REGULARIZED STEIN VARIATIONAL GRADIENT FLOW

YE HE [1], KRISHNAKUMAR BALASUBRAMANIAN [2], BHARATH K. SRIPERUMBUDUR[3], AND JIANFENG LU[4]

ABSTRACT. The Stein Variational Gradient Descent (SVGD) algorithm is a deterministic particle method for sampling. However, a mean-field analysis reveals that the gradient flow corresponding to the SVGD algorithm (i.e., the Stein Variational Gradient Flow) only provides a constant-order approximation to the Wasserstein Gradient Flow corresponding to the KL-divergence minimization. In this work, we propose the Regularized Stein Variational Gradient Flow, which interpolates between the Stein Variational Gradient Flow and the Wasserstein Gradient Flow. We establish various theoretical properties of the Regularized Stein Variational Gradient Flow (and its time-discretization) including convergence to equilibrium, existence and uniqueness of weak solutions, and stability of the solutions. We provide preliminary numerical evidence of the improved performance offered by the regularization.

MSC Subject Classification. 35Q62, 35Q68, 65C60, 82C22.

Keywords. Wasserstein gradient flow, Stein variational gradient descent, particle-based sampling, convergence to equilibrium, mean-field analysis, reproducing kernel Hilbert space, regularization.

1. INTRODUCTION

Given a potential function $V : \mathbb{R}^d \to \mathbb{R}$, the sampling problem involves generating samples from the density

$$\pi(x) \coloneqq Z^{-1} e^{-V(x)}, \qquad \text{with} \qquad Z \coloneqq \int e^{-V(x)} dx \qquad (1)$$

being the normalization constant, which is typically assumed to be unknown or hard to compute. The task of sampling arises in several fields of applied mathematics, including Bayesian statistics and machine learning in the context of numerical integration. There are two widely-used approaches for sampling: (i) diffusion-based *randomized* algorithms, which are based on discretizations of certain diffusion processes, and (ii) particle-based *deterministic* algorithms, which are discretizations of certain *approximate* gradient flows. A central idea connecting the two approaches is the seminal work by [JKO98] which provided a variational interpretation of the Langevin diffusion as the Wasserstein Gradient Flow (WGF),

$$\partial_t \mu_t = \nabla \cdot (\mu_t \, \nabla_{W_2} F(\mu_t)) = \nabla \cdot \left(\mu_t \, \nabla \log \frac{\mu_t}{\pi} \right), \qquad (2)$$

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[1] SCHOOL OF MATHEMATICS, GEORGIA INSTITUTE OF TECHNOLOGY, 686 CHERRY STREET, ATLANTA, GA, 30332. EMAIL: YHE367@GATECH.EDU

[2] DEPARTMENT OF STATISTICS, UNIVERSITY OF CALIFORNIA, DAVIS, 399 CROCKER LANE, ONE SHIELDS AVENUE DAVIS, CA 95616. EMAIL: KBALA@UCDAVIS.EDU

[3] DEPARTMENT OF STATISTICS, PENNSYLVANIA STATE UNIVERSITY, 314, THOMAS BUILDING, UNIVERSITY PARK, PA 16802. EMAIL: BKS18@PSU.EDU

[4] MATHEMATICS DEPARTMENT, DUKE UNIVERSITY, BOX 90320, 120 SCIENCE DR., DURHAM, NC 27708-0320. EMAIL: JIANFENG@MATH.DUKE.EDU

where the term $\nabla_{W_2} F(\mu_t) = \nabla \log \frac{\mu_t}{\pi}$ could be interpreted as the Wasserstein gradient[1] of the relative entropy functional (also called as the Kullback–Leibler divergence), defined by

$$F(\mu_t) = \mathrm{KL}(\mu_t|\pi) \coloneqq \int_{\mathbb{R}^d} \log \frac{\mu_t(x)}{\pi(x)} \mu_t(x) dx,$$

evaluated at μ_t. This leads to the idea that sampling could be viewed as *optimization on the space of densities/measures*, a viewpoint that has provided a deeper understanding of the sampling problem [Wib18, TSA20].

There are several merits and disadvantages to both the randomized and deterministic discretizations of the (approximate) WGF. First, note that obtaining exact space-time discretization of the WGF in (2) is not possible. Indeed, due to the presence of the diffusion term, when initialized with a N-particle based empirical measure, the particles do not remain as particles for any time $t > 0$. Hence, on the one hand, randomized discretizations like the Langevin Monte Carlo algorithm, are used as implementable space-time discretizations of the WGF. On the other hand, motivated by applications where the randomness in the discretization is undesirable, in the applied mathematics literature, other discretizations of *approximate* WGF were developed. Such methods are predominantly based on using mollifiers and we refer the reader to [Rav85, Rus90, DM90, CB16, CCP19] for a partial list and to [Che17], for a comprehensive overview.

Recently, in the machine learning community, the Stein Variational Gradient Descent [LW16, Liu17] was proposed as another deterministic discretization of approximate WGF, and has gathered significant attention due to applications in reinforcement learning [LRLP17], graphical modeling [WZL18], measure quantization [XKS22], and other fields of machine learning and applied mathematics [WTBL19, CLGL+20, CLGL+20, KSA+20]. Due to the use of the reproducing kernels, the Stein Variational Gradient Descent (SVGD) algorithm provides a space-time discretization of the following *approximate* Wasserstein Gradient Flow (which we refer to as the Stein Variational Gradient Flow (SVGF) for simplicity)

$$\partial_t \mu_t = \nabla \cdot \left(\mu_t \; \mathcal{T}_{k,\mu_t} \nabla \log \frac{\mu_t}{\pi} \right), \tag{3}$$

where $\mathcal{T}_{k,\mu} : L_2^d(\mu) \to L_2^d(\mu)$[2] is the integral operator defined as $\mathcal{T}_{k,\mu} f(x) = \int k(x,y) f(y) \mu(y) dy$ for any function $f \in L_2^d(\mu)$, and for a kernel $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$; see, for example [LLN19]. Hence, SVGD (which is based on the SVGF), in this context, while being deterministic only provides a discretization of a *constant-order approximation* to the Wasserstein Gradient Flow due to the presence of the kernel integral operator. Indeed, if $\mathrm{supp}(\mu_t) = \mathbb{R}^d$ and k is a bounded continuous translation invariant *characteristic* kernel [SGF+10] on $\mathbb{R}^d$ (e.g., Gaussian, Laplacian kernels), then

$$\|\mathcal{T}_{k,\mu_t} - I\|_{\mathrm{op}} = \sup\{\|\mathcal{T}_{k,\mu_t} f - f\|_{L_2^d(\mu_t)} : \|f\|_{L_2^d(\mu_t)} = 1\} \geq \|\mathcal{T}_{k,\mu_t}\mathbf{1} - \mathbf{1}\|_{L_2^d(\mu_t)}$$
$$\geq \|1 - \int k(\cdot, x)\mu_t(x)\, dx\|_{L_2(\mu_t)} > 0,$$

where $\mathbf{1} = (1, \ldots, 1)^{\mathsf{T}} \in \mathbb{R}^d$. This shows that the order of the error is crucially dependent on the choice of the kernel k.

To overcome the above issue with the SVGF, in this work, we propose the Regularized Stein Variational Gradient Flow (R-SVGF). To motivate the proposed flow, we first note that the Wasserstein gradient $\nabla \log(\mu_t/\pi)$ lives in $L_2^d(\mu_t)$, while the kernelized Wasserstein gradient $\mathcal{T}_{k,\mu_t} \nabla \log(\mu_t/\pi)$ *morally* lives in the reproducing kernel Hilbert space[3] $\mathcal{H}_k^d \subset L_2^d(\mu_t)$. If $\nabla \log(\mu_t/\pi) \in \overline{\mathrm{Ran}(\mathcal{T}_{k,\mu_t})}$, then it is easy to verify that

$$\|((1-\nu)\mathcal{T}_{k,\mu_t} + \nu I)^{-1}\mathcal{T}_{k,\mu_t}\nabla \log(\mu_t/\pi) - \nabla \log(\mu_t/\pi)\|_{L_2^d(\mu_t)} \to 0, \quad \text{as} \quad \nu \to 0.$$

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[1]See, for example, [AGS05, San17] for the exact definition.
[2]Defined in Section 1.3.
[3]Defined in Section 2.

Additionally, if $\nabla \log(\mu_t/\pi)$ is sufficiently smooth, i.e., there exists $\gamma \in \left(0, \frac{1}{2}\right]$ such that $\nabla \log(\mu_t/\pi) = \mathcal{T}_{k,\mu_t}^{\gamma} h$, for some $h \in L_2^d(\mu_t)$ (see, for example, [CZ07]), then

$$\left\| ((1-\nu)\mathcal{T}_{k,\mu_t} + \nu I)^{-1} \mathcal{T}_{k,\mu_t} \nabla \log(\mu_t/\pi) - \nabla \log(\mu_t/\pi) \right\|_{L_2^d(\mu_t)} = O(\nu^{2\gamma}), \quad \text{as} \quad \nu \to 0.$$

In other words, $((1-\nu)\mathcal{T}_{k,\mu_t} + \nu I)^{-1} \mathcal{T}_{k,\mu_t} \nabla \log(\mu_t/\pi)$ is a good approximation to $\nabla \log(\mu_t/\pi)$ for small ν. With this motivation, we propose the following R-SVGF given by

$$\partial_t \mu_t = \nabla \cdot \left(\mu_t \; ((1-\nu)\mathcal{T}_{k,\mu_t} + \nu I)^{-1} \; \mathcal{T}_{k,\mu_t} \left(\nabla \log \frac{\mu_t}{\pi} \right) \right), \tag{4}$$

for some regularization parameter $\nu \in (0, 1]$, where R-SVGF arbitrarily approximates the WGF as $\nu \to 0$. It is important to note that in the case of $\gamma = 1/2$, we have $\nabla \log(\mu_t/\pi) \in \mathcal{H}_k^d$, yet, (3) suffers from the drawback of providing only a constant-order approximation to (2).

1.1. **Summary of Contributions.** Our contributions in this work are as follows:

(1) We propose the Regularized SVGF (R-SVGF) that interpolates between the Wasserstein Gradient Flow and the SVGF. The advantage of the proposed flow is that one could obtain an implementable space-time discretization as long as the regularization parameter is bounded away from zero. The main intuition behind the proposed flow is to pick an appropriately small regularization parameter so that we could arbitrarily approximate the WGF (Theorems 1 and 3).

(2) For the R-SVGF, we provide rates of convergence to the equilibrium density in two cases: (i) in the Fisher Information metric under no further assumptions on the target $\pi \in \mathcal{P}(\mathbb{R}^d)$ (Theorem 2) and (ii) in the KL-divergence metric under an LSI assumption on the target (Theorem 4). We also establish similar results for the time-discretized R-SVGF (Theorems 5 and 6).

(3) We characterize the existence and uniqueness (Theorem 7), and stability (Theorem 8) of solutions to the R-SVGF.

(4) We provide preliminary numerical experiments demonstrating the advantage of the space-time discretization of the R-SVGF, which we call the Regularized Stein Variational Gradient Descent (R-SVGD) algorithm, over the standard SVGD algorithm.

1.2. **Organization.** The rest of the paper is organized as follows. In Section 1.3, we introduce the notations used in the rest of the paper. In Section 2, we provide the preliminaries on reproducing kernel Hilbert spaces required for our work. In Section 3, we introduce the R-SVGF, along with the notion of regularized Stein-Fisher information, required for our analysis. Due to the technical nature of the proofs, we postpone the results on existence and uniqueness of the R-SVGF, and related stability results respectively to Sections 5 and 6. In Section 4, we provide convergence results on the R-SVGF and its time-discretized version. We conclude in Section 7 with a space-time discretization which provides a practically implementable algorithm, and provide preliminary empirical results.

1.3. **Notations.** We use the following notations throughout this work:

- For a matrix, $\|\cdot\|_2$ denotes the matrix 2-norm (spectral norm) and $\|\cdot\|_{HS}$ denotes the Hilbert-Schmidt norm which is defined as $\|A\|_{HS}^2 = \sum_{i,j=1}^{d} |a_{ij}|^2$ for any matrix $A = (a_{ij})_{i,j \in [d]}$.
- The term id denotes the $d \times d$ identity matrix. I_d corresponds to the identity operator in the RKHS. I corresponds to the identity operator in $L_2(\mu)$.
- $\left(L_\infty(\mathbb{R}^d), \|\cdot\|_{L_\infty(\mathbb{R}^d)} \right)$ denotes the space of all essentially bounded measurable functions on $\mathbb{R}^d$ with $\|f\|_{L_\infty(\mathbb{R}^d)} := \inf\{C : |f(x)| \leq C \text{ for almost every } x \in \mathbb{R}^d\}$ for any $f \in L_\infty(\mathbb{R}^d)$.
- $\mathcal{C}(\mathbb{R}^d; \mathbb{R}^d)$ is the space of all $\mathbb{R}^d$-valued continuous functions on $\mathbb{R}^d$.

- $\mathcal{C}_0^\infty([0,\infty)\times\mathbb{R}^d)$ is the space of all $\mathbb{R}$-valued measurable functions on $[0,\infty)\times\mathbb{R}^d$ that vanish at infinity, i.e., for any $f \in \mathcal{C}_0^\infty([0,\infty)\times\mathbb{R}^d)$, $f(t,x) \to 0$ as $t \to \infty$ and $f(t,x) \to 0$ as $x \to \infty$.
- For any function space $\mathcal{H}$ on $\mathbb{R}^d$, $\mathcal{C}([0,T];\mathcal{H})$ is the space of functions f such that for any fixed $t \in [0,T]$, $f(t,\cdot) \in \mathcal{H}$ and for any fixed $x \in \mathbb{R}^d$, $f(\cdot,x)$ is a continuous function on $[0,T]$. $\mathcal{C}^1([0,T];\mathcal{H})$ is the space of functions f such that for any fixed $t \in [0,T]$, $f(t,\cdot) \in \mathcal{H}$ and for any fixed $x \in \mathbb{R}^d$, $f(\cdot,x)$ is a continuous function with a continuous first order derivative on $[0,T]$.
- Let $\mathcal{P}(\mathbb{R}^d)$ denote the space of all probability densities (with respect to the Lebesgue measure) on $\mathbb{R}^d$ that are twice continuously differentiable with full supports on $\mathbb{R}^d$ and finite second moments.
- For any $\mu_1,\mu_2 \in \mathcal{P}(\mathbb{R}^d)$ and any $p \geq 1$, $\mathcal{W}_p(\mu_1,\mu_2)$ denotes the Wasserstein-p distance between μ_1 and μ_2 defined as $\mathcal{W}_p(\mu_1,\mu_2) := \inf_{X\sim\mu_1,Y\sim\mu_2}\mathbb{E}[|X-Y|^p]^{\frac{1}{p}}$.
- For any $\mu \in \mathcal{P}(\mathbb{R}^d)$, $\left(L_2(\mu),\|\cdot\|_{L_2(\mu)}\right)$ is the space of all μ-square integrable measurable function on $\mathbb{R}^d$ with $\|f\|_{L_2(\mu)}^2 := \int_{\mathbb{R}^d}|f(x)|^2\mu(x)dx$.
- For any function space $\mathcal{H}$, we say $f \in \mathcal{H}^d$ if $f = [f_1,\cdots,f_d]^\mathsf{T}$ such that $f_i \in \mathcal{H}$ for all $i \in [d]$. If the function space $(\mathcal{H},\|\cdot\|_{\mathcal{H}})$ is further a Hilbert space, $(\mathcal{H}^d,\|\cdot\|_{\mathcal{H}^d})$ denotes the Hilbert space of all vector valued functions whose entries are in $(\mathcal{H},\|\cdot\|_{\mathcal{H}})$ with $\|f\|_{\mathcal{H}^d}^2 := \sum_{i=1}^d\|f_i\|_{\mathcal{H}}^2$ for any $f = [f_1,\cdots,f_d]^\mathsf{T} \in \mathcal{H}^d$.
- Let $(\mathcal{H},\|\cdot\|_{\mathcal{H}})$ and $(\mathcal{G},\|\cdot\|_{\mathcal{G}})$ be two function spaces. For an operator $A : \mathcal{H} \to \mathcal{G}$, we denote the adjoint operator of A by A^*. We denote the operator norm by $\|A\|_{\mathcal{H}\to\mathcal{G}}$, which is defined as $\|A\|_{\mathcal{H}\to\mathcal{G}} := \sup_{\|u\|_{\mathcal{H}}\leq 1}\|Au\|_{\mathcal{G}}$. When we don't emphasize the spaces, we denote the operator norm of A by $\|A\|_{\mathrm{op}}$ for simplicity.
- Let $(\mathcal{H},\|\cdot\|_{\mathcal{H}})$ and $(\mathcal{G},\|\cdot\|_{\mathcal{G}})$ be two Hilbert spaces. For an operator $A : \mathcal{H} \to \mathcal{G}$, we denote the Hilbert-Schmidt norm by $\|A\|_{HS}$ which is defined as $\|A\|_{HS}^2 := \sum_{i\in I}\|Ae_i\|_{\mathcal{G}}^2$ where $\{e_i\}_{i\in I}$ is an orthonormal basis of $\mathcal{H}$. We denote the nuclear norm by $\|A\|_{nuc}$ which is defined as $\|A\|_{nuc} := \sum_{i\in I}\langle(A^*A)^{\frac{1}{2}}e_i,e_i\rangle_{\mathcal{H}}$ where $\{e_i\}_{i\in I}$ is an orthonormal basis of $\mathcal{H}$.
- For a smooth function $f : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, $\nabla_1 f$ denotes the gradient of f in the first variable and $\nabla_2 f$ denotes the gradient of f in the second variable.
- For a map $\phi : \mathbb{R}^d \to \mathbb{R}^d$, ϕ_i denotes the i-th component of the function value and $\nabla\phi$ denotes the Jacobian, i.e., $(\nabla\phi)_{ij} = \partial_j\phi_i$ for all $i,j \in [d]$.
- $T_\#\rho$ represents the push-forward of the density ρ under a map T.
- $\langle\cdot,\cdot\rangle_{\mathcal{H}}$ denotes inner-product in the Hilbert space $\mathcal{H}$. $\langle\cdot,\cdot\rangle$ denotes inner-product in the Euclidean space $\mathbb{R}^d$.

2. Preliminaries on Reproducing Kernel Hilbert Space

In this section, we introduce some properties of RKHS which would be used later in the formulation and analysis of R-SVGF. We refer the reader to [SC08, BTA11, PR16] for the basics of RKHS. We let $\mathcal{H}_k$ be a separable RKHS over $\mathbb{R}^d$ with the reproducing kernel $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}_{>0}$ and with $\|\cdot\|_{\mathcal{H}_k}$ denoting the associated RKHS norm. We make the following assumption on the kernel function k throughout the paper.

Assumption A1. The kernel function $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is symmetric, strictly positive definite and continuous.

Additional assumptions on the kernel will be introduced when they are required. The following results are essentially based on [SC08, Lemma 4.23, and Theorems 4.26 and 4.27].

Proposition 1 ([SC08]). *The following holds.*

(i) *The kernel function k is bounded if and only if every $f \in \mathcal{H}_k$ is bounded. Moreover, the inclusion $\iota_d : \mathcal{H}_k \to L_\infty(\mathbb{R}^d)$ is continuous and $\|\iota_d\|_{\mathcal{H}_k \to L_\infty(\mathbb{R}^d)} = \|k\|_\infty$, where $\|k\|_\infty := \sup_{x \in \mathbb{R}^d} \sqrt{k(x,x)}$.*

(ii) *Let μ be a σ-finite measure on $\mathbb{R}^d$ and k be a measurable kernel. Assume that*

$$\|k\|_{L_2(\mu)} := \left(\int_{\mathbb{R}^d} k(x,x) d\mu(x) \right)^{\frac{1}{2}} < \infty.$$

Then $\mathcal{H}_k$ consists of 2-integrable functions and the inclusion $\iota_{k,\mu} : \mathcal{H}_k \to L_2(\mu)$ is continuous with $\|\iota_{k,\mu}\|_{\mathcal{H}_k \to L_2(\mu)} \leq \|k\|_{L_2(\mu)}$. Moreover, the adjoint of this inclusion is the operator $\iota_{k,\mu}^* : L_2(\mu) \to \mathcal{H}_k$ defined by

$$\iota_{k,\mu}^* g(x) := \int_{\mathbb{R}^d} k(x,y) g(y) d\mu(y), \qquad g \in L_2(\mu), \ x \in \mathbb{R}^d.$$

(iii) *Under the assumptions in (ii), $\mathcal{H}_k$ is dense in $L_2(\mu)$ if and only if $\iota_{k,\mu}^* : L_2(\mu) \to \mathcal{H}_k$ is injective. Alternatively, $\iota_{k,\mu}^* : L_2(\mu) \to \mathcal{H}_k$ has a dense image if and only if $\iota_{k,\mu} : \mathcal{H}_k \to L_2(\mu)$ is injective.*

(iv) *Under the assumptions in (ii), $\iota_{k,\mu} : \mathcal{H}_k \to L_2(\mu)$ is a Hilbert-Schmidt operator with $\|\iota_{k,\mu}\|_{HS} = \|k\|_{L_2(\mu)}$. Moreover, the integral operator $\mathcal{T}_{k,\mu} = \iota_{k,\mu} \iota_{k,\mu}^* : L_2(\mu) \to L_2(\mu)$ is compact, positive, self-adjoint, and nuclear with $\|\mathcal{T}_{k,\mu}\|_{nuc} = \|\iota_{k,\mu}\|_{HS} = \|k\|_{L_2(\mu)}$.*

When $f \in \mathcal{H}_k^d$ with $f = [f_1, \cdots, f_d]^\mathsf{T}$ and $g \in \mathcal{H}_k$, we define $\langle f, g \rangle_{\mathcal{H}_k}$ as a vector in $\mathbb{R}^d$ and $(\langle f, g \rangle_{\mathcal{H}_k})_i = \langle f_i, g \rangle_{\mathcal{H}_k}$ for all $i \in [d]$. When $f \in L_2^d(\mu)$ with $f = [f_1, \cdots, f_d]^\mathsf{T}$ and $g \in L_2(\mu)$, we define $\langle f, g \rangle_{L_2(\mu)}$ as a vector in $\mathbb{R}^d$ and $(\langle f, g \rangle_{L_2(\mu)})_i = \langle f_i, g \rangle_{L_2(\mu)}$ for all $i \in [d]$. Note also that $\mathcal{T}_{k,\mu} = \iota_{k,\mu} \iota_{k,\mu}^*$ and $\mathrm{Ran}(\mathcal{T}_{k,\mu}^{1/2}) = \mathcal{H}_k \subset L_2(\mu)$. We refer the interested reader to [CZ07] for more details.

Finally, we remark that by letting $(\lambda_i, e_i)_{i=1}^\infty$ be the set of eigenvalues and eigenfunctions of the operator $\mathcal{T}_{k,\mu}$ where $\lambda_1 \geq \lambda_2 \geq \cdots > 0$ and $(e_i)_{i=1}^\infty$ form an orthonormal system in $\mathrm{Ran}(\mathcal{T}_{k,\mu})$, we have the following spectral representation that, for all $f \in L_2(\mu)$,

$$\mathcal{T}_{k,\mu} f = \sum_{i=1}^\infty \lambda_i \langle f, e_i \rangle_{L_2(\mu)} e_i. \tag{5}$$

Computing the spectral representation, in general for any given μ and kernel k is a non-trivial task. Results are only known on a case-by-case basis; see, for example, [MNY06, AM14, CX20, SH21]. However, we use the decomposition only in our analysis. For the purely practical algorithm that we describe eventually in Section 7, we do not need to know the decomposition explicitly.

Remark 1. Strictly speaking, the above notation implicitly assumes that the operator $\mathcal{T}_{k,\mu}$ has a trivial null space, in which case $\overline{\mathrm{Ran}(\mathcal{T}_{k,\mu})} \equiv L_2(\mu)$ and hence the eigenfunctions $(e_i)_{i=1}^\infty$ form an orthonormal basis to $L_2(\mu)$. However, our analysis does not require this condition on $\mathcal{T}_{k,\mu}$. In particular, if $\mathcal{T}_{k,\mu}$ has a non-trivial null-space, then $\overline{\mathrm{Ran}(\mathcal{T}_{k,\mu})} \subset L_2(\mu)$. In this case, our analysis still holds true. For example, with a slight abuse of notation, if we let e_i, for certain values of i, also denote the basis of the null-space of $\mathcal{T}_{k,\mu}$, conclusions similar to our results hold.

3. REGULARIZED SVGF

We now introduce the formulation of the Regularized-SVGF and discuss its connection with the SVGF and the WGF. Recall that in the mean-field limit, the SVGF in (3) only provides a constant order approximation to the WGF in (2), due to the presence of the operator $\mathcal{T}_{k,\mu}$. As the operator $\mathcal{T}_{k,\mu}$ is not invertible, we seek to obtain a regularized inverse so that we end up with the following Regularized-SVGF, as in (4), for some regularization parameter $\nu \in (0,1]$. Note in particular that,

as $\nu \to 0$, the Regularized-SVGF gets arbitrarily close to the WGF. Our goal in this section is to derive the above-mentioned R-SVGF from first principles.

The central operator required in our formulation is the following *Stein operator*, which is defined for all $p \in \mathcal{P}(\mathbb{R}^d)$, and for all smooth maps $\phi : \mathbb{R}^d \to \mathbb{R}^d$, as

$$\mathcal{A}_p \phi(x) = \phi(x) \otimes \nabla \log p(x) + \nabla \phi(x),$$

where $\otimes$ denotes the outer-product. Generally speaking, the Stein operator can also be defined for some densities that are outside of $\mathcal{P}(\mathbb{R}^d)$. We restrict to $p \in \mathcal{P}(\mathbb{R}^d)$ in the paper for the purpose of our analysis. Now, the Wasserstein Gradient Flow in (2) could be thought of as follows. Consider moving a particle $x \sim \rho$ (for some $\rho \in \mathcal{P}(\mathbb{R}^d)$) based on the mapping $x \mapsto T(x) \coloneqq x + h\phi(x)$, where $h > 0$ is a step-size parameter, and ϕ is a vector-field chosen so that the KL-divergence between the pushforward of ρ according to T, denoted as $T_\#\rho$, and the target density π in minimal. Liu and Wang [LW16, Theorem 3.1], showed that

$$\nabla_h \mathrm{KL}(T_\#\rho|\pi)|_{h=0} = -\mathbb{E}_{x \sim \rho}[\mathrm{trace}(\mathcal{A}_\pi \phi(x))].$$

We also refer to [JKO98] for an earlier version of the same result. Based on this observation, if we try to find the vector-field ϕ in the unit-ball of $L_2^d(\rho)$ that maximizes the quantity $[\mathbb{E}_{x \sim \rho}[\mathrm{trace}(\mathcal{A}_\pi \phi(x))]]^2$, a straight-forward calculation based on integration-by-parts, results in the optimal ϕ being the Wasserstein gradient $\nabla \log \frac{\rho}{\pi}$. To have a practical implementation, [LW16] considered maximizing $[\mathbb{E}_{x \sim \rho}[\mathrm{trace}(\mathcal{A}_\pi \phi(x))]]^2$ over the unit-ball in the RKHS $\mathcal{H}_k^d$, which results in the optimal vector-field being equal to $\mathcal{T}_{k,\rho} \nabla \log \frac{\rho}{\pi}$, and correspondingly results in the SVGF in (3).

In this work, we propose to find the vector field ϕ that maximizes $[\mathbb{E}_{x \sim \rho}[\mathrm{trace}(\mathcal{A}_\pi \phi(x))]]^2$ over the unit-ball with respect to an interpolated norm between $L_2^d(\rho)$ and $\mathcal{H}_k^d$. Specifically, the interpolation norm that we consider is of the form $\nu \|\cdot\|_{\mathcal{H}_k^d}^2 + (1 - \nu) \|\cdot\|_{L_2^d(\rho)}^2$, for some regularization parameter $\nu \in (0, 1]$, which trades-off between $\| \cdot \|_{\mathcal{H}_k^d}^2$ and $\| \cdot \|_{L_2^d(\rho)}^2$. We also remark here that a similar idea has been leveraged in the context of RKHS-based statistical hypothesis testing [BLY21]. Formally, for $\rho, \pi \in \mathcal{P}(\mathbb{R}^d)$, we consider the following optimization problem.

$$S(\rho, \pi) \coloneqq \max_{\phi \in \mathcal{H}_k^d} \left\{ [\mathbb{E}_{x \sim \rho}[\mathrm{trace}(\mathcal{A}_\pi \phi(x))]]^2 \qquad \text{such that} \quad \nu \|\phi\|_{\mathcal{H}_k^d}^2 + (1 - \nu) \|\phi\|_{L_2^d(\rho)}^2 \leq 1 \right\}.$$

For any $\rho \in \mathcal{P}(\mathbb{R}^d)$, the optimal vector field, ϕ that minimizes $\mathrm{KL}(T_\#\rho|\pi)$ can be described via the following result. To make the statements more consistent with the analysis (and proofs), we will denote $\mathcal{T}_{k,\cdot}$ explicitly as $\iota_{k,\cdot} \iota_{k,\cdot}^*$ in the rest of the paper. Before we proceed, we also recall that the Fisher information between two densities $\rho, \pi \in \mathcal{P}(\mathbb{R}^d)$, is defined as

$$I(\rho|\pi) \coloneqq \left\| \nabla \log \frac{\rho}{\pi} \right\|_{L_2(\rho)}^2 = \sum_{i=1}^{\infty} \left| \left\langle \nabla \log \frac{\rho}{\pi}, e_i \right\rangle_{L_2(\rho)} \right|^2, \tag{6}$$

with $(e_i)_{i=1}^{\infty}$ being an orthonormal basis to $L_2(\rho)$.

