

ON THE RANDOM WALK METROPOLIS ALGORITHM FOR GAUSSIAN RANDOM FIELD PRIORS AND THE GRADIENT FLOW

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We study random walk based algorithms for posterior simulation in a large class of Bayesian nonparametric problems with Gaussian random field or Gaussian process priors. Our emphasis is both on developing practical guidelines for the design and implementation of efficient algorithms for these naturally high dimensional problems, and on the development of rigorous underpinning theory. We illustrate via an example that, in designing algorithms for nonparametric problems, it is important to take advantage of the infinite dimensional structure inherent in both the prior and likelihood. Algorithms which ignore this structure can be very inefficient, even with large computing power. The novelty of our work is twofold. (i) We give one of the first results rigorously quantifying the efficiency of random walk based algorithms in infinite dimensional Bayesian nonparametric problems; in particular this work describes a modification of the standard random walk Metropolis algorithm which results in an order of magnitude efficiency gain, when measured in terms of the dimension of the approximation space. (ii) We develop a theory of simulated annealing for posterior simulation in an infinite dimensional framework and show how a noisy gradient descent algorithm can emerge, without explicitly computing the gradient, from certain carefully specified random walks when combined with a Metropolis-Hastings accept-reject mechanism. This theory extends results known in finite dimensions for finding local maxima using a gradient flow and hence is of independent interest.

1. Introduction. Bayesian nonparametrics have witnessed rapid growth in the last decade, both in the construction of novel prior distributions [DPP07, WCT11] and obtaining results on posterior consistency and sharp convergence rates, *e.g.*, [GVDV11, VDVZ08]. Nonparametric methods are increasingly popular in many applications due to their flexibility to model a wide variety of statistical problems when the parameter is naturally infinite dimensional. In such problems, the posterior distribution usually does not have a closed form solution (except in special cases) and therefore one needs to resort to computational methods such as the Markov Chain Monte Carlo (MCMC) algorithms to get samples from the posterior distribution. In this regard, a wide array of fast computational algorithms have been developed for obtaining posterior draws [RC04, PR08, IZ00].

However there has not been much research dedicated to understanding the computational complexity of MCMC algorithms in the nonparametric setting. Doing so will lead to concrete guidelines that practitioners can use while selecting and implementing these algorithms and it is this viewpoint which motivates our work. In this paper, we study random walk based algorithms on a large class of Bayesian nonparametric problems with Gaussian random field (Gaussian process being a particular case when the unknown function depends on one variable) prior distributions. Gaussian random fields are ubiquitous in nonparametric modeling due their remarkable sample path properties and the fact that they can be characterized entirely by the mean function and covariance operator [RW06]. Due to their conceptual simplicity and ease of implementation, the random walk metropolis (RWM) algorithm and its variants are the basic building blocks of entire families of

more sophisticated MCMC algorithms. Since the parameter space is infinite dimensional, practical implementation of the RWM involves discretizing the parameter space. Discretization can be equivalently viewed as restricting the infinite dimensional parameter space to \mathbb{R}^N , with N being a very large number, which is chosen so as to resolve adequately the features of parameters under the posterior distribution. It is well known that such discretization schemes might suffer from the curse of dimensionality: the efficiency of the algorithm decreases as the dimension N of the discretized space grows large.

The main message of our work is that it is important to invest some care in designing and implementing MCMC algorithms for nonparametric problems to avoid this curse. More concretely a useful design principle is: “first design an algorithm which evolves on the entire (infinite dimensional) parameter space and then discretize the space” rather than “discretize the space and apply an off-the-shelf finite dimensional sampler”. In following the “sample then discretize” design principle it is possible to take advantage of the underlying infinite dimensional structure in both the prior distribution and the likelihood to increase the efficiency of the algorithm by an order of magnitude. On the contrary, algorithms which ignore this structure can turn out to be very inefficient, even with large computing power. In this paper, we illustrate this idea by exhibiting two nearly identical looking variants of the RWM MCMC method (with near identical implementations and cost per step), where one has the computational complexity of $O(N)$, and the other has the complexity of $O(1)$ (in a sense made more precise later). These results hold for a large class of routinely used models in Bayesian nonparametrics. The practical consequence of our results is that practitioners have a concrete guideline for the choice of random walk based algorithms for posterior simulation with Gaussian random field priors in Bayesian nonparametric problems.

Let us describe the class of models to which our main results are applicable. We denote the prior and posterior distributions respectively by π_0 and π and consider models in which both π_0 and π are measures on a Hilbert space \mathcal{H} . Furthermore π_0 is assumed to be a Gaussian random field on \mathcal{H} . The posterior π is given by the identity

$$\frac{d\pi}{d\pi_0}(x) = M_\Psi \exp(-\Psi(x)), \quad x \in \mathcal{H} \quad (1.1)$$

for a real valued π_0 -measurable functional Ψ (which denotes the log-likelihood) and M_Ψ a normalizing constant. Although the above formulation might seem slightly abstract, it encompasses a very large class of models arising in practice ranging from nonparametric regression to diffusion processes. Let us briefly elaborate on one concrete application. Consider estimating an unknown function x observed at discrete points on a compact set:

$$y_k = x(t_k) + \epsilon_k \quad (1.2)$$

where $t_k \in \mathcal{T} \subset \mathbb{R}^d$ and ϵ_k are i.i.d errors, which are mean 0 and have a smooth density $g(\cdot)$. The unknown function x is assumed to be in the Hilbert space $\mathcal{H} = L_2(\mathcal{T})$. We assume a centered Gaussian random field prior on the function x , $\pi_0 \sim \text{No}(0, C)$, where C is a self-adjoint, positive and trace-class operator on \mathcal{H} . Let $\{\varphi_j, \lambda_j^2\}_{j \geq 1}$ be the eigenfunctions and eigenvalues of C respectively, so that

