Convergence of Noise-Free Sampling Algorithms with Regularized Wasserstein Proximals

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Abstract

In this work, we investigate the convergence properties of the backward regularized Wasserstein proximal (BRWP) method for sampling a target distribution. The BRWP approach can be shown as a semi-implicit time discretization for a probability flow ODE with the score function whose density satisfies the Fokker-Planck equation of the overdamped Langevin dynamics. Specifically, the evolution of the score function is computed using a kernel formula derived from the regularized Wasserstein proximal operator. By applying the Laplace method to obtain the asymptotic expansion of this kernel formula, we establish guaranteed convergence in terms of the Kullback–Leibler divergence for the BRWP method towards a strongly log-concave target distribution. Our analysis also identifies the optimal and maximum step sizes for convergence. Furthermore, we demonstrate that the deterministic and semi-implicit BRWP scheme outperforms many classical Langevin Monte Carlo methods, such as the Unadjusted Langevin Algorithm (ULA), by offering faster convergence and reduced bias. Numerical experiments further validate the convergence analysis of the BRWP method.

Keywords: Entropy dissipation; Regularized Wassertein proximal; Laplace methods; Score functions; Optimal time stepsize.

1 Introduction

Sampling from complex and potentially high-dimensional distributions is increasingly crucial in data science Andrieu et al. (2003), computational mathematics Durmus and Moulines (2018), and engineering Leimkuhler and Matthews (2015). Efficient sampling algorithms are central to numerous real-world applications, including identifying global optimizers for high-dimensional functions Ma et al. (2019), generating samples from latent spaces in generative modeling Song and Ermon (2019), and solving Bayesian inverse problems to estimate posterior distributions Stuart (2010); Garbuno-Inigo et al. (2020). The success of these applications heavily relies on the efficiency, reliability, and theoretical convergence guarantees of the employed sampling algorithms.

Given the importance of sampling from known distributions, various algorithms have been developed and analyzed. Markov Chain Monte Carlo (MCMC) methods are widely used Ma et al. (2021); Mengersen and Tweedie (1996); Bélisle et al. (1993); Carrillo et al. (2022); Betancourt (2017). A well-known example is the overdamped Langevin dynamics, which relies on a gradient drift vector field and a simple diffusion process introduced by Gaussian noise. Theoretical results show that the continuous-time Langevin Monte Carlo (LMC) method can converge to a stationary distribution under appropriate assumptions Otto and Villani (2000). In practice, challenges arise with LMC when discretizing the Langevin dynamics in time, particularly due to the dimension dependence caused by the random walk component and the bias introduced by finite time stepsize. Notable LMC methods include the Unadjusted Langevin Algorithm (ULA), which employs an explicit Euler time discretization Parisi (1981), the Metropolis-Adjusted Langevin Algorithm (MALA), which incorporates an acceptance-rejection step Xifara et al. (2014), and the Proximal Langevin Algorithm, which utilizes an implicit time update in the drift vector field Liang and Chen (2022).

In recent years, studies such as Song and Ermon (2019); Lu et al. (2022); Chen et al. (2024); Huang et al. (2024) have focused on the probability flow ODE derived from Langevin dynamics. This approach involves expressing the diffusion process, driven by Brownian motion, in terms of the score function, which is the gradient of the logarithm of the density function. The density itself satisfies the Fokker-Planck equation associated with overdamped Langevin dynamics. This reformulation also connects to the gradient flow of the Kullback–Leibler (KL) divergence in the Wasserstein space, which is the probability density space endowed with the Wasserstein-2 metric Otto and Villani (2000). In this context, the score function represents the Wasserstein gradient of the negative Boltzmann-Shannon entropy. It has been shown that utilizing the score function is an effective method for sampling a target distribution, particularly from a numerical standpoint Lu et al. (2022); Zhang and Chen (2022); Zhao et al. (2024); Wang and Li (2022).

The application of probability flow ODEs into sampling problems presents several significant challenges. Firstly, the computation or approximation of the score function can be both computationally intensive and inaccurate from finite samples. Secondly, the time discretization of the probability flow ODE is crucial. The time-implicit Jordan–Kinderlehrer–Otto (JKO) scheme addresses this by iteratively solving the proximal operator of the KL divergence in Wasserstein space. However, the JKO scheme is computationally demanding due to the absence of a closed-form update for the Wasserstein proximal operator, which typically requires an additional minimization procedure. To mitigate these issues, a regularization term can be introduced to the Wasserstein proximal operator, as demonstrated in Li et al. (2023), leading to a system that admits a closed-form solution via the Hopf-Cole transformation. This solution, known as the kernel formula, enables a semi-implicit time discretization of the evolution of the score function, forming the basis of the Backward Regularized Wasserstein Proximal (BRWP) scheme. The BRWP scheme, initially introduced in Tan et al. (2023) using empirical distribution to approximate density function, was later enhanced in Han et al. (2024) using tensor train approximation for high-dimensional distributions. Analysis in Han et al. (2024); Tan et al. (2023) demonstrates that, for Gaussian target distributions, the BRWP scheme achieves faster convergence and exhibits less sensitivity to dimensionality in terms of mixing time, suggesting its potential applicability to a broader class of non-Gaussian distributions.

In this work, we explore the convergence properties of the BRWP scheme for sampling from strongly log-concave distributions. By leveraging the Laplace method on the kernel formula, we show that the BRWP algorithm is a semi-implicit discretization of the probability flow ODE, where the score function is evaluated at the next time point and free from Brownian motion. This implicit approach enhances the robustness and stability of the sampling process. Moreover, since the probability flow ODE in the BRWP scheme is deterministic, we can conduct higher-order numerical analysis, which enables faster convergence by optimizing the step size, as demonstrated in our upcoming analysis.

We informally demonstrate the main results as below. We aim to sample a target distribution $\rho^* := \frac{1}{Z}\exp(-\beta V)$ with a given potential function $V \in C^2(\mathbb{R}^d;\mathbb{R})$, a normalization constant $Z = \int_{\mathbb{R}^d}\exp(-\beta V(x))dx < \infty$, a constant inverse temperature β, and an initial density ρ_0. In particular, in section 3, we show that the following kernel formula from the regularized Wasserstein proximal operator

$$\rho_T(x) = \int_{\mathbb{R}^d} \frac{\exp\left[-\frac{\beta}{2}\left(V(x) + \frac{\|x-y\|_2^2}{2T}\right)\right]}{\int_{\mathbb{R}^d}\exp\left[-\frac{\beta}{2}\left(V(z) + \frac{\|z-y\|_2^2}{2T}\right)\right]dz}\rho_0(y)dy\,, \tag{1}$$

provides a one-step time approximation of the Fokker-Planck equation:

$$\frac{\partial \rho}{\partial t} = \nabla\cdot(\nabla V\rho) + \beta^{-1}\Delta\rho\,.$$

Here, the stepsize is given as $T > 0$.

Theorem 1 *(Informal, see Theorem 4) For fixed $x \in \mathbb{R}^d$ and stepsize $T > 0$, suppose ρ_0 satisfies the Fokker-Planck equation at time t_0. Then we have*

$$\rho_T(x) = \rho_0(x) + T\frac{\partial \rho_0}{\partial t}\bigg|_{t=t_0}(x) + \mathcal{O}(T^2)\,. \tag{2}$$

With the help of the kernel formula (1) and assume that it can be computed accurately, we implement the following semi-implicit discretization with the stepsize $h > 0$ of the score dynamic to sample from ρ^*:

$$x_{k+1} = x_k - h(\nabla V(x_k) + \beta^{-1}\nabla\log\rho_T(x_k))\,, \tag{3}$$

where $\rho_T(x) = \rho(t_k + T, x)$. Considering the evolution of the density function associated with x_k, denoted as ρ_k, in section 4, we show the convergence guarantees of the proposed sampling method in terms of the KL divergence where $\mathrm{D}_{\mathrm{KL}}(\rho_k\|\rho^*) = \int \rho_k \log\frac{\rho_k}{\rho^*}dx$.

Theorem 2 *(Informal, see Theorem 12) Assume ρ^* is strongly log-concave with constant α. For a sufficient small constant $\delta > 0$, the BRWP algorithm will achieve an error of $\mathrm{D}_{\mathrm{KL}}(\rho_k\|\rho^*) \le \delta$, with*

$$k = \mathcal{O}\left(\frac{|\ln\delta|}{2\alpha\sqrt{\delta}}\right),$$

where the stepsize is chosen as $T = h = \sqrt{\delta}$ when $\sqrt{\delta} < 2/(3\alpha)$.

The convergence of Langevin dynamics-based methods has been extensively studied under various assumptions in the literature Balasubramanian et al. (2022); Durmus and Moulines (2018); Dwivedi et al. (2019); Chewi et al. (2024). In comparison to methods like ULA, proximal Langevin, and other Langevin dynamics-based sampling algorithms, our scheme—being free from noise—offers a sampling complexity that is independent of the dimension d and has a bias that is only on the order of $\sqrt{\delta}$. Additionally, the explicit decay results facilitate the selection of an optimal step size, which is achievable due to the deterministic nature of our approach. Similarly, the convergence of sampling algorithms derived from the probability flow ODE has been investigated in Gao and Zhu (2024); Chen et al. (2023, 2022). However, these results are often unstable, with errors tending to infinity as time progresses, and they generally rely on the assumption of an accurately estimated score function at each time step Yang and Wibisono (2022). In this work, we provide a precise choice of stepsize and offer a detailed analysis of how to approximate the evolution of the density function using the regularized Wasserstein proximal operator which is depicted in detail in section 5.

Finally, in Section 6, we present numerical experiments to validate our theoretical results and briefly outline several future research directions in conclusion.

2 Review on Probability Flow ODE with Score Function, Regularized Wasserstein Proximal Operator, and BRWP Algorithm

In this section, we begin by outlining the sampling problem for a given target distribution and reviewing classical sampling algorithms derived from overdamped Langevin dynamics, along with their convergence analysis in Wasserstein space. We then discuss various sampling algorithms based on discrete-time approximations of the Fokker-Planck equation, including the ULA, JKO scheme, and BRWP. To provide a comprehensive comparison, we summarize the sampling complexity and optimal stepsize for BRWP and several popular existing methods in Table 1.

2.1 Sampling problem

We aim to generate a collection of samples $\{x_{k,j}\}_{j=1}^N \in \mathbb{R}^d$, with $k \in \mathbb{Z}$ representing the iteration steps, and $j = 1, \cdots N$ forming the number of samples, drawn from a known probability distribution, also named a Gibbs distribution

$$\rho^*(x) = \frac{1}{Z}\exp(-\beta V(x))\,,$$

where $Z = \int_{\mathbb{R}^d} \exp(-\beta V(x))dx < +\infty$ is the normalization constant, $\beta > 0$ is the inverse temperature, and $V \in C^2(\mathbb{R}^d;\mathbb{R})$ represents the potential function. The collection $\{x_{0,j}\}_{j=1}^N$ is an arbitrary set of initial particles, and the objective of the sampling algorithm is to ensure that, as k increases, the distribution of $\{x_{k,j}\}_{j=1}^N$ approximates the density function ρ^*.

The classical sampling algorithm is to consider the Langevin dynamics, which is described by the stochastic differential equation

$$dX_t = -\nabla V(X_t)dt + \sqrt{2\beta^{-1}}dB_t\,, \tag{4}$$

where B_t denotes the standard Brownian motion in $\mathbb{R}^d$. The density function of X_t evolves according to the Kolmogorov forward equation, also named Fokker-Planck equation:

$$\begin{aligned}\frac{\partial\rho}{\partial t} =& \nabla\cdot(\rho\nabla V) + \beta^{-1}\Delta\rho \\ =& \nabla\cdot(\rho\nabla V) + \beta^{-1}\nabla\cdot(\rho\nabla\log\rho) \\ =& \beta^{-1}\nabla\cdot\left(\rho\nabla\log\frac{\rho}{\rho^*}\right)\,,\end{aligned} \tag{5}$$

where the second equality is based on the fact that $\nabla\log\rho = \nabla\rho/\rho$. Clearly, ρ^* is an equilibrium of the Fokker-Planck equation (5). Thus, the invariant distribution of Langevin dynamics follows ρ^*.

A known fact is that the Fokker-Planck equation corresponds to the Wasserstein-2 gradient flow of the KL divergence

$$\mathrm{D}_{\mathrm{KL}}(\rho\|\rho^*) := \int \rho\log\frac{\rho}{\rho^*}dx\,.$$

This means that the Fokker-Planck equation (5) can be formulated as

$$\frac{\partial \rho}{\partial t} = \beta^{-1}\nabla \cdot \left(\rho \nabla \frac{\delta}{\delta \rho}\mathrm{D}_{\mathrm{KL}}(\rho \| \rho^*)\right),$$

where $\frac{\delta}{\delta\rho}$ is the L^2 first variation w.r.t. the density function ρ. Furthermore, in the Wasserstein space, the squared norm of the gradient of the KL divergence, also known as the relative Fisher information, is written as

$$\mathcal{I}(\rho\|\rho^*) = \int \left\| \nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \rho dx\,.$$

From any initial distributions, the probability density of Langevin dynamics converges to the target distribution ρ^*. Specifically, we have

$$\frac{d}{dt}\mathrm{D}_{\mathrm{KL}}(\rho\|\rho^*) = -\beta^{-1}\mathcal{I}(\rho\|\rho^*) < 0\,.$$

Moreover, when ρ^* satisfies the log-Sobolev inequality (LSI) with constant α, we can establish the relationship between the KL divergence and Fisher information

$$\mathrm{D}_{\mathrm{KL}}(\rho\|\rho^*) \le \frac{1}{2\beta\alpha}\mathcal{I}(\rho\|\rho^*)\,. \tag{6}$$

This inequality can be viewed as the gradient-dominated condition, commonly known as the Polyak-Lojaciewicz (PL) inequality in the Wasserstein space. From now on, we assume that $\nabla^2 V \succeq \alpha I$, or ρ^* is strongly log-concave, such that the LSI holds Gross (1975); Bakry and Émery (2006).

Utilizing the PL inequality, one can show that the KL divergence converges exponentially along the Wasserstein gradient flow (see Lemma 17 in the appendix for more details)

$$\mathrm{D}_{\mathrm{KL}}(\rho_t\|\rho^*) \le \exp(-2\alpha t)\mathrm{D}_{\mathrm{KL}}(\rho_0\|\rho^*)\,,$$

where $\rho_t(x) = \rho(t, x)$.

Although the convergence at the continuous time level is promising, numerical analysis of the particle trajectory in the discrete Langevin dynamics reveals a bias and a dependence on the dimensionality of the problem. This issue arises due to the evolution of Brownian motions in approximating Langevin dynamics, which can slow down convergence in high-dimensional sampling problems, as its variance is proportional to the dimension. More details will be provided in the next subsection.

Given these difficulties, in this work, we instead consider a probability flow ODE, where the diffusion is generated by the score function:

$$dX_t = -\nabla V(X_t)dt - \beta^{-1}\nabla \log \rho_t(X_t)dt\,. \tag{7}$$

The trajectory of (7) differs from the Langevin dynamics (4). However, using the identity $\nabla \log \rho = \nabla\rho/\rho$, it is straightforward to show the corresponding Liouville equation remains the Fokker-Planck equation (5). Consequently, the corresponding probability flow continues to be the Wasserstein gradient flow for the KL divergence. In continuous time, the KL divergence still converges exponentially fast along the flow given by (7).

Moreover, since the ODE (7) is deterministic, it is feasible to perform higher-order numerical analysis under finite time stepsizes to explore the higher-order error terms introduced by discretization and optimal stepsize associated with the discretization. This analysis will be the main focus of Section 4, where we demonstrate the improved convergence rate and accuracy.

2.2 Discrete time approximation

Although the KL divergence converges exponentially fast in continuous time along the flow given by the Fokker-Planck equation, discretizing Langevin dynamics slows down convergence. It also introduces a bias term due to the discretization error. For example, applying explicit Euler discretization with stepsize h to (4) results in the ULA

$$x_{k+1} = x_k - h\nabla V(x_k) + \sqrt{2\beta^{-1}h}z_k \,, \tag{8}$$

where $z_k \sim \mathcal{N}(0, I)$. The convergence of ULA is well studied, and Vempala and Wibisono (2019) shows

$$\mathrm{D}_{\mathrm{KL}}(\rho_k \| \rho^*) \leq \exp(-\alpha hk)\mathrm{D}_{\mathrm{KL}}(\rho_0 \| \rho^*) + \frac{8hdL^2}{\alpha} \,,$$

where ρ_k represents the density at time $t_k = kh$ and $-LI \preceq \nabla^2 V \preceq LI$. The discretization induces an error term of order h, which depends on the dimension d that arises from the Brownian motion term. This makes high-dimensional cases particularly challenging and limits the optimal selection of stepsize.

Then we turn to study the discretization of the probability flow ODE (7) and note that one of the primary challenges is the approximation of the score function. It becomes increasingly difficult and inaccurate in high-dimensional spaces. As a result, a straightforward explicit Euler discretization can be highly unstable, potentially causing ρ_k to become concentrated around the global minimum of $V(x)$ due to the drift term $\nabla V(x)$. Hence, an implicit discretization to (7) becomes highly demanding.