Proposition 2. *Let $T(x) = x + h\phi(x)$ and $T_\#\rho(z)$ be the density of $z = T(x)$ for any $\rho \in \mathcal{P}(\mathbb{R}^d)$. For $\nu \in (0, 1]$, define*

$$\mathcal{B} \coloneqq \{\phi \in \mathcal{H}_k^d : \nu \|\phi\|_{\mathcal{H}_k^d}^2 + (1 - \nu) \|\phi\|_{L_2^d(\rho)}^2 \leq 1\}.$$

Let $\pi \propto e^{-V}$ and $\pi \in \mathcal{P}(\mathbb{R}^d)$. If $I(\rho|\pi) < \infty$ and k satisfies Assumption A1 with $\int k(x, x)\rho(x)dx < \infty$, then the direction of steepest descent in $\mathcal{B}$ that maximizes

$$-\nabla_h \mathrm{KL}(T_\#\rho|\pi)|_{h=0}$$

is given by

$$\phi_{\rho,\pi}^*(\cdot) \propto \left((1 - \nu)\iota_{k,\rho}^* \iota_{k,\rho} + \nu I_d \right)^{-1} \mathbb{E}_{x \sim \rho}[-\nabla V(x)k(x, \cdot) + \nabla k(x, \cdot)],$$

where $\iota_{k,\rho} : \mathcal{H}_k^d \to L_2^d(\rho)$ *is the inclusion operator and* $\iota_{k,\rho}^*$ *is its adjoint, as in Proposition* 1. *Furthermore, under the optimal vector field* $\phi_{\rho,\pi}^*$, *we have* $-\nabla_h \mathrm{KL}(T_\# \rho | \pi)|_{h=0} = S(\rho, \pi)$.

Proof. First note that according to [LW16, Theorem 3.1], we have

$$\nabla_h \mathrm{KL}(T_\# \rho | \pi)|_{h=0} = -\mathbb{E}_{x \sim \rho}[\mathrm{trace}(\mathcal{A}_\pi \phi(x))].$$

Therefore, we have

$$\phi_{\rho,\pi}^* = \underset{\phi \in \mathcal{H}_k^d}{\arg\max} \left\{ [\mathbb{E}_{x \sim \rho}[\mathrm{trace}(\mathcal{A}_\pi \phi(x))]]^2 \quad \text{such that} \quad \nu \|\phi\|_{\mathcal{H}_k^d}^2 + (1-\nu) \|\phi\|_{L_2^d(\rho)}^2 \leq 1 \right\}.$$

Next, observe that we have

$$\mathbb{E}_{x \sim \rho}[\mathrm{trace}(\mathcal{A}_\pi \phi(x))] = \sum_{i=1}^d \mathbb{E}_{x \sim \rho}[-\partial_i V(x) \phi_i(x) + \partial_i \phi_i(x)]$$

$$= \sum_{i=1}^d \mathbb{E}_{x \sim \rho}[-\partial_i V(x) \langle \phi_i, k(x, \cdot) \rangle_{\mathcal{H}_k} + \langle \phi_i, \partial_i k(x, \cdot) \rangle_{\mathcal{H}_k}]$$

$$= \langle \phi, \mathbb{E}_{x \sim \rho}[-\nabla V(x) k(x, \cdot) + \nabla k(x, \cdot)] \rangle_{\mathcal{H}_k^d}.$$

The term $\mathbb{E}_{x \sim \rho}[-\nabla V(x) k(x, \cdot) + \nabla k(x, \cdot)]$ is finite for all $x \in \mathbb{R}^d$ due to the following inequality:

$$|\mathbb{E}_{x \sim \rho}[-\nabla V(x) k(x, \cdot) + \nabla k(x, \cdot)]| = |\iota_{k,\rho}^* \nabla \log \frac{\rho}{\pi}(x)| = \left| \int k(x, y) \nabla \log \frac{\rho(y)}{\pi(y)} \rho(y) dx \right|$$

$$\leq I(\rho | \pi)^{\frac{1}{2}} \sqrt{k(x, x)} \left(\int k(y, y) \rho(y) dy \right)^{\frac{1}{2}} < \infty,$$

where the first inequality follows from the Cauchy-Schwartz inequality and the reproducing property of the RKHS. The second inequality follows from conditions on k and ρ. Meanwhile, the constraint can be written as

$$\nu \|\phi\|_{\mathcal{H}_k^d}^2 + (1-\nu) \|\phi\|_{L_2^d(\rho)}^2 = \nu \langle \phi, \phi \rangle_{\mathcal{H}_k^d} + (1-\nu) \langle \iota_{k,\rho} \phi, \iota_{k,\rho} \phi \rangle_{L_2^d(\rho)}$$

$$= \langle (\nu I_d + (1-\nu) \iota_{k,\rho}^* \iota_{k,\rho}) \phi, \phi \rangle_{\mathcal{H}_k^d}$$

$$= \left\| ((1-\nu) \iota_{k,\rho}^* \iota_{k,\rho} + \nu I_d)^{\frac{1}{2}} \phi \right\|_{\mathcal{H}_k^d}^2,$$

where $I_d : \mathcal{H}_k \to \mathcal{H}_k$ is the identity operator. Now, note that $\left((1-\nu) \iota_{k,\rho}^* \iota_{k,\rho} + \nu I_d \right)^{\frac{1}{2}}$ is well-defined since $\iota_{k,\rho}^* \iota_{k,\rho} : \mathcal{H}_k^d \to \mathcal{H}_k^d$ is positive, compact and self-adjoint. Therefore, based on the above display, the constraint $\{\phi \in \mathcal{H}_k^d : \nu \|\phi\|_{\mathcal{H}_k^d}^2 + (1-\nu) \|\phi\|_{L_2^d(\rho)}^2 \leq 1\}$ is equivalent to

$$\{\phi \in \mathcal{H}_k^d : \psi = ((1-\nu) \iota_{k,\rho}^* \iota_{k,\rho} + \nu I_d)^{\frac{1}{2}} \phi \quad and \quad \|\psi\|_{\mathcal{H}_k^d} \leq 1\}.$$

Since the spectrum of $\iota_{k,\rho}^* \iota_{k,\rho}$ is positive and $\nu \in (0, 1]$, $(1-\nu) \iota_{k,\rho}^* \iota_{k,\rho} + \nu I_d$ is invertible. For all $\phi \in \mathcal{H}_k^d$, there exists a unique $\psi \in \mathcal{H}_k^d$ such that $\left((1-\nu) \iota_{k,\rho}^* \iota_{k,\rho} + \nu I_d \right)^{-\frac{1}{2}} \psi = \phi$. Applying this fact along with the equivalent form of the constraint, we have

$$\mathbb{E}_{x \sim \rho}(\mathrm{trace}(\mathcal{A}_\pi \phi(x))) = \left\langle ((1-\nu) \iota_{k,\rho}^* \iota_{k,\rho} + \nu I_d)^{-\frac{1}{2}} \psi, \mathbb{E}_{x \sim \rho}[-\nabla V(x) k(x, \cdot) + \nabla k(x, \cdot)] \right\rangle_{\mathcal{H}_k^d}$$

$$= \left\langle \psi, ((1-\nu) \iota_{k,\rho}^* \iota_{k,\rho} + \nu I_d)^{-\frac{1}{2}} \mathbb{E}_{x \sim \rho}[-\nabla V(x) k(x, \cdot) + \nabla k(x, \cdot)] \right\rangle_{\mathcal{H}_k^d}$$

$$\leq \left\| ((1-\nu) \iota_{k,\rho}^* \iota_{k,\rho} + \nu I_d)^{-\frac{1}{2}} \mathbb{E}_{x \sim \rho}[-\nabla V(x) k(x, \cdot) + \nabla k(x, \cdot)] \right\|_{\mathcal{H}_k^d}$$

where the second identity follows from the fact that $\left((1-\nu)\iota_{k,\rho}^*\iota_{k,\rho}+\nu I_d\right)^{-\frac{1}{2}}$ is self-adjoint and the upper bound in the last inequality is achieved when

$$\psi^* \propto \left((1-\nu)\iota_{k,\rho}^*\iota_{k,\rho}+\nu I_d\right)^{-\frac{1}{2}} \mathbb{E}_{x\sim\rho}[-\nabla V(x)k(x,\cdot)+\nabla k(x,\cdot)],$$

and the result hence follows. $\square$

With the optimal-vector field as derived above, we consider the following mean-field partial differential equation (PDE) as the R-SVGF:

$$\partial_t\rho_t = \nabla \cdot \left(\rho_t \; \iota_{k,\rho_t} \left((1-\nu)\iota_{k,\rho_t}^*\iota_{k,\rho_t}+\nu I_d\right)^{-1} \iota_{k,\rho_t}^* \left(\nabla\log\frac{\rho_t}{\pi}\right)\right). \tag{7}$$

It is important to notice that the R-SVGF interpolates between the SVGF and the WGF. However, the regime of interest for us is when $\nu \to 0$, as we get arbitrarily close to the WGF. We quantify this statement precisely in the later sections. On the other hand, when $\nu \to 1$, the R-SVGF becomes the SVGF.

Remark 2. We now make the following remarks about the above result.

   (i) We can alternatively write $\phi_{\rho,\pi}^*$ from Proposition 2 as

$$\phi_{\rho,\pi}^* \propto - \left((1-\nu)\iota_{k,\rho}^*\iota_{k,\rho}+\nu I_d\right)^{-1} \iota_{k,\rho}^* \left(\nabla\log\frac{\rho}{\pi}\right),$$

   since we have

$$\mathbb{E}_{x\sim\rho}[-\nabla V(x)k(x,\cdot)+\nabla k(x,\cdot)] = \int_{\mathbb{R}^d} k(\cdot,x)\left(-\nabla V(x) - \frac{\nabla\rho(x)}{\rho(x)}\right)\rho(x)dx$$
$$= -\iota_{k,\rho}^*\left(\nabla\log\frac{\rho}{\pi}\right).$$

  (ii) The operator in (7) has an equivalent expression, as we discuss below. First, we claim that

$$\iota_{k,\rho}\left((1-\nu)\iota_{k,\rho}^*\iota_{k,\rho}+\nu I_d\right)^{-1}\iota_{k,\rho}^* = \left((1-\nu)\iota_{k,\rho}\iota_{k,\rho}^*+\nu I\right)^{-1}\iota_{k,\rho}\iota_{k,\rho}^*.$$

   To see that, we start with the trivial identity in the first line below and proceed as

$$\left((1-\nu)\iota_{k,\rho}\iota_{k,\rho}^*+\nu I\right)\iota_{k,\rho} = \iota_{k,\rho}\left((1-\nu)\iota_{k,\rho}^*\iota_{k,\rho}+\nu I_d\right),$$
$$\implies \iota_{k,\rho} = \left((1-\nu)\iota_{k,\rho}\iota_{k,\rho}^*+\nu I\right)^{-1}\iota_{k,\rho}\left((1-\nu)\iota_{k,\rho}^*\iota_{k,\rho}+\nu I_d\right)$$
$$\implies \iota_{k,\rho}\left((1-\nu)\iota_{k,\rho}^*\iota_{k,\rho}+\nu I_d\right)^{-1} = \left((1-\nu)\iota_{k,\rho}\iota_{k,\rho}^*+\nu I\right)^{-1}\iota_{k,\rho}$$
$$\implies \iota_{k,\rho}\left((1-\nu)\iota_{k,\rho}^*\iota_{k,\rho}+\nu I_d\right)^{-1}\iota_{k,\rho}^* = \left((1-\nu)\iota_{k,\rho}\iota_{k,\rho}^*+\nu I\right)^{-1}\iota_{k,\rho}\iota_{k,\rho}^*.$$

   According to this observation, (7) can also be written in the following form

$$\partial_t\rho_t = \nabla \cdot \left(\rho_t \; \left((1-\nu)\iota_{k,\rho_t}\iota_{k,\rho_t}^*+\nu I\right)^{-1}\iota_{k,\rho_t}\iota_{k,\rho_t}^*\left(\nabla\log\frac{\rho_t}{\pi}\right)\right)$$
$$= \nabla \cdot \left(\rho_t \; \left((1-\nu)\mathcal{T}_{k,\rho_t}+\nu I\right)^{-1}\mathcal{T}_{k,\rho_t}\left(\nabla\log\frac{\rho_t}{\pi}\right)\right),$$

   thereby providing the R-SVGF introduced in (4) in Section 1.

 (iii) **Particle-based spatial discretization.** We now describe the spatial discretization of the R-SVGF. Based on the results in Proposition 2 and (ii) in Remark 2, we obtain the following ODE system:

$$\begin{cases} \dfrac{dx_i(t)}{dt} = -\left((1-\nu)\iota_{k,\rho_t^N}^*\iota_{k,\rho_t^N}+\nu I_d\right)^{-1}\left(\dfrac{1}{N}\sum_{j=1}^{N}-\nabla_2 k\left(x_i(t),x_j(t)\right)+k\left(x_i(t),x_j(t)\right)\nabla V(x_j(t))\right), \\[4mm] x_i(0) = x_i^0 \in \mathbb{R}^d, \quad i=1,2,\ldots,N \end{cases},$$

where $\{x_i(t)\}_{i=1}^N$ is the set of N particles. $\rho_t^N = \frac{1}{N}\sum_{j=1}^N \delta_{x_j(t)}$ is the empirical distribution at time t, provides a N-particle spatial discretization of the R-SVGF.

(iv) **Time discretization.** We also have the following time-discretization of the R-SVGF. Let $\{h_n\}_{n=1}^\infty$ be the sequence of time step-size. We denote the density at the n-th iterate by ρ^n for all integers $n \geq 1$. Then the time discretization of the R-SVGF can be written as

$$\rho^{n+1} = \left(id - h_{n+1} \mathcal{D}_{\nu_{n+1},\rho^n} \nabla \log \frac{\rho^n}{\pi} \right)_{\#\rho^n}, \tag{8}$$

where $\mathcal{D}_{\nu_n,\rho^n} = \left((1-\nu_n)\iota_{k,\rho^n}\iota_{k,\rho^n}^* + \nu_n I_d \right)^{-1} \iota_{k,\rho^n}\iota_{k,\rho^n}^*$.

(v) The parameter ν can also be made to be dependent on t or n; in fact, in our analysis, we pick a time-varying regularization parameter.

4. Convergence Results in Continuous and Discrete Time

Our goal in this section is to derive convergence guarantees for the R-SVGF. Before we proceed, we introduce the notion of Regularized Stein-Fisher information (or Regularized Kernel Stein Discrepancy).

4.1. **Regularized Stein-Fisher Information and its Properties.** Related to the Fisher information defined in (6), several works, for example [KSA$^+$20, DNS23, SSR22], used the notion of Stein-Fisher Information to understand the convergence properties of the SVGD algorithm. The Stein-Fisher information was introduced in [CSG16, LLJ16, GM17] under the name Kernel Stein Discrepancy. It is defined as

$$I_{Stein}(\rho|\pi) := \left\| \iota_{k,\rho}^* \nabla \log \frac{\rho}{\pi} \right\|_{\mathcal{H}_k^d}^2 = \left\langle \nabla \log \frac{\rho}{\pi}, \iota_{k,\rho}\iota_{k,\rho}^* \nabla \log \frac{\rho}{\pi} \right\rangle_{L_2^d(\rho)} = \sum_{i=1}^\infty \lambda_i \left| \left\langle \nabla \log \frac{\rho}{\pi}, e_i \right\rangle_{L_2(\rho)} \right|^2,$$

where $(\lambda_i, e_i)_{i=1}^\infty$ are the set of eigenvalues and eigenvectors of the operator $\iota_{k,\rho}\iota_{k,\rho}^*$, with $\lambda_1 \geq \lambda_2 \geq \cdots > 0$. A drawback of the Stein-Fisher information is that it is a weaker metric, for example in comparison to the Fisher information metric in (6); see [GM17, GDVM19, SGBSM23]. Indeed, comparing (6) and the above definition for the Stein-Fisher information, it is immediately clear that the Stein-Fisher information is severely restrictive, in particular when the eigenvalues of the chosen RKHS decay fast. To counter this effect, we introduce the following regularized Stein-Fisher information and show that when the regularization parameter is chosen appropriately, the regularized Stein-Fisher information upper and lower bounds the Fisher information.

Definition 1 (Regularized Stein-Fisher Information). *For any $\rho \in \mathcal{P}(\mathbb{R}^d)$, the regularized Stein Fisher information from ρ to π, denoted as $I_{\nu,Stein}(\rho|\pi)$, is defined as*

$$I_{\nu,Stein}(\rho|\pi) := \left\langle \iota_{k,\rho}^* \nabla \log \frac{\rho}{\pi}, \left((1-\nu)\iota_{k,\rho}^*\iota_{k,\rho} + \nu I_d \right)^{-1} \iota_{k,\rho}^* \nabla \log \frac{\rho}{\pi} \right\rangle_{\mathcal{H}_k^d}. \tag{9}$$

The regularized Stein Fisher information in (9) is well-defined because the operator

$$(1-\nu)\iota_{k,\rho}^*\iota_{k,\rho} + \nu I_d : \mathcal{H}_k^d \to \mathcal{H}_k^d$$

is positive and for any $f \in \mathcal{H}_k^d$, $\left((1-\nu)\iota_{k,\rho}^*\iota_{k,\rho} + \nu I_d \right) f = 0$ if and only if $f = 0$.

Remark 3. The regularized Stein Fisher information has the following alternative representation:

$$I_{\nu,Stein}(\rho|\pi) = \sum_{i=1}^\infty \frac{\lambda_i}{(1-\nu)\lambda_i + \nu} \left| \left\langle \nabla \log \frac{\rho}{\pi}, e_i \right\rangle_{L_2(\rho)} \right|^2. \tag{10}$$

For $\nu > 0$, with the fact that λ_i decreases to zero as $i \to \infty$, the regularized Stein Fisher information and the Stein Fisher information both encode the spectral decay information of $\iota_{k,\rho}\iota_{k,\rho}^*$. However, note that the regularized Stein Fisher information tends to the Fisher information as $\nu \to 0$. Hypothetically speaking, if ν is set to zero, then the regularized Stein Fisher information actually becomes the Fisher information. In our analysis, we will take advantage of the relation between the regularized Stein Fisher information and the Fisher information, while studying the convergence properties of R-SVGF under Log-Sobolev inequality assumptions on the target π. A precise relation between the regularized Stein Fisher information and the Fisher information is stated in the following result. Before stating the result, we introduce the following notation for convenience. For $\gamma \in (0, \frac{1}{2}]$, we denote the pre-image of $\nabla \log \frac{\rho}{\pi} \in L_2^d(\rho)$ under $(\iota_{k,\rho}\iota_{k,\rho}^*)^\gamma$ as

$$\mathfrak{I}(\rho, \gamma) := (\iota_{k,\rho}\iota_{k,\rho}^*)^{-\gamma} \nabla \log \frac{\rho}{\pi}.$$

Note that $\|\mathfrak{I}(\rho, \gamma)\|_{L_2^d(\rho)}$ is finite if and only if $\nabla \log \frac{\rho}{\pi} \in \mathrm{Ran}((\iota_{k,\rho}\iota_{k,\rho}^*)^\gamma)$.

Proposition 3 (Equivalence relation between $I(\rho|\pi)$ and $I_{\nu,Stein}(\rho|\pi)$). *Let $\rho, \pi \in \mathcal{P}(\mathbb{R}^d)$ and suppose there exists $\gamma \in (0, \frac{1}{2}]$ such that $\|\mathfrak{I}(\rho, \gamma)\|_{L_2^d(\rho)} < \infty$. If the regularization parameter is chosen to satisfy the following condition,*

$$\frac{\nu}{1 - \nu} \leq \left(\frac{I(\rho|\pi)}{2 \|\mathfrak{I}(\rho, \gamma)\|_{L_2^d(\rho)}^2} \right)^{\frac{1}{2\gamma}}, \tag{11}$$

then we have that

$$\frac{1}{2}(1 - \nu)^{-1} I(\rho|\pi) \leq I_{\nu,Stein}(\rho|\pi) \leq (1 - \nu)^{-1} I(\rho|\pi).$$

Proof of Proposition 3. According to (10), we have

$$I_{\nu,Stein}(\rho|\pi) = \sum_{i=1}^\infty \frac{\lambda_i}{(1 - \nu)\lambda_i + \nu} \left| \left\langle \nabla \log \frac{\rho}{\pi}, e_i \right\rangle_{L_2(\rho)} \right|^2$$

$$\leq (1 - \nu)^{-1} \sum_{i=1}^\infty \left| \left\langle \nabla \log \frac{\rho}{\pi}, e_i \right\rangle_{L_2(\rho)} \right|^2 \leq (1 - \nu)^{-1} I(\mu|\pi).$$

On the other hand, since $\|\mathfrak{I}(\rho, \gamma)\|_{L_2^d(\rho)} < \infty$ for some $\gamma \in (0, \frac{1}{2}]$, there exists $h = \mathfrak{I}(\rho, \gamma) \in L_2^d(\rho)$ such that

$$\nabla \log \frac{\rho}{\pi} = (\iota_{k,\rho}\iota_{k,\rho}^*)^\gamma h.$$

Therefore

$$(1 - \nu)^{-1} I(\rho|\pi) - I_{\nu,Stein}(\rho|\pi) = \sum_{i=1}^\infty \frac{(1 - \nu)^{-1}\nu}{(1 - \nu)\lambda_i + \nu} \left| \langle (\iota_{k,\rho}\iota_{k,\rho}^*)^\gamma h, e_i \rangle_{L_2(\rho)} \right|^2 \tag{12}$$

$$= \sum_{i=1}^\infty \frac{(1 - \nu)^{-1}\nu\lambda_i^{2\gamma}}{(1 - \nu)\lambda_i + \nu} |\langle h, e_i \rangle_{L_2(\rho)}|^2$$

$$\leq (1 - \nu)^{-1-2\gamma}\nu^{2\gamma} \|\mathfrak{I}(\rho, \gamma)\|_{L_2^d(\rho)}^2$$

$$\leq \frac{1}{2}(1 - \nu)^{-1} I(\rho|\pi),$$

where the second to last inequality follows from the fact that

$$\sup_i \left(\frac{(1 - \nu)^{-1}\nu\lambda_i^{2\gamma}}{(1 - \nu)\lambda_i + \nu} \right) = (1 - \nu)^{-1-2\gamma}\nu^{2\gamma} \sup_i \left(\frac{(1 - \nu)\lambda_i}{(1 - \nu)\lambda_i + \nu} \right)^{2\gamma} \left(\frac{\nu}{(1 - \nu)\lambda_i + \nu} \right)^{1-2\gamma}$$

$$\leq (1 - \nu)^{-1-2\gamma}\nu^{2\gamma},$$

and the last inequality follows from the condition in (11). □

4.2. Convergence results for R-SVGF.

4.2.1. *Relationship between R-SVGF and WGF.* Assuming the existence and uniqueness of the R-SVGF (see Section 5) and WGF (see [JKO98] for sufficient conditions) we now provide the relationship between the R-SVGF and the WGF in various metrics. We first start with the relationship in the Fisher information metric, without any stringent assumptions on the target density (thereby allowing for multi-modal and complex densities that arise in practice). Note that the Fisher information metric corresponds to the first-order stationarity metric for the WGF, obtained by minimizing the KL divergence. This metric has been recently proposed as a meaningful metric to consider in the case of sampling from general non-log-concave densities in [BCE+22]. Note in particular under mild conditions on q (e.g., connected support) that having the Fisher information $I(p|q) = 0$ implies $p \equiv q$. However, even when $I(p|q) \leq \epsilon$, for some $\epsilon > 0$, we have that the modes of the two densities are well-aligned, as argued in [BCE+22]. In order to state our next result, we denote by $(\lambda_{i,t}, e_{i,t})_{i=1}^{\infty}$, the set of eigenvalues and eigenvectors of the operator $\iota_{k,\rho_t} \iota_{k,\rho_t}^*$ for any $t \geq 0$, with $\lambda_{1,t} \geq \lambda_{2,t} \geq \cdots > 0$.

Theorem 1 (Relation to the WGF in Relative Fisher Information). *Let (ρ_t) be the solution to* (7) *and (μ_t) be the solution to the WGF, i.e.,*

$$\begin{cases} \partial_t \mu = \nabla \cdot \left(\mu \nabla \log \frac{\mu}{\pi} \right), \\ \mu(0, \cdot) = \mu_0(\cdot). \end{cases} \tag{13}$$

For any $t > 0$, suppose there exists $\gamma_t \in (0, \frac{1}{2}]$ such that $\|\mathfrak{I}(\rho_t, \gamma_t)\|_{L_2^d(\rho_t)} < \infty$. Then, for any initial density $\mu_0 \in \mathcal{P}(\mathbb{R}^d)$, and for any $T \in (0, \infty)$, we have

$$\int_0^T I(\rho_t|\mu_t) dt \leq \frac{4}{3} \mathrm{KL}(\rho_0|\mu_0) + \frac{4}{3} \int_0^T (\lambda_{1,t} \vee 1)^2 \nu^{2\gamma_t} (1 - \nu)^{-2\gamma_t} \|\mathfrak{I}(\rho_t, \gamma_t)\|_{L_2^d(\rho_t)}^2 dt, \tag{14}$$

where $\lambda_{1,t}$ is the largest eigenvalue of $\iota_{k,\rho_t} \iota_{k,\rho_t}^*$ for all $t \geq 0$.