$$C\varphi_j = \lambda_j^2 \varphi_j \quad \text{for} \quad j \in \mathbb{N}.$$

We assume a normalization under which $\{\varphi_j\}_{j \geq 1}$ forms a complete orthonormal basis in \mathcal{H} . For every $x \in \mathcal{H}$ we have the representation $x = \sum_j x_j \varphi_j$, where $x_j = \langle x, \varphi_j \rangle$. This representation makes it apparent that, constructing a Gaussian random field prior on \mathcal{H} leads to a Gaussian

prior distribution $x_j \sim \text{No}(0, \lambda_j^2)$ on the basis coefficients. The prior assumption on the regularity of the function x can be invoked by assuming appropriate decay on the eigenvalues of the C . Some researchers construct prior distributions using covariance functions, instead of a covariance operator. These are equivalent approaches and similar results to those developed in this paper will hold in this setting as well, using the connection between the covariance function and the Green's function of the precision C^{-1} .

From Bayes' rule, we have that the posterior distribution π is given by

$$d\pi(x) \propto \prod_k g(y_k - x(t_k)) d\pi_0(x) \quad (1.3)$$

where g is the density of the noise. Due to the remarkable properties of the sample paths of Gaussian random fields, models constructed above are one of the simplest but fundamental tools in Bayesian nonparametrics capturing a huge number of useful and practical models in various applications; see [HSV10, Stu10a] for some examples. Notice that if the noise ϵ_k were Gaussian, the model is conjugate and thus the posterior distribution is Gaussian. As mentioned above the theoretical properties of these models are very well studied. In fact sharp rates of posterior concentration are known, and remarkable connections are established between the convergence rates of the posterior distribution and the small ball probabilities of the prior distribution [VDVZ08, Cas08] which in turn is related to the eigenvalues of the covariance operator. Interesting results are also known from a minimax perspective [Zha00]. However, not much is known about the computational efficiency of RWM algorithms on these target distributions.

In Section 2.3 and 2.4 we will specify, and discuss, the precise assumptions on Ψ which we adopt in this paper. In the above example, roughly speaking, our theory will apply if the density g has tails which are Gaussian or heavier than Gaussian. Furthermore we do not need an additive error model as in (2.11); for example the main results are applicable if we had binary or Poisson regression. All of our assumptions can be further relaxed for the results to go through, but the choices we make here help to keep the exposition simple.

Now we turn to describing the class of algorithms studied in this paper, which are based on Metropolis-Hastings MCMC methods [RC04]. Recall that, to sample from π , the RWM algorithm creates a π -reversible Markov chain $\{x^n\}_{n=0}^\infty$ which moves from a current state x^0 to a new state x^1 via *proposing* a candidate y , using a symmetric Markov transition kernel such as a random walk, and accepting y with probability $\alpha(x^0, y)$, where $\alpha(x, y) = 1 \wedge \frac{\pi(y)q(y, x)}{\pi(x)q(x, y)}$ where q is the proposal density.

Consider the following two proposals: (i) the standard random walk (S-RWM)

$$y = x + \sqrt{2\delta} \xi \quad (1.4)$$

and the preconditioned random walk (P-RWM)

$$y = (1 - 2\delta)^{\frac{1}{2}} x + \sqrt{2\delta} \xi \quad (1.5)$$

where $\xi \sim \text{No}(0, C)$ is chosen independently of x and δ is the time step; (ii) the P-RWM algorithm, introduced in [BRSV08], belongs to a family of Metropolis-Hastings methods defined on the Hilbert space \mathcal{H} which are reversible and invariant with respect to π . As can be seen above, the two proposals are nearly identical (the only difference being that the S-RWM has a symmetric proposal and the P-RWM doesn't). However, as will be seen below, the S-RWM is *extremely inefficient*, compared to the P-RWM.

In our set-up, a natural way to perform the discretization is to consider the N -dimensional space spanned by the first N basis functions $\varphi_j, 1 \leq j \leq N$, project the target density into this

basis and let the Markov chain evolve in \mathbb{R}^N . This is easy to implement as well, by setting in $\xi \sim \text{No}(0, C^N)$ in (1.4) and (1.5), where the diagonal elements of the covariance matrix C^N are the first N eigenvalues of C and the off-diagonal elements are 0. A key question for practitioners is this: what is the relationship between the time step δ and the dimension N required to get efficient mixing in the limit $N \rightarrow \infty$. In particular how should δ decay to zero as N grows? Since δ measures the size of the proposed moves, this has direct bearing on understanding complexity of the RWM algorithms.