Implicit methods for solving Langevin dynamics have also been extensively studied, including proximal Langevin Wibisono (2019), proximal sampler with restricted Gaussian oracle Liang and Chen (2022), and implicit Langevin Hodgkinson et al. (2021). In particular, from the density level, the implicit method usually corresponds to a certain splitting Bernton (2018) of the classical JKO scheme for the Fokker-Planck equation

$$\rho_{k+1} = \underset{\rho \in \mathcal{P}_2(\mathbb{R}^d)}{\arg\min} \; \beta^{-1}\mathrm{D}_{\mathrm{KL}}(\rho \| \rho^*) + \frac{1}{2h}W_2(\rho, \rho_k)^2 \,, \tag{9}$$

where $W_2(\rho, \rho_k)$ is the Wasserstein-2 distance between densities ρ and ρ_k.

However, the aforementioned implicit implementation requires solving certain proximal operators or a system of nonlinear equations, which could be time-consuming and difficult for general families of density functions. In light of this, a semi-implicit Euler discretization method was proposed in Tan et al. (2023); Han et al. (2024) for the particle evolution equation (7) at time t_k:

$$x_{k+1} = x_k - h\left(\nabla V(x_k) + \beta^{-1}\nabla \log \rho_T(x_k)\right) , \tag{10}$$

where $\rho_T(x) = \rho(t_k + T, x)$, and for simplicity, we omit t_k in ρ_T when there is no confusion. In other words, we only evaluate the score function in the next time step.

2.3 Regularized Wasserstein proximal operator and kernel formula

Concerning (10), one may note approximating the terminal density $\rho_T := \rho(t_k + T, \cdot)$ is challenging due to non-linearity concerning the initial density and high dimensional nature of the density function ρ. The classical JKO scheme in (9) also requires an expensive optimization operation.

To address this, we first note that the JKO scheme can be regarded as a Wasserstein proximal operator with KL divergence. Then by considering a regularized Wasserstein proximal operator Li et al. (2023), a kernel formula can be obtained to compute its solution.

The solution can be adapted to approximate the evolution of the density function along the Fokker-Planck equation with a small stepsize.

Assume $t_k = 0$ for simplicity. Specifically, we first recall the Wasserstein proximal with linear energy

$$\rho_T = \arg\min_q \left[\frac{1}{2T} W_2(\rho_0, q)^2 + \int_{\mathbb{R}^d} V(x)q(x)dx \right] . \tag{11}$$

Note that this is slightly different from the Wasserstein proximal operator with KL divergence as we will later add a Laplacian regularization to this. Additionally, by the Benamou-Brenier formula Benamou and Brenier (2000), the Wasserstein-2 distance can be expressed as an optimal transport problem, leading to

$$\frac{W_2(\rho_0, q)^2}{2T} = \inf_{\rho, v} \int_0^T \int_{\mathbb{R}^d} \frac{1}{2} \|v(t,x)\|_2^2 \rho(t,x)\, dx\, dt\,,$$

where the minimizer is taken over all vector fields $v : [0,T] \times \mathbb{R}^d \to \mathbb{R}^d$, density functions $\rho : [0,T) \times \mathbb{R}^d \to \mathbb{R}$, such that

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0\,, \quad \rho(0,x) = \rho_0(x)\,, \quad \rho(T,x) = q(x)\,.$$

Solving (11) is usually a challenging optimization problem. In Li et al. (2023), motivated by Schrödinger bridge systems, the authors introduce a regularized Wasserstein proximal operator by adding a Laplacian regularization term, leading to

$$\rho_T = \arg\min_q \inf_{v, \rho} \int_0^T \int_{\mathbb{R}^d} \frac{1}{2} \|v(t,x)\|_2^2 \rho(t,x)\, dx\, dt + \int_{\mathbb{R}^d} V(x)q(x)\, dx\,, \tag{12}$$

with

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = \beta^{-1} \Delta \rho\,, \quad \rho(0,x) = \rho_0(x)\,, \quad \rho(T,x) = q(x)\,. \tag{13}$$

Introducing a Lagrange multiplier function Φ, we find that solving ρ_T is equivalent to computing the solution of the coupled PDEs

$$\begin{cases} \partial_t \rho + \nabla_x \cdot (\rho \nabla_x \Phi) = \beta^{-1} \Delta_x \rho\,, \\ \partial_t \Phi + \frac{1}{2} ||\nabla_x \Phi||_2^2 = -\beta^{-1} \Delta_x \Phi\,, \\ \rho(0,x) = \rho_0(x)\,, \quad \Phi(T,x) = -V(x)\,. \end{cases} \tag{14}$$

Comparing the first equation in (14) with the Fokker-Planck equation defined in (5), we observe that the solution to the regularized Wasserstein proximal operator (12) approximates the terminal density ρ when T is small. In other words, by solving the coupled PDE (14), we can approximate the evolution of the Fokker-Planck equation. This approximation will be justified rigorously in Section 3.

The motivation for considering the regularized Wasserstein proximal operator as an approximate solution lies in the fact that the coupled PDEs (14) can be solved using a Hopf-Cole type transformation. Then $\rho(t,x)$ can be computed by solving a system of backward-forward heat equations

$$\rho(t,x) = \eta(t,x)\hat{\eta}(t,x)\,, \tag{15}$$

where $\hat{\eta}$ and η satisfy

$$\begin{aligned} &\partial_t \hat{\eta}(t,x) = \beta^{-1} \Delta_x \hat{\eta}(t,x)\,, \\ &\partial_t \eta(t,x) = -\beta^{-1} \Delta_x \eta(t,x)\,, \\ &\eta(0,x)\hat{\eta}(0,x) = \rho_0(x), \quad \eta(T,x) = \exp\left(-\beta V(x)\right)\,. \end{aligned} \tag{16}$$

Denote $G_t(x,y) = 1/(4\pi\frac{t}{\beta})^{\frac{d}{2}} \exp(-\|x-y\|_2^2/(4\frac{t}{\beta}))$ as the heat kernel with thermal diffusivity β. The solution to the regularised Wasserstein proximal operator (12) can be computed as

$$\begin{cases} \rho(t,x) = (G_{T-t} * \exp(-\frac{V}{2\beta})) \cdot (G_t * \frac{\rho_0}{G_T * \exp(-\frac{V}{2\beta})})(x)\,, \\ v(t,x) = 2\beta^{-1}\nabla \log(G_{T-t} * \exp(-\frac{V}{2\beta}))\,, \\ \rho_T = \exp(-\frac{V}{2\beta})(x) * (G_T * \frac{\rho_0}{G_T * \exp(-\frac{V}{2\beta})})(x)\,. \end{cases}$$

In particular, we are mostly interested in the terminal density ρ_T which is an approximation to the density function that evolves from the Fokker-Planck equation with initial density ρ_0 at time T. We write down the explicit formula of ρ_T for the convenience of the upcoming discussion

$$\rho_T(x) = \mathrm{Prox}_{T,V}(\rho_0)(x) := \int_{\mathbb{R}^d} \frac{\exp\big[-\frac{\beta}{2}\big(V(x) + \frac{\|x-y\|_2^2}{2T}\big)\big]}{\int_{\mathbb{R}^d} \exp\big[-\frac{\beta}{2}\big(V(z) + \frac{\|z-y\|_2^2}{2T}\big)\big] dz} \rho_0(y) dy. \tag{17}$$

2.4 BRWP algorithm

We now present the complete BRWP algorithm for sampling based on the semi-implicit discretization of the probability flow ODE.

Algorithm 1 BRWP for Sampling from $\rho^* = \frac{1}{Z}\exp(-\beta V)$

Input: Initial particle set $\{x_{0,j}\}_{j=1}^N$
for $k = 1, 2, 3, \dots$ **do**
  Given ρ_k as the density function for $\{x_{k,j}\}$, compute $\rho_{t_k+T}(x_{k,j})$ using the kernel formula.
  for each particle $j = 1, 2, \dots, N$ **do**
    Update particle:

$$x_{k+1,j} = x_{k,j} - h\left(\nabla V(x_{k,j}) + \beta^{-1}\nabla \log \rho_{t_k+T}(x_{k,j})\right)$$

  end for
end for

Here, T represents the stepsize for the evolution of the Fokker-Planck equation in (5), and h represents the discretization stepsize for the score dynamics (7). In our discussion, we are primarily interested in the case where $T = h$. We use different notations to emphasize that these are discretization parameters for two distinct processes.

The goal of this work is to establish results on the sampling complexity and maximum stepsize h required for the convergence of the interacting particle system generated by (10) under the following assumptions on ρ^*

- **Strony log-concavity:** The target distribution ρ^* is log-concave, i.e., there exists a constant $\alpha > 0$ such that $\nabla^2 V \succeq \alpha I$.
- **Bounded derivatives:** The second and third derivatives of the function V are bounded. Specifically, there exist constants $L, M > 0$ such that $\|\nabla^2 V\|_\infty \le L$ and $\|\nabla^3 V\|_\infty \le M$.

We note that the first assumption ensures the existence of a log-Sobolev inequality, while the second assumption facilitates the convergence of second and third order Taylor expansions involving V. The bounded derivative assumptions are for theoretical convenience and do not appear in the final expression of sampling complexity or mixing time. Moreover, we only require that $\|\nabla^2 V\|_\infty$ and $\|\nabla^3 V\|_\infty$ are bounded in a neighborhood of the particles $\{x_{k,j}\}$, where the neighborhood size is proportional to the discretization stepsize. Our numerical experiments (see Section 6) demonstrate that the proposed methods work for a general family of distributions.

We first summarize the theoretical results we will prove in Section 4 in Table 1, where we compare BRWP with other popular methods. Sampling complexity refers to the number of iterations needed to achieve at a given level of accuracy.

Algorithm	**Sampling complexity when** $\mathrm{D}_{\mathrm{KL}}(\rho_k\|\rho^*) \le \delta$	**Maximum stepsize** h
BRWP (this paper)	$\mathcal{O}\left(\frac{\|\ln\delta\|}{2\alpha\delta^{1/2}}\right)$	$\frac{2}{3\alpha}$
ULA (Vempala and Wibisono (2019))	$\mathcal{O}\left(\frac{dL^2}{\alpha^2\delta}\right)$	$\frac{\alpha}{4L^2}$
Underdamped Langevin (Ma et al. (2021))	$\mathcal{O}\left(\frac{d^{1/2}(L^{3/2}+d^{1/2}K)}{\alpha^2\delta^{1/2}}\right)$	$\mathcal{O}\left(\frac{\alpha}{L^{3/2}}\right)$
Proximal Langevin (Wibisono (2019))	$\mathcal{O}\left(\frac{d^{1/2}(L^{3/2}+dK)}{\alpha^{3/2}\delta^{1/2}}\right)$	$\min\left\{\frac{1}{8L}, \frac{1}{K}, \frac{3\alpha}{32L^2}\right\}$

Table 1: Iteration complexities for Langevin algorithms under log-Sobolev inequality with constant α. Here $-LI \preceq \nabla^2 V \preceq LI$ and K is the upper bound for $\|\nabla^3 V\|_{op}$.

In the next section, we shall assume that we know exactly ρ_k at time t_k and focus on investigating the approximate density given by the kernel formula (17).

3 Laplace Approximation to the kernel formula

In this section, we demonstrate that the solution to the regularized Wasserstein proximal operator (17) approximates the evolution of the Fokker-Planck equation (5) when T is small by utilizing the Laplace method. The proof shows that the solution to the Fokker-Planck equation can be approximated using the kernel formula without the need for inversion or optimization.

Our strategy is to employ the **Laplace method** up to two terms Bleistein and Handelsman (1986)

$$\int_\Omega g(x)\exp\left(-\frac{f(x)}{T}\right)dx = (2\pi T)^{d/2}\exp\left(-\frac{f(x^*)}{T}\right)\left[\frac{g(x^*)}{|\nabla^2 f(x^*)|^{1/2}} + \frac{T}{2}H_1(x^*) + \mathcal{O}(T^2)\right], \quad (18)$$

where $x^* = \arg\min_x f(x)$ is the unique minimizer of f in Ω, $|\nabla^2 f|$ is the determinant of the Hessian matrix of f, and H_1 is the first-order term of the expansion. The explicit form for H_1 is given below, with its detailed derivation available in Section 8.3 of Bleistein and Handelsman (1986). Writing $f_p = \frac{\partial}{\partial x_p} f$ for $p = 1, \cdots, d$, we have

$$\begin{aligned} H_1(x^*) = -|\nabla^2 f(x^*)|^{-1/2}\Big\{ & - f_{srq}B_{sq}B_{rp}g_p + \mathrm{Tr}(CB) \\ & + g\left[f_{pqr}f_{stu}\left(\frac{1}{4}B_{ps}B_{qr}B_{tu} + \frac{1}{6}B_{ps}B_{qt}B_{ru}\right) - \frac{1}{4}f_{pqrs}B_{pr}B_{qs}\right]\Big\}_{x=x^*}, \end{aligned} \quad (19)$$

where we use the summation convention to sum over all indices from 1 to d. The matrices in the expression are defined as

$$C = \{g_{pq}\}\,, \quad B = \{B_{pq}\}\,, \quad \sum B_{pq} f_{qr}(x^*) = \delta_{pr}\,.$$

We can then apply this approximation to the kernel formula of the regularized Wasserstein proximal operator in (17) to obtain the asymptotic expansion when T is small. In Theorem 4, we will show that ρ_T, computed from the kernel formula satisfies

$$\rho_T(x) = \rho_0(x) + T \frac{\partial \rho_0}{\partial t}\bigg|_{t=t_0}(x) + \mathcal{O}(T^2)\,,$$

where ρ_0 satisfies the Fokker-Planck equation at time t_0. The proof relies on exploring the explicit representations of the first two terms in the approximation (18), the Taylor expansion of the potential function V (by the bounded derivative assumption), and the uniqueness of the minimizer x^* in (19), which follows from the log-concavity assumption.

3.1 Approximation to the normalization term

Firstly, we derive the approximation result for the denominator in the kernel formula (17), as shown in the following lemma.

Lemma 3 *For any y, assuming $T\Delta V(s_y) \le 1$, we have*

$$\begin{aligned} &\left(\frac{\beta}{4\pi T}\right)^{d/2} \int_{\mathbb{R}^d} \exp\left(-\frac{\beta}{2}\left(V(z) + \frac{\|z-y\|_2^2}{2T}\right)\right) dz \\ =&\frac{1}{1 + T/2\Delta V(\tilde{s}_y)} \exp\left(-\frac{\beta}{2}\left(V(\tilde{s}_y) + \frac{\|\tilde{s}_y - y\|_2^2}{2T}\right)\right) + \mathcal{O}(T^2)\,, \end{aligned} \tag{20}$$

where

$$s_y = y - T\nabla V(s_y)\,, \quad \tilde{s}_y = y - T\nabla V(y)\,.$$

Proof For the normalization term in (17) and fixed y, we have

$$\begin{aligned} &\left(\frac{\beta}{4\pi T}\right)^{d/2} \int_{\mathbb{R}^d} \exp\left(-\frac{\beta}{2}\left(V(z) + \frac{\|z-y\|_2^2}{2T}\right)\right) dz \\ =&\left(\frac{\beta}{4\pi T}\right)^{d/2} \int_{\mathbb{R}^d} \exp\left(-\frac{\beta}{2T}\left(TV(z) + \frac{\|z-y\|_2^2}{2}\right)\right) dz \\ =&\exp\left(-\frac{\beta}{2T}\left(TV(s_y) + \frac{\|s_y-y\|_2^2}{2}\right)\right)\left[\frac{1}{|1 + T\nabla^2 V(s_y)|^{1/2}} + \frac{T}{\beta} H_1(s_y) + \mathcal{O}\left(\frac{2T}{\beta}\right)^2\right]\,, \end{aligned} \tag{21}$$

where s_y is defined as the arg min of the exponent

$$s_y := \arg\min_z \left\{TV(z) + \frac{\|y-z\|_2^2}{2}\right\}\,.$$

Next, we verify that $H_1(s_y)$ is of order $\mathcal{O}(T)$. Concerning the general form of Laplace method (18), we note

$$g(z) = 1\,, \quad f(z) = TV(z) + \frac{\|z-y\|_2^2}{2}\,, \quad f_{pq}(z) = T\frac{\partial^2 V}{\partial z_p \partial z_q}(z) + \delta_{pq}\,, \quad f_{pqr}(z) = T\frac{\partial^3 V}{\partial z_p \partial z_q \partial z_r}(z)\,,$$

where the quadratic term becomes a constant after taking the second-order partial derivative and vanishes after taking the third-order partial derivative. Given that the B matrix in (19) is the inverse of a diagonal matrix plus $T\nabla^2 V$, the magnitude of the diagonal entries of B is $\mathcal{O}(1)$.

