

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

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ABSTRACT. 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 [12, 21], the zigzag process [7] and the bouncy particle sampler [14, 33]. 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, 23, 37]. The zigzag and bouncy particle samplers are also suitable for the big data situation, as they can be unbiased even if 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 satisfies 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 fixed 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 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

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

Here 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

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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 [33] 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 given by

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

where κ is the Gaussian distribution and

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

Other PDMPs have been proposed for sampling purposes, including Hamiltonian BPS [38], the Coordinate Sampler [34], the Gibbs zigzag sampler [36], the Boomerang sampler [8], and more general bounces involving randomization [29, 38, 40]. While our framework can be generalized, 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 [2] and our previous work for the underdamped Langevin dynamics [15], the idea of which originates from the pioneering work [28]. 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], however without explicit convergence rate estimates. The work [1] established explicit convergence rate 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, 30] in one-dimension and [25] for the metastable regime.

More generally, convergence result of type (7) for hypocoercive equations was established in $H^1(\rho_\infty)$ in [31, 39] for a class of kinetic equations. Hypocoercivity estimate in terms of a

modified L^2 space was developed in [19, 20, 26] and a series of works based on this framework [3, 24, 35].

Notations. 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 . 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

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

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 is 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

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

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 . Throughout the paper, we use the notation $A = \Theta(B)$ to indicate that there exists universal constants $c, C > 0$ independent of all parameters such that $cB \leq A \leq CB$.

1.1. Assumptions and Main Results. Below are three fundamental assumptions that $U(x)$ must satisfy in our framework. The convergence rate gets better if we have stronger assumptions on U .

Assumption 1 (Poincaré inequality for μ_U). *The measure μ_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 e.g., the books [32, 39] 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 [27] for a proof). While previous works on hypocoercivity [20] and works following its framework [1, 3, 35] use elliptic regularity estimate in x for which Assumption 1

suffices, our proof, in particular the construction of test functions in Lemma 2.1, relies on spectral decomposition of the operator $\nabla_x^* \nabla_x$, which is only guaranteed through the slightly stronger Assumption 3.

Below we present the main result of this work.

Theorem 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*

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

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

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

Then, the convergence rate ν can be explicitly estimated for the three PDMPs as

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

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

This theorem will be proved in Section 2.

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

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

Therefore the optimal convergence rate is given by

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

Table 1 summarizes the result under the assumption $m\mathcal{I} \leq \nabla_x^2 U \leq LI$ (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 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 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 $\nabla_x^2 U \geq -LI$ is still an improvement from the rate in [1], whose estimate provides a rate of $O(d^{-(1+\omega)/2})$ under the assumption $\Delta_x U(x) \leq cd^{1+\omega} + |\nabla_x U(x)|^2/2$. As suggested in [9], a dimension independent convergence rate might not be possible for BPS.

	convergence rate ν	optimal γ
RHMC	$\Theta(\sqrt{m})$	$\Theta(\sqrt{m})$
ZZ	$\Theta(\frac{m}{\sqrt{L}})$	$\Theta(\sqrt{L})$
BPS	$\Theta(\sqrt{\frac{m}{d}})$	$\Theta(\sqrt{dm})$

TABLE 1. Summary of 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 $m \ll 1 \ll L$.

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. *There exists a constant C independent of all parameters such that for all functions f ,*

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

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

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

where R and R_{ZZ} are the same quantities as defined in Theorem 1.

To prove Theorem 2, 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.

Lemma 2.1 ([15, Lemma 2.6]). *For any function $g = g(t, x) \in L^2(\lambda \times \mu_U)$ with $(g)_{\lambda \times \mu_U} = 0$, there exist $\bar{\phi} = (\phi_0, \phi_1, \dots, \phi_d)^\top \in H^1(\lambda \times \mu_U)^{d+1}$ solving*

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

with estimates

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

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

Here we use the convention $\partial_{x_0} := \partial_t$, C is a universal constant and R is the ‘‘convexity barrier’’ parameter for potential U defined in Theorem 1.

Before proceeding to the proof of Theorem 2, 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 2.2. *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 in 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 use a change of variables $\tilde{v} := v - 2(v \cdot n_k)n_k$, so that $v \cdot F_k = -\tilde{v} \cdot F_k$, and $\kappa(\tilde{v}) = \kappa(v)$:

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

Lemma 2.3. *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 , 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 line, and the symmetry of Gaussian $\kappa(v)$ in the sense that $\kappa(v) = \kappa(-v)$ in the third line:

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

We are now ready to prove Theorem 2.

Proof of Theorem 2. 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 2.1 with $g = \Pi_v f$.

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 2.4. *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.