We answer this question by establishing a diffusion limit for P-RWM, and compare the required conditions on δ , as a function of N , with those obtained for S-RWM in the recent paper [MPS11], which generalizes the pioneering works on optimal scaling for i.i.d distributions in [RGG97]. Given a discrete time Markov chain x^k on the time intervals $t_k = k\delta$, define its piecewise linear interpolation to be:

$$z^\delta(t) = \frac{1}{\delta} (t - t_k) x^{k+1, \delta} + \frac{1}{\delta} (t_{k+1} - t) x^{k, \delta} \quad \text{for} \quad t_k \leq t < t_{k+1}. \quad (1.6)$$

THEOREM 1.1. [MPS11]: *Let $\{x^k\}$ be the Markov chain on \mathbb{R}^N corresponding to the S-RWM proposal and z^δ be as defined in (1.6). Then the following hold:*

1. *If the chain is started in stationarity then, for any fixed $\delta > 0$, the expected acceptance probability converges to zero as the dimension $N \rightarrow \infty$, faster than any algebraic power of N .*
2. *If the chain is started in stationarity for the “optimal scale” $\delta = O(1/N)$ the expected acceptance probability converges to a non-zero number, as the dimension $N \rightarrow \infty$. Furthermore for this choice of δ , started at stationarity, the linear interpolation process z^δ converges weakly to the diffusion*

$$(1.7) \quad dz(t) = -\left(z(t) + C\nabla\Psi(z)\right) dt + \sqrt{2}dW$$

on the space of paths, $C([0, T], \mathcal{H})$ with $z(0) = x$ and W is a Wiener process on \mathcal{H} with covariance operator C .

3. *For the chain started at stationarity with the optimal scale $\delta = O(1/N)$, the “optimal acceptance” probability, which maximizes the one-step mean squared distance of the Markov chain, is 0.234.*

The general idea behind the theory of *optimal scaling* [RGG97] encoded in Theorem 1.1 is the following. In the proposal (1.4), the step size δ (as a function of the dimension N) cannot be too large or too small. Smaller values of δ lead to frequent acceptance leading to local moves and is clearly inefficient. Larger values of δ lead to proposals which are accepted only rarely. So, if one uses the same step-size for all dimensions, the acceptance rates are near 0 even in moderate dimensions like $N = 50$ or 100. Thus the theory of optimal scaling finds the right balance by choosing $\delta = O(1/N)$ (so the step-size decreases as the dimensions grows) so as to keep the acceptance probability a constant. At this choice of scaling, there is a diffusion limit for the algorithm which gives rise to the following two conclusions:

1. The diffusion in (1.7) is ergodic with stationary measure π . Thus if we run the diffusion to compute Monte Carlo averages of a function f by setting:

$$\hat{f} = \frac{1}{T} \int f(z(t)) dt, \quad (1.8)$$

using ergodicity, we may find a $T = T$ so that \hat{f} approximates $\int f d\pi$ to a desired precision. Note that this time T is *independent of any discretization dimension N* , since the diffusion z is defined on the infinite dimensional space \mathcal{H} . Now, the diffusion limit in Theorem 1.1 implies the desired

continuous time average can be approximated by S-RWM Markov and the corresponding estimator should be

$$\hat{f}_{N,\text{S-RWM}} = \frac{\delta}{T} \sum_{k=1}^{\lfloor T/\delta \rfloor} f(x^k)$$

provided that $\delta = \mathcal{O}(N^{-1})$. The optimal scaling results also imply that the scale δ cannot be greater than $\mathcal{O}(N^{-1})$ (as a function of N) for the algorithm to have $\mathcal{O}(1)$ acceptance probability. Thus the S-RWM in dimension N needs $\mathcal{O}(N)$ steps to explore the target distribution for any preset value of the Monte Carlo error. In this sense, the computational work needed from the S-RWM is $\mathcal{O}(N)$.

2. One of the celebrated aspects of the optimal scaling theory, widely cited and used by applied workers in many fields, is that the optimal acceptance probability corresponding to the optimal scale turns out to be 0.234. This implies that practitioners can simply tune the S-RWM algorithm to obtain the acceptance probability to be around 20 – 30%. There are even adaptive algorithms which are automated to obtain this acceptance probability.

An important point to be noticed is that the optimal scaling theory and the S-RWM algorithms are constructed with a “discretize then design a sampler” viewpoint: firstly, the problem (target distribution) is discretized, secondly, a standard Random Walk Metropolis algorithm applied and then the algorithm is tuned to achieve optimality. The advantage is that the algorithms need not be defined on the entire Hilbert space \mathcal{H} , but only on finite dimensional subspaces. In fact, the S-RWM is not well-defined on all of \mathcal{H} . One of our key observations in this paper is that, this also turns out to be the key disadvantage of the S-RWM algorithm in high dimensions.

In contrast, the P-RWM algorithms adhere to the “design a sampler then discretize” principle (see [HPUU08], Chapter 3, for discussion of similar issues for optimization problems on function spaces), where the algorithms are defined on all of \mathcal{H} , and therefore, unlike S-RWM, do not suffer from the degeneracy due to discretization. Our first main result encapsulates this idea:

Main Result 1: *Let $\{x^k\}$ be the Markov chain corresponding to the P-RWM proposal and z^δ be as defined in (1.6). Then the following hold:*

1. *If the chain is started in stationarity in \mathbb{R}^N then, for any $\delta > 0$, the expected acceptance probability of the Markov chain converges to a non-zero number as $N \rightarrow \infty$.*
2. *If the chain is started at any arbitrary point $x^0 \in \mathcal{H}$ (the infinite dimensional Hilbert space) then as $\delta \rightarrow 0$, the linear interpolation process z^δ converges weakly to the diffusion process given by (1.7).*

The following are the implications of the above result:

1. Since the algorithm is defined on all of \mathcal{H} , it is robust to finite dimensional approximations: the step-size δ needs to be small to see the diffusion limit, but this measure of smallness *is independent of N* , since the limit theorem holds in \mathcal{H} itself. Furthermore, the acceptance probability doesn’t decay to 0 as the dimension grows large. This fact is demonstrated in numerical experiments in [BRSV08] for Langevin based proposals and also confirmed for the P-RWM in [CRSW11].
2. The diffusion limit implies that the estimator

$$\hat{f}_{N,\text{P-RWM}} = \frac{\delta}{T} \sum_{k=1}^{\lfloor T/\delta \rfloor} f(x^k)$$

will have the same precision as that of \hat{f} given by (1.8), uniformly with respect to dimension. Thus the P-RWM algorithm explores the target distribution π in $\mathcal{O}(1)$ time regardless of the discretization

dimension N , in stark contrast with the S-RWM.