Proof of Theorem 1. First note that we have the following upper bound on $\frac{d}{dt} \mathrm{KL}(\rho_t|\mu_t)$:

$$\frac{d}{dt} \mathrm{KL}(\rho_t|\mu_t)$$

$$= \frac{d}{dt} \int_{\mathbb{R}^d} \log \frac{\rho_t(x)}{\mu_t(x)} \rho_t(x) dx$$

$$= \int_{\mathbb{R}^d} \partial_t \rho_t(x) \log \frac{\rho_t(x)}{\mu_t(x)} dx + \int_{\mathbb{R}^d} \left(\frac{\partial_t \rho_t(x)}{\mu_t(x)} + \rho_t(x) \partial_t \left(\frac{1}{\mu_t(x)} \right) \right) \frac{\mu_t(x)}{\rho_t(x)} \rho_t(x) dx$$

$$= \int_{\mathbb{R}^d} \partial_t \rho_t(x) \log \frac{\rho_t(x)}{\mu_t(x)} dx + \int_{\mathbb{R}^d} \partial_t \rho_t(x) dx - \int_{\mathbb{R}^d} \partial_t \mu_t(x) \frac{\rho_t(x)}{\mu_t(x)} dx$$

$$= -\int_{\mathbb{R}^d} \left\langle \iota_{k,\rho_t} \left((1 - \nu) \iota_{k,\rho_t}^* \iota_{k,\rho_t} + \nu I_d \right)^{-1} \iota_{k,\rho_t}^* \nabla \log \frac{\rho_t(x)}{\pi(x)}, \nabla \log \frac{\rho_t(x)}{\mu_t(x)} \right\rangle \rho_t(x) dx$$

$$\quad + 0 + \int_{\mathbb{R}^d} \left\langle \mu_t(x) \nabla \log \frac{\mu_t(x)}{\pi(x)}, \nabla \left(\frac{\rho_t(x)}{\mu_t(x)} \right) \right\rangle dx$$

$$= -\int_{\mathbb{R}^d} \left\langle \iota_{k,\rho_t} \left((1 - \nu) \iota_{k,\rho_t}^* \iota_{k,\rho_t} + \nu I_d \right)^{-1} \iota_{k,\rho_t}^* \nabla \log \frac{\rho_t(x)}{\pi(x)}, \nabla \log \frac{\rho_t(x)}{\mu_t(x)} \right\rangle \rho_t(x) dx$$

$$\quad + \int_{\mathbb{R}^d} \left\langle \nabla \log \frac{\rho_t(x)}{\mu_t(x)}, \nabla \log \frac{\mu_t(x)}{\pi(x)} \right\rangle \rho_t(x) dx$$

$$
\begin{aligned}
&= -\int_{\mathbb{R}^d} \left\langle \nabla \log \frac{\rho_t(x)}{\mu_t(x)}, \nabla \log \frac{\rho_t(x)}{\pi(x)} - \nabla \log \frac{\mu_t(x)}{\pi(x)} \right\rangle \rho_t(x)dx \\
&\quad - \int_{\mathbb{R}^d} \left\langle \left(\iota_{k,\rho_t} \left((1-\nu)\iota_{k,\rho_t}^* \iota_{k,\rho_t} + \nu I_d \right)^{-1} \iota_{k,\rho_t}^* - I \right) \nabla \log \frac{\rho_t(x)}{\pi(x)}, \nabla \log \frac{\rho_t(x)}{\mu_t(x)} \right\rangle \rho_t(x)dx \\
&\leq -\int_{\mathbb{R}^d} \left| \nabla \log \frac{\rho_t(x)}{\mu_t(x)} \right|^2 \rho_t(x)dx \\
&\quad + \frac{1}{4}\int_{\mathbb{R}^d} \left| \nabla \log \frac{\rho_t(x)}{\mu_t(x)} \right|^2 \rho_t(x)dx + \left\| \left(\iota_{k,\rho_t} \left((1-\nu)\iota_{k,\rho_t}^* \iota_{k,\rho_t} + \nu I_d \right)^{-1} \iota_{k,\rho_t}^* - I \right) \nabla \log \frac{\rho_t}{\pi} \right\|_{L_2^d(\rho_t)}^2 \\
&= -\frac{3}{4}I(\rho_t|\mu_t) + \sum_{i=1}^{\infty} \frac{(1-\lambda_{i,t})^2 \nu^2}{((1-\nu)\lambda_{i,t}+\nu)^2} \left| \left\langle \nabla \log \frac{\rho_t}{\pi}, e_{i,t} \right\rangle_{L_2(\rho_t)} \right|^2.
\end{aligned}
$$

In the above calculation, the fourth equality follows by integration-by-parts. The inequality follows by Young's inequality for the inner product (i.e., $\langle p, q \rangle \leq \frac{1}{2}c|p|^2 + \frac{1}{2c}|q|^2$ for any $p, q \in \mathbb{R}^d$) and the last equality follows from the proof of Proposition 3. Since $\nabla \log \frac{\rho_t}{\pi} = (\iota_{k,\rho_t}\iota_{k,\rho_t}^*)^{\gamma_t} h_t$ for some $\gamma_t \in (0, 1/2]$ with $h_t := \Im(\rho_t, \gamma_t) \in L_2^d(\rho_t)$, we obtain

$$
\begin{aligned}
\frac{d}{dt}\mathrm{KL}(\rho_t|\mu_t) &\leq -\frac{3}{4}I(\rho_t|\mu_t) + \left(\max_i (1-\lambda_{i,t})^2 \right) \left(\max_i \frac{\lambda_{i,t}^{\gamma_t}\nu}{(1-\nu)\lambda_{i,t}+\nu} \right)^2 \|h_t\|_{L_2^d(\rho_t)}^2 \\
&\leq -\frac{3}{4}I(\rho_t|\mu_t) + (\lambda_{1,t} \vee 1)^2 \nu^{2\gamma_t}(1-\nu)^{-2\gamma_t} \|\Im(\rho_t, \gamma_t)\|_{L_2^d(\rho_t)}^2,
\end{aligned}
$$

where the last inequality follows from the facts that

$$
\max_i (1-\lambda_{i,t})^2 \leq (\max_i \lambda_{i,t} \vee 1)^2 \quad \text{and} \quad \frac{\lambda_{i,t}^{\gamma_t}\nu}{(1-\nu)\lambda_{i,t}+\nu} \leq \nu^{\gamma_t}(1-\nu)^{-\gamma_t}.
$$

Integrating from $t = 0$ to $t = T$, we get

$$
\mathrm{KL}(\rho_T|\mu_T) - \mathrm{KL}(\rho_0|\mu_0) \leq -\frac{3}{4}\int_0^T I(\rho_t|\mu_t)dt + \int_0^T (\lambda_{1,t} \vee 1)^2 \nu^{2\gamma_t}(1-\nu)^{-2\gamma_t} \|\Im(\rho_t, \gamma_t)\|_{L_2^d(\rho_t)}^2 dt.
$$

Since KL-divergence is non-negative, (14) is proved. $\qquad\square$

Remark 4. The sequence $\{\lambda_{1,t}\}_{t\geq 0}$ in Theorem 1 is the largest eigenvalue of $\iota_{k,\rho_t}\iota_{k,\rho_t}^*$ for all $t \geq 0$. Note that it depends on both the kernel k and the solution (ρ_t) to (7). If the kernel function k is assumed to be uniformly bounded, according to Proposition 1, $\lambda_{1,t}^2$ is uniformly upper bounded by $\sup_{x\in\mathbb{R}^d} k(x, x)$ for all $t \geq 0$. For specific choices of kernel function, initial and target distributions, it is required to track $\lambda_{1,t}$ for all $t \geq 0$. We will illustrate this further with an example in Remark 10.

Remark 5. The above result shows that as long as $\rho_0 = \mu_0$, i.e., both the WGF and the R-SVGF are initialized with the same density, and ν is chosen such that

$$
T^{-1}\int_0^T (\lambda_{1,t} \vee 1)^2 \nu^{2\gamma_t}(1-\nu)^{-2\gamma_t} \|\Im(\rho_t, \gamma_t)\|_{L_2^d(\rho_t)}^2 dt \to 0,
$$

the *averaged* Fisher information along the path tends to zero. This shows the benefit of regularizing the SVGF – it enables one to closely approximate the WGF with appropriate choice of the regularization parameters.

4.2.2. *Convergence to Equilibrium along the Fisher Information.* We now provide results on the convergence to equilibrium along the Fisher information for the R-SVGF. We re-emphasize here that our result provided below holds as long as the target $\pi \in \mathcal{P}(\mathbb{R}^d)$, without additional structural assumptions (via, say, functional inequalities).

Theorem 2 (**Convergence of Fisher information**). *Let (ρ_t) be the solution to* (7). *For any $t > 0$, suppose there exists $\gamma_t \in (0, \frac{1}{2}]$ such that $\|\Im(\rho_t, \gamma_t)\|_{L_2^d(\rho_t)} < \infty$. Then*

$$\int_0^\infty I(\rho_t|\pi)dt \leq (1-\nu)\mathrm{KL}(\rho_0|\pi) + \int_0^\infty \nu^{2\gamma_t}(1-\nu)^{-2\gamma_t} \|\Im(\rho_t, \gamma_t)\|_{L_2^d(\rho_t)}^2 dt,$$

Furthermore, if $\int_0^\infty \nu^{2\gamma_t}(1-\nu)^{-2\gamma_t} \|\Im(\rho_t, \gamma_t)\|_{L_2^d(\rho_t)}^2 dt < \infty$, then we get $I(\bar{\rho}_t|\pi) \to 0$ as $t \to \infty$, where $\bar{\rho}_t := \frac{1}{t}\int_0^t \rho_s ds$ is the averaged density of $(\rho_s)_{0 \leq s \leq t}$.

Before proving the above theorem, we introduce a few intermediate results.

Proposition 4 (Decay of the KL-divergence). *For the solution $(\rho_t)_{t \geq 0}$ to the PDE* (7), *it holds that*

$$\frac{d}{dt}\mathrm{KL}(\rho_t|\pi) = -I_{\nu,Stein}(\rho_t|\pi), \tag{15}$$

and consequently

$$\frac{d}{dt}\mathrm{KL}(\rho_t|\pi) \leq 0. \tag{16}$$

Proof of Proposition 4. Note that

$$\frac{d}{dt}\mathrm{KL}(\rho_t|\pi) = \frac{d}{dt}\int_{\mathbb{R}^d} \rho_t \log\frac{\rho_t}{\pi}dx$$
$$= \int_{\mathbb{R}^d} \partial_t\rho_t \log\frac{\rho_t}{\pi}dx + \int_{\mathbb{R}^d} \partial_t\rho_t dx$$
$$= -\int_{\mathbb{R}^d} \left\langle \nabla\log\frac{\rho_t}{\pi}(x), \iota_{k,\rho_t}\left((1-\nu)\iota_{k,\rho_t}^*\iota_{k,\rho_t} + \nu I_d\right)^{-1} \iota_{k,\rho_t}^* \left(\nabla\log\frac{\rho_t}{\pi}\right)(x) \right\rangle \rho_t(x)dx + 0$$
$$= -\left\langle \nabla\log\frac{\rho_t}{\pi}, \iota_{k,\rho_t}\left((1-\nu)\iota_{k,\rho_t}^*\iota_{k,\rho_t} + \nu I_d\right)^{-1} \iota_{k,\rho_t}^* \left(\nabla\log\frac{\rho_t}{\pi}\right) \right\rangle_{L_2^d(\rho_t)}$$
$$= -\left\langle \iota_{k,\rho_t}^*\nabla\log\frac{\rho_t}{\pi}, \left((1-\nu)\iota_{k,\rho_t}^*\iota_{k,\rho_t} + \nu I_d\right)^{-1} \iota_{k,\rho_t}^* \left(\nabla\log\frac{\rho_t}{\pi}\right) \right\rangle_{\mathcal{H}_k^d}.$$

It suffices to show that for all $\nu > 0$, $\left((1-\nu)\iota_{k,\rho_t}^*\iota_{k,\rho_t} + \nu I_d\right)^{-1}$ is a positive operator from $\mathcal{H}_k^d$ to $\mathcal{H}_k^d$. By the definition of ι_{k,ρ_t}, for any $f \in \mathcal{H}_k^d$ with $\|f\|_{\mathcal{H}_k^d} = 1$,

$$\langle f, \left((1-\nu)\iota_{k,\rho_t}^*\iota_{k,\rho_t} + \nu I_d\right) f \rangle_{\mathcal{H}_k^d} = (1-\nu)\langle \iota_{k,\rho_t}f, \iota_{k,\rho_t}f \rangle_{L_2^d(\rho_t)} + \nu \|f\|_{\mathcal{H}_k^d}^2$$
$$= (1-\nu)\|\iota_{k,\rho_t}f\|_{L_2^d(\rho_t)}^2 + \nu > 0$$

for all $\nu > 0$. Therefore, $(1-\nu)\iota_{k,\rho_t}^*\iota_{k,\rho_t} + \nu I_d$ is a positive operator from $\mathcal{H}_k^d$ to $\mathcal{H}_k^d$. So is the operator $\left((1-\nu)\iota_{k,\rho_t}^*\iota_{k,\rho_t} + \nu I_d\right)^{-1}$. Hence, we have (16). The claim in (15) follows directly from (16), (5) and Definition 1. $\square$

We now provide the proof of Theorem 2. For the proof, we recall that we use $(\lambda_{i,t}, e_{i,t})_{i=1}^\infty$ to denote the set of eigenvalues and eigenvectors of the operator $\iota_{k,\rho_t}\iota_{k,\rho_t}^*$ for any $t \geq 0$, with $\lambda_{1,t} \geq \lambda_{2,t} \geq \cdots > 0$.

Proof of Theorem 2. From Proposition 4 and (12), we know that

$$\frac{d}{dt}\mathrm{KL}(\rho_t|\pi) = -(1-\nu)^{-1}I(\rho_t|\pi) + \sum_{i=1}^{\infty}\frac{(1-\nu)^{-1}\nu}{(1-\nu)\lambda_{i,t}+\nu}\left|\left\langle\nabla\log\frac{\rho_t}{\pi}, e_{i,t}\right\rangle_{L_2(\rho_t)}\right|^2,$$

where $\nabla\log\frac{\rho_t}{\pi} = (\iota_{k,\rho_t}\iota_{k,\rho_t}^*)^{\gamma_t}h_t$ for some $\gamma_t \in (0, \frac{1}{2}]$ with $h_t := \mathfrak{I}(\rho_t, \gamma_t) \in L_2^d(\rho_t)$. Therefore, we have

$$\frac{d}{dt}\mathrm{KL}(\rho_t|\pi)$$

$$= -(1-\nu)^{-1}I(\rho_t|\pi) + \sum_{i=1}^{\infty}\frac{(1-\nu)^{-1}\nu}{(1-\nu)\lambda_{i,t}+\nu}\left|\left\langle(\iota_{k,\rho_t}\iota_{k,\rho_t}^*)^{\gamma_t}h_t, e_{i,t}\right\rangle_{L_2(\rho_t)}\right|^2$$

$$= -(1-\nu)^{-1}I(\rho_t|\pi) + \sum_{i=1}^{\infty}\frac{(1-\nu)^{-1}\nu\lambda_{i,t}^{2\gamma_t}}{(1-\nu)\lambda_{i,t}+\nu}\left|\langle h_t, e_{i,t}\rangle_{L_2(\rho_t)}\right|^2$$

$$= \sum_{i=1}^{\infty}(1-\nu)^{-1-2\gamma_t}\nu^{2\gamma_t}\left(\frac{(1-\nu)\lambda_{i,t}}{(1-\nu)\lambda_{i,t}+\nu}\right)^{2\gamma_t}\left(\frac{\nu}{(1-\nu)\lambda_{i,t}+\nu}\right)^{1-2\gamma_t}\left|\langle h_t, e_{i,t}\rangle_{L_2(\rho_t)}\right|^2$$

$$\quad - (1-\nu)^{-1}I(\rho_t|\pi)$$

$$\leq -(1-\nu)^{-1}I(\rho_t|\pi) + (1-\nu)^{-1-2\gamma_t}\nu^{2\gamma_t}\|\mathfrak{I}(\rho_t, \gamma_t)\|^2_{L_2^d(\rho_t)}.$$

The result follows by integrating over t and noting that the KL-divergence is non-negative. Now, with ρ_t denoting the solution to (9), we have that $I(\rho_t|\pi)$ is non-negative and continuous in t. The claim of convergence follows from the convexity of $\rho \mapsto I(\rho|\mu)$. $\qquad\square$

4.2.3. *Convergence in KL-divergence under LSI.* While the previous result was provided for any the target density $\pi \in \mathcal{P}(\mathbb{R}^d)$, in this section, we provide improved convergence results of the R-SVGF under the assumption that the π further satisfies the Log-Sobolev Inequality. Recall that we say that π satisfies the Log-Sobolev inequality with constant $\lambda > 0$ if for all $\mu \in \mathcal{P}(\mathbb{R}^d)$:

$$\mathrm{KL}(\mu|\pi) \leq \frac{1}{2\lambda}I(\mu|\pi).$$

Our first result below is a stronger version of the result in Theorem 1, under the assumption that the target π satisfies LSI and Assumption 1 on the initialization of the WGF.

Assumption 1. *The initial density μ_0 is chosen so that the solution (μ_t) to (13) also satisfies LSI with parameter λ, for all $t > 0$.*

Under the stronger assumption that the target density π is strongly log-concave, following the arguments in [VW19, Theorem 8], it is easy to show that Assumption 1 is satisfied as long as μ_0 is chosen such that it satisfies LSI. We conjecture that the same holds true even when the target density satisfies LSI and additional mild smoothness assumptions (i.e., LSI is preserved along the trajectory as long as the initial density μ_0 satisfies LSI, presumably with additional milder assumptions). However, a proof of this conjecture has eluded us thus far.

Theorem 3 (Relation to the WGF under LSI)**.** *Assume π satisfies the log-Sobolev inequality with parameter λ. Let (ρ_t) be the solution to (7). Let (μ_t) be the solution to the WGF, defined in (13), with μ_0 satisfying Assumption 1. For any $t > 0$, suppose there exists $\gamma_t \in (0, \frac{1}{2}]$ such that $\|\mathfrak{I}(\rho_t, \gamma_t)\|_{L_2^d(\rho_t)} < \infty$. Then, for any $T \in (0, \infty)$, we have*

$$\mathrm{KL}(\rho_T|\mu_T) \leq e^{-3\lambda T/2}\mathrm{KL}(\rho_0|\mu_0) + \int_0^T (\lambda_{1,t} \vee 1)^2\nu^{2\gamma_t}(1-\nu)^{-2\gamma_t}e^{-3\lambda(T-t)/2}\|\mathfrak{I}(\rho_t, \gamma_t)\|^2_{L_2^d(\rho_t)}\,dt,$$

(17)

where $\lambda_{1,t}$ is the largest eigenvalue of $\iota_{k,\rho_t}\iota_{k,\rho_t}^*$ for all $t \geq 0$.

Proof of Theorem 3. Following the same arguments as in the proof of Theorem 1, we obtain that for any $t > 0$,

$$\frac{d}{dt}\mathrm{KL}(\rho_t|\mu_t) \leq -\frac{3}{4}I(\rho_t|\mu_t) + \sum_{i=1}^{\infty}\frac{(1-\lambda_i)^2\nu^2}{((1-\nu)\lambda_i+\nu)^2}\left|\left\langle\nabla\log\frac{\rho_t}{\pi}, e_i\right\rangle_{L_2(\rho_t)}\right|^2$$

$$\leq -\frac{3}{4}I(\rho_t|\mu_t) + (\lambda_{1,t}\vee 1)^2\nu^{2\gamma_t}(1-\nu)^{-2\gamma_t}\nu^{2\gamma_t}\|\mathfrak{I}(\rho_t,\gamma_t)\|_{L_2^d(\rho_t)}^2.$$

Hence, under Assumption 1 we obtain

$$\frac{d}{dt}\mathrm{KL}(\rho_t|\mu_t) \leq -\frac{3\lambda}{2}\mathrm{KL}(\rho_t|\mu_t) + (\lambda_{1,t}\vee 1)^2\nu^{2\gamma_t}(1-\nu)^{-2\gamma_t}\|\mathfrak{I}(\rho_t,\gamma_t)\|_{L_2^d(\rho_t)}^2.$$

Finally, (17) follows from the Gronwall's inequality. □

Our second result is a stronger version of the result in Theorem 2, under the assumption that the target distribution π satisfies LSI. We remark that convergence to equilibrium of the related WGF under various functional inequalities is a well-studied topic. We refer the interested reader to [BGL14] for a detailed overview.

Theorem 4 (Decay of KL-divergence under LSI). *Assume that π satisfies the log-Sobolev inequality with $\lambda > 0$. Let (ρ_t) be the solution to (7). For any $t > 0$, suppose there exists $\gamma_t \in (0, \frac{1}{2}]$ such that $\|\mathfrak{I}(\rho_t,\gamma_t)\|_{L_2^d(\rho_t)} < \infty$. Then, for any $T \in (0, \infty)$, we have*

$$\mathrm{KL}(\rho_T|\pi) \leq e^{-2(1-\nu)^{-1}\lambda T}\mathrm{KL}(\rho_0|\pi) + \int_0^T \nu^{2\gamma_t}(1-\nu)^{-2\gamma_t-1}\|\mathfrak{I}(\rho_t,\gamma_t)\|_{L_2^d(\rho_t)}^2 e^{2(1-\nu)^{-1}\lambda(t-T)}dt.$$

Proof of Theorem 4. From the proof of Theorem 2, we have

$$\frac{d}{dt}\mathrm{KL}(\rho_t|\pi) \leq -(1-\nu)^{-1}I(\rho_t|\pi) + (1-\nu)^{-1-2\gamma_t}\nu^{2\gamma_t}\|\mathfrak{I}(\rho_t,\gamma_t)\|_{L_2^d(\rho_t)}^2$$

$$\leq -2(1-\nu)^{-1}\lambda\mathrm{KL}(\rho_t|\pi) + (1-\nu)^{-1-2\gamma_t}\nu^{2\gamma_t}\|\mathfrak{I}(\rho_t,\gamma_t)\|_{L_2^d(\rho_t)}^2,$$

where the last inequality follows the log-Sobolev inequality. The final statement follows from Gronwall's inequality. □

Remark 6 (Exponential Decay of KL-divergence). Yet another way to state the above result is via the introducing the following regularized Stein-LSI, similar to the introduction of Stein-LSI in [DNS23]. However, the introduction of Stein-LSI is quite restrictive in the sense that it couples assumptions on the target and the chosen RKHS. This makes verifying the conditions more delicate. To counter this effect, we now introduce the notion of Regularized Stein-LSI. We say that $\pi \in \mathcal{P}(\mathbb{R}^d)$ satisfies the regularized Stein log-Sobolev inequality with constant $\lambda > 0$ if for all $\mu \in \mathcal{P}(\mathbb{R}^d)$:

$$\mathrm{KL}(\mu|\pi) \leq \frac{1}{2\lambda}I_{\nu,Stein}(\mu|\pi). \tag{18}$$

An advantage of the above condition is that, as $\nu \to 0$ the regularized Stein-LSI inequality becomes equivalent to the standard LSI inequality. Under the condition that the target density π satisfies (18), and letting (ρ_t) be the solution to (7), it holds that

$$\mathrm{KL}(\rho_t|\pi) \leq e^{-2\lambda t}\mathrm{KL}(\rho_0|\pi). \tag{19}$$

The proof of (19) follows immediately from Proposition 4 and (18).

4.3. **Convergence results for Time-discretized R-SVGF.** In this section, we analyze the convergence properties of the time-discretized R-SVGF in (8). To do so, we require the following additional assumptions.

Assumption A2. The following conditions hold:

(1) There exists a constant $B > 0$ such that $\|\nabla_1 k(x, \cdot)\|_{\mathcal{H}_k^d} \leq B$ for all $x \in \mathbb{R}^d$.

(2) The potential function $V : \mathbb{R}^d \to \mathbb{R}$ is twice continuously differentiable and gradient Lipschitz with parameter L.

(3) Along the time discretization (8), $I(\rho^n | \pi) < \infty$ for all fixed $n \geq 0$.

The smoothness assumptions in points (1) and (2) of Assumption A2 are commonly required in analyzing any discrete-time algorithms, albeit deterministic [KSA$^+$20, SSR22] or randomized [VW19, CEL$^+$22, BCE$^+$22]. While it could be relaxed (see, for example, [SR22]), in general it is impossible to completely avoid them as in the case of analyzing the corresponding flows. Before stating our results, we also introduce some convenient notations. We let

$$\mathfrak{S}_n := \left(\sup_i \frac{\lambda_i^{(n)^{1+2\gamma_n}}}{\left((1 - \nu_{n+1}) \lambda_i^{(n)} + \nu_{n+1} \right)^2} \right) \quad \text{and} \quad R_n := \|\mathfrak{I}(\rho^n, \gamma_n)\|_{L_2^d(\rho^n)}, \tag{20}$$

where the sequence $\{\lambda_i^{(n)}\}_{i \geq 1}$ corresponds to the positive eigenvalues of the operator $\iota_{k,\rho^n} \iota_{k,\rho^n}^*$ in the order of decreasing values for all $n \geq 0$.

Theorem 5 (Convergence in Fisher Divergence). *Suppose Assumption A2 holds. Let (ρ^n) be the time discretization of the R-SVGF described in (8) with initial condition $\rho^0 = \rho_0$ such that $\mathrm{KL}(\rho_0 | \pi) \leq R$. For each n, suppose that ν_{n+1} and the step-size h_{n+1} are chosen such that,*

$$h_{n+1} < \min \left\{ \frac{1 - \nu_{n+1}}{L}, \frac{\alpha - 1}{\alpha B R_n \sqrt{\mathfrak{S}_n}} \right\}, \tag{21}$$

where $\alpha \in (1, 2]$ is some constant, and suppose that there exists $\gamma_n \in (0, \frac{1}{2}]$, such that $\mathfrak{I}(\rho^n, \gamma_n) \in L_2^d(\rho^n)$. Then,

$$\sum_{n=0}^{\infty} \frac{h_{n+1}}{2(1 - \nu_{n+1})} I(\rho^n | \pi) \leq \sum_{n=0}^{\infty} \nu_{n+1}^{2\gamma_n} (1 - \nu_{n+1})^{-2\gamma_n - 1} h_{n+1} \left(1 + \frac{1}{2} \nu_{n+1}^{-1} \alpha^2 B^2 h_{n+1} \right) R_n^2 + R. \tag{22}$$

Before proving Theorem 5, we first prove the following intermediate result. For the proofs, we let $(\lambda_i^{(n)}, e_i^{(n)})_{i=1}^{\infty}$ to denote the set of eigenvalues and eigenvectors of the operator $\iota_{k,\rho^n} \iota_{k,\rho^n}^*$, with $\lambda_1^{(n)} \geq \lambda_2^{(n)} \geq \cdots > 0$.

Lemma 1. *For each $n \geq 1$, define $g = \mathcal{D}_{\nu_{n+1}, \rho^n} \nabla \log \frac{\rho^n}{\pi}$. Under the conditions in Theorem 5, we have that, for any $x \in \mathbb{R}^d$ and $t \in [0, h_{n+1}]$,*

$$\|\nabla g(x)\|_{HS}^2 \leq B^2 R_n^2 \mathfrak{S}_n \quad and \quad \left\| (id - t\nabla g(x))^{-1} \right\|_2 \leq \alpha.$$

Proof of Lemma 1. Since for each n, there exists $\gamma_n \in (0, 1/2)$ and a function $h = \mathfrak{I}(\rho^n, \gamma_n) \in L_2^d(\rho^n)$ such that $(\iota_{k,\rho^n} \iota_{k,\rho^n}^*)^{2\gamma_n} h_j = \partial_j \log \frac{\rho^n}{\pi}$, where h_j is the j-th component of the function value of h, we have

$$\|\nabla g(x)\|_{HS}^2 = \sum_{j,l=1}^{d} \left| \frac{\partial g_j(x)}{\partial x_l} \right|^2$$

$$= \sum_{j,l=1}^{d} \left(\sum_{i=1}^{\infty} \frac{\lambda_i^{(n)}}{(1 - \nu_{n+1}) \lambda_i^{(n)} + \nu_{n+1}} \left\langle \partial_j \log \frac{\rho^n}{\pi}, e_i^{(n)} \right\rangle_{L_2(\rho^n)} \partial_l e_i^{(n)}(x) \right)^2$$

$$= \sum_{j,l=1}^{d} \left(\sum_{i=1}^{\infty} \frac{\lambda_i^{(n)1+\gamma_n}}{(1-\nu_{n+1})\lambda_i^{(n)}+\nu_{n+1}} \left\langle h_j, e_i^{(n)} \right\rangle_{L_2(\rho^n)} \partial_l e_i^{(n)}(x) \right)^2$$

$$\leq \sum_{j,l=1}^{d} \left(\sum_{i=1}^{\infty} \left\langle h_j, e_i^{(n)} \right\rangle_{L_2(\rho^n)}^2 \right) \left(\sum_{i=1}^{\infty} \frac{\lambda_i^{(n)2+2\gamma_n}}{\left((1-\nu_{n+1})\lambda_i^{(n)}+\nu_{n+1}\right)^2} \left| \partial_l e_i^{(n)}(x) \right|^2 \right)$$

$$= \left(\sum_{i=1}^{\infty} \left| \left\langle h, e_i^{(n)} \right\rangle_{L_2(\rho^n)} \right|^2 \right) \left(\sum_{i=1}^{\infty} \frac{\lambda_i^{(n)2+2\gamma_n}}{\left((1-\nu_{n+1})\lambda_i^{(n)}+\nu_{n+1}\right)^2} \left| \nabla e_i^{(n)}(x) \right|^2 \right)$$

$$\leq \sup_i \left(\frac{\lambda_i^{(n)1+2\gamma_n}}{\left((1-\nu_{n+1})\lambda_i^{(n)}+\nu_{n+1}\right)^2} \right) \|\nabla_1 k(x,\cdot)\|_{\mathcal{H}_k^d}^2 R_n^2$$

$$\leq B^2 R_n^2 \sup_i \left(\frac{\lambda_i^{(n)1+2\gamma_n}}{\left((1-\nu_{n+1})\lambda_i^{(n)}+\nu_{n+1}\right)^2} \right).$$

In the above, the first inequality follows from Cauchy-Schwartz inequality, the second inequality follows from the fact that

$$\sum_{i=1}^{\infty} \lambda_i^{(n)} \left| \nabla e_i^{(n)}(x) \right|^2 = \sum_{i=1}^{\infty} \langle \nabla_1 k(x,\cdot), \sqrt{\lambda_i^{(n)}} e_i^{(n)} \rangle_{\mathcal{H}_k^d}^2 = \|\nabla_1 k(x,\cdot)\|_{\mathcal{H}_k^d}^2,$$

and the last inequality follows from Assumption A2. Meanwhile, since $\|\nabla g(x)\|_2 \leq \|\nabla g(x)\|_{HS}$ for all $x \in \mathbb{R}^d$, for every $t \in [0, h_{n+1}]$, we have

$$\left\|(id - t\nabla g(x))^{-1}\right\|_2 \leq \sum_{m=0}^{\infty} \|t\nabla g(x)\|_2^m \leq \sum_{m=0}^{\infty} \|t\nabla g(x)\|_{HS}^m$$

$$\leq \sum_{m=0}^{\infty} \left(h_{n+1} B R_n \sup_i \left(\frac{\lambda_i^{(n)1+2\gamma_n}}{\left((1-\nu_{n+1})\lambda_i^{(n)}+\nu_{n+1}\right)^2} \right)^{\frac{1}{2}} \right)^m$$

$$\leq \sum_{m=0}^{\infty} \left(\frac{\alpha-1}{\alpha} \right)^m = \alpha.$$

where the last inequality follows from (21). □

Proof of Theorem 5. We start from studying the single step along (8). In the following analysis, for each $n \geq 1$, we denote $g = \mathcal{D}_{\nu_{n+1},\rho^n} \nabla \log \frac{\rho^n}{\pi}$, $\phi_t(x) = x - tg(x)$ for all $x \in \mathbb{R}^d$, $t \in [0, h_{n+1}]$ and $\tilde{\rho}_t = (\phi_t)_{\#}\rho^n$. Therefore, we have

$$\rho^n = \tilde{\rho}_0 \quad \text{and} \quad \rho^{n+1} = (\phi_{h_{n+1}})_{\#}\rho^n = \tilde{\rho}_{h_{n+1}}.$$