Before proceeding with the proof of Theorem 2, let us provide a heuristic justification for Lemma 2.4: 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 , $\nabla_{x_i} \phi_j$ or $\phi_k \nabla_x U$. Therefore, integrating out the v component against Gaussian, and by Lemma 2.1 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 later part of the paper.

Now let us return to the proof of Theorem 2 assuming Lemma 2.4. To simplify notations, we define the operator

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

We now estimate the L^2 norm of $\Pi_v f$. Using Lemma 2.3 for $q = -F_k$, $\varphi(v \cdot q) = v \cdot q$ and $\psi(v) = (v \cdot n_k)(\phi \cdot n_k)$ and then integrate out v , we have

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

Therefore, by the construction of the test functions $\bar{\phi}$, we have

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

where the third equality follows from introducing a dummy v variable and noting that by the basic properties of Gaussian measure κ , $\int_{\mathbb{R}^d} v_i d\kappa(v) = 0$, $\int_{\mathbb{R}^d} v_i v_j d\kappa(v) = \delta_{ij}$, and $\int_{\mathbb{R}^d} v_i^4 d\kappa(v) = 3$.

To estimate the first term on the RHS of (28) we use integration by parts:

$$\begin{aligned}
& \int_{I \times \mathbb{R}^d \times \mathbb{R}^d} f \mathcal{J} dt d\rho_\infty \\
& \stackrel{(24)}{=} \int_{I \times \mathbb{R}^d \times \mathbb{R}^d} \left(\partial_t f \phi_0 - v \cdot \nabla_x f \phi_0 + f \phi_0 v \cdot \sum_{k=0}^K F_k - \partial_t f v \cdot \phi + (v \cdot \nabla_x f)(v \cdot \phi) \right. \\
& \quad \left. - (v \cdot \nabla_x U)(v \cdot \phi) f + f \phi \cdot F_0 - 2 \sum_{k=1}^K (-v \cdot F_k)_+ (v \cdot n_k)(\phi \cdot n_k) f \right) dt d\rho_\infty \\
& = \int_{I \times \mathbb{R}^d \times \mathbb{R}^d} \left((\partial_t f - v \cdot \nabla_x f)(\phi_0 - v \cdot \phi) + f \phi_0 v \cdot F_0 + f \phi \cdot F_0 - (v \cdot F_0)(v \cdot \phi) f \right. \\
& \quad \left. + (v \cdot \sum_{k=1}^K F_k)(\phi_0 - v \cdot \phi) f - 2 \sum_{k=1}^K (-v \cdot F_k)_+ (v \cdot n_k)(\phi \cdot n_k) f \right) dt d\rho_\infty \\
& = \int_{I \times \mathbb{R}^d \times \mathbb{R}^d} \left((\partial_t f - v \cdot \nabla_x f + \sum_{k=1}^K (v \cdot F_k)_+ f)(\phi_0 - v \cdot \phi) + \phi_0 F_0 \cdot \nabla_v f - (F_0 \cdot \nabla_v f)(v \cdot \phi) \right. \\
& \quad \left. - \sum_{k=1}^K (-v \cdot F_k)_+ (\phi_0 - v \cdot \phi) f - 2 \sum_{k=1}^K (-v \cdot F_k)_+ (v \cdot n_k)(\phi \cdot n_k) f \right) dt d\rho_\infty \\
& = \int_{I \times \mathbb{R}^d \times \mathbb{R}^d} \left((\partial_t f - v \cdot \nabla_x f + \sum_{k=1}^K (v \cdot F_k)_+ f + F_0 \cdot \nabla_v f)(\phi_0 - v \cdot \phi) \right. \\
& \quad \left. - \sum_{k=1}^K (-v \cdot F_k)_+ \mathcal{B}_k(\phi_0 - v \cdot \phi) \mathcal{B}_k^2 f \right) dt d\rho_\infty \\
& \stackrel{(21), (22)}{=} \int_{I \times \mathbb{R}^d \times \mathbb{R}^d} \left((\partial_t f - v \cdot \nabla_x f - \sum_{k=1}^K (v \cdot F_k)_+ (\mathcal{B}_k - I) f + F_0 \cdot \nabla_v f)(\phi_0 - v \cdot \phi) \right) dt d\rho_\infty \\
& \stackrel{(26)}{\leq} \|\phi_0 - v \cdot \phi\|_{L^2(\lambda \times \rho_\infty)} \|\mathcal{A}f\|_{L^2(\lambda \times \rho_\infty)}.
\end{aligned}$$

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

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

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 triangle inequality

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

□

With Theorem 2, the proof of exponential convergence reduces to a standard energy estimate with $\gamma(\Pi_v - \mathcal{I})$ playing the role of “diffusion”, in line with the moral “hypo-coercivity is simply coercivity with respect to the correct norm”, quoted from [2, Page 4].