3. One of the key technical novelties in this paper is that the diffusion limit in (1.7) for the P-RWM is derived for *any* initial condition for the Markov chain, unlike the optimal scaling results where the results hold *only at stationarity*.

4. In contrast to the situation with S-RWM there is no unambiguous notion of optimal acceptance probability. The user has freedom to determine the optimal choice for (small δ) in a problem-dependent fashion.

5. Our main result also calls for a shift of focus from *optimal scaling* to *optimal design* of algorithms for bayesian nonparametric problems. For instance, our results suggest that the P-RWM for any scale δ is much more efficient than the S-RWM in high dimensions, even at its optimal scale.

To illustrate our point on optimal design, let us give some intuition behind the efficiency gain of P-RWM relative to that of S-RWM. The key observation is that the P-RWM “inherits” the structure of the prior distribution (and hence the posterior) better than the S-RWM. Indeed, imagine that the log-likelihood $\Psi = 0$, so that we have $\pi = \pi_0$. Then it is known that the Ornstein-Uhlenbeck (OU) process

$$\begin{aligned} dz &= -z dt + \sqrt{2}dW \\ z_0 &= x, \end{aligned} \tag{1.9}$$

is reversible and ergodic with respect to π [DPZ96], where W is a Brownian motion in \mathcal{H} with covariance operator equal to C . If $t > 0$ then the exact solution of this equation has the form, for $\delta = \frac{1}{2}(1 - e^{-2t})$,

$$\begin{aligned} z(t) &= e^{-t}x + \sqrt{(1 - e^{-2t})}\xi \\ &= (1 - 2\delta)^{\frac{1}{2}}x + \sqrt{2\delta}\xi, \end{aligned} \tag{1.10}$$

where $\xi \sim \text{No}(0, C)$. Given a current state x of our Markov chain the P-RWM proposes exactly according to the above formula, for some choice of $t > 0$, or equivalently $\delta \in (0, \frac{1}{2})$. Thus if $\Psi = 0$, the P-RWM algorithm started at stationarity has an acceptance probability of 1, where as the stationary measure of the S-RWM proposal without the accept/reject mechanism is not π . Thus in the case $\Psi = 0$, the Gaussian posterior distribution suggests that the right way to proceed is via P-RWM proposals. For $\Psi \neq 0$, our result shows that even if the posterior is not Gaussian, the Gaussian prior distribution still suggests that P-RWM should be used instead of S-RWM. More generally, it illuminates the point that even within the same family of MCMC algorithms (in our set-up, algorithms based on random walk), the ones (P-RWM) which inherit the infinite dimensional structure of the prior/posterior distribution have huge computational advantages over those (S-RWM) which ignore this structure. This interplay between the statistical properties of the posterior distribution and the efficiency of the algorithms is well documented in finite dimensions, but ours is one of the first efforts pointing this out for nonparametric applications.

Now we proceed to the second motivation behind studying algorithms for the target distributions of the kind (1.1). There are many applications ([EHN96]) where it is of natural interest to find global or local minima of a functional

$$(1.11) \quad J(x) = \frac{1}{2}\|C^{-1/2}x\|^2 + \Psi(x),$$

where C is the self-adjoint, positive and trace-class linear operator described above, on the Hilbert space $(\mathcal{H}, \langle \cdot, \cdot \rangle, \|\cdot\|)$. Gradient flow or steepest descent is a natural approach to this problem, but

in its basic form requires computation of the gradient $\nabla\Psi$ which, in some applications, may be an expensive or complex task. In addition, when multiple minima are present, it may be important to include noise within the algorithm in order to allow escape from local minima. The second goal of this paper is to show how a noisy gradient descent can emerge, *without explicitly computing the gradient*, from certain carefully specified random walks, when combined with a Metropolis-Hastings accept-reject mechanism [Tie98], with tunable noise level τ . In the finite state [KJV83, Čer85] or finite dimensional context [Gem85, GH86, HKS89] the idea of using random walks, with accept-reject, to perform global optimization is a well-known idea which goes by the name of simulated-annealing; see the review [BT93] for further references. The novelty of our work is that the theory is developed on an infinite dimensional Hilbert space, and the applications of the theory are particularly tailored towards practical problems arising in Bayesian nonparametrics. In this context, minimization of J given by (1.11) corresponds to finding the MAP estimator.