The following analysis is motivated by [SSR22, Proposition 3.1]. According to [Vil21, Theorem 5.34], the velocity field ruling the evolution of $\tilde{\rho}_t$ is $\omega_t \in L_2^d(\tilde{\rho}_t)$ and $\omega_t(x) = -g(\phi_t^{-1}(x))$. Define $\psi(t) = \mathrm{KL}(\tilde{\rho}_t|\pi)$. According to the chain rule in [Vil21, Section 8.2],

$$\psi'(t) = \langle \nabla_{W_2} \mathrm{KL}(\tilde{\rho}_t|\pi), \omega_t \rangle_{L_2^d(\tilde{\rho}_t)},$$

$$\psi''(t) = \left\langle \omega_t, \mathrm{Hess}_{\mathrm{KL}(\cdot|\pi)}(\tilde{\rho}_t)\omega_t \right\rangle_{L_2^d(\tilde{\rho}_t)}.$$

where $\mathrm{Hess}_{\mathrm{KL}(\cdot|\pi)}(\tilde\rho_t)$ is the Wasserstein Hessian of $\mathrm{KL}(\cdot|\pi)$ at $\tilde\rho_t$. For any $\mu \in \mathcal{P}(\mathbb{R}^d)$ and any v in the Wasserstein tangent space at μ, the Wasserstein Hessian is given by [KSA+20],

$$\langle v, \mathrm{Hess}_{\mathrm{KL}(\cdot|\pi)}(\mu)v \rangle_{L_2^d(\mu)} = \langle v, \nabla^2 V v \rangle_{L_2^d(\mu)} + \mathbb{E}_\mu[\|\nabla v(X)\|_{HS}^2].$$

Therefore we can expand the difference in KL-divergence between the two consecutive iterations as

$$\psi(h_{n+1}) - \psi(0)$$
$$= \psi'(0)h_{n+1} + \int_0^{h_{n+1}} (h_{n+1} - t)\psi''(t)dt$$
$$= -h_{n+1} \langle \nabla_{W_2}\mathrm{KL}(\rho^n|\pi), g \rangle_{L_2^d(\rho^n)} + \int_0^{h_{n+1}} (h_{n+1} - t)\langle \omega_t, \mathrm{Hess}_{\mathrm{KL}(\cdot|\pi)}(\tilde\rho_t)\omega_t \rangle_{L_2^d(\tilde\rho_t)}dt. \qquad (23)$$

The first term on the right-hand side of (23) can be studied via the spectrum of the operator $\iota_{k,\rho^n}\iota_{k,\rho^n}^*$.

$$-h_{n+1}\langle \nabla_{W_2}\mathrm{KL}(\rho^n|\pi), g \rangle_{L_2^d(\rho^n)}$$
$$= -h_{n+1}\left\langle \nabla\log\frac{\rho^n}{\pi}, \left((1-\nu_{n+1})\iota_{k,\rho^n}^*\iota_{k,\rho^n} + \nu_{n+1}I_d\right)^{-1}\iota_{k,\rho^n}^*\nabla\log\frac{\rho^n}{\pi}\right\rangle_{L_2^d(\rho^n)}$$
$$= -h_{n+1}\sum_{i=1}^\infty \frac{\lambda_i^{(n)}}{(1-\nu_{n+1})\lambda_i^{(n)} + \nu_{n+1}}\left|\left\langle \nabla\log\frac{\rho^n}{\pi}, e_i^{(n)}\right\rangle_{L_2(\rho^n)}\right|^2$$
$$= -h_{n+1}I_{\nu_{n+1},Stein}(\rho^n|\pi).$$

Since $\tilde\rho_t = (\phi_t)_{\#}\rho^n$, for any function h we have $\mathbb{E}_{X\sim\tilde\rho_t}[h(X)] = \mathbb{E}_{Y\sim\rho^n}[h(\phi_t(Y))]$. Hence, for the second term on the right side of (23), we obtain

$$\langle \omega_t, \mathrm{Hess}_{\mathrm{KL}(\cdot|\pi)}(\tilde\rho_t)\omega_t \rangle_{L_2^d(\tilde\rho_t)} = \langle \omega_t, \nabla^2 V \omega_t \rangle_{L_2^d(\tilde\rho_t)} + \mathbb{E}_{\tilde\rho_t}[\|\nabla\omega_t(x)\|_{HS}^2]$$
$$= \langle g(\phi_t^{-1}), \nabla^2 V g(\phi_t^{-1}) \rangle_{L_2^d(\tilde\rho_t)} + \mathbb{E}_{\rho^n}[\|\nabla\omega_t\circ\phi_t(x)\|_{HS}^2]$$
$$= \mathbb{E}_{\rho^n}\left[g(x)^T\nabla V^2(\phi_t(x))g(x)\right] + \mathbb{E}_{\rho^n}\left[\|\nabla g(x)(\nabla\phi_t(x))^{-1}\|_{HS}^2\right]$$
$$\leq L\|g\|_{L_2^d(\rho^n)}^2 + \mathbb{E}_{\rho^n}\left[\|\nabla g(x)(\nabla\phi_t(x))^{-1}\|_{HS}^2\right],$$

where the last inequality follows from Assumption A2-(2). Therefore, we obtain

$$\mathrm{KL}(\rho^{n+1}|\pi) - \mathrm{KL}(\rho^n|\pi) \leq -h_{n+1}I_{\nu_{n+1},Stein}(\rho^n|\pi) + \frac{Lh_{n+1}^2}{2}\|g\|_{L_2^d(\rho^n)}^2$$
$$+ \frac{h_{n+1}^2}{2}\max_{t\in[0,h_{n+1}]}\mathbb{E}_{\rho^n}\left[\|\nabla g(x)(\nabla\phi_t(x))^{-1}\|_{HS}^2\right],$$

where

$$\|g\|_{L_2^d(\rho^n)}^2 = \left\|\mathcal{D}_{\nu_{n+1},\rho^n}\nabla\log\frac{\rho^n}{\pi}\right\|_{L_2^d(\rho^n)}^2$$
$$= \left\|\left((1-\nu_{n+1})\iota_{k,\rho^n}\iota_{k,\rho^n}^* + \nu_{n+1}I_d\right)^{-1}\iota_{k,\rho^n}\iota_{k,\rho^n}^*\nabla\log\frac{\rho^n}{\pi}\right\|_{L_2^d(\rho^n)}^2$$
$$= \sum_{i=1}^d \left(\frac{\lambda_i^{(n)}}{(1-\nu_{n+1})\lambda_i^{(n)} + \nu_{n+1}}\right)^2\left|\left\langle \nabla\log\frac{\rho^n}{\pi}, e_i^{(n)}\right\rangle_{L_2(\rho^n)}\right|^2$$
$$\leq (1-\nu_{n+1})^{-2}I(\rho_n|\pi),$$

with $(\lambda_i^{(n)}, e_i^{(n)})_{i=1}^\infty$ being the sequence of eigenvalues and eigenvectors to the operator $\iota_{k,\rho^n}\iota_{k,\rho^n}^*$ such that $\lambda_1^{(n)} \geq \cdots \geq \lambda_i^{(n)} \geq \cdots > 0$ and $(e_i^{(n)})_{i=1}^\infty$ is an orthonormal basis of $L_2(\rho^n)$. According to Lemma 1 and Assumption A2,

$$\|\nabla g(x)\|_{HS}^2$$

$$\leq \sup_i \left(\frac{\lambda_i^{(n)1+2\gamma_n}}{\left((1-\nu_{n+1})\lambda_i^{(n)} + \nu_{n+1} \right)^2} \right) B^2 R_n^2$$

$$\leq \sup_i \left(\frac{\nu_{n+1}^{2\gamma_n-1}}{(1-\nu_{n+1})^{2\gamma_n+1}} \left(\frac{(1-\nu_{n+1})\lambda_i^{(n)}}{(1-\nu_{n+1})\lambda_i^{(n)} + \nu_{n+1}} \right)^{1+2\gamma_n} \left(\frac{\nu_{n+1}}{(1-\nu_{n+1})\lambda_i^{(n)} + \nu_{n+1}} \right)^{1-2\gamma_n} \right) B^2 R_n^2$$

$$\leq \nu_{n+1}^{2\gamma_n-1}(1-\nu_{n+1})^{-2\gamma_n-1} B^2 R_n^2,$$

and furthermore according to Lemma 1, $\left\| (id - t\nabla g(x))^{-1} \right\|_2^2 \leq \alpha^2$. Therefore, we get

$$\mathrm{KL}(\rho^{n+1}|\pi) - \mathrm{KL}(\rho^n|\pi) \leq -h_{n+1}I_{\nu_{n+1},Stein}(\rho^n|\pi) + \frac{Lh_{n+1}^2(1-\nu_{n+1})^{-2}}{2}I(\rho^n|\pi)$$

$$+ \frac{1}{2}\alpha^2 B^2 \nu_{n+1}^{2\gamma_n-1}(1-\nu_{n+1})^{-2\gamma_n-1}R_n^2 h_{n+1}^2$$

$$\leq -h_{n+1}(1-\nu_{n+1})^{-1}\left(1 - \frac{Lh_{n+1}(1-\nu_{n+1})^{-1}}{2} \right)I(\rho^n|\pi)$$

$$+ h_{n+1}\nu_{n+1}^{2\gamma_n}(1-\nu_{n+1})^{-2\gamma_n-1}R_n^2\left(1 + \frac{1}{2}h_{n+1}\nu_{n+1}^{-1}\alpha^2 B^2 \right)$$

$$\leq -\frac{1}{2}h_{n+1}(1-\nu_{n+1})^{-1}I(\rho^n|\pi)$$

$$+ h_{n+1}\nu_{n+1}^{2\gamma_n}(1-\nu_{n+1})^{-2\gamma_n-1}R_n^2\left(1 + \frac{1}{2}h_{n+1}\nu_{n+1}^{-1}\alpha^2 B^2 \right),$$

where the last inequality follows from (21) and the second inequality follows from the fact that

$$I(\rho^n|\pi) - (1-\nu_{n+1})I_{\nu_{n+1},Stein}(\rho^n|\pi) \leq \nu_{n+1}^{2\gamma_n}(1-\nu_{n+1})^{-2\gamma_n}R_n^2,$$

which is proved in Proposition 3. Lastly, summing over n and we obtain

$$\sum_{n=0}^\infty \frac{h_{n+1}}{2(1-\nu_{n+1})}I(\rho^n|\pi) \leq \sum_{n=0}^\infty \left(\mathrm{KL}(\rho^n|\pi) - \mathrm{KL}(\rho^{n+1}) \right)$$

$$+ \sum_{n=0}^\infty h_{n+1}\nu_{n+1}^{2\gamma_n}(1-\nu_{n+1})^{-2\gamma_n-1}R_n^2\left(1 + \frac{1}{2}h_{n+1}\nu_{n+1}^{-1}\alpha^2 B^2 \right)$$

$$\leq \mathrm{KL}(\rho^0|\pi) + \sum_{n=0}^\infty h_{n+1}\nu_{n+1}^{2\gamma_n}(1-\nu_{n+1})^{-2\gamma_n-1}R_n^2\left(1 + \frac{1}{2}h_{n+1}\nu_{n+1}^{-1}\alpha^2 B^2 \right),$$

where the last inequality follows from the fact that KL divergence is non-negative. Therefore, (22) is proved. □

Remark 7. We emphasize that the above result does not make any assumptions on the target density π, except for $\pi \in \mathcal{P}(\mathbb{R}^d)$ and the Lipschitz gradient assumption. In particular, it holds for multi-modal densities. However, the metric of convergence is the weaker Fisher information metric.

We now provide a stronger result under the LSI assumption.

Theorem 6. *Suppose Assumption A2 holds and π satisfies the log-Sobolev inequality with parameter λ. Let (ρ^n) be as described in (8) with initial condition $\rho^0 = \rho_0$ such that $\mathrm{KL}(\rho_0|\pi) \leq R$. Assume the regularization parameter and the step-size parameters are chosen such that for all $n \geq 0$, they satisfy*

$$h_{n+1} \leq \min\left\{\frac{1 - \nu_{n+1}}{L}, \frac{\alpha - 1}{\alpha B R_n \sqrt{\mathfrak{S}_n}}, \frac{2\nu_{n+1}}{\alpha^2 B^2}, \frac{2(1 - \nu_{n+1})}{\lambda}\right\}, \quad \frac{\nu_{n+1}}{1 - \nu_{n+1}} \leq \left(\frac{I(\rho^n|\pi)}{2R_n^2}\right)^{\frac{1}{2\gamma_n}}, \quad (24)$$

where $\alpha \in (1, 2]$ is a constant, $\gamma_n \in (0, \frac{1}{2}]$, and $\mathfrak{I}(\rho^n, \gamma_n) \in L_2^d(\rho^n)$. Then, for all $n \geq 1$,

$$\mathrm{KL}(\rho^n|\pi) \leq R \prod_{i=1}^{n}\left(1 - \frac{1}{2}\lambda(1 - \nu_i)^{-1}h_i\right). \quad (25)$$

Proof of Theorem 6. From the proof of Theorem 5, we can bound the difference in KL-divergence between two consecutive iterations by

$$\begin{aligned}
&\mathrm{KL}(\rho^{n+1}|\pi) - \mathrm{KL}(\rho^n|\pi) \\
&\leq -\frac{1}{2}h_{n+1}(1 - \nu_{n+1})^{-1}I(\rho^n|\pi) + h_{n+1}\nu_{n+1}^{2\gamma_n}(1 - \nu_{n+1})^{-2\gamma_n - 1}R_n^2\left(1 + \frac{1}{2}h_{n+1}\nu_{n+1}^{-1}\alpha^2 B^2\right) \\
&= -\frac{1}{4}h_{n+1}(1 - \nu_{n+1})^{-1}I(\rho^n|\pi)\left(2 - \frac{\nu_{n+1}^{2\gamma_n}}{(1 - \nu_{n+1})^{2\gamma_n}}\frac{R_n^2\left(1 + \frac{1}{2}h_{n+1}\nu_{n+1}^{-1}\alpha^2 B^2\right)}{I(\rho^n|\pi)}\right) \\
&\leq -\frac{1}{4}h_{n+1}(1 - \nu_{n+1})^{-1}I(\rho^n|\pi)\left(2 - \frac{\nu_{n+1}^{2\gamma_n}}{(1 - \nu_{n+1})^{2\gamma_n}}\frac{2R_n^2}{I(\rho^n|\pi)}\right) \\
&\leq -\frac{1}{4}h_{n+1}(1 - \nu_{n+1})^{-1}I(\rho^n|\pi),
\end{aligned}$$

where the second inequality follows from the fact that $\frac{1}{2}h_{n+1}\nu_{n+1}^{-1}\alpha^2 B^2 \leq 1$, and the last inequality follows from (24). Last, since π satisfies the log-Sobolev inequality with parameter λ, we get

$$\mathrm{KL}(\rho^{n+1}|\pi) \leq \left(1 - \frac{1}{2}\lambda(1 - \nu_{n+1})^{-1}h_{n+1}\right)\mathrm{KL}(\rho^n|\pi),$$

and (25) follows from the above recursive inequality. $\square$

Remark 8 (Choice of $\{\nu_n\}_{n\geq 1}$). From (24) and (25), we observe that there is a trade-off in terms of $\{\nu_n\}_{n\geq 1}$, as smaller $\{\nu_n\}_{n\geq 1}$ will result in slower convergence of the time-discretized R-SVGF in KL-divergence. Indeed, if $\{\nu_n\}_{n\geq 1}$ are chosen to be small, (24) requires the step-size $\{h_n\}_{n\geq 1}$ to be small as well. And, as shown in (25), $\mathrm{KL}(\rho_n|\pi)$ decays at a slower rate when $\{h_n\}_{n\geq 1}$ are smaller. We also refer to Remark 10 below and Remark 12 for further trade-offs with respect to the parameter $\{\nu_n\}_{n\geq 1}$.

Remark 9. According to (25), to reach an ϵ-accuracy in KL-divergence, we need the number of iterations to be at least n_ϵ such that $\prod_{i=1}^{n_\epsilon}\left(1 - \frac{1}{2}\lambda(1 - \nu_i)^{-1}h_i\right)R \leq \epsilon$. With the fact that $\log(1 - x) < -x$ for all $x \in (0, 1)$, we get n_ϵ satisfies

$$\sum_{i=1}^{n_\epsilon}(1 - \nu_i)^{-1}h_i \geq \frac{2}{\lambda}\log\left(\frac{R}{\epsilon}\right).$$

Under (24), if we can choose the time step sizes $(h_i)_{i=1}^{\infty}$ to be a constant $h > 0$, then we have $n_\epsilon = O(\log(R/\epsilon))$. For comparison, in Table 4.3, we provide the iteration complexity results for different methods, to obtain $\mathrm{KL}(\rho_n|\pi) \leq \epsilon$, under the assumption that the target π satisfies LSI.

Method	Source	Type	Iterations
SVGF	NA	Deterministic	unknown
LMC	[VW19, CEL$^+$22]	Randomized	$\mathcal{O}(\frac{1}{\epsilon})$
MALA	NA	Randomized	unknown
Proximal sampler	[CCSW22]	Randomized	$\mathcal{O}\left(\log^\lambda(\frac{1}{\epsilon})\right)$
Regularized SVGF	Theorem 6	Deterministic	$\mathcal{O}\left(\log\left(\frac{1}{\epsilon}\right)\right)$

TABLE 1. The results for SVGF and Regularized SVGF are strictly non-algorithmic, as the stated results require that the initial density supplied to the method must have finite KL divergence to π. The results from [VW19, CEL$^+$22, CCSW22] are for LMC, MALA and the proximal sampler are algorithmic, and are presented in a simplified manner to convey the dependency on the accuracy parameter ϵ. The result for the proximal sampler holds only in expectation. Currently, it is not clear how to obtain a high-probability result in KL-divergence; see [CCSW22] for details.

We also emphasize that prior results on the analysis of time-discretization of the SVGF under functional inequality assumptions are established only in the weaker Stein-Fisher information metric [KSA$^+$20, SSR22]. Our results above are established for the KL-divergence and is more in line with similar results established for other randomized Monte Carlo algorithms [VW19, CEL$^+$22, BCE$^+$22]. We end this section with the following remark on an illustrative example.

Remark 10 (An illustrative example). Consider sampling from a Gaussian target $\pi = \mathcal{N}(0, Q)$, where Q is strictly positive definite and $k(x, y) = \langle x, y \rangle + 1$, the linear kernel. This model has recently been studied in [LGBP24] motivated by connections to Gaussian variational inference. Note that the above target π satisfies LSI with λ being the minimal eigenvalue of Q. Based on the results established in [LGBP24], our results on the R-SVGF and the time-discretized R-SVGF can be interpreted as follows. Before we proceed, we point out a subtle fact. To establish existence and uniqueness later in Section 5 we assume that the kernel is bounded, which is not satisfied by the linear kernel. However, based on an explicit calculation, existence and uniqueness results were shown for the linear kernel in [LGBP24].

R-SVGF: If $\rho_0 = \mathcal{N}(0, \Sigma_0)$, then note that we have for all $t \geq 0$, $\rho_t = \mathcal{N}(0, \Sigma_t)$, $\gamma_t = 1/2$, $\lambda_{1,t} \leq 1 + \|\Sigma_t\|_F^2$ and $\|\mathcal{J}(\rho_t, \gamma_t)\|_{L_2(\rho_t)} = \left\|Q^{-1} - \Sigma_t^{-1}\right\|_F$. It follows from [LGBP24, Equation 9] that

$$\frac{\mathrm{d}}{\mathrm{d}t}\Sigma_t = 2\big((1-\nu)\Sigma_t + \nu I_d\big)^{-1}\Sigma_t - \big((1-\nu)\Sigma_t + \nu I_d\big)^{-1}\Sigma_t^2 Q^{-1} - Q^{-1}\big((1-\nu)\Sigma_t + \nu I_d\big)^{-1}\Sigma_t^2.$$

Further assuming that $\Sigma_0 Q = Q\Sigma_0$, there exists an orthonormal matrix P such that we have $Q = P^\mathsf{T}\mathrm{diag}\{q_1, \cdots, q_d\}P$ and $\Sigma_t = P^\mathsf{T}\mathrm{diag}\{\sigma_1(t), \cdots, \sigma_d(t)\}P$ with $q_1 \geq q_2 \geq \cdots \geq q_d$. According to [LGBP24, page 45], we also have that $\lambda = q_d$, $\|\Sigma_t - Q\| = O\big(\exp(-\frac{2t}{(1-\nu)q_1+\nu})\big)$ and

$$\lambda_{1,t} \leq 1 + O\bigg(\sum_{i=1}^d \big(q_i + \exp(-\frac{2t}{(1-\nu)q_i+\nu})\big)^2\bigg),$$

$$\|\mathcal{J}(\rho_t, \gamma_t)\|_{L_2(\rho_t)}^2 = O\left(\sum_{i=1}^d \sigma_i(0)^{-\frac{2\nu}{(1-\nu)q_i+\nu}} q_i^{-4+\frac{2\nu}{(1-\nu)q_i+\nu}}(\sigma_i(0) - q_i)^2 e^{-\frac{4t}{(1-\nu)q_i+\nu}}\right).$$

Our convergence result in Theorem 4, hence translates as

$$\mathrm{KL}(\rho_T|\pi) \le e^{-2(1-\nu)^{-1}\lambda T}\mathrm{KL}(\rho_0|\pi) + \int_0^T \nu(1-\nu)^{-2}\|\mathfrak{I}(\rho_t,\gamma_t)\|_{L_2^d(\rho_t)}^2 e^{2(1-\nu)^{-1}\lambda(t-T)}dt$$

$$= e^{-2(1-\nu)^{-1}q_d T}\mathrm{KL}(\rho_0|\pi) + O\left(\nu(1-\nu)^{-2}T\exp\left(-\min\left\{\frac{4}{(1-\nu)q_1+\nu}, \frac{2q_d}{1-\nu}\right\}T\right)\right),$$

for $T \in (0,\infty)$. The first term in the above bound indicates the exponential convergence of the R-SVGF and the convergence rate is proportional to $1/(1-\nu)$. The second term characterizes the bias between ρ_T and π. For any fixed values of T, the bias term vanishes as $\nu \to 0$. Therefore, in order to obtain an optimal upper bound on $\mathrm{KL}(\rho_T|\pi)$, there is a trade-off between choosing large ν (i.e., $\nu \to 1$) and small ν (i.e., $\nu \to 0$), which depends on T and eigenvalues of Σ_0 and Q.

Time-discretized R-SVGF: Note that if $\rho^0 = \mathcal{N}(0, S_0)$, then for all $n \ge 0$, $\rho^n = \mathcal{N}(0, S_n)$, $\gamma_n = 1/2$. $R_n = \|\mathcal{J}(\rho^n, \gamma_n)\|_{L_2(\rho^n)} = \|Q^{-1} - S_n^{-1}\|_F$ and $I(\rho^n|\pi) = \mathrm{trace}(S_n(Q^{-1} - S_n^{-1})^\mathsf{T}(Q^{-1} - S_n^{-1}))$, where $(S_n)_{n\ge 0}$ is updated as:

$$\begin{aligned}
S_{n+1} - S_n = {} & h_{n+1}\big((1-\nu_{n+1})S_n + \nu_{n+1}I_d\big)^{-1}(S_n^{-1} - Q^{-1})S_n^2 \\
& h_{n+1}S_n\big((1-\nu_{n+1})S_n + \nu_{n+1}I_d\big)^{-1}(S_n^{-1} - Q^{-1})S_n \\
& + h_{n+1}^2\big((1-\nu_{n+1})S_n + \nu_{n+1}I_d\big)^{-1}(S_n^{-1} - Q^{-1})S_n^3 \times \\
& \qquad\qquad \times (S_n^{-1} - Q^{-1})\big((1-\nu_{n+1})S_n + \nu_{n+1}I_d\big)^{-1}.
\end{aligned} \tag{26}$$

Since $\nabla_1 k(x,y) = y$, the RKHS norm of $\nabla_1 k(x,y)$ is obtained as follows

$$\|\nabla_1 k(x,y)\|_{\mathcal{H}_k^d}^2 = \sum_{i=1}^d \langle y_i, y_i \rangle_{\mathcal{H}_k} = \sum_{i=1}^d \partial_i \partial_{i+d} k(y,y) = d.$$

Therefore, we have $\gamma_n = 1/2$, $B = \sqrt{d}$ and $\mathfrak{S}_n \le (1-\nu_{n+1})^{-2}$ for all $n \ge 0$. Now, the convergence result in Theorem 6 translates as:

$$\mathrm{KL}(\rho^n|\pi) \le \mathrm{KL}(\rho^0|\pi)\Pi_{i=1}^n\left(1 - \frac{q_d}{2(1-\nu_i)}h_i\right),$$

where for all $i \ge 1$,

$$\frac{\nu_i}{1-\nu_i} \le \frac{\mathrm{trace}(S_{i-1}(Q^{-1} - S_{i-1}^{-1})^\mathsf{T}(Q^{-1} - S_{i-1}^{-1}))}{2\|Q^{-1} - S_{i-1}^{-1}\|_F^2},$$

$$h_i \le \min\left\{\frac{1-\nu_i}{q_1}, \frac{2(1-\nu_i)}{q_d}, \frac{2(1-\nu_i)}{\sqrt{d}\|Q^{-1} - S_{i-1}^{-1}\|_F}, \frac{\nu_i}{2d}\right\}.$$

We now show that such a choice of $\{\nu_i, h_i\}_{i\ge 1}$ exists. Assuming $QS_0 = S_0Q$, there exists an orthonormal matrix P such that $Q = P^\mathsf{T}\mathrm{diag}\{q_1, \cdots, q_d\}P$ and $S_i = P^\mathsf{T}\mathrm{diag}\{\sigma_{1,i}, \cdots, \sigma_{d,i}\}P$ with $q_1 \ge q_2 \ge \cdots \ge q_d$. Then, (26) implies that for any $k = 1, \cdots, d$,

$$q_k^{-1}\sigma_{k,i+1} = \big(1 + h_{i+1}((1-\nu_{i+1})\sigma_{k,i} + \nu_{i+1})^{-1}(1 - q_k^{-1}\sigma_{k,i})\big)^2 q_k^{-1}\sigma_{k,i}.$$

Now, we pick

$$h_{i+1} = \delta\min_k\big((1-\nu_{i+1})\sigma_{k,i} + \nu_{i+1}\big), \quad \frac{\nu_i}{1-\nu_i} = \frac{\mathrm{trace}(S_{i-1}(Q^{-1}-S_{i-1}^{-1})^\mathsf{T}(Q^{-1}-S_{i-1}^{-1}))}{2\|Q^{-1}-S_{i-1}^{-1}\|_F^2}, \tag{27}$$

with $\delta \in (0, 1/2)$. According to [LGBP24, Theorem 3.10], if $q_k^{-1}\sigma_{k,0} \in [u_\delta, 1/3 + 1/(3\delta)]$ for all $k = 1, \cdots, d$, we have $\|S_i - Q\|_2 \le e^{-i\delta}\|S_0 - Q\|$. Here u_δ is the smaller root of $f_\delta'(u) = 1 - \delta$ with

$f_\delta(x) = (1 + \delta(1-x))^2 x$. According to the convergence of S_i and the fact that

$$\|S_{i-1}\|_2 \left\|Q^{-1} - S_{i-1}^{-1}\right\|_F^2 \geq \text{trace}(S_{i-1}(Q^{-1} - S_{i-1}^{-1})^\intercal (Q^{-1} - S_{i-1}^{-1})) \geq \left\|S_{i-1}^{-1}\right\|_2^{-1} \left\|Q^{-1} - S_{i-1}^{-1}\right\|_F^2,$$

we have that $\{\nu_i\}_{i\geq 1}$ and $\{1 - \nu_i\}_{i\geq 1}$ have uniform positive lower bounds, i.e., $\inf_i \nu_i > 0$ and $\inf_i 1 - \nu_i > 0$. Therefore, we can further choose

$$\delta = \inf_i \left\{ \left((1-\nu_i)\|S_{i-1}^{-1}\|_2^{-1} + \nu_i\right)^{-1} \min\{\frac{1-\nu_i}{q_1}, \frac{2(1-\nu_i)}{q_d}, \frac{2(1-\nu_i)}{\sqrt{d} \left\|Q^{-1} - S_{i-1}^{-1}\right\|_F}, \frac{\nu_i}{2d}\} \right\} > 0,$$

where the positivity of the third term follows from the fact that

$$\left\|Q^{-1} - S_{i-1}^{-1}\right\|_F \leq \left\|Q^{-1}\right\|_2 \left\|S_{i-1}^{-1}\right\|_2 \|Q - S_{i-1}\|_F.$$

Therefore, we have shown that there exists $\delta \in (0, 1/2)$ such that $\{\nu_i, h_i\}_{i\geq 1}$ defined in (27) satisfies the assumptions in Theorem 6 and $\inf_i h_i > 0$.

Last, we discuss the iteration complexity under the choice of $\{\nu_i, h_i\}_{i\geq 1}$ in (27). According to Remark 9, $\text{KL}(\rho^n | \pi) \leq \epsilon$ if n satisfies

$$\sum_{i=1}^{n} \frac{h_i}{1 - \nu_i} \geq \frac{2}{q_d} \log \frac{\text{KL}(\rho^0 | \pi)}{\epsilon}.$$

Since $\inf_i h_i > 0$ and $\inf_i 1 - \nu_i > 0$, we obtain $n = O(\log(\text{KL}(\rho^0 | \pi)/\epsilon))$.