Proof of Theorem 1. We first notice that

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

for all $t > 0$. Indeed, this follows from (10) and

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

which is a result of the PDE evolution (1) and

$$\begin{aligned} \int_{\mathbb{R}^d \times \mathbb{R}^d} \mathcal{L}f d\rho_\infty(x, v) &= \int_{\mathbb{R}^d \times \mathbb{R}^d} f v \cdot \nabla_x U - f v \cdot F_0 - \sum_{k=1}^K (v \cdot F_k)_+ f + \sum_{k=1}^K \mathcal{B}_k (v \cdot F_k)_+ f d\rho_\infty \\ &= \int_{\mathbb{R}^d \times \mathbb{R}^d} f v \cdot \left(\sum_{k=1}^K F_k \right) - \sum_{k=1}^K (v \cdot F_k)_+ f + \sum_{k=1}^K (-v \cdot F_k)_+ f d\rho_\infty = 0, \end{aligned}$$

where the first equality follows from integration by parts and the second from the definition and property of \mathcal{B}_k , proved in Lemma 2.2.

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 2.2,

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

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 $\int_{(s,t) \times \mathbb{R}^d \times \mathbb{R}^d} f \mathcal{L} f \, dt \, d\rho_\infty$:

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

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 $0 < s < t$,

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

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 monotonicity (33), we obtain

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

The prefactor

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

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

$$(35) \quad \nu = \sup_{T>0} \frac{1}{2T} \log\left(1 + \frac{2\gamma T}{(1 + C_{\mathcal{J}} + C\gamma(\frac{1}{\sqrt{m}} + T))^2}\right) = \Theta\left(\sup_{T>0} \frac{\gamma}{(1 + C_{\mathcal{J}} + \gamma(\frac{1}{\sqrt{m}} + T))^2}\right).$$

Substituting (17) into (35), we get

$$(36) \quad \nu = \begin{cases} \Theta\left(\frac{\gamma}{(1 + \frac{1}{\sqrt{m}T} + \frac{R}{\sqrt{m}} + RT + \frac{\gamma}{\sqrt{m}} + \gamma T)^2}\right), & \text{for RHMC;} \\ \Theta\left(\frac{\gamma}{(1 + \frac{1}{\sqrt{m}T} + \frac{R_{ZZ}}{\sqrt{m}} + R_{ZZ}T + \frac{\gamma}{\sqrt{m}} + \gamma T)^2}\right), & \text{for ZZ;} \\ \Theta\left(\frac{\gamma}{(\sqrt{d}(1 + \frac{1}{\sqrt{m}T} + \frac{R}{\sqrt{m}} + RT) + \gamma(\frac{1}{\sqrt{m}} + T))^2}\right), & \text{for BPS.} \end{cases}$$

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

The rest of the work is to prove Lemma 2.4. For RHMC,

$$\mathcal{J} = -\partial_t \phi_0 + v \cdot \nabla_x \phi_0 + v \cdot \partial_t \phi - \sum_i v_i v \cdot \partial_{x_i} \phi + \phi \cdot \nabla_x U.$$

The norm $\|\mathcal{J}\|_{L^2(\lambda \times \rho_x)}$ 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

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

Lemma 2.5. *Let ϕ_i , $i = 0, \dots, d$ be test functions as in Lemma 2.1. Then*

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

Here R_{ZZ} is defined as in Theorem 1.

Proof. Using integration by parts,

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

After rearranging, we have

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

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

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

Therefore, by Cauchy-Schwarz inequality,

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

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

Proof of Lemma 2.4 for zigzag process. To estimate $\|\mathcal{J}\|_{L^2(\lambda \times \rho_\infty)}^2$, we expand its terms, categorize them according to its power 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 0-th power of v :

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

Terms with 2-nd power of v :

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

Terms with 4-th power on v :

$$\int_{I \times \mathbb{R}^d \times \mathbb{R}^d} \sum_{i,j,p,q} v_i v_j v_p v_q \partial_{x_i} \phi_j \partial_{x_p} \phi_q \, dt \, d\rho_\infty$$

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

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

Terms where $(-v_k \partial_{x_k} U)_+$ appearing twice, in which case the overall power of v is even and thus Lemma 2.3 is applicable:

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

Cross terms with $(-v_k \partial_{x_k} U)_+$ where we could still use Lemma 2.3 due to an overall even power of v :

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

Finally cross terms with $(-v_k \partial_{x_k} U)_+$ where one cannot use Lemma 2.3 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:

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

$$\leq \int_{I \times \mathbb{R}^d} \left(6 \sum_{k=1}^d ((\partial_t \phi_k)^2 + (\partial_{x_k} \phi_0)^2) + 2 \sum_{k=1}^d \phi_k^2 (\partial_{x_k} U)^2 \right) dt d\mu_U(x).$$