Thus, looking at the expression of $H_1(s_y)$, we confirm that

$$H_1(s_y) = \mathcal{O}(T)\,,$$

as all terms in (19) are of the order $\mathcal{O}(T)$. Then the approximation in (21) is simplified to

$$\begin{aligned}&\left(\frac{\beta}{4\pi T}\right)^{d/2}\int_{\mathbb{R}^d}\exp\left(-\frac{\beta}{2}\left(V(z)+\frac{||z-y||_2^2}{2T}\right)\right)dz \\ =&\frac{1}{|1+T\nabla^2 V(s_y)|^{1/2}}\exp\left(-\frac{\beta}{2T}\left(TV(s_y)+\frac{\|s_y-y\|_2^2}{2}\right)\right)+\mathcal{O}(T^2)\,.\end{aligned} \tag{22}$$

Next, we compute s_y more explicitly. Since $V(z)$ is convex, so is $TV(z)+\|z-y\|_2^2$ for any y and T with respect to z. This ensures s_y is unique. By the first-order optimality condition, s_y satisfies

$$T\nabla V(s_y)+s_y = y\,.$$

To further simplify the expression and compute the integral explicitly, we define an approximation for s_y as

$$\tilde{s}_y := y - T\nabla V(y)\,. \tag{23}$$

By definition of $\tilde{s}_y$, we have

$$\|\tilde{s}_y - s_y\|_2 = T\|\nabla V(s_y)-\nabla V(y)\|_2 \le LT\|s_y-y\|_2 = LT^2\|\nabla V(s_y)\|_2 = \mathcal{O}(T^2)\,.$$

The inequality holds when ∇V is Lipschitz continuous with constant L which can be implied by $\nabla^2 V$ is bounded by L along the line segment connecting y and s_y.

Finally, for the determinant of the Hessian matrix, we apply the Taylor expansion of the determinant operator and the square root function to obtain

$$\begin{aligned}|I+T\nabla^2 V(s_y)| &= I + T\Delta V(s_y)+\mathcal{O}(T^2)\,,\\ |I+T\nabla^2 V(s_y)|^{1/2} &= I+\frac{T}{2}\Delta V(s_y)+\mathcal{O}(T^2)\,,\end{aligned} \tag{24}$$

which converges when $T\Delta V(s_y)\le 1$.

We arrive at the desired result by combining equations (21) to (24). ■

3.2 Approximation to the kernel formula

In this subsection, we will present the approximation to the complete kernel formula for ρ_T and discuss several implications of the approximation. Letting

$$V_0(x) = -\beta^{-1}\log\rho_0(x)\,,$$

we follow a similar approach as in the proof of Lemma 3 to derive the asymptotic approximation of ρ_T. Due to the similarity in the proof of the following theorem, we will highlight the key steps and leave the complete proof in the appendix.

Theorem 4 *For fixed x, assume that ΔV_0 is bounded above on the line segment connecting x and r_x, where r_x satisfies $r_x = x + T\nabla(V - 2V_0)(r_x)$. Moreover, when $T\Delta V(r_x) \leq 1$ and $T\Delta V_0(r_x) \leq 1$, we have*

$$\rho_T(x) = \rho_0(x)\big[1 - \beta T\nabla(V - V_0)\cdot\nabla V_0(x) + T\Delta(V - V_0)(x)\big] + \mathcal{O}(T^2)\,. \tag{25}$$

If ρ_0 satisfies the Fokker-Planck equation at time t_0, we have

$$\rho_T = \rho_0 + T\beta^{-1}\nabla\cdot\left(\nabla\log\frac{\rho_0}{\rho^*}\rho_0\right) + \mathcal{O}(T^2) = \rho_0 + T\frac{\partial\rho}{\partial t}\bigg|_{t=t_0} + \mathcal{O}(T^2)\,. \tag{26}$$

Proof The main proof is divided into three steps.

Step 1: Substituting (20) into the expression for ρ_T in (17), we obtain

$$\begin{aligned}\rho_T(x) =& \exp\left(-\frac{\beta}{2}V(x)\right)\cdot \\ & \int_{\mathbb{R}^d}\frac{1+\frac{T}{2}\Delta V(\tilde{s}_y)}{(4\pi T/\beta)^{d/2}}\exp\left[-\frac{\beta}{2}\left(\frac{||x-y||_2^2}{2T} + 2V_0(y) - V(\tilde{s}_y) - \frac{||y-\tilde{s}_y||_2^2}{2T}\right)\right]dy + \mathcal{O}(T^2)\,,\end{aligned}$$

where $\tilde{s}_y = y - T\nabla V(y)$.

Step 2: Applying the Laplace method to approximate the integral obtained in Step 1, we arrive at

$$\begin{aligned}\rho_T(x) =& \frac{\exp\left(-\frac{\beta}{2}V(x)\right)\left[1+\frac{T}{2}\Delta V(\tilde{s}_{\tilde{r}_x})\right]}{1+\frac{T}{2}\Delta(2V_0 - V)(\tilde{r}_x)}\cdot \\ & \exp\left[-\frac{\beta}{2}\left(\frac{||x-\tilde{r}_x||_2^2}{2T} - \frac{||\tilde{r}_x - \tilde{s}_{\tilde{r}_x}||_2^2}{2T} + 2V_0(\tilde{r}_x) - V(\tilde{s}_{\tilde{r}_x})\right)\right] + \mathcal{O}(T^2)\,,\end{aligned}$$

where

$$\tilde{r}_x := x + T\nabla(V - 2V_0)(x)\,,$$

being the minimizer of the exponent.

Step 3: Using a Taylor expansion on the exponent again and the definitions of $\tilde{s}_{\tilde{r}_x}$ and $\tilde{r}_x$, we derive

$$2V_0(\tilde{r}_x) - V(\tilde{s}_{\tilde{r}_x}) + \frac{||x-\tilde{r}_x||_2^2}{2T} - \frac{||\tilde{r}_x - \tilde{s}_{\tilde{r}_x}||_2^2}{2T} = 2V_0(x) - V(x) + 2T\nabla(V - V_0)\cdot\nabla V_0(x) + \mathcal{O}(T^2)\,,$$

which leads directly to the desired result after substitution.

Finally, the relation (26) comes from

$$\frac{\partial\rho}{\partial t}\bigg|_{t=t_0} = \beta^{-1}\nabla\cdot\left(\nabla\log\frac{\rho_0}{\rho^*}\rho_0\right) = \left(\Delta(V - V_0) - \beta\nabla V_0\cdot\nabla(V - V_0)\right)\rho_0\,.$$

■

We observe that it is sufficient for the Hessian of V_0 to be bounded only within a T-neighborhood around the sampling point x, rather than requiring global boundedness, which can be challenging to verify in practice. Additionally, since most sampling points are typically situated near the high-density regions of ρ^*, it is adequate for V_0 to exhibit reasonable smoothness specifically within these high-density areas.

We remark that (26) implies ρ_T computed from the kernel formula serves as a first-order approximation to the solution of the Fokker-Planck equation. Before proceeding to the particle formulation of our sampling algorithm, we present two direct corollaries of the approximation in Theorem 4. These corollaries demonstrate that if the kernel formula (17) is successfully applied for a small time stepsize T, i.e.,

$$\rho_{k+1} = \mathrm{Prox}_{T,V}(\rho_k)\,, \quad k = 0, 1, 2, \cdots\,, \tag{27}$$

the KL divergence and Fisher information between ρ_k and ρ^* will converge exponentially with an error term of $\mathcal{O}(T^2)$.

Firstly, for the convergence of the KL divergence, we have the following lemma whose proof can be found in Appendix A.2.

Lemma 5 *For ρ_k at iteration k defined by (27), we have*

$$\mathrm{D}_{\mathrm{KL}}(\rho_k\|\rho^*) - \mathrm{D}_{\mathrm{KL}}(\rho_{k+1}\|\rho^*) = T\beta^{-1}\mathcal{I}(\rho_k\|\rho^*) + \mathcal{O}(T^2)\,.$$

Applying the PL inequality (6), we obtain a lower bound for the decay of the KL energy

$$\mathrm{D}_{\mathrm{KL}}(\rho_k\|\rho^*) - \mathrm{D}_{\mathrm{KL}}(\rho_{k+1}\|\rho^*) \geq 2\alpha T\mathrm{D}_{\mathrm{KL}}(\rho_k\|\rho^*) + \mathcal{O}(T^2)\,.$$

Using Grönwall's inequality, we then establish the exponential convergence of the KL divergence.

Theorem 6 *Under the same assumptions as in Theorem 4, with ρ_k from (27), we have*

$$\mathrm{D}_{\mathrm{KL}}(\rho_k\|\rho^*) \leq \mathrm{D}_{\mathrm{KL}}(\rho_0\|\rho^*)\exp(-2\alpha kT) + \mathcal{O}(T)\,. \tag{28}$$

Similarly, the convergence of the Fisher information can be derived by applying the Taylor expansion to $\int \|\nabla \log \frac{\rho_k}{\rho^*}\|_2^2 \rho_k dx$, alongside the exponential convergence of the Fisher information along the flow of Fokker-Planck equation as proved in Lemma 17 in the appendix. This leads to the following corollary.

Corollary 7 *Under the same assumptions as in Theorem 4, with ρ_k from (27), we have*

$$\mathcal{I}(\rho_k\|\rho^*) \leq \mathcal{I}(\rho_0\|\rho^*)\exp(-2\alpha kT) + \mathcal{O}(T)\,. \tag{29}$$

4 Rapid Convergence of BRWP

In this section, we analyze the convergence of the BRWP presented in Algorithm 1, where the particle evolves according to

$$x_{k+1} = x_k - h(\nabla V(x_k) + \beta^{-1}\nabla \log \rho_T(x_k))\,, \tag{30}$$

with $\nabla \log \rho_T$ being a first-order approximation to the score function at time $t_k + T$ for $T \leq h$, where ρ_T satisfies

$$\rho_T = \rho_k + T\beta^{-1}\nabla\cdot\left(\nabla \log \frac{\rho_k}{\rho^*}\rho_k\right) + \mathcal{O}(T^2)\,. \tag{31}$$

According to Theorem 4, the kernel formula (17) provides a feasible way to compute ρ_T without any optimization and inversion. Since ρ_k and ρ^* are independent of T, the order of the error term will remain the same after taking the gradient on (31). More practical considerations of evaluating this formula will be addressed in Section 5.

Our primary objective is to determine the sampling complexity and maximum step size outlined in Table 1 at the end of Section 2, as well as to analyze the mixing time of the BRWP algorithm. Specifically, we will first analyze the evolution of the density function under discretization and then derive the rate of decay for the KL divergence between the density function of the generated particles and ρ^*.

4.1 Evolution of density function of the particle system

In the next lemma, we will first derive the evolution of the density function for the discrete particle system (30). Since most of the derivation is Taylor expansion and standard integration by parts, we will highlight key steps in the following proof and leave the complete derivation in the Appendix A.3.

Lemma 8 *The evolution of the density function corresponding to* (30) *is given by*

$$\begin{aligned}\rho_{k+1} =&\rho_k + h\beta^{-1}\nabla\cdot\left(\nabla\log\frac{\rho_k}{\rho^*}\rho_k\right) + hT\beta^{-2}\nabla\cdot\left[\nabla\left(\frac{\nabla\cdot(\nabla\log\frac{\rho_k}{\rho^*}\rho_k)}{\rho_k}\right)\rho_k\right] \\ &+\frac{h^2}{2}\nabla\cdot(\tilde{\phi}\rho_k) + \mathcal{O}(h^3)\,,\end{aligned} \tag{32}$$

where

$$\tilde{\phi} := \left[\nabla\cdot(\nabla\phi\nabla\phi^T) + (\nabla\phi)^T(\nabla\phi\cdot\nabla\log\rho_k)\right]\,,\quad \phi := \beta^{-1}(\log\rho_T - \log\rho^*)\,. \tag{33}$$

Proof [Sketch of the proof] The outline of the proof is given as follows.

Step 1. Let $\phi(x) = V(x) + \beta^{-1}\log\rho_T(x)$. For any smooth function u, we have

$$\begin{aligned}\int u\rho_{k+1}\,dx &= \int\left[u - h\nabla\phi\cdot\nabla u + \frac{h^2}{2}\nabla\phi^T\nabla^2 u\nabla\phi\right]\rho_k\,dx + \mathcal{O}(h^3) \\ &= \int u\left[\rho_k + h\nabla\cdot(\nabla\phi\rho_k) + \frac{h^2}{2}\sum_{i,j}\frac{\partial^2}{\partial x_i\partial x_j}\left(\frac{\partial\phi}{\partial x_i}\frac{\partial\phi}{\partial x_j}\rho_k\right)\right]dx + \mathcal{O}(h^3)\,.\end{aligned} \tag{34}$$

Step 2. The term involving the Hessian can be simplified to

$$\sum_i\frac{\partial}{\partial x_i}\left(\frac{\partial\phi}{\partial x_i}\frac{\partial\phi}{\partial x_j}\rho_k\right) = \left[\nabla\cdot(\nabla\phi\nabla\phi^T) + (\nabla\phi)^T(\nabla\phi\cdot\nabla\log\rho_k)\right]\rho_k = \tilde{\phi}\cdot\rho_k\,.$$

Step 3. The desired result follows by noting that

$$\log\rho_T = \rho_k + T\beta^{-1}\frac{\nabla\cdot\left(\nabla\log\frac{\rho_k}{\rho^*}\rho_k\right)}{\rho_k} + \mathcal{O}(T^2)\,.$$

■

To simplify notation, we define

$$\mathcal{D}_k^\beta(u) := \frac{\beta^{-1}}{\rho_k}\nabla\cdot(\nabla u\rho_k)\,. \tag{35}$$

Equation (32) can then be rewritten more compactly as

$$\rho_{k+1} = \rho_k + h\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right)\rho_k + hT\mathcal{D}_k^\beta\circ\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right)\rho_k + \frac{h^2}{2}\nabla\cdot(\tilde{\phi}\rho_k) + \mathcal{O}(h^3)\,. \tag{36}$$

Next, we can substitute (36) into the definition of KL divergence and apply the definition of $\mathcal{D}_k^\beta$ to obtain the decay of KL divergence at each time step. The result is summarized in the following lemma and is derived using integration by parts and the Taylor expansion of the logarithmic function. The detailed proof is provided in Appendix A.3.

Lemma 9 *For the density function evolves from* (30) *from time* t_k *to* $t_{k+1} = t_k + h$*, we have*

$$\mathrm{D}_{\mathrm{KL}}(\rho_k\|\rho^*) - \mathrm{D}_{\mathrm{KL}}(\rho_{k+1}\|\rho^*) = h\beta^{-1}\mathcal{I}(\rho_k\|\rho^*) - \frac{h(h+2T)}{2}\int \left|\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right)\right|^2 \rho_k dx \qquad (37)$$
$$- \frac{h^2}{2}\beta^{-2}\int\left\langle \nabla\log\frac{\rho_k}{\rho^*},\, \nabla^2\log\frac{\rho_k}{\rho^*}\nabla\log\frac{\rho_k}{\rho^*}\right\rangle \rho_k\, dx + \mathcal{O}(h^3)\,.$$

4.2 Convergence of KL divergence and the mixing time

In the expansion presented in Lemma 9, the first term, associated with Fisher information, induces the exponential decay due to the PL inequality (6), which is also common in the analysis of time-discretizations of Langevin dynamics. Thus, the second and third terms, which result from discretization errors, are crucial for comparing the convergence rates of different schemes.

Given that our expansion includes terms up to $\mathcal{O}(h^2)$, it is natural to consider identities related to the second-order time derivative of KL divergence along the flow of the Fokker-Planck equation. Assuming ρ_k satisfies the Fokker-Planck equation at time t_k, Lemma 18 in the appendix provides the well known identity

$$\frac{d^2}{dt^2}\mathrm{D}_{\mathrm{KL}}(\rho_k\|\rho^*) = 2\beta^{-1}\int\left\langle\nabla\log\frac{\rho_k}{\rho^*},\, \nabla^2 V\nabla\log\frac{\rho_k}{\rho^*}\right\rangle\rho_k\, dx + 2\beta^{-2}\int\left\|\nabla^2\log\frac{\rho_k}{\rho^*}\right\|_{\mathrm{F}}^2\rho_k\, dx\,.$$

Additionally, using the definition of $\mathcal{D}_k^\beta$ in (35), Lemma 19 in the appendix shows another representation of the second-order derivative of KL divergence

$$\frac{1}{2}\frac{d^2}{dt^2}\mathrm{D}_{\mathrm{KL}}(\rho_k\|\rho^*) = \int\left|\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right)\right|^2\rho_k\, dx + \beta^{-2}\int\left\langle\nabla\log\frac{\rho_k}{\rho^*},\, \nabla^2\log\frac{\rho_k}{\rho^*}\nabla\log\frac{\rho_k}{\rho^*}\right\rangle\rho_k\, dx\,.$$

Substituting these results into (37), we obtain

$$\begin{aligned}
&\mathrm{D}_{\mathrm{KL}}(\rho_k\|\rho^*) - \mathrm{D}_{\mathrm{KL}}(\rho_{k+1}\|\rho^*) \qquad (38)\\
&\geq h\beta^{-1}\mathcal{I}(\rho_k\|\rho^*) - \frac{h(h+2T)}{4}\frac{d^2}{dt^2}\mathrm{D}_{\mathrm{KL}}(\rho_k\|\rho^*)\\
&\quad - \frac{hT}{2}\beta^{-2}\left[\int\left\|\nabla^2\log\frac{\rho_k}{\rho^*}\right\|_{\mathrm{F}}^2\rho_k\, dx + \int\left\|\nabla\log\frac{\rho_k}{\rho^*}\right\|_2^4\rho_k\, dx\right] + \mathcal{O}(h^3)\\
&= h\beta^{-1}\mathcal{I}(\rho_k\|\rho^*) - \frac{h(h+3T)}{4}\frac{d^2}{dt^2}\mathrm{D}_{\mathrm{KL}}(\rho_k\|\rho^*)\\
&\quad + \frac{hT\beta^{-1}}{2}\int\left\langle\nabla\log\frac{\rho_k}{\rho^*},\, \nabla^2 V\nabla\log\frac{\rho_k}{\rho^*}\right\rangle\rho_k\, dx - \frac{hT\beta^{-2}}{2}\int\left\|\nabla\log\frac{\rho_k}{\rho^*}\right\|_2^4\rho_k\, dx + \mathcal{O}(h^3)\,,
\end{aligned}$$

where we used the inequality

$$\|A\|_{\mathrm{F}}^2 + \|x\|_2^4 \geq -2\sum_{ij} x_i a_{ij} x_j = -2x^T A x\,,$$

in the second line. Regarding the terms in the final line of (38), the second-order time derivative can be bounded using the PL inequality by writing it as the difference of the Fisher information at t_k and t_{k+1}, while the third term can be bounded below by the strong log-concavity assumption. This leaves us with the task of bounding the term with the fourth power, which involves detailed calculations using vector calculus identities. In Lemma 20 in the appendix, we show that for continuous time, where ρ satisfies the Fokker-Planck equation

$$\frac{\partial}{\partial t} \int \left\| \nabla \log \frac{\rho}{\rho^*} \right\|_2^4 \rho \, dx \leq -4\alpha \int \left\| \nabla \log \frac{\rho}{\rho^*} \right\|_2^4 \rho \, dx \,,$$

which implies that the fourth-order term also decays exponentially.