In finite dimensions the basic idea behind simulated annealing is built from Metropolis-Hastings methods which have an invariant measure with Lebesgue density proportional to $\exp(-\tau^{-1}J(x))$. By adapting the temperature $\tau \in (0, \infty)$ according to an appropriate cooling schedule it is possible to locate global minima of J . The essential challenge in transferring this idea to infinite dimensions is that there is no Lebesgue measure. However, our key observation in this paper is that, the above issue can be circumvented by working with measures defined via their density with respect to a Gaussian measure like the posterior measure like those of π defined in (1.1). To introduce the parameter τ , we modify our prior distribution π_0 and write

$$\pi_0^\tau = N(0, \tau C), \quad (1.12)$$

so that the posterior distribution π^τ takes the form:

$$\frac{d\pi^\tau}{d\pi_0^\tau}(x) \propto \exp\left(-\frac{\Psi(x)}{\tau}\right). \quad (1.13)$$

Note that if \mathcal{H} is finite dimensional then π^τ has Lebesgue density proportional to $\exp(-\tau^{-1}J(x))$. It is also known that small ball probabilities are asymptotically maximized (in the small radius limit), under π^τ , on balls centred at minimizers of J [DS11]. To further incorporate the parameter τ , we modify the P-RWM proposal to be

$$y = (1 - 2\delta)^{\frac{1}{2}}x + \sqrt{2\delta\tau}\xi \quad (1.14)$$

where $\xi \sim N(0, C)$ and the “proposed move” (1.14) will be accepted or rejected with probability found from pointwise evaluation of Ψ given by,

$$\alpha^\delta(x, \xi) = 1 \wedge \exp\left(-\frac{1}{\tau}(\Psi(y) - \Psi(x))\right) \quad (1.15)$$

(see Section 3 for more details) resulting in a Markov chain $\{x^{k,\delta}\}_{k \in \mathbb{Z}^+}$.

As mentioned earlier, our of our main results state that as δ goes to 0, the linear interpolation process $z^\delta(t)$ given by (1.6) converges to the diffusion

$$dz(t) = -\left(z(t) + C\nabla\Psi(z)\right)dt + \sqrt{2\tau}dW.$$

This equation is reversible, ergodic and satisfies a law of large numbers with respect to the measure π^τ [DPZ96, HSV07b]. Since small ball probabilities under π^τ are maximized when centred at

minimizers of J , the result thus shows that the algorithm will generate sequences which concentrate near minimizers of J . Varying τ according to a cooling schedule then results in a simulated annealing method on Hilbert space. Weak convergence results for the approximation of stochastic equations in infinite dimensions may be found in the numerical analysis literature. For the heat equation and variants see [Sha03, DP09, GKL09, KLL10], for dispersive and nondispersive wave problems see [Hau10, dBD06] and for delay equations see [BS05, BKMS08]. These papers rely on use of the Kolmogorov equation to establish weak convergence and do not typically deliver convergence on pathspace, but rather convergence of functionals at a given fixed time. In contrast our approach, which is much simpler, proves weak convergence on pathspace, and does not use the Kolmogorov equation; rather we use an invariance principle for Brownian motion in Hilbert space [Ber86], coupled with the preservation of weak convergence under continuous mappings. Our approach as it stands, does not deliver rates of weak convergence, but can be made more quantitative to obtain convergence rates. Since we are only interested in qualitative properties and their statistical applications, we do not venture in this direction.

Let us give a quick heuristic to see why the gradient flow emerges through the pointwise computation of Ψ and the accept-reject mechanism. Note that for $\delta \ll 1$, we see from (1.15) that

$$(1.16) \quad \alpha^\delta(x, \xi) \approx 1 \wedge \exp\left(-\sqrt{\frac{2\delta}{\tau}} \Psi(x) \xi\right).$$

This induces a bias towards accepting moves for which the Gaussian random variable ξ , which is independent of x , aligns with the negative gradient of Ψ . Formalizing this heuristic is the content of Section 4.¹

Because the SDE (1.7) and the Markov chain are not started at stationarity, and because neither possess a smoothing property (they are only asymptotically strong Feller [HSV07a]), almost sure fine scale properties under its' invariant measure π^τ are not necessarily reflected at any finite time. For example if C is the covariance operator of Brownian motion or Brownian bridge then the quadratic variation of draws from the invariant measure, an almost sure quantity, is not reproduced at any finite time in (1.7) unless $z(0)$ has this quadratic variation; the almost sure property is approached only asymptotically as $t \rightarrow \infty$. This behaviour is reflected in the underlying Metropolis-Hastings Markov chain P-RWM which approximates (1.7), where the almost sure property is only reached asymptotically as $k \rightarrow \infty$. The second main result (informally stated here and rigorously formulated and proved in Section 5) gives quantitative information about the rate at which the P-RWM algorithm approaches statistical equilibrium.

Main Result 2: *The almost sure quantities such as the quadratic variation under P-RWM satisfy a limiting linear ordinary differential equation (ODE) with globally exponentially attractive steady*

¹As discussed previously, the S-RWM would use the proposal

$$x + \sqrt{\delta\tau} \xi,$$

in place of (1.10) leading to the accept-reject formula

$$\alpha^\delta(x, \xi) = 1 \wedge \exp\left(-\frac{1}{\tau} (I(x + \sqrt{2\delta\tau}\xi) - I(x))\right)$$

in place of (1.15) for a function $I(x)$. Unfortunately $I(x)$ is almost surely infinite with respect to x drawn from π^τ if \mathcal{H} is infinite dimensional; consequently the S-RWM algorithm is only defined after finite dimensional approximation of the space and consequently the time-step δ suffers from a Courant-like restriction as the dimension is increased which in turn leads to the decay of acceptance probability.

state given by the value of the quantity under π^τ .

Let us conclude the introduction with the following note. The diffusion limit results obtained here are entirely self-contained and the proof technique is analogous to the of diffusion limits of Markov chains in finite dimensions. We believe therefore that the methods of analysis that we introduce may be used to understand other MCMC algorithms and other nonparametric problems.