Therefore, combining these calculations, we obtain finally

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

Remark 2.6. Our bound in Lemma 2.5 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 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 2.5. We will follow the notations of the proof of [15, Lemma 2.6]. Let us decompose

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

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 $g \in H^2(\lambda \times \mu_U)$,

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

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 $\Pi_v f = f^\perp$ and $\Pi_v f = e^{\alpha t} w_\alpha(x)$ (note in the case $\Pi_v f = t - \frac{T}{2}$ the corresponding $\phi_k = 0$ for $k \geq 1$, and thus (40) trivially holds), the corresponding functions ϕ_k satisfy

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

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

$$(41) \quad \begin{cases} -\partial_{tt} u + \nabla_x^* \nabla_x u = f^\perp & \text{in } I \times \mathbb{R}^d, \\ \partial_t u(t=0, \cdot) = \partial_t u(t=T, \cdot) = 0 & \text{in } \mathbb{R}^d. \end{cases}$$

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

$$\begin{aligned} \sum_{i,j=0}^d \|\partial_{x_i x_j} u\|_{L^2(\lambda \times \mu_U)}^2 &= \|-\partial_{tt} u + \nabla_x^* \nabla_x u\|_{L^2(\lambda \times \mu_U)}^2 - \int_{I \times \mathbb{R}^d} \nabla_x u^\top \nabla_x^2 U \nabla_x u dt d\mu_U(x) \\ &= \|f^\perp\|_{L^2(\lambda \times \mu_U)}^2 - \sum_{k=1}^d \int_{I \times \mathbb{R}^d} (\partial_{x_k} u)^2 U_k''(x_k) dt d\mu_U(x), \end{aligned}$$

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

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

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

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

$$\mathbf{n}_i = \frac{\partial_{x_i} U}{|\nabla_x U|}$$

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

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

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

Lemma 2.7. *Let ϕ_i , $i = 0, \dots, d$ be the test functions as in Lemma 2.1. Then*

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

Here R is defined as in Theorem 1.

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

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

where the first inequality follows from Cauchy-Schwartz. \square

Proof of Lemma 2.4 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 its power 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 2.3 can be applied:

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

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

$$\begin{aligned}
& \int_{I \times \mathbb{R}^d \times \mathbb{R}^d} \left(4\partial_t \phi_0 (-v \cdot \mathbf{n})_+ (v \cdot \mathbf{n}) (\phi \cdot \nabla_x U) + 4 \sum_{i,j} 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}^d \times \mathbb{R}^d} \left(\partial_t \phi_0 (v \cdot \mathbf{n})^2 + \sum_{i,j} 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}^d \times \mathbb{R}^d} \left(\partial_t \phi_0 \sum_i \mathbf{n}_i^2 + \sum_{i,j,p,q} v_i v_j v_p v_q \mathbf{n}_p \mathbf{n}_q \partial_{x_i} \phi_j \right) (\phi \cdot \nabla_x U) dt d\rho_\infty \\
&= -2 \int_{I \times \mathbb{R}^d \times \mathbb{R}^d} \left(\partial_t \phi_0 + \sum_i v_i^4 \mathbf{n}_i^2 \partial_{x_i} \phi_i + \sum_{i \neq j} v_i^2 v_j^2 \mathbf{n}_j^2 \partial_{x_i} \phi_i \right. \\
&\quad \left. + 2 \sum_{i \neq j} v_i^2 v_j^2 \mathbf{n}_i \mathbf{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 \mathbf{n}_i^2 \partial_{x_i} \phi_i + \sum_{i \neq j} \mathbf{n}_j^2 \partial_{x_i} \phi_i + 2 \sum_{i \neq j} \mathbf{n}_i \mathbf{n}_j \partial_{x_i} \phi_j \right) (\phi \cdot \nabla_x U) dt d\mu_U(x) \\
&= -2 \int_{I \times \mathbb{R}^d} \left(\partial_t \phi_0 + \sum_i \partial_{x_i} \phi_i + 2 \sum_{i,j} \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(-(\partial_t \phi_0 + \sum_i \partial_{x_i} \phi_i) (\phi \cdot \nabla_x U) + \sum_{i,j} (\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(-(\partial_t \phi_0 + \sum_i \partial_{x_i} \phi_i) (\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

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

$$\stackrel{(43)}{\leq} \int_{I \times \mathbb{R}^d} \left(4|\partial_t \phi|^2 + 4|\nabla_x \phi_0|^2 + 9(\phi \cdot \nabla_x U)^2 \right) dt d\mu_U(x).$$

Therefore, combining these calculations, we obtain

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

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