Hence, for the density function evolving according to (32), we have the following result.

Lemma 10 *For ρ_k satisfying the iterative relationship* (32)*, we have*

$$\int \left\| \nabla \log \frac{\rho_k}{\rho^*} \right\|_2^4 \rho_k \, dx \leq \exp(-4\alpha hk) \int \left\| \nabla \log \frac{\rho_0}{\rho^*} \right\|_2^4 \rho_0 \, dx + \mathcal{O}(h) \,. \tag{39}$$

Proof The result follows from combining the findings in Lemma 20, the relation

$$\rho_{k+1} = \rho_k + h \frac{\partial \rho_k}{\partial t} + \mathcal{O}(h^2) = \rho_{t_k+h} + \mathcal{O}(h^2) \,,$$

where ρ_{t_k+h} is the density evolving according to the exact Fokker-Planck equation at time $t_k + h$ with initial density ρ_k at time t_k, and Grönwall's inequality. ■

The next Lemma will describe the relation of KL divergence at t_k and t_{k+1} whose proof follows from the results established in Lemma 10 and the application of the PL inequality to (38), as detailed in Appendix A.3.

Lemma 11 *Let $M_0 := \beta^{-2} \int \|\nabla \log \frac{\rho_0}{\rho^*}\|_2^4 \rho_0 \, dx$, $t_k = kh$, and $T = sh$ for $s \in [0,1]$. Then, the decay of KL divergence in one step is given by*

$$\mathrm{D_{KL}}(\rho_{k+1} \| \rho^*) \leq \left[1 - 2\alpha h + (1+2s)\alpha^2 h^2\right] \mathrm{D_{KL}}(\rho_k \| \rho^*) + \frac{h^2 s}{2} M_0 \exp(-4\alpha hk) + \mathcal{O}(h^3) \,. \tag{40}$$

We are now ready to present the main theorem concerning the convergence guarantee of the BRWP algorithm in terms of KL divergence.

Theorem 12 *Suppose $T = sh$ for $s \in [0,1]$. The KL divergence at the k-th time step satisfies*

$$\begin{aligned} \mathrm{D_{KL}}(\rho_k \| \rho^*) \leq &\exp\left[-\alpha kh \left(2 - (1+2s)\alpha h\right)\right] \mathrm{D_{KL}}(\rho_0 \| \rho^*) \\ &+ \frac{h^2}{2} \frac{s M_0 \exp(-4\alpha kh)}{\exp(-4\alpha h) - (1 - 2h\alpha + (1+2s)\alpha^2 h^2)} + \mathcal{O}(h^2) \,. \end{aligned} \tag{41}$$

When $s = 1$, the algorithm achieves an error $\mathrm{D_{KL}}(\rho_k \| \rho^*) \leq \delta$ with

$$k = \mathcal{O}\left(\frac{|\ln \delta|}{2\alpha\sqrt{\delta}}\right),$$

and the stepsize $h = \sqrt{\delta}$ when $\sqrt{\delta} < \frac{2}{3\alpha}$ and $\delta \ll 1$.

Proof By applying results in Lemma 21 regarding the convergence of general sequences of the form (40), we obtain the inequality (41).

We note that since

$$\frac{h}{\exp(-4\alpha h) - (1 - 2h\alpha + (1+2s)\alpha^2 h^2)} = \frac{1}{-2\alpha + \mathcal{O}(h)} \,,$$

the second term in (41) is of order $h\exp(-4\alpha t_k)$ and much smaller than the first term for small h. Hence, let $h^2 = \delta$, $s = 1$, and require the first term in (41) to be of order $\mathcal{O}(\delta)$. This implies

$$k \geq \frac{\ln(\mathrm{D}_{\mathrm{KL}}(\rho_0\|\rho^*)) - \ln\delta}{h\alpha(2-3\alpha h)}\,.$$

Substituting $h^2 = \delta$ into the above, we obtain the desired result on sampling complexity. ■

We remark that from Han et al. (2024); Tan et al. (2023), the bias of BRWP for target Gaussian distribution is of order h^2, which coincides with our current analysis and is better than ULA whose bias is of order $\mathcal{O}(h)$.

However, in practice, we usually choose a small stepsize to make the bias term small. We present the following corollary on the maximum and optimal stepsize. The result is based on the explicit decay result in Theorem 12, which is useful for the case α is large or adaptive step size, i.e., using a larger stepsize for the first few iterations.

Corollary 13 *For $T = h$, regarding the convergence of the KL divergence with the BRWP algorithm:*

- *The maximum allowable step size is $h = \frac{2}{3\alpha}$.*
- *The step size that yields the fastest convergence is $h = \frac{1}{3\alpha}$.*

Some other quantities are also often useful for measuring the efficiency of a sampling algorithm including the Wasserstein-2 distance between ρ_k and ρ^* and the mixing time. In particular, the mixing time is defined as

$$t_{mix}(\delta,\rho_0) = \min\{k \mid d_{TV}(\rho_k,\rho^*) \leq \delta\}\,, \tag{42}$$

where ρ_k is the density function at time t_k starting from ρ_0 and

$$d_{TV}(\rho_k,\rho^*) = \int_{\mathbb{R}^d} |\rho_k(x) - \rho^*(x)|\,dx\,. \tag{43}$$

Recalling the Pinsker's inequality

$$d_{TV}(\rho_k,\rho^*)^2 \leq \frac{1}{2}\mathrm{D}_{\mathrm{KL}}(\rho_k\rho^*\|\rho^*)\,,$$

and the Talagrand's inequality

$$\frac{\alpha}{2}W_2(\rho_k,\rho^*)^2 \leq \mathrm{D}_{\mathrm{KL}}(\rho_k\|\rho^*)\,,$$

we obtain the following direct corollary of Theorem 12.

Corollary 14 *When $T = h$ for the BRWP algorithm, the convergence of the Wasserstein-2 distance between ρ_k and ρ^* is given by*

$$W_2(\rho_k,\rho^*)^2 \leq \frac{2\exp\left(-\alpha kh(2-3\alpha h)\right)}{\alpha}\mathrm{D}_{\mathrm{KL}}(\rho_0\|\rho^*) + \frac{h^2M_0\exp(-4\alpha kh)}{\alpha(\exp(-4\alpha h) - (1-2h\alpha+3\alpha^2h^2))} + \mathcal{O}(h^2).$$

The mixing time will be $t_{mix}(\delta,\rho_0) = \mathcal{O}\left(\frac{|\ln\delta|}{2\alpha\delta}\right)\mathrm{D}_{\mathrm{KL}}(\rho_0\|\rho^*)$ with $h = \delta$.

5 Estimation of Score function and Practical Consideration

In this section, we analyze the impact of numerical errors arising from approximating the score function, $\nabla \log \rho_T$, at each iteration of the interacting particle system described in (7). These errors can significantly affect the overall numerical performance. One common approach for estimating the score function is kernel density estimation, as employed in Tan et al. (2023); Han et al. (2024). Based on existing accuracy results for score estimation (e.g., Wibisono et al. (2024); Jiang and Zhang (2009)), the score function can be approximated with high accuracy, provided that a sufficiently large number of particles is used. This assumption underlies the results presented in Section 4.

For example, if the error in the score function estimation is of order $\mathcal{O}(h^2)$, then the previous discussions remain valid, as this would introduce an additional error term of order $\mathcal{O}(h^3)$. However, if the score function estimation lacks sufficient accuracy, our results in Section 4 will be weakened due to the introduction of an additional error term from the score function estimation itself.

Additionally, we explore an alternative method for computing the score function by iteratively applying the kernel formula (17). This approach circumvents the need to estimate the score function at each iteration, potentially improving efficiency and stability.

5.1 Score function from successive approximation

We denote the sequence of density functions $\tilde{\rho}_k$ as the density generated by evaluating the regularized proximal operator (27)

$$\tilde{\rho}_{k+1} = \mathrm{Prox}_{T,V}(\tilde{\rho}_k)\,, \tag{44}$$

with $\tilde{\rho}_0 = \rho_0$ as the initial density. As discussed previously, we also denote ρ_k as the density function generated by BRWP as in (7).

We propose a direct computation of the score function in each iteration using the regularized Wasserstein proximal operator, bypassing the need to construct an empirical distribution or perform kernel density estimation from the particles $\{x_{k,j}\}$. This approach leads to the following algorithm.

Algorithm 2 BRWP for Sampling from $\rho^* = \frac{1}{Z}\exp(-\beta V)$ with successively evaluating the regularized Wasserstein proximal operator.

```
Let ρ̃_0 = ρ_0.
for k = 1, 2, 3, ... do
    Compute ρ̃_{k+1} with (44) and ∇ρ̃_{k+1} with (45).
    for each particle j = 1, 2, ..., N do
        x_{k+1,j} = x_{k,j} − h(∇V(x_{k,j}) + β^{-1} ∇ log ρ̃_{k+1}(x_{k,j})).
    end for
end for
```

Since $\nabla \log \tilde{\rho}_{k+1} = \nabla \tilde{\rho}_k / \tilde{\rho}_k$, computing the score function requires us to also compute the evolution of the gradient of $\tilde{\rho}_k$, which can be derived by taking the gradient of the kernel formula (17). The gradient formula is expressed as follows

$$\begin{aligned}\nabla\tilde{\rho}_{k+1}(x) =& -\frac{\beta}{2}\nabla V(x)\tilde{\rho}_{k+1}(x) - \beta\int_{\mathbb{R}^d} \frac{\frac{(x-y)}{2T}\exp\left[-\frac{\beta}{2}\left(V(x)+\frac{\|x-y\|_2^2}{T}\right)\right]}{\int_{\mathbb{R}^d}\exp\left[-\frac{\beta}{2}\left(V(z)+\frac{\|z-y\|_2^2}{2T}\right)\right]dz}\tilde{\rho}_k(y)\,dy \\ =& -\beta\left(\frac{1}{2}\nabla V(x)+\frac{x}{2T}\right)\tilde{\rho}_{k+1}(x) + \frac{\beta}{2T}\int_{\mathbb{R}^d}\frac{y\exp\left[-\frac{\beta}{2}\left(V(x)+\frac{\|x-y\|_2^2}{2T}\right)\right]}{\int_{\mathbb{R}^d}\exp\left[-\frac{\beta}{2}\left(V(z)+\frac{\|z-y\|_2^2}{2T}\right)\right]dz}\tilde{\rho}_k(y)\,dy\,.\end{aligned} \tag{45}$$

The asymptotic value of $\nabla\tilde{\rho}_{k+1}$ can be obtained using the Laplace method, as summarized in the first statement of the following lemma. Additionally, the difference between the two sequences of density functions, ρ_k and $\tilde{\rho}_k$, is addressed in the second statement.

Lemma 15 *For $\tilde{\rho}_k$ from* (44) *and ρ_k from* (7) *with the same initial density ρ_0, we have:*

1. *The gradient of $\tilde{\rho}_k$ obtained from the gradient of kernel formula* (45) *satisfies*

$$\nabla\tilde{\rho}_{k+1}(x) = \nabla\tilde{\rho}_k(x) + T\nabla\frac{\partial\tilde{\rho}_k}{\partial t}\bigg|_{t=t_k}(x) + \mathcal{O}(T^2)\,; \tag{46}$$

2. *The difference between the two sequences of density functions satisfies*

$$\tilde{\rho}_k - \rho_k = \mathcal{O}(h^2)\,, \quad \nabla\log\tilde{\rho}_k - \nabla\log\rho_k = \mathcal{O}(h^2)\,.$$

Proof The proof of the first statement follows similar lines to those in Section 3, so we defer it to the Appendix A.4.

For the second statement, we use induction. By Lemma 8 and Theorem 4, we have

$$\rho_1 = \rho_0 + h\frac{\partial\rho_0}{\partial t} + \mathcal{O}(h^2)\,, \quad \tilde{\rho}_1 = \rho_0 + h\frac{\partial\rho_0}{\partial t} + \mathcal{O}(h^2)\,,$$

where the time derivative is the derivative along the flow of the Fokker-Planck equation. Thus, $\tilde{\rho}_1 - \rho_1 = \mathcal{O}(h^2)$.

Inductively, at the k-th iteration, we have

$$\rho_{k+1} - \tilde{\rho}_{k+1} = \rho_k - \tilde{\rho}_k + h\frac{\partial(\rho_k - \tilde{\rho}_k)}{\partial t} + \mathcal{O}(h^2) = \mathcal{O}(h^2)\,.$$

Hence, the result for the score function follows similarly. ■

The significance of Lemma 15 is that we can use the approximate score function $\nabla\log\tilde{\rho}_{k+1}$ in each iteration to avoid repeatedly approximating the density function. Since our approximate score function is accurate up to the order $\mathcal{O}(T^2)$, all discussions in Section 4 still hold. This is summarized in the following corollary.

Corollary 16 *For sampling with the particle evolution equation*

$$x_{k+1} = x_k - h(\nabla V(x_k) + \beta^{-1}\nabla\log\tilde{\rho}_{k+1}(x_k))\,, \quad \tilde{\rho}_{k+1} = \mathrm{Prox}_{h,V}(\tilde{\rho}_k)\,, \quad \tilde{\rho}_0 = \rho_0\,, \tag{47}$$

the results in Lemma 8 and Theorem 12 also hold for the corresponding density function.

In particular, to evaluate high-dimensional integrals in kernel formulas, we can utilize tensor train approximations as applied in Han et al. (2024). This approach essentially shifts the difficulty from high-dimensional sampling problems to evaluating high-dimensional integrals, which can be efficiently tackled using advanced tensor methods due to the structure of the kernel formula as it involves heat kernels that can be evaluated dimension by dimension.

6 Numerical Experiments

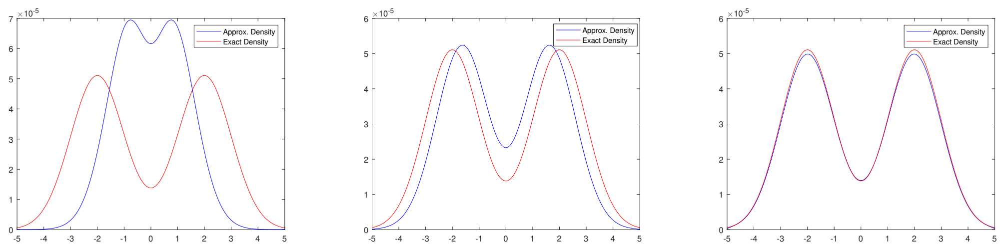
In this section, we present several numerical experiments to illustrate the theoretical results derived in the previous sections. All below numerical experiments are conducted in a 10-dimensional sample space, i.e., $\mathbb{R}^d$ with $d = 10$ and we only plot the result in the first dimension for the purpose of presentation.

Example 1. In this example, we explore the evolution of density functions over several iterations using the kernel formula (17). Consistent with Theorem 4, we numerically demonstrate that the computed density converges to the target density under an appropriately chosen step size. To efficiently manage the high-dimensional integrations involved, we employ tensor train approximation for the density functions. Further details on this approach can be found in our previous work Han et al. (2024).