The rest of the paper is organized as follows. In section 2 we describe some notation used throughout the paper, discuss the required properties of Gaussian measures and Hilbert-space valued Brownian motions, and state our assumptions. In this section, we also exhibit a large class of statistical problems arising in practice which satisfy our assumptions. Section 3 contains a precise definition of the Markov chain $\{x^{k,\delta}\}_{k \in \mathbb{Z}^+}$, together with statement and proof of the weak convergence theorem that is the main result of the paper. Section 4 contains proof of the lemmas which underly the weak convergence theorem. In section 5 we state and prove the limit theorem for almost sure quantities such as quadratic variation; such results are often termed “fluid limits” in the applied probability literature. An simulation example illustrating the main result is presented in section 6. We conclude in section 7. Proofs of some technical lemmas are deferred to the Appendices A and B.

2. Preliminaries. In this section we define some notational conventions, Gaussian measure and Brownian motion in Hilbert space, and state our assumptions concerning the operator C and the functional Ψ .

2.1. *Notation.* Let $(\mathcal{H}, \langle \cdot, \cdot \rangle, \|\cdot\|)$ denote a separable Hilbert space of real valued functions with the canonical norm derived from the inner-product. Let C be a positive, trace class operator on \mathcal{H} and $\{\varphi_j, \lambda_j^2\}_{j \geq 1}$ be the eigenfunctions and eigenvalues of C respectively, so that

$$C\varphi_j = \lambda_j^2 \varphi_j \quad \text{for} \quad j \in \mathbb{N}.$$

We assume a normalization under which $\{\varphi_j\}_{j \geq 1}$ forms a complete orthonormal basis in \mathcal{H} . For every $x \in \mathcal{H}$ we have the representation $x = \sum_j x_j \varphi_j$, where $x_j = \langle x, \varphi_j \rangle$. Using this notation, we define Sobolev-like spaces $\mathcal{H}^r, r \in \mathbb{R}$, with the inner-products and norms defined by

$$\langle x, y \rangle_r \stackrel{\text{def}}{=} \sum_{j=1}^{\infty} j^{2r} x_j y_j \quad \text{and} \quad \|x\|_r^2 \stackrel{\text{def}}{=} \sum_{j=1}^{\infty} j^{2r} x_j^2. \quad (2.1)$$

Notice that $\mathcal{H}^0 = \mathcal{H}$. Furthermore $\mathcal{H}^r \subset \mathcal{H} \subset \mathcal{H}^{-r}$ for any $r > 0$. The Hilbert-Schmidt norm $\|\cdot\|_C$ is defined as

$$\|x\|_C^2 = \sum_j \lambda_j^{-2} x_j^2.$$

For $r \in \mathbb{R}$, let $B_r : \mathcal{H} \mapsto \mathcal{H}$ denote the operator which is diagonal in the basis $\{\varphi_j\}_{j \geq 1}$ with diagonal entries j^{2r} , i.e.,

$$B_r \varphi_j = j^{2r} \varphi_j$$

so that $B_r^{\frac{1}{2}} \varphi_j = j^r \varphi_j$. The operator B_r lets us alternate between the Hilbert space \mathcal{H} and the interpolation spaces \mathcal{H}^r via the identities:

$$\langle x, y \rangle_r = \langle B_r^{\frac{1}{2}} x, B_r^{\frac{1}{2}} y \rangle \quad \text{and} \quad \|x\|_r^2 = \|B_r^{\frac{1}{2}} x\|^2. \quad (2.2)$$

Since $\|B_r^{-1/2}\varphi_k\|_r = \|\varphi_k\| = 1$, we deduce that $\{B_r^{-1/2}\varphi_k\}_{k \geq 1}$ forms an orthonormal basis for \mathcal{H}^r . For a positive, self-adjoint operator $D : \mathcal{H}^r \mapsto \mathcal{H}^r$, its trace in \mathcal{H}^r is defined as

$$\text{Trace}_{\mathcal{H}^r}(D) \stackrel{\text{def}}{=} \sum_{j=1}^{\infty} \langle B_r^{-\frac{1}{2}} \varphi_j, D B_r^{-\frac{1}{2}} \varphi_j \rangle_r.$$

Since $\text{Trace}_{\mathcal{H}^r}(D)$ does not depend on the orthonormal basis, the operator D is said to be trace class in \mathcal{H}^r if $\text{Trace}_{\mathcal{H}^r}(D) < \infty$ for some, and hence any, orthonormal basis of \mathcal{H}^r . Let $\otimes_{\mathcal{H}^r}$ denote the outer product operator in \mathcal{H}^r defined by

$$(x \otimes_{\mathcal{H}^r} y)z \stackrel{\text{def}}{=} \langle y, z \rangle_r x \quad \forall x, y, z \in \mathcal{H}^r. \quad (2.3)$$

For an operator $L : \mathcal{H}^r \mapsto \mathcal{H}^l$, we denote its operator norm by $\|\cdot\|_{\mathcal{L}(\mathcal{H}^r, \mathcal{H}^l)}$ defined by

$$\|L\|_{\mathcal{L}(\mathcal{H}^r, \mathcal{H}^l)} \stackrel{\text{def}}{=} \sup_{\|x\|_r=1} \|Lx\|_l.$$

For self-adjoint L and $r = l = 0$ this is, of course, the spectral radius of L .

Throughout we use the following notation.