5. EXISTENCE AND UNIQUENESS

The existence and uniqueness of the SVGF was studied in [LLN19]. Motivated by their approach, in this section we study the existence and uniqueness of solutions to (7) under appropriate assumptions. Our main difficulty is in handling the non-linear operator $((1 - \nu)\mathcal{T}_{k,\mu} + \nu I)^{-1} \mathcal{T}_{k,\mu}$ in the R-SVGF.

We first introduce the definition of weak solutions to (7). We restrict the initial conditions in the probability measure space $\mathcal{P}_V$ which is defined as

$$\mathcal{P}_V := \left\{ \rho \in \mathcal{P} \ : \ \|\rho\|_{\mathcal{P}_V} := \int_{\mathbb{R}^d} (1 + V(x)) d\rho(x) < \infty \right\},$$

where, in this section, with a slight overload of notations, we use $\mathcal{P}$ to denote the set of all probability measures on $\mathbb{R}^d$. We emphasize here that that $\mathcal{P}_V$ is a space of probability *measures* because the weak solutions do not necessarily have densities even if the target measure and the initial measure has a density; see [LLN19] for additional details. We say that a measure-valued function $\rho \in \mathcal{C}([0, \infty), \mathcal{P}_V)$ is a weak solution to (7) with initial condition $\rho_0 \in \mathcal{P}_V$ if

$$\sup_{t \in [0,T]} \|\rho_t\|_{\mathcal{P}_V} < \infty, \ \forall \ T > 0,$$

and

$$\int_0^\infty \int_{\mathbb{R}^d} (\partial_t \phi(t, x) + \nabla\phi(t, x) \cdot U[\rho_t](x)) d\rho_t(x) dt + \int_{\mathbb{R}^d} \phi(0, x) d\rho_0(x) = 0,$$

for all $\phi \in \mathcal{C}_0^\infty([0, \infty) \times \mathbb{R}^d)$ and $U[\rho] := -\left((1 - \nu)\iota_{k,\rho}\iota_{k,\rho}^* + \nu I\right)^{-1} \iota_{k,\rho}\iota_{k,\rho}^* (\nabla \log \frac{\rho}{\pi})$.

In order to study the existence of weak solutions, we consider the characteristic flow (see, for example, [MRZ16] and [LLN19, Definition 3.1]) induced by (7), which is written as

$$\begin{cases} \dfrac{d}{dt}\Phi(t, x, \rho_0) = -\mathcal{D}_{\nu,\rho_t}\nabla\log\dfrac{\rho_t}{\pi}(\Phi(t, x, \rho_0)), \\ \rho_t = (\Phi(t, \cdot, \rho_0))_{\#}\rho_0, \\ \Phi(0, x, \rho_0) = x, \end{cases} \tag{28}$$

where $\mathcal{D}_{\nu,\rho_t} = \left((1-\nu)\iota_{k,\rho_t}\iota_{k,\rho_t}^* + \nu I\right)^{-1} \iota_{k,\rho_t}\iota_{k,\rho_t}^*$ for all $t > 0$. Here, the expression $\rho_t = \Phi(t,\cdot,\rho_0)_{\#}\rho_0$ means that the measure ρ_t is the push-forward measure of ρ_0 under the map $x \to \Phi(t,x,\rho_0)$. We think of $\{X(t,\cdot,\rho_0)\}_{t\geq 0,\rho_0}$ as a family of maps from $\mathbb{R}^d$ to $\mathbb{R}^d$ parameterized by t and ρ_0. The existence and uniqueness of the weak solutions of (7) is equivalent to the existence and uniqueness of solutions to (28). In Theorem 7, we first prove that the mean field characteristic flow in (28) is well-defined. To do so, we also require the following additional assumptions on the kernel and the potential functions.

Assumption K1. The kernel $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is symmetric, positive definite and fourth continuously differentiable in both variables with bounded derivatives up to fourth order. More explicitly, we assume

(1) $\|k\|_\infty := \sup_{x\in\mathbb{R}^d} \sqrt{k(x,x)} < \infty$
(2) $\|\nabla k\|_\infty := \sup_{x,y\in\mathbb{R}^d} |\nabla_1 k(x,y)| = \sup_{x,y\in\mathbb{R}^d} |\nabla_2 k(x,y)| < \infty$
(3) $\|\nabla_1 \cdot \nabla_2 k\|_\infty := \sup_{x,y\in\mathbb{R}^d} |\nabla_x \cdot \nabla_y k(x,y)| < \infty$.
(4) $\|\nabla^2 k\|_\infty := \sup_{x,y\in\mathbb{R}^d} \|\nabla_x^2 k(x,y)\|_2 < \infty$.
(5) $\|\nabla_1\nabla_2 k(x,y)\|_\infty := \sup_{x,y\in\mathbb{R}^d} \|\nabla_x\nabla_y k(x,y)\|_2 < \infty$.
(6) $\|\nabla^2(\nabla_1 \cdot \nabla_2 k)\|_\infty := \sup_{x,y\in\mathbb{R}^d} \|\nabla_x^2(\nabla_x \cdot \nabla_y k(x,y))\|_2 < \infty$.
(7) $\|\nabla_1\nabla_2(\nabla_1 \cdot \nabla_2 k)\|_\infty := \sup_{x,y\in\mathbb{R}^d} \|\nabla_x\nabla_y(\nabla_x \cdot \nabla_y k(x,y))\|_2 < \infty$.
(8) $\|\nabla_1^2 \cdot \nabla_2^2 k\|_\infty := \sup_{x,y\in\mathbb{R}^d} \sum_{i,j=1}^d |\partial_{x_i}\partial_{x_j}\partial_{y_i}\partial_{y_j} k(x,y)| < \infty$.

We emphasize here that [LLN19] required that the kernel is radial for their analysis. However, our analysis does not require this assumption. A classical example of a kernel satisfying the above conditions is the Gaussian kernel.

Assumption V1. The potential function $V : \mathbb{R}^d \to \mathbb{R}$ satisfies

(1) $V \in \mathcal{C}^2(\mathbb{R}^d)$, $V \geq 0$ and $V(x) \to +\infty$ as $|x| \to +\infty$.
(2) For any $\alpha, \beta > 0$, there exists a constant $C_{\alpha,\beta} > 0$ such that if $|y| \leq \alpha|x| + \beta$, then

$$(1 + |x|)(|\nabla V(y)| + \|\nabla^2 V(y)\|_2) \leq C_{\alpha,\beta}(1 + V(x)).$$

(3) V is gradient Lipschitz with parameter L_V, i.e., for all $x \in \mathbb{R}^d$, $\|\nabla^2 V(x)\|_2 \leq L_V$.

To present our result, we define the set of functions

$$Y := \left\{ u \in \mathcal{C}(\mathbb{R}^d; \mathbb{R}^d) \mid \sup_{x\in\mathbb{R}^d} |u(x) - x| < \infty \right\},$$

which is a complete metric space with the uniform metric $d_Y(u,v) = \sup_{x\in\mathbb{R}^d} |u(x) - v(x)|$.

Theorem 7. *Let k satisfy Assumption K1, V satisfy Assumption V1 and $\rho_0 \in \mathcal{P}_V$.*

(i) *For any $T > 0$, there exists a unique solution $\Phi(\cdot,\cdot,\rho_0) \in \mathcal{C}^1([0,T]; Y)$ to (28). Moreover, the measure $\rho_t = \Phi(t,\cdot,\rho_0)_{\#}\rho_0$ satisfies*

$$\|\rho_t\|_{\mathcal{P}_V} \leq \|\rho_0\|_{\mathcal{P}_V} \exp(C_{1,0}\nu^{-1/2}\|k\|_\infty \mathrm{KL}(\rho_0|\pi)^{1/2} t^{1/2}).$$

(ii) *For any $\rho_0 \in \mathcal{P}_V$, there is a unique $\rho \in \mathcal{C}([0,\infty); \mathcal{P}_V)$ which is a weak solution to (7). Moreover, for all $t \geq 0$,*

$$\|\rho_t\|_{\mathcal{P}_V} \leq \|\rho_0\|_{\mathcal{P}_V} \exp(C_{1,0}\nu^{-1/2}\|k\|_\infty \mathrm{KL}(\rho_0|\pi)^{1/2} t^{1/2}).$$

Remark 11. In Theorem 7, we introduce an upper bound to the $\mathcal{P}_V$-norm of the solution to (7) for any $\nu \in (0,1]$. A similar result is established for the case of SVGF, i.e., when $\nu = 1$ in [LLN19, Theorem 2.4]. In comparison to [LLN19, Theorem 2.4], our result requires that the initial KL-divergence to the target is bounded. Furthermore, if we set $\nu = 1$ in our result, we do not end up recovering their result. When $\nu = 1$, there is an explicit integral formula to $\mathcal{D}_{1,\rho_t}\nabla \log \frac{\rho_t}{\pi}$ which is

leveraged in [LLN19] for their proof. For $\nu \in (0,1)$, due to the absence of an explicit representation, we get the result in Theorem 7 by carefully analyzing the quantity $\mathcal{D}_{\nu,\rho_t}(\nabla \log \frac{\rho_t}{\pi})$ along with the decay of KL-divergence property introduced in Proposition 4.

Proof of Theorem 7. Our proof leverages the approach of [LLN19, Theorem 3.2] for the case of SVGF. In comparison to [LLN19], we handle various difficulties arising with the non-linear operator in R-SVGF. We first prove claim (i) based on the following two steps. Claim (ii) follows directly from claim (i) and [Vil21, Theorem 5.34].

Step 1 (Local well-posedness): Fix $r > 0$ and define

$$Y_r := \left\{ u \in Y \mid \sup_{x \in \mathbb{R}^d} |u(x) - x| \le r \right\}. \tag{29}$$

We will prove that there exists $T_0 > 0$ such that (28) has a unique solution $\Phi(t, x, \rho_0)$ in the set $S_r = \mathcal{C}([0, T_0]; Y_r)$ which is a complete metric space with metric

$$d_S(u, v) = \sup_{t \in [0, T_0]} d_Y(u(t, \cdot), v(t, \cdot)).$$

The integral formulation of (28) is

$$\Phi(t, x, \rho_0) = x - \int_0^t \mathcal{D}_{\nu,\rho_s} \nabla \log \frac{\rho_s}{\pi} (\Phi(s, x, \rho_0)) ds$$

$$= x + \int_0^t \left((1-\nu) \iota_{k,\rho_s} \iota_{k,\rho_s}^* + \nu I \right)^{-1} \mathbb{E}_{y \sim \rho_s}[-\nabla V(y)k(y, \cdot) + \nabla k(y, \cdot)](\Phi(s, x, \rho_0)) ds. \tag{30}$$

Let us define the operator $\mathcal{F} : u(t, \cdot) \mapsto \mathcal{F}(u)(t, \cdot)$ by

$$\mathcal{F}(u)(t, x) = x + \int_0^t \left((1-\nu) \iota_{k,\rho_{u,s}} \iota_{k,\rho_{u,s}}^* + \nu I \right)^{-1} \mathbb{E}_{y \sim \rho_{u,s}}[-\nabla V(y)k(y, \cdot) + \nabla k(y, \cdot)](u(s, x)) ds, \tag{31}$$

where $\rho_{u,t} = (u(t, \cdot))_{\#} \rho_0$. For the simplicity of notation, we will denote the map defined in (31) by $\mathcal{F}(u)(t, x) = x - \int_0^t \mathcal{D}_{\nu,\rho_{u,s}} \nabla \log \frac{\rho_{u,s}}{\pi} (u(s, x)) ds$ for any $u \in S_r$. We now show that $\mathcal{F}$ is a contraction from S_r to S_r and thus has a unique fixed point. First, we show that $\mathcal{F}$ maps S_r into S_r for some $T_0 > 0$. For any $u \in S_r$, checking that $(t, x) \mapsto \mathcal{F}(u)(t, x)$ is continuous is straightforward. We need to show that $\sup_{x \in \mathbb{R}^d} |\mathcal{F}(u)(t, x) - x| \le r$ for any $u \in S_r$.

Note that there is an equivalent representation for $\mathcal{D}_{\nu,\rho_{u,s}}$:

$$\mathcal{D}_{\nu,\rho_{u,s}} = \iota_{k,\rho_{u,s}} \left((1-\nu) \iota_{k,\rho_{u,s}}^* \iota_{k,\rho_{u,s}} + \nu I_d \right)^{-1} \iota_{k,\rho_{u,s}}^*.$$

We then analyze the operators $\iota_{k,\rho_{u,s}}$ and $\left((1-\nu) \iota_{k,\rho_{u,s}}^* \iota_{k,\rho_{u,s}} + \nu I_d \right)^{-1} \iota_{k,\rho_{u,s}}^*$ respectively. Since $\|k\|_\infty < \infty$, according to Proposition 1, $\iota_{k,\rho_{u,s}}$ is the inclusion operator from $\mathcal{H}_k^d$ to $L_\infty^d(\mathbb{R}^d)$. The corresponding operator norm, denoted as $\left\| \iota_{k,\rho_{u,s}} \right\|_{\mathcal{H}_k^d \to L_\infty^d}$ can be bounded in the following way:

$$\left\| \iota_{k,\rho_{u,s}} \right\|_{\mathcal{H}_k^d \to L_\infty^d} := \sup_{\|f\|_{\mathcal{H}_k^d} = 1} \sup_{x \in \mathbb{R}^d} |f(x)|$$

$$= \sup_{\|f\|_{\mathcal{H}_k^d} = 1} \sup_{x \in \mathbb{R}^d} |\langle k(x, \cdot), f \rangle_{\mathcal{H}_k}|$$

$$\le \sup_{x \in \mathbb{R}^d} \sqrt{k(x, x)} := \|k\|_\infty. \tag{32}$$

Meanwhile, let $(\lambda_i, e_i)_{i=1}^{\infty}$ be the spectrum of $\iota_{k,\rho_{u,s}} \iota_{k,\rho_{u,s}}^*$ with $(e_i)_{i=1}^{\infty}$ being an orthonormal basis of $L_2^d(\rho_{u,s}) \equiv \overline{\mathrm{Ran}(\iota_{k,\rho_{u,s}} \iota_{k,\rho_{u,s}}^*)}$. According to Proposition 1, $(\sqrt{\lambda_i} e_i)_{i=1}^{\infty}$ is an orthonormal basis of $\mathcal{H}_k^d$; see also Remark 1. Hence, we have

$$
\left\| \left((1-\nu)\iota_{k,\rho_{u,s}}^* \iota_{k,\rho_{u,s}} + \nu I_d \right)^{-1} \iota_{k,\rho_{u,s}}^* \nabla \log \frac{\rho_{u,s}}{\pi} \right\|_{\mathcal{H}_k^d}^2
$$

$$
\leq \left\| \left((1-\nu)\iota_{k,\rho_{u,s}}^* \iota_{k,\rho_{u,s}} + \nu I_d \right)^{-\frac{1}{2}} \right\|_{\mathcal{H}_k^d \to \mathcal{H}_k^d}^2 \left\| \left((1-\nu)\iota_{k,\rho_{u,s}}^* \iota_{k,\rho_{u,s}} + \nu I_d \right)^{-\frac{1}{2}} \iota_{k,\rho_{u,s}}^* \nabla \log \frac{\rho_{u,s}}{\pi} \right\|_{\mathcal{H}_k^d}^2
$$

$$
\leq \nu^{-1} I_{\nu,Stein}(\rho_{u,s}|\pi). \tag{33}
$$

where the last inequality follows from (9) and the fact that $(1-\nu)\iota_{k,\rho_{u,s}}^* \iota_{k,\rho_{u,s}}$ is positive. With (32) and (33), we get the following uniform bound on $|\mathcal{D}_{\nu,\rho_{u,s}} \nabla \log \frac{\rho_{u,s}}{\pi}(x)|$ for all $x \in \mathbb{R}^d$,

$$
\left| \mathcal{D}_{\nu,\rho_{u,s}} \nabla \log \frac{\rho_{u,s}}{\pi}(x) \right| \leq \left\| \mathcal{D}_{\nu,\rho_{u,s}} \nabla \log \frac{\rho_{u,s}}{\pi} \right\|_{L_\infty^d}
$$

$$
\leq \left\| \iota_{k,\rho_{u,s}} \right\|_{\mathcal{H}_k^d \to L_\infty^d} \left\| \left((1-\nu)\iota_{k,\rho_{u,s}}^* \iota_{k,\rho_{u,s}} + \nu I_d \right)^{-1} \iota_{k,\rho_{u,s}}^* \nabla \log \frac{\rho_{u,s}}{\pi} \right\|_{\mathcal{H}_k^d}
$$

$$
\leq \nu^{-\frac{1}{2}} \left\| k \right\|_\infty I_{\nu,Stein}(\rho_{u,s}|\pi)^{\frac{1}{2}}.
$$

Therefore, for all $t \in [0,T]$ and all $x \in \mathbb{R}^d$:

$$
|\mathcal{F}(u)(t,x) - x| \leq \nu^{-\frac{1}{2}} \left\| k \right\|_\infty \int_0^T I_{\nu,Stein}(\rho_{u,s}|\pi)^{\frac{1}{2}} ds. \tag{34}
$$

According to Lemma 2, there exists $T_0 > 0$ such that for all $u \in S_r$,

$$
\int_0^{T_0} I_{\nu,Stein}(\rho_{u,t}|\pi)^{\frac{1}{2}} dt < \nu^{1/2} \left\| k \right\|_\infty^{-1} r,
$$

which along with (34) implies $|\mathcal{F}(u)(t,x) - x| \leq r$ for all $u \in S_r$.

Next we show that $\mathcal{F}$ is a contraction on S_r. Our goal is to show that there exists $T_0 > 0$ and $C \in (0,1)$ such that for any $u, v \in S_r$,

$$
\sup_{t \in [0,T_0]} \sup_{x \in \mathbb{R}^d} |\mathcal{F}(u)(t,x) - \mathcal{F}(v)(t,x)| < C \sup_{t \in [0,T_0]} \sup_{x \in \mathbb{R}^d} |u(t,x) - v(t,x)|.
$$

Let $\rho_{u,t} = (u(t,\cdot))_{\#}\rho_0$, $\rho_{v,t} = (v(t,\cdot))_{\#}\rho_0$, we have that

$$
|\mathcal{F}(u)(t,x) - \mathcal{F}(v)(t,x)| = \left| \int_0^t \mathcal{D}_{\nu,\rho_{u,s}} \nabla \log \frac{\rho_{u,s}}{\pi}(u(s,x)) - \mathcal{D}_{\nu,\rho_{v,s}} \nabla \log \frac{\rho_{v,s}}{\pi}(v(s,x)) \, ds \right|
$$

$$
\leq \left| \int_0^t \mathcal{D}_{\nu,\rho_{u,s}} \nabla \log \frac{\rho_{u,s}}{\pi}(u(s,x)) - \mathcal{D}_{\nu,\rho_{v,s}} \nabla \log \frac{\rho_{v,s}}{\pi}(u(s,x)) ds \right|
$$

$$
+ \left| \int_0^t \mathcal{D}_{\nu,\rho_{v,s}} \nabla \log \frac{\rho_{v,s}}{\pi}(u(s,x)) - \mathcal{D}_{\nu,\rho_{2,s}} \nabla \log \frac{\rho_{2,s}}{\pi}(v(s,x)) ds \right|
$$

$$
\leq d_S(u,v) \int_0^{T_0} C_1(t) dt + \int_0^{T_0} L(t) dt \sup_{t \in [0,T_0]} \sup_{x \in \mathbb{R}^d} |u(t,x) - v(t,x)|
$$

$$
= d_S(u,v) \int_0^{T_0} C_1(t) + L(t) \, dt,
$$

where the second inequality follows from Lemma 3 and Lemma 4. Furthermore, according to (38) and (39), there exists $T_0 > 0$ such that

$$\int_0^{T_0} C_1(t) + L(t) \ dt < 1.$$

Therefore we have proved that there exists $T_0 > 0$ such that $\mathcal{F}$ is a contraction from S_r into S_r. According to the contraction theorem, $\mathcal{F}$ has a unique fixed point $\Phi(\cdot, \cdot, \rho_0) \in S_r$ which solves (28). Defining $\rho_t = (\Phi(t, \cdot, \rho_0))_\# \rho_0$, one sees that $\Phi(t, x, \rho_0)$ solves (28) in the time interval $[0, T_0]$.

Step 2 (Extension of local solution): According to (37) and (39), we can extend the local solution beyond time T_0 as long as the quantity

$$\|\rho_t\|_{\mathcal{P}_V} = \int_{\mathbb{R}^d} (1 + V(\Phi(t, x, \rho_0))) d\rho_0(x)$$

remains finite. Next we establish a bound on this quantity showing that the local solution can be extended to any $t > 0$.

$$\partial_t \int_{\mathbb{R}^d} (1 + V(\Phi(t, x, \rho_0))) \rho_0(dx) = -\int_{\mathbb{R}^d} \left\langle \nabla V(\Phi(t, x, \rho_0)), \mathcal{D}_{\nu, \rho_t} \nabla \log \frac{\rho_t}{\pi}(\Phi(t, x, \rho_0)) \right\rangle d\rho_0(x)$$

$$= -\left\langle \nabla V, \iota_{k, \rho_t} \left((1-\nu)\iota_{k, \rho_t}^* \iota_{k, \rho_t} + \nu I_d\right)^{-1} \iota_{k, \rho_t}^* \nabla \log \frac{\rho_t}{\pi} \right\rangle_{L_2^d(\rho_t)}$$

$$= -\left\langle \iota_{k, \rho_t}^* \nabla V, \left((1-\nu)\iota_{k, \rho_t}^* \iota_{k, \rho_t} + \nu I_d\right)^{-1} \iota_{k, \rho_t}^* \nabla \log \frac{\rho_t}{\pi} \right\rangle_{\mathcal{H}_k^d}$$

$$\leq \left\| \iota_{k, \rho_t}^* \nabla V \right\|_{\mathcal{H}_k^d} \left\| \left((1-\nu)\iota_{k, \rho_t}^* \iota_{k, \rho_t} + \nu I_d\right)^{-1} \iota_{k, \rho_t}^* \nabla \log \frac{\rho_t}{\pi} \right\|_{\mathcal{H}_k^d},$$

where

$$\left\| \iota_{k, \rho_t}^* \nabla V \right\|_{\mathcal{H}_k^d}^2 = \left\langle \nabla V, \iota_{k, \rho} \iota_{k, \rho_t}^* \nabla V \right\rangle_{L_2^d(\rho_t)}$$

$$= \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} k(y, z) \left\langle \nabla V(y), \nabla V(z) \right\rangle d\rho_t(y) d\rho_t(z)$$

$$= \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} k(\Phi(t, y, \rho_0), \Phi(t, z, \rho_0)) \left\langle \nabla V(\Phi(t, y, \rho_0)), \nabla V(\Phi(t, z, \rho_0)) \right\rangle d\rho_0(y) d\rho_0(z)$$

$$\leq \|k\|_\infty^2 \left(\int_{\mathbb{R}^d} |\nabla V(\Phi(t, y, \rho_0))| d\rho_0(y) \right)^2$$

$$\leq \|k\|_\infty^2 C_{1,0}^2 \|\rho_t\|_{\mathcal{P}_V}^2,$$

where the last inequality follows from Assumption V1. Therefore,

$$\partial_t \|\rho_t\|_{\mathcal{P}_V} \leq C_{1,0} \|k\|_\infty \|\rho_t\|_{\mathcal{P}_V} \left\| \left((1-\nu)\iota_{k, \rho_t}^* \iota_{k, \rho_t} + \nu I_d\right)^{-1} \iota_{k, \rho_t}^* \nabla \log \frac{\rho_t}{\pi} \right\|_{\mathcal{H}_k^d}$$

$$\leq C_{1,0} \|k\|_\infty \nu^{-\frac{1}{2}} I_{\nu, Stein}(\rho_t | \pi)^{\frac{1}{2}} \|\rho_t\|_{\mathcal{P}_V},$$

where the last inequality follows from (33). It follows from Gronwall's inequality that

$$\|\rho_t\|_{\mathcal{P}_V} \leq \|\rho_0\|_{\mathcal{P}_V} \exp\left(C_{1,0} \nu^{-\frac{1}{2}} \|k\|_\infty \int_0^t I_{\nu, Stein}(\rho_s | \pi)^{\frac{1}{2}} ds \right)$$

$$\leq \|\rho_0\|_{\mathcal{P}_V} \exp\left(C_{1,0} \nu^{-\frac{1}{2}} \|k\|_\infty \sqrt{t \int_0^t I_{\nu, Stein}(\rho_s | \pi) ds} \right)$$

$$\leq \|\rho_0\|_{\mathcal{P}_V} \exp\left(C_{1,0} \nu^{-\frac{1}{2}} \|k\|_\infty \sqrt{t \text{KL}(\rho_0 | \pi)} \right), \tag{35}$$

where the second inequality follows from Jensen's inequality and the last inequality follows from (15). With this bound, we can iterate the argument to extend the local solution defined on $[0, T_0] \times \mathbb{R}^d$ to all of $[0, \infty) \times \mathbb{R}^d$, so that (35) holds for all $t > 0$. Finally, $\Phi(\cdot, x, \rho_0)$ has continuous first order derivative due to the integral formulation in (30), Assumption K1 and Assumption V1. The proof is thus complete. $\square$

Lemma 2. *Let $\rho_0 \in \mathcal{P}_V$ and suppose the assumptions in Theorem 7 hold. Then, for any $\epsilon > 0$, there exists a constant $T > 0$ such that for all $u \in S_r$ and $t \in [0, T]$, with $\rho_{u,t} = u(t, \cdot)_{\#}\rho_0$, we have*

$$\int_0^T I_{\nu, Stein}(\rho_{u,t}|\pi)^{\frac{1}{2}} dt < \epsilon. \tag{36}$$

Proof of Lemma 2. According to Proposition 2, the regularized kernelized Stein discrepancy can be written as

$$S(\rho_{u,t}|\pi)^2 = \left(\mathbb{E}_{x \sim \rho_{u,t}} \left[\text{trace}(\mathcal{A}_\pi \phi^*_{\rho_{u,t},\pi}(x)) \right] \right)^2$$

$$= \left\| \left((1-\nu)\iota^*_{k,\rho_{u,t}}\iota_{k,\rho_{u,t}} + \nu I_d \right)^{-\frac{1}{2}} \iota^*_{k,\rho_{u,t}} \nabla \log \frac{\rho_{u,t}}{\pi} \right\|^2_{\mathcal{H}^d_k}$$

$$= \left\langle \iota^*_{k,\rho_{u,t}} \nabla \log \frac{\rho_{u,t}}{\pi}, \left((1-\nu)\iota^*_{k,\rho_{u,t}}\iota_{k,\rho_{u,t}} + \nu I_d \right)^{-1} \iota^*_{k,\rho_{u,t}} \nabla \log \frac{\rho_{u,t}}{\pi} \right\rangle_{\mathcal{H}^d_k} = I_{\nu, Stein}(\rho_{u,t}, \pi).$$

Meanwhile, since $\rho_{u,t} = u(t, \cdot)_{\#}\rho_0$ with $u \in S_r$, for any $\mathbb{R}^d$-valued random vector X, $u(t, X) \sim \rho_{u,t}$ and $|u(t, X) - X| \leq r$ almost surely. Therefore,

$$\mathcal{W}_1(\rho_{u,t}, \pi) \leq \mathcal{W}_1(\rho_0, \rho_{u,t}) + \mathcal{W}_1(\rho_0, \pi) = \inf_{X \sim \rho_0, Y \sim \rho_{u,t}} \mathbb{E}[|X - Y|] + \mathcal{W}_1(\rho_0, \pi) \leq r + \mathcal{W}_1(\rho_0, \pi),$$

where $\mathcal{W}_1$ is the Wasserstein-1 distance defined in Section 1.3. Next, we upper bound the regularized kernelized Stein discrepancy by the Wasserstein-1 distance. According to [GM17, Lemma 18], for any general vector field $\phi \in \mathcal{H}^d_k$, we have

$$\left| \mathbb{E}_{x \sim \rho_{u,t}} \left[\text{trace}(\mathcal{A}_\pi \phi(x)) \right] \right| \leq \left(M_0(\phi)M_1(\nabla V) + M_2(\phi)d \right) \mathcal{W}_1(\rho_{u,t}, \pi)$$

$$+ \sqrt{2M_0(\phi)M_1(\phi)\mathbb{E}_{x \sim \pi}[|\nabla V(x)|^2]} \, \mathcal{W}_1(\rho_{u,t}, \pi),$$

where for any $g : \mathbb{R}^d \to \mathbb{R}^d$ and $g \in C^1(\mathbb{R}^d)$,

$$M_0(g) := \sup_{x \in \mathbb{R}^d} |g(x)|, \quad M_1(g) := \sup_{x \neq y} \frac{|g(x) - g(y)|}{|x - y|}, \quad M_2(g) := \sup_{x \neq y} \frac{\|\nabla g(x) - \nabla g(y)\|_2}{|x - y|}.$$