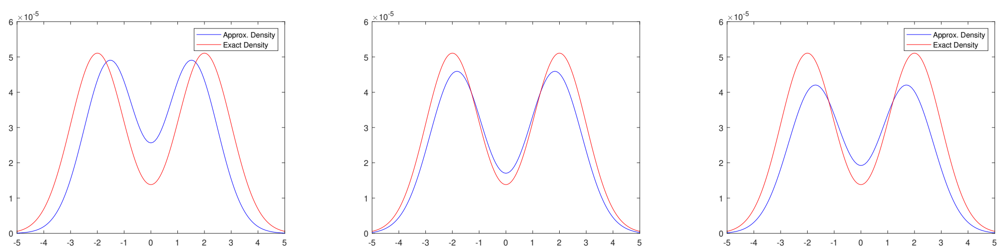
The first distribution we consider is a mixed Gaussian distribution defined as

$$\rho^*(x) = \frac{1}{2(2\pi\sigma^2)^{d/2}} \left[\exp\left(-\frac{\|x-a\|_2^2}{2\sigma^2} \right) + \exp\left(-\frac{\|x+a\|_2^2}{2\sigma^2} \right) \right], \tag{48}$$

where $a = 2$.



(a) $T = 0.01$, 20 iterations. (b) $T = 0.01$, 100 iterations. (c) $T = 0.01$, 400 iterations.



(d) $T = 0.05$, 20 iterations. (e) $T = 0.05$, 40 iterations. (f) $T = 0.1$, 15 iterations.

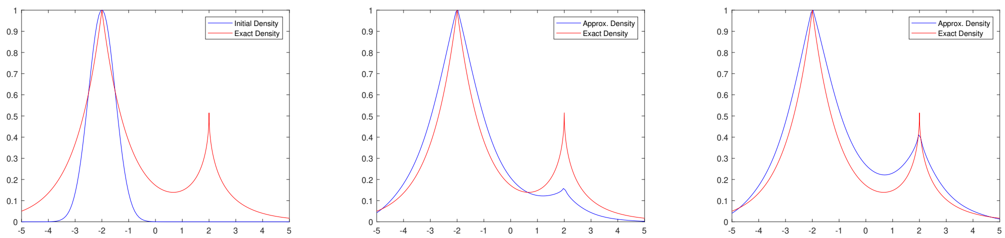
Figure 1: Evolution of the density function (blue) with (17) for different stepsizes T for the first dimension. The initial density is $\mathcal{N}(0, 2)$. The target density is a mixed Gaussian (red).

From Fig. 1, we observe that for sufficiently small stepsizes, the generated density converges to the target density very satisfactorily. Furthermore, comparing the first and last plots, we note that a larger time stepsize results in faster convergence while having a larger approximation error.

Next, we consider a mixture of L_1 and $L_{1/2}$ norms, where

$$\rho^*(x) = \frac{1}{Z} \left[\exp(-\|x + 2\vec{e}_1\|_1) + \frac{1}{2} \exp(-\|x - 2\vec{e}_1\|_{1/2}^2) \right],$$

$\vec{e}_1$ is the vector with the first entry equal to 1 and all other entries equal to 0, and Z is the normalization constant.



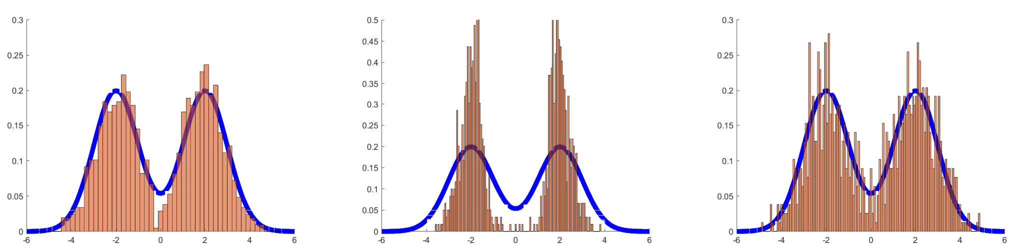
(a) Initial distribution. (b) $T = 0.05$, 20 iterations. (c) $T = 0.05$, 50 iterations.

Figure 2: Evolution of the density function (blue) for the first dimension with (17) as the target density with a mixture of L_1 and $L_{1/2}$ norms (red).

From Fig. 2, we observe that even for the non-smooth potential function, which exceeds the assumptions made in the previous analysis, the density still converges to the target distribution satisfactorily using the kernel formula.

Example 2: In the second example, we assess the convergence of the BRWP algorithm by computing the score function based on the density function evolved using the regularized Wasserstein proximal operator, as outlined in Algorithm 2. We compare the performance of the BRWP method with that of the explicit Euler discretization of the probability flow ODE, which utilizes the score function at time t_k approximated by a kernel density estimation with Gaussian kernel from particles, and the ULA described in (8).

The figure below shows the distribution of particles after 50 iterations for the mixed Gaussian distribution defined in (48).



(a) BRWP (b) Explicit Euler. (c) ULA.

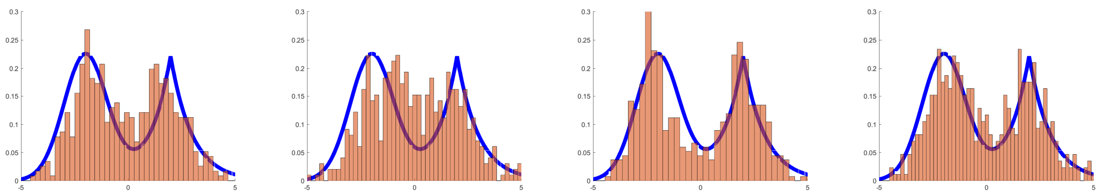
Figure 3: Histogram of 500 particles after 50 iterations in the first dimension for a Gaussian mixture distribution with $h = T = 0.02$.

Comparing the first and second graphs in Fig. 3, it is evident that the semi-implicit discretization (BRWP) improves the robustness of sampling and mitigates the variance reduction phenomenon observed in the explicit Euler discretization. Additionally, comparing the first and last plots, we note that the BRWP algorithm provides a more accurate and structured approximation to the target distribution due to its noise-free nature.

In the second experiment, we consider a mixture of Gaussian and Laplace distributions defined as

$$\rho^*(x) = \frac{1}{Z}\left[\exp\left(-\frac{\|x-2\|_2^2}{2\sigma^2}\right) + \exp\left(-\frac{\|x+2\|_1}{2b}\right)\right],$$

where Z is the normalization constant.



(a) BRWP
10 iterations

(b) ULA
10 iterations

(c) BRWP
20 iterations

(d) ULA
20 iterations

Figure 4: Histogram of 500 particles in the first dimension for the mixture of Gaussian and Laplace distributions with $h = T = 0.02$.

In Fig. 4, the TT-BRWP algorithm exhibits faster convergence to the target distribution compared to ULA, which is consistent with our previous theoretical results.

7 Conclusion and discussion

In this work, we present the convergence analysis of the BRWP algorithm, which is designed to sample from a known distribution up to a normalization constant. The algorithm relies on a semi-implicit time discretization of a noise-free probability flow ODE with the diffusion generated by the score function. The corresponding Liouville equation is still the Fokker-Planck equation of the overdamped Langevin dynamic. To address the challenge of approximating the evolution of the density function which usually involves intensive optimization, we apply the regularized Wasserstein proximal operator, whose solution is represented by a simple kernel formula. Using the Laplace method, we first demonstrate that the kernel formula serves as a first-order approximation to the evolution of the Fokker-Planck equation. Given the noise-free nature of the new sampling algorithm, we then conduct a high-order numerical analysis to study the KL divergence convergence guarantee of the BRWP algorithm. The analysis shows that the new approach offers faster convergence in high-dimensional settings and exhibits less bias than many existing methods. Additionally, we derive the optimal and maximum stepsizes required for convergence.

Our BRWP sampling method can be viewed as an interacting particle system based on a kernel derived from the regularized Wasserstein proximal operator. This concept shares similar motivations with sampling algorithms from interacting particle systems proposed in Garbuno-Inigo et al. (2020); Carrillo et al. (2022); Reich and Weissmann (2021); Carrillo et al. (2019); Liu and Wang (2016). However, we apply and evaluate these kernels differently. Here, we apply the interacting particle systems to approximate the linear Fokker-Planck equation, while other methods generate new interacting particle samplers from nonlinear Fokker-Planck equations. It is essential to highlight that a major challenge of our algorithm in practice is accurately approximating the density function and efficiently simulating the kernel formula, particularly as the dimension increases.

There are several interesting future directions to explore from this work. First, it would be valuable to extend the discussion to more general non-log-concave distributions and investigate the convergence of the algorithm. Second, the current analysis and numerical framework can be extended and generalized to different schemes, addressing challenges such as constrained sampling problems, sampling from group symmetric distribution, and sampling under different metrics. Lastly, we are also applying this approach to broader fields, including global optimization, time-reversible diffusion, and solving high-dimensional Hamilton-Jacobi equations.

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Appendix A. Postponed Proofs and Lemmas

In this section, we provide proofs for lemmas and theorems that are used in our analysis. Some of the results in Section A.1 are well-known. We include them in the appendix for the sake of completeness.

A.1 Identities and inequalities along the flow of the Fokker-Planck equation

Let $\rho^*(x) = \frac{1}{Z}\exp(-\beta V(x))$. When $\nabla^2 V \succeq \alpha I$, it is known that ρ^* satisfies the log-Sobolev inequality. Specifically, for any smooth function g with $E_{\rho^*}(g^2) \leq \infty$, we have

$$\int g^2 \log g^2 \rho^* \, dx - \int g^2 \rho^* \, dx \log \int g^2 \rho^* \, dx \leq \frac{2}{\beta\alpha} \int \|\nabla g\|^2 \rho^* \, dx \,. \tag{49}$$

Note that the factor of β arises from the definition $\rho^* = \frac{1}{Z}\exp(-\beta V)$, and our assumption applies to the function V.

Using the log-Sobolev inequality, we can derive the following dissipation result for Fokker-Planck equation (5).

Lemma 17 *If ρ^* satisfies the log-Sobolev inequality* (49) *and ρ is the solution to the Fokker-Planck equation* (5)*, then*

$$\frac{d}{dt}\mathrm{D_{KL}}(\rho\|\rho^*) = -\beta^{-1}\mathcal{I}(\rho) \leq -2\alpha \mathrm{D_{KL}}(\rho\|\rho^*) \,.$$

Proof By definition of KL divergence, we have

$$\frac{d}{dt}\mathrm{D_{KL}}(\rho\|\rho^*) = \int \frac{\partial}{\partial t}\rho \log\frac{\rho}{\rho^*} \, dx = \beta^{-1} \int \nabla\cdot\left(\nabla \log\frac{\rho}{\rho^*}\rho\right)\log\frac{\rho}{\rho^*} \, dx = -\beta^{-1}\int \left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \rho \, dx \,.$$

Substituting $g^2 = \frac{\rho}{\rho^*}$ to (49), we further obtain the following inequality relating KL divergence and Fisher information

$$\mathrm{D_{KL}}(\rho\|\rho^*) = \int \log\frac{\rho}{\rho^*}\rho \, dx \leq \frac{1}{2\beta\alpha}\int \left\|\nabla \log\frac{\rho}{\rho^*}\right\|_2^2 \rho \, dx = \frac{1}{2\beta\alpha}\mathcal{I}(\rho\|\rho^*) \,.$$

■

Then, for the second-order time derivative of the KL divergence, we can derive the following two relations using the definition and integration by parts. These relations are crucial for the proof of Lemma 11.

Lemma 18 *When ρ^* satisfies the log-Sobolev inequality and ρ is the solution to the Fokker-Planck equation, the second-order time derivative of KL divergence satisfies*

(i)

$$\frac{d^2}{dt^2}\mathrm{D}_{\mathrm{KL}}(\rho\|\rho^*) = 2\beta^{-2}\int \left\|\nabla^2 \log\frac{\rho}{\rho^*}\right\|_{\mathrm{F}}^2 \rho\, dx + 2\beta^{-1}\int \left\langle \nabla \log\frac{\rho}{\rho^*}, \nabla^2 V \nabla \log \frac{\rho}{\rho^*}\right\rangle \rho\, dx\,.$$

(ii)

$$\frac{d^2}{dt^2}\mathrm{D}_{\mathrm{KL}}(\rho\|\rho^*) = -\beta^{-1}\frac{d}{dt}\mathcal{I}(\rho) \geq 2\beta^{-1}\alpha\mathcal{I}(\rho) \geq 4\beta^{-1}\alpha^2\mathrm{D}_{\mathrm{KL}}(\rho\|\rho^*)\,.$$

Proof Using the fact that ρ satisfies the Fokker-Planck equation, and recall our definitions of $\mathcal{D}^\beta$ and the generator $\mathcal{L}$ as used in Section 4 which are

$$\mathcal{D}^\beta(u) = \frac{\beta^{-1}}{\rho}\nabla\cdot(\nabla u\,\rho)\,, \quad \mathcal{L}(v) = \beta^{-1}\Delta v - \nabla V\cdot\nabla v\,. \tag{50}$$

Using integration by parts, we then get

$$\begin{aligned}
&\frac{d^2}{dt^2}\mathrm{D}_{\mathrm{KL}}(\rho\|\rho^*) = \frac{d}{dt}\int \frac{\partial}{\partial t}\rho \log\frac{\rho}{\rho^*}\, dx = \int \frac{\partial^2\rho}{\partial t^2}\log\frac{\rho}{\rho^*}\, dx + \int \left|\frac{\partial \rho}{\partial t}\right|^2 \frac{1}{\rho}\, dx \qquad (51)\\
=&\int \left[\beta^{-1}\Delta\frac{\partial\rho}{\partial t} + \nabla\cdot\left(\nabla V\frac{\partial \rho}{\partial t}\right)\right]\log\frac{\rho}{\rho^*}\, dx + \int \left|\mathcal{D}^\beta\left(\log\frac{\rho}{\rho^*}\right)\right|^2\rho\, dx\\
=&\int \mathcal{D}^\beta\left(\log\frac{\rho}{\rho^*}\right)\mathcal{L}\left(\log\frac{\rho}{\rho^*}\right)\rho\, dx + \int \left|\mathcal{D}^\beta\left(\log\frac{\rho}{\rho^*}\right)\right|^2\rho\, dx\\
=&2\int \mathcal{D}^\beta\left(\log\frac{\rho}{\rho^*}\right)\mathcal{L}\left(\log\frac{\rho}{\rho^*}\right)\rho\, dx + \int \mathcal{D}^\beta\left(\log\frac{\rho}{\rho^*}\right)\left[\mathcal{D}^\beta\left(\log\frac{\rho}{\rho^*}\right) - \mathcal{L}\left(\log\frac{\rho}{\rho^*}\right)\right]\rho\, dx\\
=&-2\beta^{-1}\int \nabla\log\frac{\rho}{\rho^*}\cdot\nabla\mathcal{L}\left(\log\frac{\rho}{\rho^*}\right)\rho\, dx + \beta^{-1}\int \mathcal{D}^\beta\left(\log\frac{\rho}{\rho^*}\right)\left\|\nabla\log\frac{\rho}{\rho^*}\right\|_2^2\rho\, dx\\
=&-2\beta^{-1}\int \nabla\log\frac{\rho}{\rho^*}\cdot\nabla\mathcal{L}\left(\log\frac{\rho}{\rho^*}\right)\rho\, dx + \beta^{-1}\int \mathcal{L}\left\|\nabla\log\frac{\rho}{\rho^*}\right\|_2^2\rho\, dx\,,
\end{aligned}$$

where the last inequality comes from the fact that $D^\beta\left(\log\frac{\rho}{\rho^*}\right)\rho = \beta^{-1}\Delta\rho + \nabla\cdot(\nabla V\rho)$.

The commutator between $\mathcal{L}$ and ∇ for a smooth function f can be written as

$$\nabla\mathcal{L}f - \mathcal{L}\nabla f = \nabla\left(\beta^{-1}\Delta f - \nabla V\cdot\nabla f\right) - \beta^{-1}\Delta(\nabla f) + \nabla V\cdot\nabla^2 f = -\nabla^2 V\nabla f\,.$$

Using the Bochner's formula

$$\frac{1}{2}\Delta\left(\|\nabla f\|_2^2\right) = \Delta\nabla f\cdot\nabla f + \|\nabla^2 f\|_{\mathrm{F}}^2\,,$$

we note that

$$\begin{aligned}
&\frac{1}{2}\mathcal{L}\|\nabla f\|_2^2 - \nabla f\cdot\nabla\mathcal{L}(f) \qquad (52)\\
=&\frac{1}{2}\mathcal{L}\|\nabla f\|_2^2 - \nabla f\cdot\mathcal{L}\nabla f + \left\langle\nabla f, \nabla^2 V\nabla f\right\rangle\\
=&\beta^{-1}\left(\frac{1}{2}\Delta\|\nabla f\|_2^2 - \nabla f\cdot\Delta\nabla f\right) - \frac{1}{2}\nabla V\cdot\nabla\|\nabla f\|_2^2 + \langle\nabla f, \nabla^2 f\nabla V\rangle + \left\langle\nabla f, \nabla^2 V\nabla f\right\rangle\\
=&\beta^{-1}\|\nabla^2 f\|_{\mathrm{F}}^2 + \left\langle\nabla f, \nabla^2 V\nabla f\right\rangle\,,
\end{aligned}$$

Combining the final equality in (52) with (51), we obtain the first statement.