- Two sequences $\{\alpha_n\}_{n \geq 0}$ and $\{\beta_n\}_{n \geq 0}$ satisfy $\alpha_n \lesssim \beta_n$ if there exists a constant $K > 0$ satisfying $\alpha_n \leq K\beta_n$ for all $n \geq 0$. The notations $\alpha_n \asymp \beta_n$ means that $\alpha_n \lesssim \beta_n$ and $\beta_n \lesssim \alpha_n$.
- Two sequences of real functions $\{f_n\}_{n \geq 0}$ and $\{g_n\}_{n \geq 0}$ defined on the same set Ω satisfy $f_n \lesssim g_n$ if there exists a constant $K > 0$ satisfying $f_n(x) \leq K g_n(x)$ for all $n \geq 0$ and all $x \in \Omega$. The notations $f_n \asymp g_n$ means that $f_n \lesssim g_n$ and $g_n \lesssim f_n$.
- The notation $\mathbb{E}_x[f(x, \xi)]$ denotes expectation with variable x fixed, while the randomness present in ξ is averaged out.

2.2. Gaussian Measure on Hilbert Space. The following facts concerning Gaussian measure on Hilbert space, and Brownian motion in Hilbert space, may be found in [DPZ92]. Since C is self-adjoint, positive and trace-class we may associate with it a centred Gaussian measure π_0 on \mathcal{H} with covariance operator C , i.e., $\pi_0 \stackrel{\text{def}}{=} \mathcal{N}(0, C)$. If $x \stackrel{\mathcal{D}}{\sim} \pi_0$ then we may write (Karhunen-Lo  ve)

$$x = \sum_{j=1}^{\infty} \lambda_j \rho_j \varphi_j \quad \text{with} \quad \rho_j \stackrel{\mathcal{D}}{\sim} \mathcal{N}(0, 1) \text{ i.i.d.} \quad (2.4)$$

If we let $(\Omega, \mathcal{F}, \mathbb{P})$ denote the probability space for the iid sequence $\{\varphi_j\}_{j \geq 1}$ then, since C is trace-class, the sum converges in $L^2(\Omega; \mathcal{H})$.

Since $\{B_r^{-1/2}\varphi_j\}_{j \geq 1}$ forms an orthonormal basis for \mathcal{H}^r , we may write (2.4) as

$$x = \sum_{j=1}^{\infty} (\lambda_j j^r) \rho_j (B_r^{-1/2} \varphi_j) \quad \text{with} \quad \rho_j \stackrel{\mathcal{D}}{\sim} \mathcal{N}(0, 1) \text{ i.i.d.} \quad (2.5)$$

Define

$$C_r = B_r^{1/2} C B_r^{1/2}. \quad (2.6)$$

If $\text{Trace}_{\mathcal{H}^r}(C_r) = \sum_{j=1}^{\infty} \lambda_j^2 j^{2r} < \infty$ for some $r > 0$ then the sum (2.5), and hence the sum (2.4), converges in $L^2(\Omega; \mathcal{H}^r)$ to a centred Gaussian random variable x with covariance operator C_r in

\mathcal{H}^r , and C in \mathcal{H} . Then for any $u, v \in \mathcal{H}^r$, if $x \stackrel{\mathcal{D}}{\sim} \pi_0$, we have $\mathbb{E}[\langle x, u \rangle_r \langle x, v \rangle_r] = \langle u, C_r v \rangle_r$. Thus in what follows, we freely alternate between the Gaussian measures $N(0, C)$ on \mathcal{H} and $N(0, C_r)$ on \mathcal{H}^r . We note that

$$\mathbb{E}[\|x\|_r^2] = \sum_{j=1}^{\infty} \lambda_j^2 j^{2r} = \text{Trace}_{\mathcal{H}^r}(C_r).$$

Frequently in applications the functional Ψ arising in (1.11) may not be defined on all of \mathcal{H} , but only on a subspace $\mathcal{H}^s \subset \mathcal{H}$, for some exponent $s > 0$. Even though the Gaussian measure π_0 is defined on \mathcal{H} , depending on the decay of the eigenvalues of C , there exists an entire range of values of r such that $\text{Trace}_{\mathcal{H}^r}(C_r) < \infty$: in that case the measure π_0 has full support on \mathcal{H}^r , i.e., $\pi_0(\mathcal{H}^r) = 1$. Indeed, the condition $\text{Trace}_{\mathcal{H}^r}(C_r) < \infty$ also implies that for any $\tau > 0$ the measure π_0^τ has full support on \mathcal{H}^r . From now onwards we fix a distinguished exponent $s > 0$ and assume that $\Psi : \mathcal{H}^s \rightarrow \mathbb{R}$ and that $\text{Trace}_{\mathcal{H}^s}(C_s) < \infty$. Then $\pi_0 \stackrel{\mathcal{D}}{\sim} N(0, C)$ on \mathcal{H} and $\pi(\mathcal{H}^s) = 1$. For ease of notations we introduce

$$\hat{\varphi}_j = B_s^{-\frac{1}{2}} \varphi_j \quad \text{for} \quad j \geq 1.$$

The family $\{\hat{\varphi}_j\}_{j \geq 1}$ forms an orthonormal basis for $(\mathcal{H}^s, \langle \cdot, \cdot \rangle_s)$. We may view the Gaussian measure $\pi_0 \stackrel{\mathcal{D}}{\sim} N(0, C)$ on $(\mathcal{H}, \langle \cdot, \cdot \rangle)$ as a Gaussian measure $N(0, C_s)$ on $(\mathcal{H}^s, \langle \cdot, \cdot \rangle_s)$.