For any $\phi \in \mathcal{H}^d_k$ and $\phi = [\phi_1, \cdots, \phi_d]^T$, according to [SC08, Lemma 4.34],

$$\sup_{x \in \mathbb{R}^d} |D^\alpha \phi_i(x)| = \sup_{x \in \mathbb{R}^d} \left| D^\alpha \langle \phi_i, k(x, \cdot) \rangle_{\mathcal{H}_k} \right| \leq \|\phi_i\|_{\mathcal{H}^d_k} \sup_{x \in \mathbb{R}^d} |D_1^\alpha D_2^\alpha k(x, x)|^{\frac{1}{2}}.$$

Therefore,

$$M_0(\phi) = \sup_{x \in \mathbb{R}^d} \sqrt{\sum_{i=1}^d \phi_i(x)^2} \leq \sqrt{\sum_{i=1}^d \|\phi_i\|^2_{\mathcal{H}_k} \sup_{x \in \mathbb{R}^d} k(x, x)} = \|k\|_\infty \|\phi\|_{\mathcal{H}^d_k},$$

$$M_1(\phi) = \sup_{x \neq y} \frac{\sqrt{\sum_{i=1}^d (\phi_i(x) - \phi_i(y))^2}}{|x - y|} \leq \sqrt{\sum_{i=1}^d \sup_{x \in \mathbb{R}^d} |\nabla \phi_i(x)|^2}$$

$$\leq \sqrt{\sum_{i=1}^{d}\sum_{j=1}^{d}\|\phi_i\|_{\mathcal{H}_k}^2 \sup_{x\in\mathbb{R}^d} D_1^{e_j}D_2^{e_j}k(x,x)} = \left(\sup_{x\in\mathbb{R}^d}\operatorname{trace}\left(\nabla_1\nabla_2 k(x,x)\right)\right)^{\frac{1}{2}}\|\phi\|_{\mathcal{H}_k^d}$$

$$\leq \|\nabla_1\cdot\nabla_2 k\|_\infty^{\frac{1}{2}}\|\phi\|_{\mathcal{H}_k^d},$$

$$M_2(\phi) = \sup_{x\neq y}\frac{\|\nabla\phi(x)-\nabla\phi(y)\|_2}{|x-y|} \leq \sup_{x\neq y}\frac{\|\nabla\phi(x)-\nabla\phi(y)\|_F}{|x-y|} \leq \sqrt{\sum_{i,j=1}^{d}\sup_{x\neq y}\frac{|\partial_j\phi_i(x)-\partial_j\phi_i(y)|^2}{|x-y|^2}}$$

$$\leq \sqrt{\sum_{i,j,l=1}^{d}\sup_{x\in\mathbb{R}^d} D_1^{e_j+e_l}D_2^{e_j+e_l}k(x,x)\|\phi_i\|_{\mathcal{H}_k}^2} \leq \|\nabla_1^2\cdot\nabla_2^2 k\|_\infty^{\frac{1}{2}}\|\phi\|_{\mathcal{H}_k^d}.$$

According to Assumption V1, $M_1(\nabla V) = L_V$ and $\mathbb{E}_{x\sim\pi}\left[|\nabla V(x)|^2\right] \leq C_{1,0}\|\pi\|_{\mathcal{P}_V}$. Therefore,

$$\left|\mathbb{E}_{x\sim\rho_{u,t}}\left[\operatorname{trace}(\mathcal{A}_\pi\phi(x))\right]\right| \leq \left(\|k\|_\infty L_V + \|\nabla_1^2\cdot\nabla_2^2 k\|_\infty^{\frac{1}{2}}d\right)\|\phi\|_{\mathcal{H}_k^d}\left(\mathcal{W}_1(\rho_0,\pi)+r\right)$$

$$+ \sqrt{2\|k\|_\infty\|\nabla_1\cdot\nabla_2 k\|_\infty^{\frac{1}{2}}C_{1,0}\|\pi\|_{\mathcal{P}_V}}\left(\mathcal{W}_1(\rho_0,\pi)+r\right)\|\phi\|_{\mathcal{H}_k^d}.$$

Note that $\phi_{k,\rho_{u,t}}^*$ satisfies that $\nu\left\|\phi_{k,\rho_{u,t}}^*\right\|_{\mathcal{H}_k^d}^2 + (1-\nu)\left\|\phi_{k,\rho_{u,t}}^*\right\|_{L_2^d(\rho_{u,t})^d} \leq 1$. Therefore,

$$\left\|\phi_{k,\rho_{u,t}}^*\right\|_{\mathcal{H}_k^d} \leq \nu^{-1/2},$$

and

$$I_{\nu,Stein}(\rho_{u,t}|\pi)^{\frac{1}{2}} = S(\rho_{u,t},\pi) = \left|\mathbb{E}_{x\sim\rho_{u,t}}\left[\operatorname{trace}(\mathcal{A}_\pi\phi_{k,\rho_{u,t}}^*(x))\right]\right|$$

$$\leq \nu^{-\frac{1}{2}}\left(\|k\|_\infty L_V + \|\nabla_1^2\cdot\nabla_2^2 k\|_\infty^{\frac{1}{2}}d\right)\left(\mathcal{W}_1(\rho_0,\pi)+r\right)$$

$$+ \nu^{-\frac{1}{2}}\sqrt{2\|k\|_\infty\|\nabla_1\cdot\nabla_2 k\|_\infty^{\frac{1}{2}}C_{1,0}\|\pi\|_{\mathcal{P}_V}}\left(\mathcal{W}_1(\rho_0,\pi)+r\right).$$

Since the upper bound is independent of the choice of $u(t,\cdot)\in S_r$ and the time variable t, for any $\epsilon > 0$, we can choose a small enough T such that (36) holds. $\qquad\square$

Lemma 3. *Under the assumptions in Theorem 7, let $S_r = \mathcal{C}([0,T];Y_r)$ with Y_r defined in (29). Then for any $t\in[0,T]$, there exists $L(t) > 0$ such that for any $u\in S_r$, for all $x,y\in\mathbb{R}^d$ and $t\in[0,T]$,*

$$\left|\mathcal{D}_{\nu,\rho_{u,t}}\nabla\log\frac{\rho_{u,t}}{\pi}(x) - \mathcal{D}_{\nu,\rho_{u,t}}\nabla\log\frac{\rho_{u,t}}{\pi}(y)\right| \leq L(t)|x-y|, \tag{37}$$

where for all $t\in[0,T]$, $\rho_{u,t} = (u(t,\cdot))_{\#}\rho_0$ and

$$L(t) = \nu^{-\frac{1}{2}}\left(2\|\nabla_1\nabla_2 k\|_\infty + 3\|\nabla^2 k\|_\infty\right)^{\frac{1}{2}} I_{\nu,Stein}(\rho_{u,t}|\pi)^{\frac{1}{2}}. \tag{38}$$

Proof of Lemma 3. Since $\mathcal{D}_{\nu,\rho_{u,t}} = \iota_{k,\rho_{u,t}}\left((1-\nu)\iota_{k,\rho_{u,t}}^*\iota_{k,\rho_{u,t}}+\nu I_d\right)^{-1}\iota_{k,\rho_{u,t}}^*$ and $\iota_{k,\rho_{u,t}}$ is the inclusion operator,

$$\left|\mathcal{D}_{\nu,\rho_{u,t}}\nabla\log\frac{\rho_{u,t}}{\pi}(x) - \mathcal{D}_{\nu,\rho_{u,t}}\nabla\log\frac{\rho_{u,t}}{\pi}(y)\right|$$

$$= \left|\left((1-\nu)\iota_{k,\rho_{u,t}}^*\iota_{k,\rho_{u,t}}+\nu I_d\right)^{-1}\iota_{k,\rho_{u,t}}^*\nabla\log\frac{\rho_{u,t}}{\pi}(x) - \left((1-\nu)\iota_{k,\rho_{u,t}}^*\iota_{k,\rho_{u,t}}+\nu I_d\right)^{-1}\iota_{k,\rho_{u,t}}^*\nabla\log\frac{\rho_{u,t}}{\pi}(y)\right|$$

$$\begin{aligned}
&= \left| \left\langle k(x,\cdot) - k(y,\cdot), \left((1-\nu)\iota^*_{k,\rho_{u,t}}\iota_{k,\rho_{u,t}} + \nu I_d \right)^{-1} \iota^*_{k,\rho_{u,t}} \nabla \log \frac{\rho_{u,t}}{\pi} \right\rangle_{\mathcal{H}_k} \right| \\
&\leq \|k(x,\cdot) - k(y,\cdot)\|_{\mathcal{H}_k} \left\| \left((1-\nu)\iota^*_{k,\rho_{u,t}}\iota_{k,\rho_{u,t}} + \nu I_d \right)^{-1} \iota^*_{k,\rho_{u,t}} \nabla \log \frac{\rho_{u,t}}{\pi} \right\|_{\mathcal{H}_k^d} \\
&\leq \nu^{-\frac{1}{2}} I_{\nu,\text{Stein}}(\rho_{u,t}|\pi)^{\frac{1}{2}} \|k(x,\cdot) - k(y,\cdot)\|_{\mathcal{H}_k^d},
\end{aligned}$$

where the second identity follows from the reproducing property and the last inequality follows from (33). Furthermore, we can write

$$\begin{aligned}
\|k(x,\cdot) - k(y,\cdot)\|^2_{\mathcal{H}_k^d} &= k(x,x) - 2k(x,y) + k(y,y) \\
&\leq \left(2\|\nabla_1\nabla_2 k\|_\infty + 3\|\nabla^2 k\|_\infty \right) |x-y|^2,
\end{aligned}$$

where the first identity follows from the RKHS property and the second identity follows from Taylor expansion and Assumption K1. Therefore, (37) holds with $L(t)$ defined in (38). $\square$

Lemma 4. *Under the assumptions in Theorem 7, let $S_r = \mathcal{C}([0,T];Y_r)$ with Y_r defined in (29). Then for any $t \in [0,T]$, there exists $C_1(t) > 0$ such that for any $u, v \in S_r$,*

$$\sup_{x\in\mathbb{R}^d} \left| \mathcal{D}_{\nu,\rho_{u,t}} \nabla \log \frac{\rho_{u,t}}{\pi}(x) - \mathcal{D}_{\nu,\rho_{v,t}} \nabla \log \frac{\rho_{v,t}}{\pi}(x) \right| \leq C_1(t) d_S(u,v), \tag{39}$$

where for all $t \in [0,T]$, $\rho_{u,t} = (u(t,\cdot))_\#\rho_0$, $\rho_{v,t} = (v(t,\cdot))_\#\rho_0$ and

$$C_1(t) = 2\nu^{-\frac{3}{2}}(1-\nu)\|k\|^2_\infty \left(2\|\nabla_1\nabla_2 k\|_\infty + 3\|\nabla^2 k\|_\infty \right)^{\frac{1}{2}} \|\nabla k\|_\infty I_{\nu,\text{Stein}}(\rho_{u,t}|\pi)^{\frac{1}{2}} + \nu^{-1}L_r \|k\|_\infty, \tag{40}$$

with L_r being defined in (44).

Proof of Lemma 4. With the facts that $\mathcal{D}_{\nu,\mu} = \iota_{k,\mu}(\iota^*_{k,\mu}\iota_{k,\mu} + \nu I)^{-1}\iota^*_{k,\mu}$ and $\iota_{k,\mu}$ is the inclusion operator we get,

$$\begin{aligned}
&\left| \mathcal{D}_{\nu,\rho_{u,t}} \nabla \log \frac{\rho_{u,t}}{\pi}(x) - \mathcal{D}_{\nu,\rho_{v,t}} \nabla \log \frac{\rho_{v,t}}{\pi}(x) \right| \\
&= \left| \left((1-\nu)\iota^*_{k,\rho_{u,t}}\iota_{k,\rho_{u,t}} + \nu I \right)^{-1} \iota^*_{k,\rho_{u,t}} \nabla \log \frac{\rho_{u,t}}{\pi}(x) \right. \\
&\qquad \left. - \left((1-\nu)\iota^*_{k,\rho_{v,t}}\iota_{k,\rho_{v,t}} + \nu I \right)^{-1} \iota^*_{k,\rho_{v,t}} \nabla \log \frac{\rho_{v,t}}{\pi}(x) \right| \\
&\leq \left| \left(\left((1-\nu)\iota^*_{k,\rho_{u,t}}\iota_{k,\rho_{u,t}} + \nu I \right)^{-1} - \left((1-\nu)\iota^*_{k,\rho_{v,t}}\iota_{k,\rho_{v,t}} + \nu I \right)^{-1} \right) \iota^*_{k,\rho_{u,t}} \nabla \log \frac{\rho_{u,t}}{\pi}(x) \right| \\
&\quad + \left| \left((1-\nu)\iota^*_{k,\rho_{v,t}}\iota_{k,\rho_{v,t}} + \nu I \right)^{-1} \left(\iota^*_{k,\rho_{u,t}} \nabla \log \frac{\rho_{u,t}}{\pi}(x) - \iota^*_{k,\rho_{v,t}} \nabla \log \frac{\rho_{v,t}}{\pi}(x) \right) \right|.
\end{aligned}$$

We then turn to study the two terms in the upper bound separately.

First term: Note that, we have

$$\begin{aligned}
&\left| \left(\left((1-\nu)\iota^*_{k,\rho_{u,t}}\iota_{k,\rho_{u,t}} + \nu I \right)^{-1} - \left((1-\nu)\iota^*_{k,\rho_{v,t}}\iota_{k,\rho_{v,t}} + \nu I \right)^{-1} \right) \iota^*_{k,\rho_{u,t}} \nabla \log \frac{\rho_{u,t}}{\pi}(x) \right| \\
&= \left| \iota_{k,\rho_{u,t}} \left((1-\nu)\iota^*_{k,\rho_{v,t}}\iota_{k,\rho_{v,t}} + \nu I \right)^{-1} \left((1-\nu)\iota^*_{k,\rho_{v,t}}\iota_{k,\rho_{v,t}} - (1-\nu)\iota^*_{k,\rho_{u,t}}\iota_{k,\rho_{u,t}} \right) \right. \\
&\qquad \left. \times \left((1-\nu)\iota^*_{k,\rho_{u,t}}\iota_{k,\rho_{u,t}} + \nu I \right)^{-1} \iota^*_{k,\rho_{u,t}} \nabla \log \frac{\rho_{u,t}}{\pi}(x) \right|
\end{aligned}$$

$$\leq \left\| \iota_{k,\rho_{u,t}} \right\|_{\mathcal{H}_k^d \to L_\infty^d} \left\| \left((1-\nu)\iota_{k,\rho_{v,t}}^* \iota_{k,\rho_{v,t}} + \nu I \right)^{-1} \right\|_{\mathcal{H}_k^d \to \mathcal{H}_k^d} (1-\nu) \left\| \iota_{k,\rho_{v,t}}^* \iota_{k,\rho_{v,t}} - \iota_{k,\rho_{u,t}}^* \iota_{k,\rho_{u,t}} \right\|_{\mathcal{H}_k^d \to \mathcal{H}_k^d}$$

$$\times \left\| \left((1-\nu)\iota_{k,\rho_{u,t}}^* \iota_{k,\rho_{u,t}} + \nu I \right)^{-1} \iota_{k,\rho_{u,t}}^* \nabla \log \frac{\rho_{u,t}}{\pi} \right\|_{\mathcal{H}_k^d}$$

$$\leq \|k\|_\infty \, \nu^{-1}(1-\nu)\nu^{-\frac{1}{2}} I_{\nu,Stein}(\rho_{u,t}|\pi)^{\frac{1}{2}}$$

$$\times \sup_{\|\phi\|_{\mathcal{H}_k^d}=1} \left\langle \int_{\mathbb{R}^d} k(\cdot,x)\phi(x)(d\rho_{u,t}(x)-d\rho_{v,t}(x)), \int_{\mathbb{R}^d} k(\cdot,y)\phi(y)(d\rho_{u,t}(y)-d\rho_{v,t}(y)) \right\rangle_{\mathcal{H}_k^d}^{\frac{1}{2}}$$

$$\leq 2\nu^{-\frac{3}{2}}(1-\nu)\|k\|_\infty^2 \left(3\left\|\nabla^2 k\right\|_\infty + 2\left\|\nabla_1\nabla_2 k\right\|_\infty \right)^{\frac{1}{2}} I_{\nu,Stein}(\rho_{u,t}|\pi)^{\frac{1}{2}} d_S(u,v). \tag{41}$$

As we are bounding the function value by its L_∞^d norm, the second step allows the function to be in the space of L_∞^d, without which we think of the function as belonging to the RKHS. The second inequality follows from (32) and (33). The last inequality follows from the fact that

$$\left\langle \int_{\mathbb{R}^d} k(\cdot,x)\phi(x)(d\rho_{u,t}(x)-d\rho_{v,t}(x)), \int_{\mathbb{R}^d} k(\cdot,y)\phi(y)(d\rho_{u,t}(y)-d\rho_{v,t}(y)) \right\rangle_{\mathcal{H}_k^d}^{\frac{1}{2}}$$

$$= \left(\sup_{\|\phi\|_{\mathcal{H}_k^d}=1} \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \left\langle k\left(u(t,x),\cdot\right)\phi\left(u(t,x)\right) - k\left(v(t,x),\cdot\right)\phi\left(v(t,x)\right), \right.\right.$$

$$\left.\left. k\left(u(t,y),\cdot\right)\phi\left(u(t,y)\right) - k\left(v(t,y),\cdot\right)\phi\left(v(t,y)\right) \right\rangle_{\mathcal{H}_k^d} d\rho_0(x)d\rho_0(y) \right)^{\frac{1}{2}}$$

$$\leq \sup_{\|\phi\|_{\mathcal{H}_k^d}=1} \int_{\mathbb{R}^d} \left\| k\left(u(t,x),\cdot\right)\phi\left(u(t,x)\right) - k\left(v(t,x),\cdot\right)\phi\left(v(t,x)\right) \right\|_{\mathcal{H}_k^d} d\rho_0(x)$$

$$\leq \sup_{\|\phi\|_{\mathcal{H}_k^d}=1} \int_{\mathbb{R}^d} \left\| \left(k\left(u(t,x),\cdot\right) - k\left(v(t,x),\cdot\right)\right)\phi\left(u(t,x)\right) \right\|_{\mathcal{H}_k^d} d\rho_0(x)$$

$$+ \sup_{\|\phi\|_{\mathcal{H}_k^d}=1} \int_{\mathbb{R}^d} \left\| k\left(v(t,x),\cdot\right)\left(\phi\left(u(t,x)\right) - \phi\left(v(t,x)\right)\right) \right\|_{\mathcal{H}_k^d} d\rho_0(x)$$

$$= \sup_{\|\phi\|_{\mathcal{H}_k^d}=1} \int_{\mathbb{R}^d} \left\| \left(k\left(u(t,x),\cdot\right) - k\left(v(t,x),\cdot\right)\right) \right\|_{\mathcal{H}_k} \left| \langle \phi(\cdot), k\left(u(t,x),\cdot\right)\rangle_{\mathcal{H}_k} \right| d\rho_0(x)$$

$$+ \sup_{\|\phi\|_{\mathcal{H}_k^d}=1} \int_{\mathbb{R}^d} \left\| k\left(v(t,x),\cdot\right) \right\|_{\mathcal{H}_k} \left| \langle \phi(\cdot), k\left(u(t,x),\cdot\right) - k\left(v(t,x),\cdot\rangle_{\mathcal{H}_k} \right| d\rho_0(x)$$

$$\leq \sup_{\|\phi\|_{\mathcal{H}_k^d}=1} \int_{\mathbb{R}^d} \left\| \left(k\left(u(t,x),\cdot\right) - k\left(v(t,x),\cdot\right)\right) \right\|_{\mathcal{H}_k} \|\phi\|_{\mathcal{H}_k^d} \left\| k\left(u(t,x),\cdot\right) \right\|_{\mathcal{H}_k} d\rho_0(x)$$

$$+ \sup_{\|\phi\|_{\mathcal{H}_k^d}=1} \int_{\mathbb{R}^d} \left\| k\left(v(t,x),\cdot\right) \right\|_{\mathcal{H}_k} \|\phi\|_{\mathcal{H}_k^d} \left\| k\left(u(t,x),\cdot\right) - k\left(v(t,x),\cdot\right) \right\|_{\mathcal{H}_k} d\rho_0(x)$$

$$= \sup_{x\in\mathbb{R}^d} \left(\sqrt{k\left(u(t,x),u(t,x)\right) + k\left(v(t,x),v(t,x)\right) - 2k\left(u(t,x),v(t,x)\right)} \right.$$

$$\left. \times \left(\sqrt{k\left(u(t,x),u(t,x)\right)} + \sqrt{k\left(v(t,x),v(t,x)\right)} \right) \right)$$

$$\leq 2\|k\|_\infty \left(3\left\|\nabla^2 k\right\|_\infty + 2\left\|\nabla_1\nabla_2 k\right\|_\infty \right)^{\frac{1}{2}} d_S(u,v),$$

where the first identity follows from the definitions of $\rho_{u,t}$ and $\rho_{v,t}$ and change of variable. The second inequality holds due to the symmetry in x and y. The second identity follows from the reproducing property of the RKHS. The last identity follows from the fact that $\|k(x,\cdot)\|_{\mathcal{H}_k} = \sqrt{k(x,x)}$ for all x and the last inequality follows from Assumption K1 and Taylor expansion on both variables in k up to second order.

Second term: Note that we have

$$
\left| \left((1-\nu)\iota^*_{k,\rho_{v,t}}\iota_{k,\rho_{v,t}} + \nu I \right)^{-1} \left(\iota^*_{k,\rho_{u,t}} \nabla \log \frac{\rho_{u,t}}{\pi}(x) - \iota^*_{k,\rho_{v,t}} \nabla \log \frac{\rho_{v,t}}{\pi}(x) \right) \right|
$$

$$
= \left| \iota_{k,\rho_{v,t}} \left((1-\nu)\iota^*_{k,\rho_{v,t}}\iota_{k,\rho_{v,t}} + \nu I \right)^{-1} \left(\iota^*_{k,\rho_{u,t}} \nabla \log \frac{\rho_{u,t}}{\pi}(x) - \iota^*_{k,\rho_{v,t}} \nabla \log \frac{\rho_{v,t}}{\pi}(x) \right) \right|
$$

$$
\leq \left\| \iota_{k,\rho_{v,t}} \right\|_{\mathcal{H}^d_k \to L^d_\infty} \left\| \left((1-\nu)\iota^*_{k,\rho_{v,t}}\iota_{k,\rho_{v,t}} + \nu I \right)^{-1} \right\|_{\mathcal{H}^d_k \to \mathcal{H}^d_k} \left\| \iota^*_{k,\rho_{u,t}} \nabla \log \frac{\rho_{u,t}}{\pi} - \iota^*_{k,\rho_{v,t}} \nabla \log \frac{\rho_{v,t}}{\pi} \right\|_{\mathcal{H}^d_k}
$$

$$
\leq \|k\|_\infty \nu^{-1} \left\| \iota^*_{k,\rho_{u,t}} \nabla \log \frac{\rho_{u,t}}{\pi} - \iota^*_{k,\rho_{v,t}} \nabla \log \frac{\rho_{v,t}}{\pi} \right\|_{\mathcal{H}^d_k},
$$

where the last inequality follows from (32) and for all $x \in \mathbb{R}^d$,

$$
\iota^*_{k,\rho_{u,t}} \nabla \log \frac{\rho_{u,t}}{\pi}(x) - \iota^*_{k,\rho_{v,t}} \nabla \log \frac{\rho_{v,t}}{\pi}(x)
$$

$$
= \int_{\mathbb{R}^d} k(x,y)\nabla \log \frac{\rho_{u,t}}{\pi}(y) d\rho_{u,t}(y) - \int_{\mathbb{R}^d} k(x,y)\nabla \log \frac{\rho_{v,t}}{\pi} d\rho_{v,t}(y)
$$

$$
= \int_{\mathbb{R}^d} \left(k(x,y)\nabla V(y) - \nabla_2 k(x,y) \right) d\rho_{u,t}(y) - \int_{\mathbb{R}^d} \left(k(x,y)\nabla V(y) - \nabla_2 k(x,y) \right) d\rho_{v,t}(y)
$$

$$
= \int_{\mathbb{R}^d} \left(k(x,u(t,y))\nabla V(u(t,y)) - k(x,v(t,y))\nabla V(v(t,y)) \right) d\rho_0(y)
$$

$$
- \int_{\mathbb{R}^d} \left(\nabla_2 k(x,u(t,y)) - \nabla_2 k(x,v(t,y)) \right) d\rho_0(y).
$$

Therefore, we have

$$
\left\| \iota^*_{k,\rho_{u,t}} \nabla \log \frac{\rho_{u,t}}{\pi} - \iota^*_{k,\rho_{v,t}} \nabla \log \frac{\rho_{v,t}}{\pi} \right\|_{\mathcal{H}^d_k}
$$

$$
\leq \int_{\mathbb{R}^d} \Bigg(\left\| k(\cdot,u(t,y))\nabla V(u(t,y)) - k(\cdot,v(t,y))\nabla V(v(t,y)) \right\|_{\mathcal{H}^d_k}
$$

$$
+ \left\| \nabla_2 k(\cdot,u(t,y)) - \nabla_2 k(\cdot,v(t,y)) \right\|_{\mathcal{H}^d_k} \Bigg) d\rho_0(y).
$$

For simplicity, in the following calculations, we denote $u(t,y)$ and $v(t,y)$ as u and v respectively. We will bound $\|k(\cdot,u)\nabla V(u) - k(\cdot,v)\nabla V(v)\|_{\mathcal{H}^d_k}$ and $\|\nabla_2 k(\cdot,u) - \nabla_2 k(\cdot,v)\|_{\mathcal{H}^d_k}$ respectively. Note that we have

$$
\|k(\cdot,u)\nabla V(u) - k(\cdot,v)\nabla V(v)\|^2_{\mathcal{H}^d_k}
$$

$$
= \langle k(\cdot,u)\nabla V(u) - k(\cdot,v)\nabla V(v), k(\cdot,u)\nabla V(u) - k(\cdot,v)\nabla V(v) \rangle_{\mathcal{H}^d_k}
$$

$$
= |\nabla V(u)|^2 k(u,u) - 2\langle \nabla V(u), \nabla V(v) \rangle k(u,v) + |\nabla V(v)|^2 k(v,v)
$$

$$
\leq |\langle \nabla V(u) - \nabla V(v), \nabla V(u)k(u,u) - \nabla V(v)k(v,v) \rangle|
$$

$$
+ |\langle \nabla V(u), \nabla V(v) \rangle (k(u,u) + k(v,v) - 2k(u,v))|,
$$

where

$$|\langle \nabla V(u) - \nabla V(v), \nabla V(u)k(u,u) - \nabla V(v)k(v,v)\rangle|$$
$$\leq |\nabla V(u) - \nabla V(v)|^2 k(u,u) + |\nabla V(u) - \nabla V(v)| |\nabla V(v)| |k(u,u) - k(v,v)|$$
$$\leq C_{1,r}^2 (1 + V(y))^2 d_{S_T}(u,v)^2 k(u,u) + C_{1,r}^2 (1 + V(y))^2 d_S(u,v) |k(u,u) - k(v,v)|$$
$$\leq C_{1,r}^2 (1 + V(y))^2 d_S(u,v)^2 \|k\|_\infty^2 + 2C_{1,r}^2 \|\nabla k\|_\infty (1 + V(y))^2 d_S(u,v)^2.$$

The second inequality follows from Assumption V1 and the last inequality follows from Assumption K1 and Taylor expansion on both variables in k up to first order. And, we also have

$$|\langle \nabla V(u), \nabla V(v)\rangle (k(u,u) + k(v,v) - 2k(u,v))|$$
$$\leq C_{1,r}^2 (1 + V(y))^2 |k(u,u) + k(v,v) - 2k(u,v)|$$
$$\leq C_{1,r}^2 (1 + V(y))^2 \left(3\left\|\nabla^2 k\right\|_\infty + 2\left\|\nabla_1 \nabla_2 k\right\|_\infty\right) d_S(u,v)^2,$$

where the first inequality follows from Assumption V1 and the last inequality follows from Assumption K1 and Taylor expansion on both variables in k up to second order. With the above two inequalities, we have

$$\|k(\cdot, u(t,y))\nabla V(u(t,y)) - k(\cdot, v(t,y))\nabla V(v(t,y))\|_{\mathcal{H}_k^d}$$
$$\leq C_{1,r}\left(\|k\|_\infty + 2\|\nabla k\|_\infty^{\frac{1}{2}} + 3\left\|\nabla^2 k\right\|_\infty^{\frac{1}{2}} + 2\|\nabla_1 \nabla_2 k\|_\infty^{\frac{1}{2}}\right) d_S(u,v)(1 + V(y)). \qquad (42)$$

Observe that, for all $x, y \in \mathbb{R}^d$

$$\langle \nabla_2 k(\cdot, x), \nabla_2 k(\cdot, y)\rangle_{\mathcal{H}_k^d} = \nabla_1 \cdot \nabla_2 \langle k(\cdot, x), k(\cdot, y)\rangle_{\mathcal{H}_k^d}$$
$$= \nabla_1 \cdot \nabla_2 k(x, y).$$

If we denote the function $\nabla_1 \cdot \nabla_2 k = D_{1,2}k$ where $D_{1,2}k$ is symmetric since k is symmetric, we get

$$\|\nabla_2 k(\cdot, u) - \nabla_2 k(\cdot, v)\|_{\mathcal{H}_k^d}^2 = D_{1,2}k(u,u) + D_{1,2}k(v,v) - 2D_{1,2}k(u,v)$$
$$\leq \left(2\left\|\nabla^2(D_{1,2}k)\right\|_\infty + \|\nabla_1 \nabla_2(D_{1,2}k)\|_\infty\right) d_S(u,v)^2.$$

where the inequality follows from Taylor expansion on both variables of $D_{1,2}k$. Therefore,

$$\|\nabla_2 k(\cdot, u) - \nabla_2 k(\cdot, v)\|_{\mathcal{H}_k^d} \leq \left(2\left\|\nabla^2(D_{1,2}k)\right\|_\infty^{\frac{1}{2}} + \|\nabla_1 \nabla_2(D_{1,2}k)\|_\infty^{\frac{1}{2}}\right) d_S(u,v). \qquad (43)$$

According to (42) and (43), we get

$$\left\|\iota_{k,\rho_{u,t}}^* \nabla \log \frac{\rho_{u,t}}{\pi} - \iota_{k,\rho_{v,t}}^* \nabla \log \frac{\rho_{v,t}}{\pi}\right\|_{\mathcal{H}_k^d} \leq L_r d_s(u,v)$$

with

$$L_r = C_{1,r} \|\rho_0\|_{\mathcal{P}_V} \left(\|k\|_\infty + 2\|\nabla k\|_\infty^{\frac{1}{2}} + 3\left\|\nabla^2 k\right\|_\infty^{\frac{1}{2}} + 2\|\nabla_1 \nabla_2 k\|_\infty^{\frac{1}{2}}\right)$$
$$+ 2\left\|\nabla^2(D_{1,2}k)\right\|_\infty^{\frac{1}{2}} + \|\nabla_1 \nabla_2(D_{1,2}k)\|_\infty^{\frac{1}{2}}. \qquad (44)$$

Therefore, the second term is bounded as

$$\left|\left((1-\nu)\iota_{k,\rho_{v,t}}^* \iota_{k,\rho_{v,t}} + \nu I\right)^{-1} \left(\iota_{k,\rho_{u,t}}^* \nabla \log \frac{\rho_{u,t}}{\pi}(x) - \iota_{k,\rho_{v,t}}^* \nabla \log \frac{\rho_{v,t}}{\pi}(x)\right)\right| \leq \nu^{-1} L_r \|k\|_\infty d_S(u,v). \qquad (45)$$

The Lemma is proved based on (41) and (45). $\qquad \square$

6. Stability

In this section, we prove a stability estimate for the weak solutions to (7). To do this, we introduce a space of probability measures on $\mathbb{R}^d$ and assumptions on V as follows,

$$\mathcal{P}_p := \left\{ \rho \in \mathcal{P} : \|\rho\|_{\mathcal{P}_p} := \int_{\mathbb{R}^d} |x|^p \rho(x)dx < \infty \right\},$$

where $\mathcal{P}$ denotes the set of all probability measures on $\mathbb{R}^d$.

