\(87\)91197-x](https://doi.org/10.1016/0370-2693(87)91197-x)
- [22] DURMUS, A., GUILLIN, A. and MONMARCHÉ, P. (2020). Geometric ergodicity of the bouncy particle sampler. *Ann. Appl. Probab.* **30** 2069–2098. [MR4149523](https://doi.org/10.1214/19-AAP1552) <https://doi.org/10.1214/19-AAP1552>
- [23] DURMUS, A., GUILLIN, A. and MONMARCHÉ, P. (2021). Piecewise deterministic Markov processes and their invariant measures. *Ann. Inst. Henri Poincaré Probab. Stat.* **57** 1442–1475. [MR4291455](https://doi.org/10.1214/20-aihp1125) <https://doi.org/10.1214/20-aihp1125>
- [24] FEARNHEAD, P., BIERKENS, J., POLLOCK, M. and ROBERTS, G. O. (2018). Piecewise deterministic Markov processes for continuous-time Monte Carlo. *Statist. Sci.* **33** 386–412. [MR3843382](https://doi.org/10.1214/18-STS648) <https://doi.org/10.1214/18-STS648>

- [25] GROTHAUS, M. and STILGENBAUER, P. (2014). Hypocoercivity for Kolmogorov backward evolution equations and applications. *J. Funct. Anal.* **267** 3515–3556. MR3266239 <https://doi.org/10.1016/j.jfa.2014.08.019>
- [26] GUILLIN, A. and NECTOUX, B. (2020). Low-lying eigenvalues and convergence to the equilibrium of some piecewise deterministic Markov processes generators in the small temperature regime. *Ann. Henri Poincaré* **21** 3575–3608. MR4163302 <https://doi.org/10.1007/s00023-020-00949-7>
- [27] HÉRAU, F. (2006). Hypocoercivity and exponential time decay for the linear inhomogeneous relaxation Boltzmann equation. *Asymptot. Anal.* **46** 349–359. MR2215889
- [28] HOOTON, J. G. (1981). Compact Sobolev imbeddings on finite measure spaces. *J. Math. Anal. Appl.* **83** 570–581. MR0641352 [https://doi.org/10.1016/0022-247X\(81\)90142-6](https://doi.org/10.1016/0022-247X(81)90142-6)
- [29] HÖRMANDER, L. (1967). Hypoelliptic second order differential equations. *Acta Math.* **119** 147–171. MR0222474 <https://doi.org/10.1007/BF02392081>
- [30] MICHEL, M., DURMUS, A. and SÉNÉCAL, S. (2020). Forward event-chain Monte Carlo: Fast sampling by randomness control in irreversible Markov chains. *J. Comput. Graph. Statist.* **29** 689–702. MR4191236 <https://doi.org/10.1080/10618600.2020.1750417>
- [31] MICLO, L. and MONMARCHÉ, P. (2013). Étude spectrale minutieuse de processus moins indécis que les autres. In *Séminaire de Probabilités XLV. Lecture Notes in Math.* **2078** 459–481. Springer, Cham. MR3185926 https://doi.org/10.1007/978-3-319-00321-4_18
- [32] MONMARCHÉ, P. (2016). Piecewise deterministic simulated annealing. *ALEA Lat. Am. J. Probab. Math. Stat.* **13** 357–398. MR3487077
- [33] MOUHOT, C. and NEUMANN, L. (2006). Quantitative perturbative study of convergence to equilibrium for collisional kinetic models in the torus. *Nonlinearity* **19** 969–998. MR2214953 <https://doi.org/10.1088/0951-7715/19/4/011>
- [34] PAVLIOTIS, G. A. (2014). *Stochastic Processes and Applications: Diffusion Processes, the Fokker–Planck and Langevin Equations. Texts in Applied Mathematics* **60**. Springer, New York. MR3288096 <https://doi.org/10.1007/978-1-4939-1323-7>
- [35] PETERS, E. A. and DE WITH, G. (2012). Rejection-free Monte Carlo sampling for general potentials. *Phys. Rev. E* **85** 026703.
- [36] ROUSSEL, J. and STOLTZ, G. (2018). Spectral methods for Langevin dynamics and associated error estimates. *ESAIM Math. Model. Numer. Anal.* **52** 1051–1083. MR3865558 <https://doi.org/10.1051/m2an/2017044>
- [37] SACHS, M., SEN, D., LU, J. and DUNSON, D. (2020). Posterior computation with the Gibbs zig-zag sampler. Preprint. Available at [arXiv:2004.04254](https://arxiv.org/abs/2004.04254).
- [38] SEN, D., SACHS, M., LU, J. and DUNSON, D. B. (2020). Efficient posterior sampling for high-dimensional imbalanced logistic regression. *Biometrika* **107** 1005–1012. MR4186502 <https://doi.org/10.1093/biomet/asaa035>
- [39] VANETTI, P., BOUCHARD-CÔTÉ, A., DELIGIANNIDIS, G. and DOUCET, A. (2017). Piecewise-deterministic Markov chain Monte Carlo. Preprint. Available at [arXiv:1707.05296](https://arxiv.org/abs/1707.05296).
- [40] VILLANI, C. (2009). Hypocoercivity. *Mem. Amer. Math. Soc.* **202** iv+141. MR2562709 <https://doi.org/10.1090/S0065-9266-09-00567-5>
- [41] WU, C. and ROBERT, C. P. (2017). Generalized bouncy particle sampler. Preprint. Available at [arXiv:1706.04781](https://arxiv.org/abs/1706.04781).
- [42] WU, C. and ROBERT, C. P. (2020). Coordinate sampler: A non-reversible Gibbs-like MCMC sampler. *Stat. Comput.* **30** 721–730. MR4065228 <https://doi.org/10.1007/s11222-019-09913-w>