Substituting $f = \log \frac{\rho}{\rho^*}$ into (52) and combined with (51), we get

$$\frac{d^2}{dt^2}\mathrm{D}_{\mathrm{KL}}(\rho\|\rho^*) = 2\beta^{-2}\int \left\|\nabla^2 \log \frac{\rho}{\rho^*}\right\|_{\mathrm{F}}^2 \rho\, dx + 2\beta^{-1}\int \left\langle \nabla \log \frac{\rho}{\rho^*}, \nabla^2 V \nabla \log \frac{\rho}{\rho^*}\right\rangle \rho\, dx$$
$$\geq 2\beta^{-1}\alpha \int \left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \rho\, dx = 2\beta^{-1}\alpha \mathcal{I}(\rho) \geq 4\alpha^2 \mathrm{D}_{\mathrm{KL}}(\rho\|\rho^*)\,,$$

where we used $\nabla^2 V \succeq \alpha I_d$ and the final inequality follows from Lemma 17. ■

Lemma 19 *Let ρ satisfy the Fokker-Planck equation* (5)*. Then, the second-order time derivative of the KL divergence satisfies*

$$\frac{1}{2}\frac{d^2}{dt^2}\mathrm{D}_{\mathrm{KL}}(\rho\|\rho^*) = \int \left|\mathcal{D}^\beta\left(\log \frac{\rho}{\rho^*}\right)\right|^2 \rho\, dx + \beta^{-2}\int \left\langle \nabla \log \frac{\rho}{\rho^*},\, \nabla^2 \log \frac{\rho}{\rho^*} \nabla \log \frac{\rho}{\rho^*}\right\rangle \rho\, dx\,,$$

where D^β is defined in (50)*.*

Proof Firstly, by the definition of KL divergence and computation in (51), we have

$$\frac{d^2}{dt^2}\mathrm{D}_{\mathrm{KL}}(\rho\|\rho^*) = \int \mathcal{D}^\beta\left(\log \frac{\rho}{\rho^*}\right)\mathcal{L}\left(\log \frac{\rho}{\rho^*}\right)\rho\, dx + \int \left|\mathcal{D}^\beta\left(\log \frac{\rho}{\rho^*}\right)\right|^2 \rho\, dx\,.$$

Moreover, we note the following relationship

$$\mathcal{D}^\beta\left(\log \frac{\rho}{\rho^*}\right) - \mathcal{L}\left(\log \frac{\rho}{\rho^*}\right) = \beta^{-1}\left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2.$$

Thus, we can express

$$\begin{aligned}\int \left|\mathcal{D}^\beta\left(\log \frac{\rho}{\rho^*}\right)\right|^2 \rho\, dx &= \frac{1}{2}\left[\int \mathcal{D}^\beta\left(\log \frac{\rho}{\rho^*}\right)\mathcal{L}\left(\log \frac{\rho}{\rho^*}\right)\rho\, dx + \int \left|\mathcal{D}^\beta\left(\log \frac{\rho}{\rho^*}\right)\right|^2 \rho\, dx\right] \\ &\quad + \frac{1}{2}\int \left(\mathcal{D}^\beta\left(\log \frac{\rho}{\rho^*}\right) - \mathcal{L}\left(\log \frac{\rho}{\rho^*}\right)\right)\mathcal{D}^\beta\left(\log \frac{\rho}{\rho^*}\right)\rho\, dx \\ &= \frac{1}{2}\frac{d^2}{dt^2}\mathrm{D}_{\mathrm{KL}}(\rho\|\rho^*) + \frac{\beta^{-1}}{2}\int \left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \mathcal{D}^\beta\left(\log \frac{\rho}{\rho^*}\right)\rho\, dx \\ &= \frac{1}{2}\frac{d^2}{dt^2}\mathrm{D}_{\mathrm{KL}}(\rho\|\rho^*) - \beta^{-2}\int \left\langle \nabla \log \frac{\rho}{\rho^*},\, \nabla^2 \log \frac{\rho}{\rho^*}\nabla \log \frac{\rho}{\rho^*}\right\rangle \rho\, dx\,,\end{aligned}$$

where the last equality uses the identity for any smooth function u

$$\int \|\nabla u\|_2^2 \mathcal{D}^\beta(u)\rho\, dx = \beta^{-1}\int \|\nabla u\|_2^2 \nabla\cdot(\nabla u \rho)\, dx$$
$$= -\beta^{-1}\int \nabla\|\nabla u\|_2^2 \cdot \nabla u \rho\, dx = -2\beta^{-1}\int \left\langle \nabla u,\, \nabla^2 u \nabla u\right\rangle \rho\, dx\,.$$

■

A.1.1 Convergence of fourth order term

We show the fourth power of $\|\nabla \log \frac{\rho}{\rho^*}\|$ also converges exponentially in Wasserstein space. The below result is used in the proof of Theorem 12.

Lemma 20 *When ρ^* is strongly log-concave with $\nabla^2 V \succeq \alpha I$ and ρ is the solution to the Fokker-Planck equation, we have*

$$\frac{\partial}{\partial t}\int \left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^4 \rho dx \leq -4\alpha \int \left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^4 \rho dx\,.$$

Proof Taking the time derivative directly, we have

$$\frac{\partial}{\partial t}\int \left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^4 \rho dx = 4\int \left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \left\langle \nabla \log \frac{\rho}{\rho^*}, \nabla \frac{\partial \rho/\partial t}{\rho}\right\rangle \rho dx + \int \left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^4 \frac{\partial \rho}{\partial t} dx\,. \quad (53)$$

Using the identity $\frac{\partial \rho}{\partial t} = \beta^{-1}\nabla\cdot\left(\nabla \log \frac{\rho}{\rho^*}\rho\right)$ and integration by parts, the first term above equals to

$$\begin{aligned}
&4\int \left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \left\langle \nabla \log \frac{\rho}{\rho^*}, \nabla \frac{\partial \rho/\partial t}{\rho}\right\rangle \rho dx \qquad (54)\\
=&-4\int \nabla\cdot\left(\left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \nabla \log \frac{\rho}{\rho^*}\right)\frac{\partial\rho/\partial_t}{\rho}\rho dx - 4\int \left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \left\langle \nabla \log \frac{\rho}{\rho^*}, \frac{\nabla\rho}{\rho}\right\rangle \frac{\partial \rho}{\partial t} dx\\
=&-4\beta^{-1}\int \nabla\cdot\left(\left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \nabla \log \frac{\rho}{\rho^*}\right)\nabla\cdot\left(\nabla \log \frac{\rho}{\rho^*}\rho\right) dx\\
&-4\beta^{-1}\int \left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \left\langle \nabla \log \frac{\rho}{\rho^*}, \frac{\nabla\rho}{\rho}\right\rangle \nabla\cdot\left(\nabla \log \frac{\rho}{\rho^*}\rho\right) dx\\
=&4\beta^{-1}\int \left\langle \nabla\nabla\cdot\left(\left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \nabla \log \frac{\rho}{\rho^*}\right), \nabla \log \frac{\rho}{\rho^*}\right\rangle \rho dx\\
&+4\beta^{-1}\int \left\langle \left[\nabla\left\langle \left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \nabla \log \frac{\rho}{\rho^*}, \frac{\nabla\rho}{\rho}\right\rangle\right], \nabla \log \frac{\rho}{\rho^*}\right\rangle \rho dx\,.
\end{aligned}$$

For the last term in (54), it can be simplified as

$$\begin{aligned}
&4\beta^{-1}\int \left\langle \left[\nabla\left\langle \left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \nabla \log \frac{\rho}{\rho^*}, \frac{\nabla\rho}{\rho}\right\rangle\right], \nabla \log \frac{\rho}{\rho^*}\right\rangle \rho dx \qquad (55)\\
=&4\beta^{-1}\int \left\langle\left\langle \nabla\left(\left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \nabla \log \frac{\rho}{\rho^*}\right), \frac{\nabla\rho}{\rho}\right\rangle, \nabla \log \frac{\rho}{\rho^*}\right\rangle \rho dx\\
&+4\beta^{-1}\int \left\langle\left\langle \left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \nabla \log \frac{\rho}{\rho^*}, \nabla\left(\frac{\nabla\rho}{\rho}\right)\right\rangle, \nabla \log \frac{\rho}{\rho^*}\right\rangle \rho dx\\
=&4\beta^{-1}\int \left\langle \left(\nabla\left(\left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \nabla \log \frac{\rho}{\rho^*}\right)\right)^T \nabla \log \frac{\rho}{\rho^*}, \nabla\rho\right\rangle dx\\
&+4\beta^{-1}\int \left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \left\langle \nabla \log \frac{\rho}{\rho^*}, \nabla\left(\frac{\nabla\rho}{\rho}\right)\nabla \log \frac{\rho}{\rho^*}\right\rangle dx\,,
\end{aligned}$$

where we have used for $u = \left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \nabla \log \frac{\rho}{\rho^*}$, $v = \frac{\nabla \rho}{\rho}$

$$(\nabla(u \cdot v))_i = \sum_j \left[\frac{\partial u_j}{\partial x_i} v_j + u_j \frac{\partial v_j}{\partial x_i}\right] = ((\nabla u) \cdot v)_i + (u \cdot (\nabla v))_i \quad \text{where } (\nabla u)_{ij} = \frac{\partial u_j}{\partial x_i},$$

in first equality. We also used

$$(A \cdot u) \cdot v = \sum_{ij} a_{ij} u_j v_i = \sum_j (\sum_i a_{ij} v_i) u_j = (A^T v) \cdot u, \quad (u \cdot A) \cdot v = (u^T A) v = u \cdot (Av),$$

in the second equality.

Noting that $\nabla(\nabla\rho/\rho) = \nabla^2 \log \rho$, the last term in (55) equals to

$$\begin{aligned} &4\beta^{-1} \int \left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \left\langle \nabla \log \frac{\rho}{\rho^*}, \nabla\left(\frac{\nabla \rho}{\rho}\right) \nabla \log \frac{\rho}{\rho^*} \right\rangle \rho dx \\ =&4\beta^{-1} \int \left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \left\langle \nabla \log \frac{\rho}{\rho^*}, \nabla^2 \log \rho \nabla \log \frac{\rho}{\rho^*} \right\rangle \rho dx . \end{aligned} \tag{56}$$

Moreover, applying integration by parts with respect to $\nabla\rho$ to the first term in the last line of (55), we get

$$\begin{aligned} &4\beta^{-1} \int \left\langle \left(\nabla\left(\left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \nabla \log \frac{\rho}{\rho^*}\right)\right)^T \nabla \log \frac{\rho}{\rho^*},\, \nabla \rho \right\rangle dx \\ =& -4\beta^{-1} \int \nabla \cdot \left[\left(\nabla\left(\left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \nabla \log \frac{\rho}{\rho^*}\right)\right)^T \nabla \log \frac{\rho}{\rho^*}\right] \rho dx \\ =& -4\beta^{-1} \int \left\langle \nabla \cdot \left(\nabla\left(\left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \nabla \log \frac{\rho}{\rho^*}\right)^T\right),\, \nabla \log \frac{\rho}{\rho^*} \right\rangle \rho dx \\ & -4\beta^{-1} \int \operatorname{Tr}\left\{\nabla\left(\left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \nabla \log \frac{\rho}{\rho^*}\right) \nabla^2 \log \frac{\rho}{\rho^*}\right\} \rho dx , \end{aligned} \tag{57}$$

where we used for $A = \nabla\left(\left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \nabla \log \frac{\rho}{\rho^*}\right)$, $b = \nabla \log \frac{\rho}{\rho^*}$, and

$$\begin{aligned} \nabla \cdot (A^T b) &= \sum_j \frac{\partial \sum_i a_{ij} b_i}{\partial x_j} = \sum_{ij} \left(\frac{\partial a_{ij}}{\partial x_j} b_i + a_{ij} \frac{\partial b_i}{\partial x_j}\right) = (\nabla \cdot A^T) \cdot b + \sum_{ij} a_{ij} (\nabla b)_{ij}^T \\ &= (\nabla \cdot A^T) \cdot b + \operatorname{Tr}\{A(\nabla b)\}, \quad (A_{ij}) = a_{ij}, \quad \nabla \cdot A^T = \sum_j \frac{\partial a_{ij}}{\partial x_j} . \end{aligned}$$

Next noting that when $u = \left\|\nabla \log \frac{\rho}{\rho^*}\right\|_2^2 \nabla \log \frac{\rho}{\rho^*}$

$$(\nabla \cdot (\nabla u)^T)_i = \sum_j \frac{\partial (\nabla u)_{ij}}{\partial x_j} = \sum_j \frac{\partial}{\partial x_j} \frac{\partial u_j}{\partial x_i} = \frac{\partial}{\partial x_i} \sum_j \frac{\partial u_j}{\partial x_j} = (\nabla(\nabla \cdot u))_i ,$$

hence the first term in both the last line of (57) and (54) cancels. Now, it only remains to look at the last term in (57). Firstly, for a scalar function $\zeta = \|\nabla \log \frac{\rho}{\rho^*}\|_2^2$ and a vector function $u = \nabla \log \frac{\rho}{\rho^*}$, we have

$$(\nabla(\zeta u))_{ij} = \frac{\partial \zeta u_j}{\partial x_i} = \frac{\partial \zeta}{\partial x_i} u_j + \zeta \frac{\partial u_j}{\partial x_i} = (\nabla \zeta u^T)_{ij} + \zeta (\nabla u)_{ij} .$$

This implies

$$
\begin{aligned}
&-4\beta^{-1}\int \mathrm{Tr}\left\{\nabla\Big(\Big\|\nabla\log\frac{\rho}{\rho^*}\Big\|_2^2\nabla\log\frac{\rho}{\rho^*}\Big)\nabla^2\log\frac{\rho}{\rho^*}\right\}\rho dx \qquad (58)\\
=&-4\beta^{-1}\int \mathrm{Tr}\left\{\Big(\nabla\Big\|\nabla\log\frac{\rho}{\rho^*}\Big\|_2^2\Big(\nabla\log\frac{\rho}{\rho^*}\Big)^T+\Big\|\nabla\log\frac{\rho}{\rho^*}\Big\|_2^2\nabla^2\log\frac{\rho}{\rho^*}\Big)\nabla^2\log\frac{\rho}{\rho^*}\right\}\rho dx\\
=&-8\beta^{-1}\int \mathrm{Tr}\Big\{\Big(\nabla^2\log\frac{\rho}{\rho^*}\cdot\nabla\log\frac{\rho}{\rho^*}\Big)\Big(\nabla^2\log\frac{\rho}{\rho^*}\cdot\nabla\log\frac{\rho}{\rho^*}\Big)^T\Big\}\rho dx\\
&-4\beta^{-1}\int\Big\|\nabla\log\frac{\rho}{\rho^*}\Big\|_2^2\Big\|\nabla^2\log\frac{\rho}{\rho^*}\Big\|_{\mathrm{F}}^2\rho dx\\
=&-8\beta^{-1}\int\Big\|\nabla^2\log\frac{\rho}{\rho^*}\nabla\log\frac{\rho}{\rho^*}\Big\|_2^2\rho dx-4\beta^{-1}\int\Big\|\nabla\log\frac{\rho}{\rho^*}\Big\|_2^2\Big\|\nabla^2\log\frac{\rho}{\rho^*}\Big\|_{\mathrm{F}}^2\rho dx\,,
\end{aligned}
$$

where we also used the fact that $\nabla^2\log\frac{\rho}{\rho^*}$ is symmetric and $Abb^TA^T=Ab(Ab)^T$.