Assumption V2. In addition to Assumption V1, there exists a constant $C_V > 0$ and $q > 1$ such that $|\nabla V(x)|^q \leq C_V(1 + V(x))$ for all $x \in \mathbb{R}^d$ and $\sup_{\theta \in [0,1]} \left\| \nabla^2 V(\theta x + (1 - \theta)y) \right\|_2^q \leq C_V(1 + V(x) + V(y))$.

Theorem 8. *Let V satisfy Assumption V2 with $q \in (1, \infty)$ and k satisfy Assumption K1. Let p be the conjugate of q, i.e., $p^{-1} + q^{-1} = 1$. Let $\rho_1, \rho_2 \in \mathcal{P}_p$ be two initial probability measures satisfying $\|\rho_i\|_{\mathcal{P}_p} \leq R$ for some constant $R > 0$ and $i = 1, 2$. Let $\rho_{1,t}$ and $\rho_{2,t}$ be the associated weak solution to (7). Then given any $T > 0$, there exists a constant $C > 0$ depending on $k, V, q, \nu, \rho_1, \rho_2$ such that,*

$$\sup_{t \in [0,T]} \mathcal{W}_p(\rho_{1,t}, \rho_{2,t}) \leq C\mathcal{W}_p(\rho_1, \rho_2).$$

More explicitly, the constant C is given by

$$C = \exp \left(\nu^{-1} \|k\|_\infty C(T, k, V, \nu, \rho_1, \rho_2, q)T + + \nu^{-\frac{1}{2}} \left(2 \|\nabla_1 \nabla_2 k\|_\infty + 3 \|\nabla^2 k\|_\infty \right)^{\frac{1}{2}} \sqrt{\mathrm{KL}(\rho_2|\pi)} T^{\frac{1}{2}} \right.$$

$$\left. + 2\nu^{-\frac{3}{2}}(1 - \nu) \|k\|_\infty^2 \left(2 \|\nabla_1 \nabla_2 k + 3 \|\nabla^2 k\|_\infty \|_\infty \right)^{\frac{1}{2}} \sqrt{\mathrm{KL}(\rho_1|\pi)} T^{\frac{1}{2}} \right), \tag{46}$$

where $C(T, k, V, \nu, \rho_1, \rho_2, q)$ is defined in (56).

Before we prove Theorem 8, we introduce the following corollary to Theorem 8.

Corollary 1. *Suppose the assumptions in Theorem 8 hold. Let $\rho_1 \in \mathcal{P}_p$ and ρ_1^N be the empirical measure formed from N samples from ρ_1. Then for any $T > 0$,*

$$\sup_{t \in [0,T]} \mathcal{W}_p(\rho_{1,t}, \rho_{1,t}^N) \to 0, \qquad as \ N \to \infty,$$

where $\rho_{1,t}$ and $\rho_{1,t}^N$ are the unique weak solutions to (7) with initial conditions ρ_1 and ρ_1^N respectively.

Since $\mathcal{W}_p(\rho_1^N, \rho_1) \to 0$ as $N \to \infty$, Corollary 1 follows directly from Theorem 8. Non-asymptotic bounds on $\sup_{t \in [0,T]} \mathcal{W}_p(\rho_{1,t}, \rho_{1,t}^N)$ that are non-uniform in time T (i.e., for $T < \infty$) in terms of N can also be obtained based on Theorem 8 and the convergence of empirical measures in $\mathcal{W}_p$ [FG15, WB19]. We leave that to the interested reader.

Remark 12. If we focus on the dependency on ν and T in (46), we have

$$C \leq C' \exp \left(\nu^{-1} T \exp \left(C' \nu^{-\frac{1}{2}} T^{\frac{1}{2}} \right) + \nu^{-\frac{3}{2}}(1 - \nu) T^{\frac{1}{2}} + \nu^{-\frac{1}{2}} T^{\frac{1}{2}} \right)$$

where C' is a constant independent of ν and T. In particular, the stability constant blows up when $\nu \to 0$, i.e. the smaller is ν, the larger is the $\mathcal{W}_p$ distance between $\rho_{1,t}$ and $\rho_{1,t}^N$ in Corollary 1. Therefore, if we choose smaller ν in the finite-particle algorithm, the R-SVGD, we will need more particles (larger N) in order to get the comparable iteration complexities.

The proof of Theorem 8 is inspired by that of [LLN19, Theorem 2.7] which in turn is motivated by the Dobrushin's coupling argument (see, for example, [Dob79] and [MRZ16, Theorem 1.4.1]). In the following proof, we mainly highlight the parts of our proof that are different from the proof of [LLN19, Theorem 2.7].

Proof of Theorem 8. First, under Assumption V2, there exists a constant $C_0 > 0$ such that $V(x) \le C_0(1 + |x|^p)$ for all $x \in \mathbb{R}^d$. Therefore, $\mathcal{P}_p \subset \mathcal{P}_V$ and $\|\rho_i\|_{\mathcal{P}_V} \le C(R) < \infty$ for $i = 1, 2$. By Theorem 7, the weak solutions take the form

$$\rho_{i,t} = (\Phi(t, \cdot, \rho_i))_{\#\rho_i}, \quad i = 1, 2$$

where $\Phi(\cdot, \cdot, \rho_i)$ solves (28) with $\rho_0 = \rho_i$. Let $\rho^{1,2}$ be a coupling measure between ρ_1 and ρ_2. Notice that, according to conditions in Theorem 8, $p > 1$. Define $\phi(x) = \frac{1}{p}|x|^p$ and observe that $p > 1$. We have that ϕ is continuously differentiable on $\mathbb{R}^d$ with

$$|\nabla\phi(x)| = |x|^{p-1}, \quad \text{for all} \quad x \in \mathbb{R}^d.$$

To see this, note that as $p > 1$, for any $x \ne 0$, $\nabla\phi(x) = |x|^{p-2}x$ and $|\nabla\phi(x)| = |x|^{p-1}$. At $x = 0$, by definition, we have $\nabla\phi(0) = 0$. Since $p > 1$, $\nabla\phi(x)$ is continuous. Then, we start from estimating the derivative of ϕ in the time variable, for which we have

$$\partial_t\phi(\Phi(t, x_1, \rho_1) - \Phi(t, x_2, \rho_2))$$
$$= -\nabla\phi(\Phi(t, x_1, \rho_1) - \Phi(t, x_2, \rho_2))\left(\mathcal{D}_{\nu,\rho_{1,t}}\nabla\log\frac{\rho_{1,t}}{\pi}(\Phi(t, x_1, \rho_1)) - \mathcal{D}_{\nu,\rho_{2,t}}\nabla\log\frac{\rho_{2,t}}{\pi}(\Phi(t, x_2, \rho_2))\right).$$

The next step is to estimate

$$\left|\mathcal{D}_{\nu,\rho_{1,t}}\nabla\log\frac{\rho_{1,t}}{\pi}(\Phi(t, x_1, \rho_1)) - \mathcal{D}_{\nu,\rho_{2,t}}\nabla\log\frac{\rho_{2,t}}{\pi}(\Phi(t, x_2, \rho_2))\right|.$$

Note that

$$\mathcal{D}_{\nu,\rho_{1,t}}\nabla\log\frac{\rho_{1,t}}{\pi}(\Phi(t, x_1, \rho_1)) - \mathcal{D}_{\nu,\rho_{2,t}}\nabla\log\frac{\rho_{2,t}}{\pi}(\Phi(t, x_2, \rho_2)) := I_1 + I_2,$$

where

$$I_1 := \mathcal{D}_{\nu,\rho_{1,t}}\nabla\log\frac{\rho_{1,t}}{\pi}(\Phi(t, x_1, \rho_1)) - \mathcal{D}_{\nu,\rho_{2,t}}\nabla\log\frac{\rho_{2,t}}{\pi}(\Phi(t, x_1, \rho_1)),$$
$$I_2 := \mathcal{D}_{\nu,\rho_{2,t}}\nabla\log\frac{\rho_{2,t}}{\pi}(\Phi(t, x_1, \rho_1)) - \mathcal{D}_{\nu,\rho_{2,t}}\nabla\log\frac{\rho_{2,t}}{\pi}(\Phi(t, x_2, \rho_2)).$$

According to Proposition 5, we have

$$|-\nabla\phi(\Phi(t, x_1, \rho_1) - \Phi(t, x_2, \rho_2)) \cdot I_1|$$
$$\le 2\nu^{-\frac{3}{2}}(1-\nu)\|k\|_\infty^2 \left(2\|\nabla_1\nabla_2 k\|_\infty + 3\|\nabla^2 k\|_\infty\right)^{\frac{1}{2}} I_{\nu,Stein}(\rho_{1,t}|\pi)^{\frac{1}{2}}|\Phi(t, x_1, \rho_1) - \Phi(t, x_2, \rho_2)|^{p-1}$$
$$\times \left(\int_{\mathbb{R}^d} |\Phi(t, y_1, \rho_1) - \Phi(t, y_2, \rho_2)|\rho^{1,2}(dy_1, dy_2)\right)$$
$$+ \nu^{-1}\|k\|_\infty C(t, k, V, \nu, \rho_1, \rho_2, q)|\Phi(t, x_1, \rho_1) - \Phi(t, x_2, \rho_2)|^{p-1}$$
$$\times \left(\int_{\mathbb{R}^d \times \mathbb{R}^d} |\Phi(t, y_1, \rho_1) - \Phi(t, y_2, \rho_2)|^p\rho^{1,2}(dy_1, dy_2)\right)^{1/p}$$

and

$$|-\nabla\phi(\Phi(t, x_1, \rho_1) - \Phi(t, x_2, \rho_2)) \cdot I_2|$$
$$\le \nu^{-\frac{1}{2}}\left(2\|\nabla_1\nabla_2 k\|_\infty + 3\|\nabla^2 k\|_\infty\right)^{\frac{1}{2}} I_{\nu,Stein}(\rho_{2,t}|\pi)^{\frac{1}{2}}|\Phi(t, x_1, \rho_1) - \Phi(t, x_2, \rho_2)|^p.$$

Now, defining

$$D_p(\rho^{1,2})(s) := \left(\int_{\mathbb{R}^d \times \mathbb{R}^d} |\Phi(s, y_1, \rho_1) - \Phi(s, y_2, \rho_2)|^p\rho^{1,2}(dy_1, dy_2)\right)^{1/p},$$

we have, for any $t \in [0, T]$ that

$$\phi(\Phi(t, x_1, \rho_1) - \Phi(t, x_2, \rho_2))$$

$$\leq \nu^{-\frac{1}{2}} \left(2 \left\|\nabla_1 \nabla_2 k\right\|_\infty + 3 \left\|\nabla^2 k\right\|_\infty\right)^{\frac{1}{2}} \int_0^t I_{\nu,Stein}(\rho_{2,s}|\pi)^{\frac{1}{2}} |\Phi(s, x_1, \rho_1) - \Phi(s, x_2, \rho_2)|^p ds$$

$$+ \phi(x_1 - x_2) + \nu^{-1} \left\|k\right\|_\infty C(T, k, V, \nu, \rho_1, \rho_2, q) \int_0^t |\Phi(s, x_1, \rho_1) - \Phi(s, x_2, \rho_2)|^{p-1} D_p(\rho^{1,2})(s) ds$$

$$+ 2\nu^{-\frac{3}{2}}(1 - \nu) \left\|k\right\|_\infty^2 \left(2 \left\|\nabla_1 \nabla_2 k\right\|_\infty + 3 \left\|\nabla^2 k\right\|_\infty\right)^{\frac{1}{2}}$$

$$\times \int_0^t I_{\nu,Stein}(\rho_{1,s}|\pi)^{\frac{1}{2}} |\Phi(s, x_1, \rho_1) - \Phi(s, x_2, \rho_2)|^{p-1} D_p(\rho^{1,2})(s) ds.$$

Integrating the above inequality w.r.t. the coupling $\rho^{1,2}$, and using the fact that

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} |\Phi(t, x_1, \rho_1) - \Phi(t, x_2, \rho_2)|^{p-1} \rho^{1,2}(dx_1, dx_2) \leq D_p(\rho^{1,2})(t)^{p-1},$$

we get

$$D_p(\rho^{1,2})(t)^p \leq D_p(\rho^{1,2})(0)^p + \nu^{-1} \left\|k\right\|_\infty C(T, k, V, \nu, \rho_1, \rho_2, q) \int_0^t D_p(\rho^{1,2})(s)^p ds$$

$$+ 2\nu^{-\frac{3}{2}}(1 - \nu) \left\|k\right\|_\infty^2 \left(2 \left\|\nabla_1 \nabla_2 k\right\|_\infty + 3 \left\|\nabla^2 k\right\|_\infty\right)^{\frac{1}{2}} \int_0^t I_{\nu,Stein}(\rho_{1,s}|\pi)^{\frac{1}{2}} D_p(\rho^{1,2})(s)^p ds$$

$$+ \left(\nu^{-\frac{1}{2}} \left(2 \left\|\nabla_1 \nabla_2 k\right\|_\infty + 3 \left\|\nabla^2 k\right\|_\infty\right)^{\frac{1}{2}}\right) \int_0^t I_{\nu,Stein}(\rho_{2,s}|\pi)^{\frac{1}{2}} D_p(\rho^{1,2})(s)^p ds.$$

By using Gronwall's inequality, we further obtain

$$D_p(\rho^{1,2})(t)^p$$
$$\leq D_p(\rho^{1,2})(0)^p \exp\left(\nu^{-1} \left\|k\right\|_\infty C(T, k, V, \nu, \rho_1, \rho_2, q) t\right)$$

$$\times \exp\left(2\nu^{-\frac{3}{2}}(1 - \nu) \left\|k\right\|_\infty^2 \left(2 \left\|\nabla_1 \nabla_2 k\right\|_\infty + 3 \left\|\nabla^2 k\right\|_\infty\right)^{\frac{1}{2}} \int_0^t I_{\nu,Stein}(\rho_{1,s}|\pi)^{\frac{1}{2}} ds\right)$$

$$\times \exp\left(\nu^{-\frac{1}{2}} \left(2 \left\|\nabla_1 \nabla_2 k\right\|_\infty + 3 \left\|\nabla^2 k\right\|_\infty\right)^{\frac{1}{2}} \int_0^t I_{\nu,Stein}(\rho_{2,s}|\pi)^{\frac{1}{2}} ds\right)$$

$$\leq D_p(\rho^{1,2})(0)^p \exp\left(\nu^{-\frac{1}{2}} \left(2 \left\|\nabla_1 \nabla_2 k\right\|_\infty + 3 \left\|\nabla^2 k\right\|_\infty\right)^{\frac{1}{2}} \sqrt{KL(\rho_2|\pi)} t^{\frac{1}{2}}\right.$$

$$+ \nu^{-1} \left\|k\right\| C(T, k, V, \nu, \rho_1, \rho_2, q) t + 2\nu^{-\frac{3}{2}}(1 - \nu) \left\|k\right\|_\infty^2 \left(2 \left\|\nabla_1 \nabla_2 k\right\|_\infty + 3 \left\|\nabla^2 k\right\|_\infty\right)^{\frac{1}{2}} \sqrt{KL(\rho_1|\pi)} t^{\frac{1}{2}}\bigg).$$

Hence, we obtain

$$\mathcal{W}_p^p(\rho_{1,t}, \rho_{2,t})$$

$$= \inf_{\pi \in \Gamma(\rho_{1,t}, \rho_{2,t})} \int_{\mathbb{R}^d \times \mathbb{R}^d} |x_1 - x_2|^p \pi(dx_1, dx_2) \leq \inf_{\rho^{1,2} \in \Gamma(\rho_1, \rho_2)} D_p(\rho^{1,2})(t)^p$$

$$\leq \exp\left(\nu^{-1} \left\|k\right\|_\infty C(T, k, V, \nu, \rho_1, \rho_2, q) t + \nu^{-\frac{1}{2}} \left(2 \left\|\nabla_1 \nabla_2 k\right\|_\infty + 3 \left\|\nabla^2 k\right\|_\infty\right)^{\frac{1}{2}} \sqrt{KL(\rho_2|\pi)} t^{\frac{1}{2}}\right.$$

$$+ 2\nu^{-\frac{3}{2}}(1 - \nu) \left\|k\right\|_\infty^2 \left(2 \left\|\nabla_1 \nabla_2 k\right\|_\infty + 3 \left\|\nabla^2 k\right\|_\infty\right)^{\frac{1}{2}} \sqrt{KL(\rho_1|\pi)} t^{\frac{1}{2}}\bigg) \inf_{\rho^{1,2} \in \Gamma(\rho_1, \rho_2)} D_p(\rho^{1,2})(0)^p$$

$$= \exp\left(\nu^{-1} \left\|k\right\|_\infty C(T, k, V, \nu, \rho_1, \rho_2, q) t + \nu^{-\frac{1}{2}} \left(2 \left\|\nabla_1 \nabla_2 k\right\|_\infty + 3 \left\|\nabla^2 k\right\|_\infty\right)^{\frac{1}{2}} \sqrt{KL(\rho_2|\pi)} t^{\frac{1}{2}}\right.$$

$$+ 2\nu^{-\frac{3}{2}}(1-\nu)\|k\|_\infty^2 \left(2\|\nabla_1\nabla_2 k\|_\infty + 3\|\nabla^2 k\|_\infty\right)^{\frac{1}{2}} \sqrt{\mathrm{KL}(\rho_1|\pi)} t^{\frac{1}{2}}\right) \mathcal{W}_p^p(\rho_1,\rho_2),$$

yielding the result. $\qquad\square$

Note that in Lemma 4, we studied perturbation bounds for (28) under two different push-forward maps. In the next result, with the existence and uniqueness of solutions proved in Theorem 7, we study perturbation results for (7) with two different initial conditions.

Proposition 5. *Under the assumptions of Theorem 8, Let $\rho^{1,2}$ be a probability measure on $\mathbb{R}^{2d}$ with marginals ρ_1 and ρ_2. Then for any $x,y \in \mathbb{R}^d$, we have*

$$\left|\mathcal{D}_{\nu,\rho_{2,t}}\nabla\log\frac{\rho_{2,t}}{\pi}(x) - \mathcal{D}_{\nu,\rho_{2,t}}\nabla\log\frac{\rho_{2,t}}{\pi}(y)\right|$$
$$\leq \nu^{-\frac{1}{2}}\left(2\|\nabla_1\nabla_2 k\|_\infty + 3\|\nabla^2 k\|_\infty\right)^{\frac{1}{2}} I_{\nu,Stein}(\rho_{2,t}|\pi)^{\frac{1}{2}} |x-y|, \tag{47}$$

and

$$\left|\mathcal{D}_{\nu,\rho_{1,t}}\nabla\log\frac{\rho_{1,t}}{\pi}(x) - \mathcal{D}_{\nu,\rho_{2,t}}\nabla\log\frac{\rho_{2,t}}{\pi}(x)\right|$$
$$\leq 2\nu^{-\frac{3}{2}}(1-\nu)\|k\|_\infty^2 \left(2\|\nabla_1\nabla_2 k\|_\infty + 3\|\nabla^2 k\|_\infty\right)^{\frac{1}{2}} I_{\nu,Stein}(\rho_{1,t}|\pi)^{\frac{1}{2}}$$
$$\times \int_{\mathbb{R}^d}|\Phi(t,x_1,\rho_1) - \Phi(t,x_2,\rho_2)|\rho^{1,2}(dx_1,dx_2)$$
$$+ \nu^{-1}\|k\|_\infty C(t,k,V,\nu,\rho_1,\rho_2,q)\left(\int_{\mathbb{R}^d\times\mathbb{R}^d}|\Phi(t,y_1,\rho_1) - \Phi(t,y_2,\rho_2)|^p \rho^{1,2}(dy_1,dy_2)\right)^{1/p}, \tag{48}$$

where $C(t,k,V,\nu,\rho_1,\rho_2,q)$ is given in (56).

Proof of Proposition 5. First, we prove (47). For any $x,y \in \mathbb{R}^d$,

$$\left|\mathcal{D}_{\nu,\rho_{2,t}}\nabla\log\frac{\rho_{2,t}}{\pi}(x) - \mathcal{D}_{\nu,\rho_{2,t}}\nabla\log\frac{\rho_{2,t}}{\pi}(y)\right|$$
$$= \left|\left((1-\nu)\iota_{k,\rho_{2,t}}^*\iota_{k,\rho_{2,t}} + \nu I_d\right)^{-1}\iota_{k,\rho_{2,t}}^*\nabla\log\frac{\rho_{2,t}}{\pi}(x)\right.$$
$$\left. - \left((1-\nu)\iota_{k,\rho_{2,t}}^*\iota_{k,\rho_{2,t}} + \nu I_d\right)^{-1}\iota_{k,\rho_{2,t}}^*\nabla\log\frac{\rho_{2,t}}{\pi}(y)\right|$$
$$= \left|\left\langle k(x,\cdot) - k(y,\cdot), \left((1-\nu)\iota_{k,\rho_{2,t}}^*\iota_{k,\rho_{2,t}} + \nu I_d\right)^{-1}\iota_{k,\rho_{2,t}}^*\nabla\log\frac{\rho_{2,t}}{\pi}(\cdot)\right\rangle_{\mathcal{H}_k}\right|$$
$$\leq \|k(x,\cdot) - k(y,\cdot)\|_{\mathcal{H}_k}\left\|\left((1-\nu)\iota_{k,\rho_{2,t}}^*\iota_{k,\rho_{2,t}} + \nu I_d\right)^{-1}\iota_{k,\rho_{2,t}}^*\nabla\log\frac{\rho_{2,t}}{\pi}\right\|_{\mathcal{H}_k^d}$$
$$\leq \nu^{-\frac{1}{2}}I_{\nu,Stein}(\rho_{2,t}|\pi)^{\frac{1}{2}}\|k(x,\cdot) - k(y,\cdot)\|_{\mathcal{H}_k^d}$$
$$\leq \nu^{-\frac{1}{2}}I_{\nu,Stein}(\rho_{2,t}|\pi)^{\frac{1}{2}}\left(2\|\nabla_1\nabla_2 k\|_\infty + 3\|\nabla^2 k\|_\infty\right)^{\frac{1}{2}}|x-y|,$$

where the second inequality follows from (33) and the last inequality follows from the reproducing property and Taylor expansion. The claim in (47) then follows from the above inequality.

To prove (48), first we have for any $x \in \mathbb{R}^d$,

$$\left|\mathcal{D}_{\nu,\rho_{1,t}}\nabla\log\frac{\rho_{1,t}}{\pi}(x) - \mathcal{D}_{\nu,\rho_{2,t}}\nabla\log\frac{\rho_{2,t}}{\pi}(x)\right|$$
$$\leq \left|\left(\left((1-\nu)\iota_{k,\rho_{1,t}}^*\iota_{k,\rho_{1,t}} + \nu I_d\right)^{-1} - \left((1-\nu)\iota_{k,\rho_{2,t}}^*\iota_{k,\rho_{2,t}} + \nu I_d\right)^{-1}\right)\iota_{k,\rho_{1,t}}^*\nabla\log\frac{\rho_{1,t}}{\pi}(x)\right|$$

$$+ \left| \left((1-\nu) \iota_{k,\rho_{2,t}}^* \iota_{k,\rho_{2,t}} + \nu I_d \right)^{-1} \left(\iota_{k,\rho_{1,t}}^* \nabla \log \frac{\rho_{1,t}}{\pi}(x) - \iota_{k,\rho_{2,t}}^* \nabla \log \frac{\rho_{2,t}}{\pi}(x) \right) \right|. \tag{49}$$

Next we bound the two terms on the right-hand side of (49).