Finally, the second term in (53) will be

$$
\int\Big\|\nabla\log\frac{\rho}{\rho^*}\Big\|_2^4\frac{\partial\rho}{\partial t}dx=-4\beta^{-1}\int\Big\|\nabla\log\frac{\rho}{\rho^*}\Big\|_2^2\Big\langle\nabla\log\frac{\rho}{\rho^*},\nabla^2\log\frac{\rho}{\rho^*}\nabla\log\frac{\rho}{\rho^*}\Big\rangle\rho dx\,. \qquad (59)
$$

Combing equations (53) to (59), we arrive

$$
\begin{aligned}
\frac{\partial}{\partial t}\int\Big\|\nabla\log\frac{\rho}{\rho^*}\Big\|_2^4\rho dx=&-4\beta^{-1}\int\Big\|\nabla^2\log\frac{\rho}{\rho^*}\Big\|_{\mathrm{F}}^2\Big\|\nabla\log\frac{\rho}{\rho^*}\Big\|_2^2\rho dx\\
&-4\int\Big\|\nabla\log\frac{\rho}{\rho^*}\Big\|_2^2\Big\langle\nabla\log\frac{\rho}{\rho^*},\,\nabla^2V\nabla\log\frac{\rho}{\rho^*}\Big\rangle\rho dx-8\beta^{-1}\int\Big\|\nabla^2\log\frac{\rho}{\rho^*}\nabla\log\frac{\rho}{\rho^*}\Big\|_2^2\rho dx\,.
\end{aligned}
$$

The desired result can now be achieved by noting the condition that $\nabla^2V\succeq\alpha I$. ■

A.2 Postponed proof for Theorems and Lemmas in section 3

Proof [Proof of Theorem 4.] Substituting (20) into the expression for ρ_T in (17), we arrive

$$
\begin{aligned}
\rho_T(x)=&\exp\Big(-\frac{\beta}{2}V(x)\Big)\int_{\mathbb{R}^d}\frac{\exp\Big(-\beta\frac{\|x-y\|_2^2}{4T}\Big)}{\int_{\mathbb{R}^d}\exp\big[-\frac{\beta}{2}\big(V(z)+\frac{\|z-y\|_2^2}{2T}\big)\big]dz}\rho_0(y)dy \qquad (60)\\
=&\exp\Big(-\frac{\beta}{2}V(x)\Big)\int_{\mathbb{R}^d}\frac{1+\frac{T}{2}\Delta V(\tilde{s}_y)}{(4\pi T/\beta)^{d/2}}\exp\Big[-\frac{\beta}{2}\Big(\frac{\|x-y\|_2^2}{2T}+2V_0(y)-V(\tilde{s}_y)-\frac{\|y-\tilde{s}_y\|_2^2}{2T}\Big)\Big]dy+\mathcal{O}(T^2)\,.
\end{aligned}
$$

For fixed x, to apply the approximation with the Laplace method as in (18), we let

$$
f(y)=\frac{\|x-y\|_2^2}{2}+2TV_0(y)-TV(\tilde{s}_y)-\frac{\|y-\tilde{s}_y\|_2^2}{2}\,,\quad g(y)=1\,. \qquad (61)
$$

Then we may write the minimizer for $f(y)$ which is a function of x as

$$
r_x=\arg\min_y f(y)=\arg\min_y\left\{\frac{\|x-y\|_2^2}{2}+2TV_0(y)-TV(\tilde{s}_y)-\frac{\|y-\tilde{s}_y\|_2^2}{2}\Big)\right\}.
$$

Similar to the derivation for Lemma 3, the first-order optimality condition leads to

$$
-(r_x-x)-2T\nabla V_0(r_x)+\Big[T\frac{\partial\tilde{s}_{r_x}}{\partial r_x}\nabla V(\tilde{s}_{r_x})+\Big(1-\frac{\partial\tilde{s}_{r_x}}{\partial r_x}\Big)(r_x-\tilde{s}_{r_x})\Big]=0\,,
$$

where $\frac{\partial \tilde{s}_{r_x}}{\partial r_x}$ is the Jacobian of $\tilde{s}_{r_x}$.

To simplify the expression for r_x, by definition of $\tilde{s}_{r_x}$ in (23) and replacing y with r_x, we have

$$r_x - \tilde{s}_{r_x} = T\nabla V(r_x)\,.$$

This leads to

$$-(r_x - x) - 2T\nabla V_0(r_x) + T\nabla V(r_x) = 0 \quad \Rightarrow \quad r_x = x + T\nabla(V - 2V_0)(r_x)\,,$$

as the term involves $\frac{\partial \tilde{s}_{r_x}}{\partial r_x}$ cancel out.

Then as a similar argument as in the proof of Lemma 3, we can define a linearized approximate solution to r_x as

$$\tilde{r}_x = x + T\nabla(V - 2V_0)(x)\,, \tag{62}$$

where $|\tilde{r}_x - r_x| = \mathcal{O}(T^2)$ under the assumption $\nabla^2(V_0 - V)$ is bounded on the line segment connection x and r_x.

Now, note that the Hessian of $f(r_x)$ in (61) will be

$$\nabla^2 f(r_x) = 1 + T\nabla^2(V_0 - V)(r_x) - \frac{T^2}{2}\nabla^3 V(r_x) = 1 + T\nabla^2(V_0 - V)(r_x) + \mathcal{O}(T^2)\,.$$

Using the Taylor expansion for the determinant function in (24) and the definition of $\tilde{r}_x$, we are ready to apply the Laplace method to ρ_T in (60) to get

$$\begin{aligned}
\rho_T(x) =& \exp\left(-\frac{\beta}{2}V(x)\right)\int_{\mathbb{R}^d} \frac{\exp\left(-\beta\frac{||x-y||_2^2}{4T}\right)}{\int_{\mathbb{R}^d}\exp\left[-\frac{\beta}{2}\left(V(z) + \frac{||z-y||_2^2}{2T}\right)\right]dz}\rho_0(y)dy \\
=&\frac{\exp\left(-\frac{\beta}{2}V(x)\right)\left[1 + \frac{T}{2}\Delta V(\tilde{s}_{r_x})\right]}{|1 + T\nabla^2(V_0 - V)(r_x) + \mathcal{O}(T^2)|^{1/2}}\exp\left[-\frac{\beta}{2}\left(\frac{||x - r_x||_2^2}{2T} - \frac{||r_x - \tilde{s}_{r_x}||_2^2}{2T} + 2V_0(r_x) - V(\tilde{s}_{r_x})\right)\right] + \mathcal{O}(T^2) \\
=&\frac{\exp\left(-\frac{\beta}{2}V(x)\right)\left[1 + \frac{T}{2}\Delta V(\tilde{s}_{\tilde{r}_x})\right]}{1 + \frac{T}{2}\Delta(2V_0 - V)(\tilde{r}_x)}\exp\left[-\frac{\beta}{2}\left(\frac{||x - \tilde{r}_x||_2^2}{2T} - \frac{||\tilde{r}_x - \tilde{s}_{\tilde{r}_x}||_2^2}{2T} + 2V_0(\tilde{r}_x) - V(\tilde{s}_{\tilde{r}_x})\right)\right] + \mathcal{O}(T^2)\,.
\end{aligned} \tag{63}$$

For the exponent in the second exponential function in the last line of (63), using the definition of $\tilde{r}_x$ and $\tilde{s}_x$ and skipping the factor $-\beta/2$, it can be simplified as

$$\begin{aligned}
&2V_0(\tilde{r}_x) - V(\tilde{s}_{\tilde{r}_x}) + \frac{T}{2}\|\nabla(V - 2V_0)(x)\|_2^2 - \frac{T}{2}\|\nabla V(\tilde{r}_x)\|_2^2 + \mathcal{O}(T^2) \\
=&2V_0\left(x + T\nabla(V - 2V_0)(x)\right) - V\left(x - 2T\nabla V_0(x)\right) + \frac{T}{2}\|\nabla(V - 2V_0)(x)\|_2^2 - \frac{T}{2}\|\nabla V(x)\|_2^2 + \mathcal{O}(T^2) \\
=&2V_0(x) + 2T\nabla V_0 \cdot \nabla(V - 2V_0)(x) - V(x) + 2T\nabla V \cdot \nabla V_0(x) \\
&+ \frac{T}{2}\|\nabla(V - 2V_0)(x)\|_2^2 - \frac{T}{2}\|\nabla V(x)\|_2^2 + \mathcal{O}(T^2) \\
=&2V_0(x) - V(x) + 2T\nabla(V - V_0)\cdot\nabla V_0(x) + \mathcal{O}(T^2)\,,
\end{aligned}$$

where we have used the Taylor expansion on V_0 and V, and the relation

$$\tilde{s}_{\tilde{r}_x} = \tilde{r}_x - T\nabla V(\tilde{r}_x) = x + T\nabla(V - 2V_0)(x) - T\nabla V(x) + \mathcal{O}(T^2) = x - 2T\nabla V_0(x) + \mathcal{O}(T^2)\,.$$

Lastly, for the coefficient before the exponential term in (63), with the help of the Neumann series, we derive

$$\frac{1 + \frac{T}{2}\Delta V(\tilde{s}_{\tilde{r}_x})}{1 + \frac{T}{2}\Delta(2V_0 - V)(\tilde{r}_x)} = \left[1 + \frac{T}{2}\Delta V(x)\right]\left[1 - \frac{T}{2}\Delta(2V_0 - V)(x)\right] + \mathcal{O}(T^2) = 1 + T\Delta(V - V_0)(x) + \mathcal{O}(T^2)\,,$$

under the assumption that $|T\Delta(2V_0 - V)(x)| \leq 2$. Combining the above expression, we arrive at the desired result in Theorem 4. ∎

Proof [Proof of Lemma 5.] Firstly, by Taylor expansion and approximation in Theorem 4, we have

$$\begin{aligned}\log \rho_{k+1} =& \log \left[\rho_k \left(1 + T\beta^{-1}\frac{\nabla \cdot (\nabla \log \frac{\rho_k}{\rho^*}\rho_k)}{\rho_k} + \mathcal{O}(T^2)\right)\right]\\ =& \log \rho_k + T\beta^{-1}\frac{\nabla \cdot (\nabla \log \frac{\rho_k}{\rho^*}\rho_k)}{\rho_k} + \mathcal{O}(T^2)\,.\end{aligned}$$

This implies

$$\rho_{k+1}\log\frac{\rho_{k+1}}{\rho^*} = \left[\rho_k + T\beta^{-1}\nabla\cdot\left(\nabla\log\frac{\rho_k}{\rho^*}\rho_k\right)\right]\left[\log\frac{\rho_k}{\rho^*} + T\beta^{-1}\frac{\nabla \cdot (\nabla \log \frac{\rho_k}{\rho^*}\rho_k)}{\rho_k}\right] + \mathcal{O}(T^2)\,.$$

Then by the definition of KL divergence, we have

$$\begin{aligned}&\mathrm{D}_{\mathrm{KL}}(\rho_k\|\rho^*) - \mathrm{D}_{\mathrm{KL}}(\rho_{k+1}\|\rho^*)\\ =& - T\beta^{-1}\int \nabla\cdot\left(\nabla\log\frac{\rho_k}{\rho^*}\rho_k\right)\left(1 + \log\frac{\rho_k}{\rho^*}\right)dx + \mathcal{O}(T^2)\\ =& T\beta^{-1}\mathcal{I}(\rho_k\|\rho^*) + \mathcal{O}(T^2)\,.\end{aligned}$$

∎

A.3 Postponed proof and additional Lemma used in Section 4

Proof [Proof of Lemma 8.] To develop the evolution of the density function for this partial evolution equation up to the third-order term $\mathcal{O}(h^3)$, we will rely on the Taylor expansion. Denote $\phi(x) = V(x) + \beta^{-1}\log\rho_T(x)$ for simplicity. Then we have $x_{k+1} = x_k - h\nabla\phi(x_k)$.

For any smooth function u, the iterative relationship between $x_{k+1} \sim \rho_{k+1}$ and $x_k \sim \rho_k$ implies

$$\begin{aligned}\mathbb{E}_{\rho_{k+1}}(u) =& \int u(x)\rho_{k+1}(x)\,dx = \int u(x - h\nabla\phi(x))\rho_k(x)\,dx\\ =& \int \left[u(x) - h\nabla\phi(x)\cdot\nabla u(x) + \frac{h^2}{2}\nabla\phi(x)^T\nabla^2(u)(x)\nabla\phi(x)\right]\rho_k(x)\,dx + \mathcal{O}(h^3)\,.\end{aligned} \tag{64}$$

For the term involving the Hessian, integration by parts leads to

$$\begin{aligned}&\int \nabla\phi(x)^T\nabla^2(u)(x)\nabla\phi(x)\rho_k(x)\,dx = \int\sum_{i,j}\left(\frac{\partial\phi}{\partial x_i}\frac{\partial\phi}{\partial x_j}\frac{\partial^2 u(x)}{\partial x_i\partial x_j}\right)\rho_k(x)\,dx\\ =& \int\sum_{i,j}\frac{\partial^2 u(x)}{\partial x_i\partial x_j}\left(\frac{\partial\phi}{\partial x_i}\frac{\partial\phi}{\partial x_j}\rho_k(x)\right)dx = \int u(x)\sum_{i,j}\frac{\partial^2}{\partial x_i\partial x_j}\left(\frac{\partial\phi}{\partial x_i}\frac{\partial\phi}{\partial x_j}\rho_k(x)\right)dx.\end{aligned}$$

Conducting integration by parts on the gradient term, (64) will become

$$\int u\rho_{k+1}\,dx = \int u\left[\rho_k + h\nabla\cdot(\nabla\phi\rho_k) + \frac{h^2}{2}\sum_{i,j}\frac{\partial^2}{\partial x_i\partial x_j}\left(\frac{\partial\phi}{\partial x_i}\frac{\partial\phi}{\partial x_j}\rho_k\right)\right]dx + \mathcal{O}(h^3).$$

For the h^2 order term, we note the summation over i index can be re-written as

$$
\begin{aligned}
&\sum_i \frac{\partial}{\partial x_i}\left(\frac{\partial \phi}{\partial x_i}\frac{\partial \phi}{\partial x_j}\rho_k\right) = \sum_i \frac{\partial}{\partial x_i}\left(\frac{\partial \phi}{\partial x_i}\frac{\partial \phi}{\partial x_j}\right)\rho_k + \frac{\partial \phi}{\partial x_j}\sum_i \frac{\partial \phi}{\partial x_i}\frac{\partial \rho_k}{\partial x_i} \\
&= \left[\nabla\cdot(\nabla\phi\nabla\phi^T) + (\nabla\phi)^T(\nabla\phi\cdot\nabla\log\rho_k)\right]\rho_k = \tilde{\phi}\cdot\rho_k\,,
\end{aligned}
$$

where we use the notation $\tilde{\phi}$ defined in (33).

In this case, since (31) implies

$$
\log\rho_T = \rho_k + T\beta^{-1}\frac{\nabla\cdot\left(\nabla\log\frac{\rho_k}{\rho^*}\rho_k\right)}{\rho_k} + \mathcal{O}(T^2)\,,
$$

we can obtain the evolution of density corresponds to (30) with an error term of order h^3 as

$$
\begin{aligned}
\rho_{k+1} &= \rho_k + h\nabla\cdot(\nabla V\rho_k + \beta^{-1}\nabla\log\rho_T\rho_k) + \frac{h^2}{2}\sum_{j=1}^d \frac{\partial}{\partial x_j}(\tilde{\phi}\rho_k) + \mathcal{O}(h^3) \\
&=\rho_k + h\nabla\cdot(\nabla V\rho_k + \beta^{-1}\nabla\rho_k) + hT\beta^{-2}\nabla\cdot\left[\nabla\left(\frac{\nabla\cdot(\nabla\log\frac{\rho_k}{\rho^*}\rho_k)}{\rho_k}\right)\rho_k\right] + \frac{h^2}{2}\sum_{j=1}^d\frac{\partial}{\partial x_j}(\tilde{\phi}\rho_k) + \mathcal{O}(h^3) \\
&=\rho_k + h\beta^{-1}\nabla\cdot\left(\nabla\log\frac{\rho_k}{\rho^*}\rho_k\right) + hT\beta^{-2}\nabla\cdot\left[\nabla\left(\frac{\nabla\cdot(\nabla\log\frac{\rho_k}{\rho^*}\rho_k)}{\rho_k}\right)\rho_k\right] + \frac{h^2}{2}\sum_{j=1}^d\frac{\partial}{\partial x_j}(\tilde{\phi}\rho_k) + \mathcal{O}(h^3)\,,
\end{aligned}
$$

which is the desired result. ■

Proof [Proof of Lemma 9.] Using the Taylor expansion of the log function, we can derive

$$
\begin{aligned}
\log\rho_{k+1} =& \log\rho_k + h\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right) - \frac{h^2}{2}\left|\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right)\right|^2 \\
&+ hT\mathcal{D}_k^\beta\circ\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right) + \frac{h^2}{2\rho_k}\nabla\cdot(\tilde{\phi}\rho_k) + \mathcal{O}(h^3)\,,
\end{aligned}
$$

and

$$
\begin{aligned}
\rho_{k+1}\log\frac{\rho_{k+1}}{\rho^*} =& \rho_k\log\frac{\rho_k}{\rho^*}\left[1 + h\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right) + hT\mathcal{D}_k^\beta\circ\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right) + \frac{h^2}{2\rho_k}\nabla\cdot(\tilde{\phi}\rho_k)\right] \\
&+ \rho_k\left[h\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right) - \frac{h^2}{2}\left|\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right)\right|^2 + hT\mathcal{D}_k^\beta\circ\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right) + \frac{h^2}{2\rho_k}\nabla\cdot(\tilde{\phi}\rho_k)\right] \\
&+ h^2\rho_k\left|\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right)\right|^2 + \mathcal{O}(h^3) \\
=&\rho_k\log\frac{\rho_k}{\rho^*} + \frac{h^2}{2}\rho_k\left|\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right)\right|^2 \\
&+ \left[h\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right) + hT\mathcal{D}_k^\beta\circ\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right) + \frac{h^2}{2\rho_k}\nabla\cdot(\tilde{\phi}\rho_k)\right]\rho_k\left(1 + \log\frac{\rho_k}{\rho^*}\right) + \mathcal{O}(h^3)\,.
\end{aligned}
$$

Then substituting the above expression into the formula of KL divergence, we have

$$
\begin{aligned}
& \mathrm{D}_{\mathrm{KL}}(\rho_k\|\rho^*) - \mathrm{D}_{\mathrm{KL}}(\rho_{k+1}\|\rho^*) \\
=& - h\left[\int \left(\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right)\rho_k + T\mathcal{D}_k^\beta\circ\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right)\rho_k + \frac{h}{2}\nabla\cdot\left(\tilde{\phi}\rho_k\right)\right)\left(1+\log\frac{\rho_k}{\rho^*}\right)dx\right] \\
& - \frac{h^2}{2}\int\left|\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right)\right|^2\rho_k\,dx + \mathcal{O}(h^3)\,.
\end{aligned} \tag{65}
$$

Next, we analyze each term in (65) carefully. Firstly, the $\mathcal{O}(h)$ term is nothing but the Fisher information

$$
-\int\mathcal{D}_k^\beta\left(\log\frac{\rho_k}{\rho^*}\right)\left(1+\log\frac{\rho_k}{\rho^*}\right)\rho_k\,dx = \beta^{-1}\int\left\|\nabla\log\frac{\rho_k}{\rho^*}\right\|_2^2\rho_k dx = \beta^{-1}\mathcal{I}(\rho_k\|\rho^*)\,.
$$

Secondly, for the $\tilde{\phi}$ term, recalling that

$$
\phi = \beta^{-1}(\log\rho_T - \log\rho^*) = \beta^{-1}\log\frac{\rho_k}{\rho^*} + \mathcal{O}(T)\,,
$$

then $\tilde{\phi}$ can be simplified as

$$
\tilde{\phi}\rho_k = \left[\nabla\cdot(\nabla\phi\nabla\phi^T) + (\nabla\phi)^T(\nabla\phi\cdot\nabla\log\rho_k)\right]\rho_k = \beta^{-2}(\rho_k\nabla\cdot\Psi + \nabla\rho_k^T\Psi)\,, \tag{66}
$$

where $\Psi := \nabla\log\frac{\rho_k}{\rho^*}(\nabla\log\frac{\rho_k}{\rho^*})^T$. The above uses the vector identifies for $u=\nabla\phi$, $v=\nabla\rho_k$, and

$$
u^T(u\cdot v) = u_j\sum_i u_iv_i = \sum_i(u_iu_j)v_i = v^T(uu^T)\,.
$$

Moreover, let $\Psi=\{\psi_{i,j}\}$, we have

$$
(\nabla\cdot(\Psi\rho_k))_j = \sum_i\frac{\partial\psi_{ij}\rho_k}{\partial x_i} = \sum_i\frac{\partial\psi_{ij}}{\partial x_i}\rho_k + \sum_i\psi_{ij}\frac{\partial\rho_k}{\partial x_i}\,,
$$

which implies $\nabla\cdot(\Psi\rho_k) = \rho_k\nabla\cdot\Psi + \nabla\rho_k^T\Psi$.