First term: we have

$$\left| \left(\left((1-\nu) \iota_{k,\rho_{1,t}}^* \iota_{k,\rho_{1,t}} + \nu I_d \right)^{-1} - \left((1-\nu) \iota_{k,\rho_{2,t}}^* \iota_{k,\rho_{2,t}} + \nu I_d \right)^{-1} \right) \iota_{k,\rho_{1,t}}^* \nabla \log \frac{\rho_{1,t}}{\pi}(x) \right|$$

$$= \left| \iota_{k,\rho_{1,t}} \left((1-\nu) \iota_{k,\rho_{2,t}}^* \iota_{k,\rho_{2,t}} + \nu I \right)^{-1} \left((1-\nu) \iota_{k,\rho_{2,t}}^* \iota_{k,\rho_{2,t}} - (1-\nu) \iota_{k,\rho_{1,t}}^* \iota_{k,\rho_{1,t}} \right) \right.$$

$$\left. \times \left((1-\nu) \iota_{k,\rho_{1,t}}^* \iota_{k,\rho_{1,t}} + \nu I \right)^{-1} \iota_{k,\rho_{1,t}}^* \nabla \log \frac{\rho_{1,t}}{\pi}(x) \right|$$

$$\leq \left\| \iota_{k,\rho_{1,t}} \right\|_{\mathcal{H}_k^d \to L_\infty^d} \left\| \left((1-\nu) \iota_{k,\rho_{2,t}}^* \iota_{k,\rho_{2,t}} + \nu I \right)^{-1} \right\|_{\mathcal{H}_k^d \to \mathcal{H}_k^d} (1-\nu) \left\| \iota_{k,\rho_{2,t}}^* \iota_{k,\rho_{2,t}} - \iota_{k,\rho_{1,t}}^* \iota_{k,\rho_{1,t}} \right\|_{\mathcal{H}_k^d \to \mathcal{H}_k^d}$$

$$\times \left\| \left((1-\nu) \iota_{k,\rho_{1,t}}^* \iota_{k,\rho_{1,t}} + \nu I \right)^{-1} \iota_{k,\rho_{1,t}}^* \nabla \log \frac{\rho_{1,t}}{\pi} \right\|_{\mathcal{H}_k^d}$$

$$\leq \|k\|_\infty \nu^{-\frac{3}{2}} (1-\nu) I_{\nu,Stein}(\rho_{1,t}|\pi)^{\frac{1}{2}}$$

$$\sup_{\|\phi\|_{\mathcal{H}_k^d}=1} \left\langle \int_{\mathbb{R}^d} k(\cdot,x)\phi(x)(d\rho_{1,t}(x) - d\rho_{2,t}(x)), \int_{\mathbb{R}^d} k(\cdot,y)\phi(y)(d\rho_{1,t}(y) - d\rho_{2,t}(y)) \right\rangle_{\mathcal{H}_k^d}^{\frac{1}{2}},$$

and

$$\sup_{\|\phi\|_{\mathcal{H}_k^d}=1} \left\langle \int_{\mathbb{R}^d} k(\cdot,x)\phi(x)(d\rho_{1,t}(x) - d\rho_{2,t}(x)), \int_{\mathbb{R}^d} k(\cdot,y)\phi(y)(d\rho_{1,t}(y) - d\rho_{2,t}(y)) \right\rangle_{\mathcal{H}_k^d}^{\frac{1}{2}}$$

$$= \left(\sup_{\|\phi\|_{\mathcal{H}_k^d}=1} \int_{\mathbb{R}^d \times \mathbb{R}^d} \int_{\mathbb{R}^d \times \mathbb{R}^d} \left\langle k\left(\Phi(t,x_1,\rho_1),\cdot\right) \phi\left(\Phi(t,x_1,\rho_1)\right) - k\left(\Phi(t,x_2,\rho_2),\cdot\right) \phi\left(\Phi(t,x_2,\rho_2)\right), \right. \right.$$

$$\left. k\left(\Phi(t,y_1,\rho_1),\cdot\right) \phi\left(\Phi(t,y_1,\rho_1)\right) - k\left(\Phi(t,y_2,\rho_2),\cdot\right) \phi\left(\Phi(t,y_2,\rho_2)\right) \right\rangle_{\mathcal{H}_k^d} \rho^{1,2}(dx_1,dx_2)\rho^{1,2}(dy_1,y_2) \right)^{\frac{1}{2}}$$

$$\leq \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \left\| k\left(\Phi(t,x_1,\rho_1),\cdot\right) \phi\left(\Phi(t,x_1,\rho_1)\right) - k\left(\Phi(t,x_2,\rho_2),\cdot\right) \phi\left(\Phi(t,x_2,\rho_2)\right) \right\|_{\mathcal{H}_k^d} \rho^{1,2}(dx_1,dx_2)$$

$$\leq 2 \|k\|_\infty \left(2 \|\nabla_1 \nabla_2 k\|_\infty + 3 \left\| \nabla^2 k \right\|_\infty \right)^{\frac{1}{2}} \int_{\mathbb{R}^d \times \mathbb{R}^d} |\Phi(t,x_1,\rho_1) - \Phi(t,x_2,\rho_2)| \rho^{1,2}(dx_1,dx_2).$$

Second term: we have

$$\left| \left((1-\nu) \iota_{k,\rho_{2,t}}^* \iota_{k,\rho_{2,t}} + \nu I \right)^{-1} \left(\iota_{k,\rho_{1,t}}^* \nabla \log \frac{\rho_{1,t}}{\pi}(x) - \iota_{k,\rho_{2,t}}^* \nabla \log \frac{\rho_{2,t}}{\pi}(x) \right) \right|$$

$$= \left| \iota_{k,\rho_{2,t}} \left((1-\nu) \iota_{k,\rho_{2,t}}^* \iota_{k,\rho_{2,t}} + \nu I \right)^{-1} \left(\iota_{k,\rho_{1,t}}^* \nabla \log \frac{\rho_{1,t}}{\pi}(x) - \iota_{k,\rho_{2,t}}^* \nabla \log \frac{\rho_{2,t}}{\pi}(x) \right) \right|$$

$$\leq \left\| \iota_{k,\rho_{2,t}} \right\|_{\mathcal{H}_k^d \to L_\infty^d} \left\| \left((1-\nu) \iota_{k,\rho_{2,t}}^* \iota_{k,\rho_{2,t}} + \nu I \right)^{-1} \right\|_{\mathcal{H}_k^d \to \mathcal{H}_k^d} \left\| \iota_{k,\rho_{1,t}}^* \nabla \log \frac{\rho_{1,t}}{\pi} - \iota_{k,\rho_{2,t}}^* \nabla \log \frac{\rho_{2,t}}{\pi} \right\|_{\mathcal{H}_k^d}$$

$$\leq \|k\|_\infty \nu^{-1} \left\| \iota_{k,\rho_{1,t}}^* \nabla \log \frac{\rho_{1,t}}{\pi} - \iota_{k,\rho_{2,t}}^* \nabla \log \frac{\rho_{2,t}}{\pi} \right\|_{\mathcal{H}_k^d}.$$

For the factor $\left\| \iota_{k,\rho_{1,t}}^* \nabla \log \frac{\rho_{1,t}}{\pi} - \iota_{k,\rho_{2,t}}^* \nabla \log \frac{\rho_{2,t}}{\pi} \right\|_{\mathcal{H}_k^d}$, notice that

$$\iota_{k,\rho_{1,t}}^* \nabla \log \frac{\rho_{1,t}}{\pi}(x) - \iota_{k,\rho_{2,t}}^* \nabla \log \frac{\rho_{2,t}}{\pi}(x)$$

$$= \int_{\mathbb{R}^d} k(x,y) \nabla \log \frac{\rho_{1,t}}{\pi}(y) d\rho_{1,t}(y) - \int_{\mathbb{R}^d} k(x,y) \nabla \log \frac{\rho_{2,t}}{\pi} d\rho_{2,t}(y)$$

$$= \int_{\mathbb{R}^d} \left(k(x,y) \nabla V(y) - \nabla_2 k(x,y) \right) d\rho_{1,t}(y) - \int_{\mathbb{R}^d} \left(k(x,y) \nabla V(y) - \nabla_2 k(x,y) \right) d\rho_{2,t}(y)$$

$$= \int_{\mathbb{R}^d \times \mathbb{R}^d} \left(k(x, \Phi(t,y_1,\rho_1)) \nabla V(\Phi(t,y_1,\rho_1)) - k(x, \Phi(t,y_2,\rho_2)) \nabla V(\Phi(t,y_2,\rho_2)) \right) d\rho^{1,2}(dy_1, dy_2)$$

$$- \int_{\mathbb{R}^d \times \mathbb{R}^d} \left(\nabla_2 k(x, \Phi(t,y_1,\rho_1)) - \nabla_2 k(x, \Phi(t,y_2,\rho_2)) \right) d\rho^{1,2}(dy_1, dy_2),$$

and we get

$$\left\| \iota_{k,\rho_{1,t}}^* \nabla \log \frac{\rho_{1,t}}{\pi} - \iota_{k,\rho_{2,t}}^* \nabla \log \frac{\rho_{2,t}}{\pi} \right\|_{\mathcal{H}_k^d}$$

$$\leq \int_{\mathbb{R}^d \times \mathbb{R}^d} \| k(\cdot, \Phi(t,y_1,\rho_1)) \nabla V(\Phi(t,y_1,\rho_1)) - k(\cdot, \Phi(t,y_2,\rho_2)) \nabla V(\Phi(t,y_2,\rho_2)) \|_{\mathcal{H}_k^d} d\rho^{1,2}(dy_1, dy_2)$$

$$+ \int_{\mathbb{R}^d \times \mathbb{R}^d} \| \nabla_2 k(\cdot, \Phi(t,y_1,\rho_1)) - \nabla_2 k(\cdot, \Phi(t,y_2,\rho_2)) \|_{\mathcal{H}_k^d} d\rho^{1,2}(dy_1, dy_2). \tag{50}$$

For simplicity, we denote $\Phi(t,y_1,\rho_1), \Phi(t,y_2,\rho_2)$ as Φ_1 and Φ_2 respectively in the following calculations. We will bound the two integrals in (50) separately.

For the first integral in (50), we have

$$\| k(\cdot, \Phi_1) \nabla V(\Phi_1) - k(\cdot, \Phi_2) \nabla V(\Phi_2) \|_{\mathcal{H}_k^d}^2$$

$$= \langle k(\cdot, \Phi_1) \nabla V(\Phi_1) - k(\cdot, \Phi_2) \nabla V(\Phi_2), k(\cdot, \Phi_1) \nabla V(\Phi_1) - k(\cdot, \Phi_2) \nabla V(\Phi_2) \rangle_{\mathcal{H}_k^d}$$

$$= |\nabla V(\Phi_1)|^2 k(\Phi_1, \Phi_1) - 2 \langle \nabla V(\Phi_1), \nabla V(\Phi_2) \rangle k(\Phi_1, \Phi_2) + |\nabla V(\Phi_2)|^2 k(\Phi_2, \Phi_2)$$

$$\leq |\langle \nabla V(\Phi_1) - \nabla V(\Phi_2), \nabla V(\Phi_1) k(\Phi_1, \Phi_1) - \nabla V(\Phi_2) k(\Phi_2, \Phi_2) \rangle|$$

$$+ |\langle \nabla V(\Phi_1), \nabla V(\Phi_2) \rangle (k(\Phi_1, \Phi_1) + k(\Phi_2, \Phi_2) - 2k(\Phi_1, \Phi_2))|,$$

where

$$|\langle \nabla V(\Phi_1) - \nabla V(\Phi_2), \nabla V(\Phi_1) k(\Phi_1, \Phi_1) - \nabla V(\Phi_2) k(\Phi_2, \Phi_2) \rangle|$$

$$\leq |\nabla V(\Phi_1) - \nabla V(\Phi_2)|^2 k(\Phi_1, \Phi_1) + |\nabla V(\Phi_1) - \nabla V(\Phi_2)||\nabla V(\Phi_2)||k(\Phi_1, \Phi_1) - k(\Phi_2, \Phi_2)|$$

$$\leq \sup_{\theta \in [0,1]} \left\| \nabla^2 (\theta \Phi_1 + (1-\theta)\Phi_2) \right\|_2^2 |\Phi_1 - \Phi_2|^2 \| k \|_\infty^2$$

$$+ \sup_{\theta \in [0,1]} \left\| \nabla^2 (\theta \Phi_1 + (1-\theta)\Phi_2) \right\|_2 |\Phi_1 - \Phi_2||\nabla V(\Phi_2)||k(\Phi_1, \Phi_1) - k(\Phi_2, \Phi_2)|$$

$$\leq C_V^{2/q} (1 + V(\Phi_1) + V(\Phi_2))^{2/q} \| k \|_\infty^2 |\Phi_1 - \Phi_2|^2$$

$$+ C_V^{1/q} (1 + V(\Phi_1) + V(\Phi_2))^{1/q} C_V^{1/q} (1 + V(\Phi_2))^{1/q} \| \nabla k \|_\infty |\Phi_1 - \Phi_2|^2$$

$$\leq C_V^{2/q} \left(\| k \|_\infty^2 + \| \nabla k \|_\infty \right) (1 + V(\Phi_1) + V(\Phi_2))^{2/q} |\Phi_1 - \Phi_2|^2. \tag{51}$$

The third inequality follows from Assumption V2 and the last inequality follows from Assumption K1 and Taylor expansion on both variables in k up to first order. Furthermore, we have

$$|\langle \nabla V(\Phi_1), \nabla V(\Phi_2) \rangle (k(\Phi_1, \Phi_1) + k(\Phi_2, \Phi_2) - 2k(\Phi_1, \Phi_2))|$$

$$\leq C_V^{2/q}(1 + V(\Phi_1))^{1/q}(1 + V(\Phi_2))^{1/q}|k(\Phi_1, \Phi_1) + k(\Phi_2, \Phi_2) - 2k(\Phi_1, \Phi_2)|$$

$$\leq C_V^{2/q}(1 + V(\Phi_1))^{1/q}(1 + V(\Phi_2))^{1/q}\left(3\left\|\nabla^2 k\right\|_\infty + 2\left\|\nabla_1 \nabla_2 k\right\|_\infty\right)|\Phi_1 - \Phi_2|^2, \tag{52}$$

where the first inequality follows from Assumption V2 and the last inequality follows from Assumption K1 and Taylor expansion on both variables in k up to second order.

From (51) and (52), we get

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} \|k(\cdot, \Phi(t, y_1, \rho_1))\nabla V(\Phi(t, y_1, \rho_1)) - k(\cdot, \Phi(t, y_2, \rho_2))\nabla V(\Phi(t, y_2, \rho_2))\|_{\mathcal{H}_k^d} d\rho^{1,2}(dy_1, dy_2)$$

$$\leq C_V^{1/q}\left(\|k\|_\infty + \|\nabla k\|_\infty^{\frac{1}{2}} + 3\|\nabla^2 k\|_\infty^{\frac{1}{2}} + 2\|\nabla_1 \nabla_2 k\|_\infty^{\frac{1}{2}}\right)$$

$$\times \int_{\mathbb{R}^d \times \mathbb{R}^d} |\Phi_1(t, y_1, \rho_1) - \Phi(t, y_2, \rho_2)|(1 + V(\Phi(t, y_1, \rho_1)) + V(\Phi(t, y_2, \rho_2)))^{1/q}\rho^{1,2}(dy_1, dy_2)$$

$$\leq C_V^{1/q}\left(\|k\|_\infty + \|\nabla k\|_\infty^{\frac{1}{2}} + 3\|\nabla^2 k\|_\infty^{\frac{1}{2}} + 2\|\nabla_1 \nabla_2 k\|_\infty^{\frac{1}{2}}\right)$$

$$\times \left(\int_{\mathbb{R}^d \times \mathbb{R}^d} |\Phi_1(t, y_1, \rho_1) - \Phi(t, y_2, \rho_2)|^p \rho^{1,2}(dy_1, dy_2)\right)^{1/p}$$

$$\times \left(\int_{\mathbb{R}^d \times \mathbb{R}^d} \left(1 + V(\Phi(t, y_1, \rho_1)) + V(\Phi(t, y_2, \rho_2))\right)\rho^{1,2}(dy_1, dy_2)\right)^{1/q}$$

$$\leq \left(\|\rho_1\|_{\mathcal{P}_V} \exp(C_{1,0}\nu^{-1/2}\|k\|_\infty \sqrt{t\mathrm{KL}(\rho_1|\pi)})\right.$$

$$\left. + \|\rho_2\|_{\mathcal{P}_V} \exp(C_{1,0}\nu^{-1/2}\|k\|_\infty \sqrt{t\mathrm{KL}(\rho_2|\pi))}\right)^{1/q}$$

$$\times C_V^{1/q}\left(\|k\|_\infty + \|\nabla k\|_\infty^{\frac{1}{2}} + 3\|\nabla^2 k\|_\infty^{\frac{1}{2}} + 2\|\nabla_1 \nabla_2 k\|_\infty^{\frac{1}{2}}\right)$$

$$\times \left(\int_{\mathbb{R}^d \times \mathbb{R}^d} |\Phi_1(t, y_1, \rho_1) - \Phi(t, y_2, \rho_2)|^p \rho^{1,2}(dy_1, dy_2)\right)^{1/p}$$

$$\leq 3C_V^{1/q}\left(\|k\|_\infty + \|\nabla k\|_\infty^{\frac{1}{2}} + \left\|\nabla^2 k\right\|_\infty^{\frac{1}{2}} + \|\nabla_1 \nabla_2 k\|_\infty^{\frac{1}{2}}\right)\left(\|\rho_1\|_{\mathcal{P}_V} + \|\rho_2\|_{\mathcal{P}_V}\right)^{1/q}$$

$$\times \exp(C_{1,0}\nu^{-1/2}q^{-1}\|k\|_\infty \sqrt{t(\mathrm{KL}(\rho_1|\pi) + \mathrm{KL}(\rho_2|\pi))})$$

$$\times \left(\int_{\mathbb{R}^d \times \mathbb{R}^d} |\Phi_1(t, y_1, \rho_1) - \Phi(t, y_2, \rho_2)|^p \rho^{1,2}(dy_1, dy_2)\right)^{1/p}$$

$$:= C_1(k, V)\left(\|\rho_1\|_{\mathcal{P}_V} + \|\rho_2\|_{\mathcal{P}_V}\right)^{\frac{1}{q}} \exp\left(D_1(k, \nu, q)\left(\mathrm{KL}(\rho_1|\pi) + \mathrm{KL}(\rho_2|\pi)\right)^{\frac{1}{2}} t^{\frac{1}{2}}\right)$$

$$\times \left(\int_{\mathbb{R}^d \times \mathbb{R}^d} |\Phi_1(t, y_1, \rho_1) - \Phi(t, y_2, \rho_2)|^p \rho^{1,2}(dy_1, dy_2)\right)^{1/p}. \tag{53}$$

where the third inequality follows from (35).

For the second integral in (50), denoting the function $\nabla_1 \cdot \nabla_2 k = D_{1,2}k$, we first notice that $D_{1,2}k$ is symmetric since k is symmetric. According to the above identity, we get

$$\|\nabla_2 k(\cdot, \Phi_1) - \nabla_2 k(\cdot, \Phi_2)\|_{\mathcal{H}_k^d}^2 = D_{1,2}k(\Phi_1, \Phi_1) + D_{1,2}k(\Phi_2, \Phi_2) - 2D_{1,2}k(\Phi_1, \Phi_2).$$

Applying Taylor's series expansion on both variables of $D_{1,2}k$, we get

$$\|\nabla_2 k(\cdot, \Phi_1) - \nabla_2 k(\cdot, \Phi_2)\|_{\mathcal{H}_k^d}^2 \leq \left(2\left\|\nabla^2(D_{1,2}k)\right\|_\infty + \|\nabla_1 \nabla_2(D_{1,2}k)\|_\infty\right)|\Phi_1 - \Phi_2|^2.$$

Therefore we obtain

$$\int_{\mathbb{R}^d} \|\nabla_2 k(\cdot, \Phi(t, y_1, \rho_1)) - \nabla_2 k(\cdot, \Phi(t, y_2, \rho_2))\|_{\mathcal{H}_k^d} \, d\rho^{1,2}(dy_1, dy_2)$$

$$\leq \left(2\|\nabla^2(D_{1,2}k)\|_\infty^{\frac{1}{2}} + \|\nabla_1\nabla_2(D_{1,2}k)\|_\infty^{\frac{1}{2}}\right) \int_{\mathbb{R}^d \times \mathbb{R}^d} |\Phi(t, y_1, \rho_1) - \Phi(t, y_2, \rho_2)| \rho^{1,2}(dy_1, dy_2). \quad (54)$$

Based on (50), (53) and (54), we then get

$$\left\| \iota_{k,\rho_{1,t}}^* \nabla \log \frac{\rho_{1,t}}{\pi} - \iota_{k,\rho_{2,t}}^* \nabla \log \frac{\rho_{2,t}}{\pi} \right\|_{\mathcal{H}_k^d}$$

$$\leq C_1(k, V) \left(\|\rho_1\|_{\mathcal{P}_V} + \|\rho_2\|_{\mathcal{P}_V}\right)^{\frac{1}{q}} \exp\left(D_1(k, \nu, q) \left(\mathrm{KL}(\rho_1|\pi) + \mathrm{KL}(\rho_2|\pi)\right)^{\frac{1}{2}} t^{\frac{1}{2}}\right)$$

$$\left(\int_{\mathbb{R}^d \times \mathbb{R}^d} |\Phi_1(t, y_1, \rho_1) - \Phi(t, y_2, \rho_2)|^p \rho^{1,2}(dy_1, dy_2)\right)^{1/p}$$

$$+ \left(2\|\nabla^2(D_{1,2}k)\|_\infty^{\frac{1}{2}} + \|\nabla_1\nabla_2(D_{1,2}k)\|_\infty^{\frac{1}{2}}\right) \int_{\mathbb{R}^d \times \mathbb{R}^d} |\Phi(t, y_1, \rho_1) - \Phi(t, y_2, \rho_2)| \rho^{1,2}(dy_1, dy_2)$$

$$\leq C(t, k, V, \nu, \rho_1, \rho_2, q) \left(\int_{\mathbb{R}^d \times \mathbb{R}^d} |\Phi_1(t, y_1, \rho_1) - \Phi(t, y_2, \rho_2)|^p \rho^{1,2}(dy_1, dy_2)\right)^{1/p}, \quad (55)$$

with

$$C(t, k, V, \nu, \rho_1, \rho_2, q)$$

$$= C_1(k, V) \left(\|\rho_1\|_{\mathcal{P}_V} + \|\rho_2\|_{\mathcal{P}_V}\right)^{\frac{1}{q}} \exp\left(D_1(k, \nu, q) \left(\mathrm{KL}(\rho_1|\pi) + \mathrm{KL}(\rho_2|\pi)\right)^{\frac{1}{2}} t^{\frac{1}{2}}\right) + C_2(k), \quad (56)$$

where

$$C_1(k, V) = 3C_V^{1/q} \left(\|k\|_\infty + \|\nabla k\|_\infty^{\frac{1}{2}} + \|\nabla^2 k\|_\infty^{\frac{1}{2}} + \|\nabla_1\nabla_2 k\|_\infty^{\frac{1}{2}}\right),$$

$$D_1(k, \nu, q) = C_{1,0}\nu^{-1/2}q^{-1}\|k\|_\infty,$$

$$C_2(k) = 2\|\nabla^2(\nabla_1 \cdot \nabla_2 k)\|_\infty^{\frac{1}{2}} + \|\nabla_1\nabla_2(\nabla_1 \cdot \nabla_2 k)\|_\infty^{\frac{1}{2}}.$$

Therefore (48) follows from our estimations on the **First term** and **Second term**. $\qquad \square$

7. Space-time Discretization: A Practical Algorithm

In this section, we introduce a practical space-time discretization to the R-SVGF described in (28). In the algorithm, we let positive integers N and n to denote the number of particles and (discrete) iterations. We denote by $(X_n^i)_{i=1}^N$ the position of the N particles at the n-th step. We let $\bar{X}_n := [X_n^1, \ldots, X_n^N]^T$. For all functions $f : \mathbb{R}^d \to \mathbb{R}^d$, we define the operator L_n as

$$L_n f := [f(X_n^1), \cdots, f(X_n^N)]^T.$$

The positions of the particles are then updated as

$$\bar{X}_{n+1} = \bar{X}_n - h_{n+1} \left(\frac{(1 - \nu_{n+1})}{N} K_n + \nu_{n+1} I_N\right)^{-1} \left(\frac{1}{N} K_n(L_n \nabla V) - \frac{1}{N} \sum_{j=1}^N L_n \nabla k(X_n^j, \cdot)\right), \quad (57)$$

where $(h_n)_{n=1}^\infty$ is the sequence of step-sizes, $I_{N \times N}$ is the $N \times N$ identity matrix and $K_n \in \mathbb{R}^{N \times N}$ is the gram matrix defined as $(K_n)_{ij} = k(X_n^i, X_n^j)$ for all $i, j \in [N]$. We call the above algorithm as the Regularized SVGD algorithm. The iterates in (57) follow from Proposition 2 and the finite-sample representations for the operators $\iota_{k,\hat{\rho}^n} \iota_{k,\hat{\rho}^n}$ where $\hat{\rho}^n$ is the empirical measure of the particles at the n-th step, i.e., $\hat{\rho}^n = \sum_{i=1}^N \delta_{X_n^i}$.
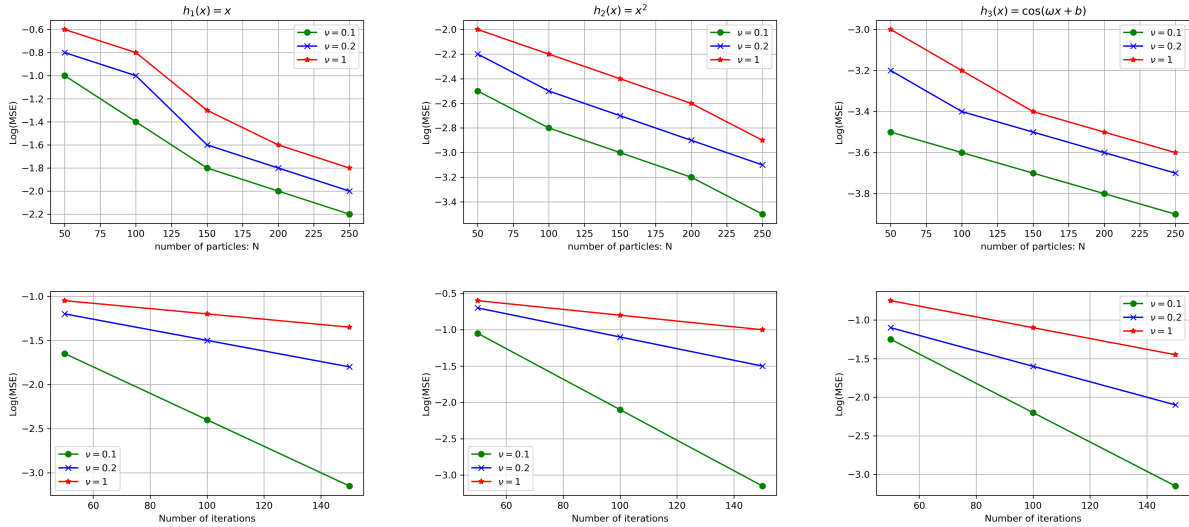
FIGURE 1. R-SVGD for various values of the regularization parameter ν. The case of $\nu = 1$ corresponds to SVGD. Left, Middle and Right columns correspond respectively to $h_1(x) := x$, $h_2(x) := x^2$ and $h_3(x) := \cos(\omega x + b)$. Top and bottom rows correspond respectively to log(MSE) versus number of particles and number of iterations.

While the convergence analysis of space-time discretization of the SVGF (i.e., the SVGD algorithm) and the R-SVGD (i.e., the regularized SVGD algorithm) is an interesting and challenging open question, in this section we demonstrate the improved performance of the regularized SVGD algorithm over the SVGD algorithm in some simulation examples. All experiments were done in MacBook Pro (2021 model). Specifically, we consider the simulation setup in [LW16]: We let the target $\pi := (1/3)\pi_1 + (2/3)\pi_2$, where $\pi_1 \equiv \text{Normal}(-2, 1)$ and $\pi_2 \equiv \text{Normal}(+2, 1)$, and we let the initial distribution to be Normal$(-10, 1)$. We now focus on numerically computing the expectations of the form $\mathbb{E}_{x \sim \pi}[h_i(x)]$, for three cases, $h_1(x) := x$, $h_2(x) := x^2$ and $h_3(x) := \cos(\omega x + b)$, where $\omega \sim \text{Normal}(0, 1)$ and $b \sim \text{Uniform}([0, 2\pi])$.

In Figure 1, we plot the mean-squared error in estimating the above expectations with the regularized and unregularized SVGD algorithm. Here, the expectation is over the initialization (and over ω and b for h_3). In the top row, we report the logarithm of the mean-squared error versus the number of particles N for a fixed number of iterations (set to 100). The corresponding average per-iteration wall-clock

N	50	100	150	200	250
$\nu = 0.1$	0.0114	0.0343	0.0861	0.1442	0.2163
$\nu = 0.2$	0.0099	0.0257	0.0586	0.1058	0.1899

TABLE 2. Average *additional* per-iteration wall-clock run-time (in seconds) for R-SVGD over SVGD.

run times are reported in Table 2. In the bottom row, we report the logarithm of the mean-squared error versus the number of iterations for a fixed number of particles (set to 200). For both algorithms, we use the Gaussian kernel $k(u, v) = \exp\left(-\frac{1}{\gamma}\|u - v\|_2^2\right)$, where the bandwidth parameter γ is set using the median heuristic [LW16]. We use the Adagrad step-size choice for both cases, following [LW16]. For the choice of the regularization parameter, we report results for various choices of ν. The case of $\nu = 1$ corresponds exactly to the SVGD algorithm. We notice that for small values of ν the regularized SVGD algorithm performs better than the SVGD algorithm.

We now discuss the per-iteration complexity of regularized SVGD and standard SVGD. SVGD requires computing the kernel matrix (which requires $\mathcal{O}(N^2)$ operations per-iterations) and the gradient of the potential (i.e., ∇V). As pointed out in [LW16] in Bayesian inference problems, typically, computing the gradient of the potential might be the main bottleneck. However, this computation could easily be done in parallel due to its finite-sum structure in Bayesian inference problems. We denote by $\mathcal{O}$(Score), the time complexity of computing/evaluating the gradient of the potential for a given target density. On top of the above computations, each iteration of regularized SVGD requires inverting a $N \times N$ matrix (or equivalently, solving a positive-definite linear system of equations), which costs $\mathcal{O}(N^3)$ complexity. With standard implementations, the per-iteration complexity regularized SVGD and standard SVGD are hence of order $\max\{\mathcal{O}(N^3), \mathcal{O}(\text{Score})\}$ and $\max\{\mathcal{O}(N^2), \mathcal{O}(\text{Score})\}$, respectively.

The matrix being inverted in regularized SVGD is the regularized kernel matrix also arising in other problems like kernel ridge regression. Hence, the rich literature on efficiently inverting kernel matrices (under various structural assumptions) could be leveraged in this context. While we leave a detailed study of speeding up the regularized SVGD algorithm as future work, we conclude here two concrete methods for provably speeding-up practical implementations of the regularized SVGD algorithms (under structural assumptions):

- *Pre-conditioned CG methods:* State-of-the-art methods on designing pre-conditioners for conjugate gradient methods for kernel ridge regression from [DEF$^+$23] could be leveraged in the context of regularized SVGD. In particular, such results may help reduce the computational complexity of regularized SVGD to $\max\{\mathcal{O}(N^2), \mathcal{O}(\text{Score})\}$, matching that of SVGD.
- *Randomized methods*: Randomized algorithms designed in the context of kernel ridge regression, namely Random Fourier Features [RR17] and sketching [YPW17] could also be leveraged to speed-up practical implementations of regularized SVGD.

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