Hence, we can simplify the term involves $\tilde{\phi}$ in (65) as

$$
\begin{aligned}
&\int\tilde{\phi}\rho_k\cdot\nabla\log\frac{\rho_k}{\rho^*}dx = \beta^{-2}\int\left\langle\nabla\log\frac{\rho_k}{\rho^*},\,\rho_k\nabla\cdot\Psi + \nabla\rho_k^T\Psi\right\rangle dx \\
=&\beta^{-2}\int\left\langle\nabla\log\frac{\rho_k}{\rho^*},\,\nabla\cdot(\Psi\rho_k)\right\rangle dx \\
=& -\beta^{-2}\int\left\langle\nabla\log\frac{\rho_k}{\rho^*},\,\nabla^2\log\frac{\rho_k}{\rho^*}\nabla\log\frac{\rho_k}{\rho^*}\right\rangle\rho_k\,dx.
\end{aligned}
$$

The last equality comes from the fact that letting $u=\log\frac{\rho_k}{\rho^*}$ and

$$
\int\sum_j\left[\partial_j u\sum_i\frac{\partial}{\partial x_i}(\partial_i u\partial_j u\rho)\right]dx = -\int\sum_{i,j}\partial_{ij}^2 u\partial_i u\partial_j u\rho dx = -\int(\nabla u)^T\nabla u^2\nabla u\rho\,dx\,,
$$

where $\partial_j u = \partial u/\partial x_j$.

Finally, for the order hT term in (65), the definition of $\mathcal{D}_k^\beta$ and integration by parts imply

$$\begin{aligned}
&\int \mathcal{D}_k^\beta \circ \mathcal{D}_k^\beta \left(\log \frac{\rho_k}{\rho^*}\right) \left(1 + \log \frac{\rho_k}{\rho^*}\right) \rho_k dx \\
=& \int \frac{\beta^{-1}}{\rho_k} \nabla \cdot \left[\nabla \mathcal{D}_k^\beta \left(\log \frac{\rho_k}{\rho^*}\right) \rho_k\right] \left(1 + \log \frac{\rho_k}{\rho^*}\right) \rho_k dx \\
=& -\int \beta^{-1} \left\langle \nabla \mathcal{D}_k^\beta \left(\log \frac{\rho_k}{\rho^*}\right), \nabla \log \frac{\rho_k}{\rho^*} \rho_k \right\rangle dx \\
=& \int \mathcal{D}_k^\beta \left(\log \frac{\rho_k}{\rho^*}\right) \beta^{-1} \nabla \cdot \left[\nabla \log \frac{\rho_k}{\rho^*} \rho_k\right] dx \\
=& \int \left|\mathcal{D}_k^\beta \left(\log \frac{\rho_k}{\rho^*}\right)\right|^2 \rho_k dx \,.
\end{aligned}$$

Combining all the above simplifications to (65), we are ready to arrive at the final expression in (37). ■

Proof [Proof for Lemma 11.] For the second-order time derivative in (37), we note that

$$\begin{aligned}
\frac{d^2}{dt^2} \mathrm{D}_{\mathrm{KL}}(\rho_k \| \rho^*) =& \frac{1}{h} \left[\frac{d\mathrm{D}_{\mathrm{KL}}(\rho_{t_k+h} \| \rho^*)}{dt} - \frac{d\mathrm{D}_{\mathrm{KL}}(\rho_k \| \rho^*)}{dt}\right] + \mathcal{O}(h) \\
=& \frac{\beta^{-1}}{h} [\mathcal{I}(\rho_k \| \rho^*) - \mathcal{I}(\rho_{k+1} \| \rho^*)] + \mathcal{O}(h) \,,
\end{aligned} \tag{67}$$

as

$$\frac{d}{dt} \mathrm{D}_{\mathrm{KL}}(\rho_k \| \rho^*) = -\beta^{-1} \mathcal{I}(\rho_k \| \rho^*) \,, \quad \mathcal{I}(\rho_{k+1} \| \rho^*) = \mathcal{I}(\rho_{t_k+h} \| \rho^*) + \mathcal{O}(h^2) \,.$$

Substituting the exponential convergence of the fourth power term (39) and discrete approximation to second order time derivative (67) into (38), we finally obtain

$$\begin{aligned}
&\mathrm{D}_{\mathrm{KL}}(\rho_{k+1} \| \rho^*) + \frac{h + 3T}{4\beta} \mathcal{I}(\rho_{k+1} \| \rho^*) \\
\leq& \mathrm{D}_{\mathrm{KL}}(\rho_k \| \rho^*) - \frac{h}{\beta} \left(1 - \frac{h + 3T}{4h} + \alpha \frac{T}{2}\right) \mathcal{I}(\rho_k \| \rho^*) + \frac{hT}{2} M_0 \exp(-4\alpha t_k) + \mathcal{O}(h^3) \,,
\end{aligned} \tag{68}$$

where $M_0 := \beta^{-2} \int \|\nabla \log \frac{\rho_0}{\rho^*}\|_2^4 \rho_0 dx$ that depends on the initial density and we have used $\nabla^2 V \succeq \alpha I$.

Since $1 - (h + 3T)/(4h) \geq 0$, using the PL inequality (6), we note (68) implies

$$\begin{aligned}
&\left(1 + \alpha \frac{h + 3T}{2}\right) \mathrm{D}_{\mathrm{KL}}(\rho_{k+1} \| \rho^*) \\
\leq& \left[1 - 2\alpha h \left(1 - \frac{h + 3T}{4h} + \alpha \frac{T}{2}\right)\right] \mathrm{D}_{\mathrm{KL}}(\rho_k \| \rho^*) + \frac{hT}{2} M_0 \exp(-4\alpha hk) + \mathcal{O}(h^3) \,,
\end{aligned}$$

which is equivalent to

$$\begin{aligned}
\mathrm{D}_{\mathrm{KL}}(\rho_{k+1} \| \rho^*) \leq& \frac{1 - 2\alpha h \left(1 - \frac{h+3T}{4h} + \alpha \frac{T}{2}\right)}{1 + \alpha \frac{h+3T}{2}} \mathrm{D}_{\mathrm{KL}}(\rho_k \| \rho^*) + \frac{hT}{2\left(1 + \alpha \frac{h+3T}{2}\right)} M_0 \exp(-4\alpha hk) + \mathcal{O}(h^3) \\
=& \left(1 - h\alpha \frac{2 + s\alpha h}{1 + \frac{\alpha}{2} h(1 + 3s)}\right) \mathrm{D}_{\mathrm{KL}}(\rho_k \| \rho^*) + \frac{h^2 s}{2} M_0 \exp(-4\alpha hk) + \mathcal{O}(h^3) \qquad (69) \\
=& \left[1 - 2h\alpha + (1 + 2s)\, \alpha^2 h^2\right] \mathrm{D}_{\mathrm{KL}}(\rho_k \| \rho^*) + \frac{h^2 s}{2} M_0 \exp(-4\alpha hk) + \mathcal{O}(h^3) \,.
\end{aligned}$$

■

The next lemma is used in the proof of Theorem 12 to derive the exponential decay of KL divergence with a bias term.

Lemma 21 *For a sequence that satisfies*

$$a_{k+1} \leq (1-c_1h)a_k + h^2 c_2 \exp(-c_3kh) + \mathcal{O}(h^3)\,,$$

where $h, c_i > 0$ *for* $i = 1,2,3$, *and* $c_1h < 1$, *we have*

$$\begin{aligned} a_k \leq& (1-c_1h)^k a_0 + h^2 \frac{c_2 \exp(-c_3kh)}{\exp(-c_3h) - (1-c_1h)} + \mathcal{O}(h^3) \\ \leq& \exp(-c_1kh)a_0 + h^2 \frac{c_2 \exp(-c_3kh)}{\exp(-c_3h) - (1-c_1h)} + \mathcal{O}(h^3)\,. \end{aligned} \tag{70}$$

Proof We first show the sequence satisfies the following inductive relationship

$$a_{k+1} \leq (1-c_1h)^{k+1} a_0 + h^2 c_2 \sum_{j=0}^{k} (1-c_1h)^j \exp(-c_3(k-j)h) + \mathcal{O}(h^3)\,.$$

It is true for $k = 0$. And for the case $k \geq 1$, we have

$$\begin{aligned} &a_{k+1} \leq (1-c_1h)a_k + h^2 c_2 \exp(-c_3kh) + \mathcal{O}(h^3) \\ \leq& (1-c_1h)^{k+1} a_0 + h^2 c_2 \left[\sum_{j=0}^{k-1} (1-c_1h)^j \exp(-c_3(k-1-j)h) + \exp(-c_3kh) \right] + \mathcal{O}(h^3) \\ =& (1-c_1h)^{k+1} a_0 + h^2 c_2 \sum_{j=0}^{k} (1-c_1h)^j \exp(-c_3(k-j)h) + \mathcal{O}(h^3)\,. \end{aligned}$$

For the term under summation, using geometric series, we derive

$$\begin{aligned} &\sum_{j=0}^{k} (1-c_1h)^j \exp(-c_3(k-j)h) = \exp(-c_3kh) \sum_{j=0}^{k} [(1-c_1h)\exp(c_3h)]^j \\ =& \exp(-c_3kh) \frac{1 - (1-c_1h)^{k+1} \exp(c_3(k+1)h)}{1 - (1-c_1h)\exp(c_3h)} \\ =& \frac{\exp(-c_3kh) - (1-c_1h)^{k+1} \exp(c_3h)}{1 - (1-c_1h)\exp(c_3h)} = \frac{\exp(-c_3(k+1)h) - (1-c_1h)^{k+1}}{\exp(-c_3h) - (1-c_1h)} \\ \leq& \frac{\exp(-c_3(k+1)h)}{\exp(-c_3h) - (1-c_1h)}\,. \end{aligned}$$

Then we arrive

$$a_{k+1} \leq (1-c_1h)^{k+1} a_0 + h^2 \frac{c_2 \exp(-c_3(k+1)h)}{\exp(-c_3h) - (1-c_1h)} + \mathcal{O}(h^3)\,.$$

■

A.4 Postponed proof for Theorems and Lemmas in section 5

Proof [Proof of the first statement in Lemma 15] We recall the proof of Theorem 4 and denote $\tilde{V}_k = -\beta^{-1}\log\tilde{\rho}_k$. We adopt the same definitions for r_x, s_{r_x}, $\tilde{r}_x$, and $\tilde{s}_{r_x}$ as in Section 3. Replacing ρ_0 with $\tilde{\rho}_k$, we derive the following

$$
\nabla\tilde{\rho}_{k+1}(x) = -\frac{\beta}{2}\int_{\mathbb{R}^d} \frac{\left[\nabla V(x) + \frac{(x-y)}{T}\right]\exp\left[-\frac{\beta}{2}(V(x)+\frac{\|x-y\|_2^2}{2T})\right]}{\int_{\mathbb{R}^d}\exp\left[-\frac{\beta}{2}\left(V(z)+\frac{\|z-y\|_2^2}{2T}\right)\right]dz}\tilde{\rho}_k(y)\,dy \tag{71}
$$

$$
\begin{aligned}
&= -\frac{\beta}{2}\nabla V(x)\tilde{\rho}_{k+1}(x) - \frac{\beta}{2T}\int_{\mathbb{R}^d}(x-y)\frac{\exp\left[-\frac{\beta}{2}(V(x)+\frac{\|x-y\|_2^2}{2T})\right]}{\int_{\mathbb{R}^d}\exp\left[-\frac{\beta}{2}\left(V(z)+\frac{\|z-y\|_2^2}{2T}\right)\right]dz}\tilde{\rho}_k(y)\,dy + \mathcal{O}(T^2)\\
&= -\frac{\beta}{2T}\int_{\mathbb{R}^d}(x-y)\left(1+\frac{T}{2}\Delta V(s_y)\right)\exp\left[-\frac{\beta}{2}\left(V(x)+\frac{\|x-y\|_2^2}{2T}+2\tilde{V}_k(y)-V(s_y)-\frac{\|y-s_y\|_2^2}{2T}\right)\right]dy\\
&\quad -\frac{\beta}{2}\nabla V(x)\tilde{\rho}_{k+1}(x) + \mathcal{O}(T^2)\,.
\end{aligned}
$$

To apply the Laplace method in (18) to the integral in (71), we write

$$
g(y) = (x-y)\left(1+\frac{T}{2}\Delta V(s_y)\right), \quad f(y) = \frac{\|x-y\|_2^2}{2} + T(2\tilde{V}_k(y) - V(s_y)) - T^2\frac{\|\nabla V(y)\|_2^2}{2},
$$

as in (18). Given the factor $\frac{1}{T}$ preceding this integral, we have to consider all the $\mathcal{O}(T)$ term in (19).

Firstly, for the leading-order term in the expansion (18), using the definition $x - r_x = T\nabla(2\tilde{V}_k - V)(r_x)$ and the expression from Theorem 4, it will be

$$
-\frac{\beta}{2}\tilde{\rho}_{k+1}(x)g(x^*) = -\frac{\beta}{2}\tilde{\rho}_{k+1}(x)\nabla\left[(2\tilde{V}_k - V)(x) - 2T\nabla(V-\tilde{V}_k)\cdot\nabla(\tilde{V}_k)(x)\right] + \mathcal{O}(T^2)\,.
$$

Next, for the first-order term $H_1(x^*)$ in (19), we note that since $f_{pqr} = \mathcal{O}(T)$ and $g(x^*)f_{pqrs}(x^*) = \mathcal{O}(T^2)$, the last two terms are of order $\mathcal{O}(T^2)$. Additionally, for the matrix B, since $f_{qr} = \delta_{qr} + \mathcal{O}(T)$, the Neumann series leads to $B_{qr} = \delta_{qr} + \mathcal{O}(T)$ as $B = \{f_{qr}(x^*)\}^{-1}$. Therefore, the first two terms in $H_1(x^*)$ are

$$
\mathrm{Tr}(CB) = \frac{T}{2}\sum_p \frac{\partial^2}{\partial y_p^2}\left[(x-y)\Delta V(y)\right] + \mathcal{O}(T^2) = -T\nabla\Delta V(y) + \mathcal{O}(T^2)\,,
$$

and

$$
-f_{srq}B_{sq}B_{rp}g_p = -f_{qqp}g_p + \mathcal{O}(T^2) = T\nabla\Delta(2\tilde{V}_k(y) - V(y)) + \mathcal{O}(T^2)\,.
$$

Hence, the second term in the expansion (18) is

$$
\frac{2T}{\beta}\frac{\beta}{4T}\tilde{\rho}_{k+1}2T\nabla\Delta(\tilde{V}_k(x) - V(x)) = \tilde{\rho}_{k+1}(x)T\nabla\Delta(\tilde{V}_k - V)(x)\,.
$$

Finally, substituting the above into (71) and recalling our expression for $\tilde{\rho}_{k+1}$ in Theorem 4, we derive

$$
\nabla\tilde{\rho}_{k+1} = \nabla\tilde{\rho}_k + T\nabla\frac{\partial\tilde{\rho}_k}{\partial t} + \mathcal{O}(T^2)\,.
$$

■

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