A Brownian motion $\{W(t)\}_{t \geq 0}$ in \mathcal{H}^s with covariance operator $C_s : \mathcal{H}^s \rightarrow \mathcal{H}^s$ is a continuous Gaussian process with stationary increments satisfying $\mathbb{E}[\langle W(t), x \rangle_s \langle W(t), y \rangle_s] = t \langle x, C_s y \rangle_s$. For example, taking $\{\beta_j(t)\}_{j \geq 1}$ independent standard real Brownian motions, the process

$$W(t) = \sum_j (j^s \lambda_j) \beta_j(t) \hat{\varphi}_j \tag{2.7}$$

defines a Brownian motion in \mathcal{H}^s with covariance operator C_s ; equivalently, this same process $\{W(t)\}_{t \geq 0}$ can be described as a Brownian motion in \mathcal{H} with covariance operator equal to C since Equation (2.7) may also be expressed as $W(t) = \sum_{j=1}^{\infty} \lambda_j \beta_j(t) \varphi_j$.

2.3. Assumptions. In this section we describe the assumptions on the covariance operator C of the Gaussian measure $\pi_0 \stackrel{\mathcal{D}}{\sim} N(0, C)$ and the functional Ψ . For each $x \in \mathcal{H}^s$ the derivative $\nabla \Psi(x)$ is an element of the dual $(\mathcal{H}^s)^*$ of \mathcal{H}^s , comprising the linear functionals on \mathcal{H}^s . However, we may identify $(\mathcal{H}^s)^* = \mathcal{H}^{-s}$ and view $\nabla \Psi(x)$ as an element of \mathcal{H}^{-s} for each $x \in \mathcal{H}^s$. With this identification, the following identity holds

$$\|\nabla \Psi(x)\|_{\mathcal{L}(\mathcal{H}^s, \mathbb{R})} = \|\nabla \Psi(x)\|_{-s}$$

and the second derivative $\partial^2 \Psi(x)$ can be identified with an element of $\mathcal{L}(\mathcal{H}^s, \mathcal{H}^{-s})$. To avoid technicalities we assume that $\Psi(x)$ is quadratically bounded, with first derivative linearly bounded and second derivative globally bounded. Weaker assumptions could be dealt with by use of stopping time arguments.

ASSUMPTIONS 2.1. *The functional Ψ and the covariance operator C satisfy the following assumptions.*

1. Decay of Eigenvalues λ_j^2 of C : *there exists a constant $\kappa > \frac{1}{2}$ such that*

$$\lambda_j \asymp j^{-\kappa}. \tag{2.8}$$

2. **Domain of Ψ :** *there exists an exponent $s \in [0, \kappa - 1/2)$ such Ψ is defined on \mathcal{H}^s .*
3. **Size of Ψ :** *the functional $\Psi : \mathcal{H}^s \rightarrow \mathbb{R}$ satisfies the growth conditions*

$$0 \leq \Psi(x) \lesssim 1 + \|x\|_s^2.$$

4. **Derivatives of Ψ :** *The derivatives of Ψ satisfy*

$$\|\nabla \Psi(x)\|_{-s} \lesssim 1 + \|x\|_s \quad \text{and} \quad \|\partial^2 \Psi(x)\|_{\mathcal{L}(\mathcal{H}^s, \mathcal{H}^{-s})} \lesssim 1.$$

REMARK 2.2. *The condition $\kappa > \frac{1}{2}$ ensures that $\text{Trace}_{\mathcal{H}^r}(C_r) < \infty$ for any $r < \kappa - \frac{1}{2}$: this implies that $\pi_0^\tau(\mathcal{H}^r) = 1$ for any $\tau > 0$ and $r < \kappa - \frac{1}{2}$.*

REMARK 2.3. *The functional $\Psi(x) = \frac{1}{2}\|x\|_s^2$ is defined on \mathcal{H}^s and its derivative at $x \in \mathcal{H}^s$ is given by $\nabla \Psi(x) = \sum_{j \geq 0} j^{2s} x_j \varphi_j \in \mathcal{H}^{-s}$ with $\|\nabla \Psi(x)\|_{-s} = \|x\|_s$. The second derivative $\partial^2 \Psi(x) \in \mathcal{L}(\mathcal{H}^s, \mathcal{H}^{-s})$ is the linear operator that maps $u \in \mathcal{H}^s$ to $\sum_{j \geq 0} j^{2s} \langle u, \varphi_j \rangle \varphi_j \in \mathcal{H}^{-s}$: its norm satisfies $\|\partial^2 \Psi(x)\|_{\mathcal{L}(\mathcal{H}^s, \mathcal{H}^{-s})} = 1$ for any $x \in \mathcal{H}^s$.*

The Assumptions 2.1 ensure that the functional Ψ behaves well in a sense made precise in the following lemma.

LEMMA 2.4. *Let Assumptions 2.1 hold.*

1. *The function $d(x) \stackrel{\text{def}}{=} -(x + C \nabla \Psi(x))$ is globally Lipschitz on \mathcal{H}^s :*

$$\|d(x) - d(y)\|_s \lesssim \|x - y\|_s \quad \forall x, y \in \mathcal{H}^s. \quad (2.9)$$

2. *The second order remainder term in the Taylor expansion of Ψ satisfies*

$$|\Psi(y) - \Psi(x) - \langle \nabla \Psi(x), y - x \rangle| \lesssim \|y - x\|_s^2 \quad \forall x, y \in \mathcal{H}^s. \quad (2.10)$$

PROOF. See [MPS11]. □

2.4. *Statistical Models satisfying our assumptions .* We now demonstrate a few class of models which satisfy our assumptions. All of the assumptions made above may be relaxed for our general results to go through. The choices we made here are to keep the exposition simple but still good enough to capture a large class of models.

2.4.1. *Nonparametric Regression..* This example is discussed in the introduction, we briefly recall it here. Consider estimating an unknown function x observed at discrete points on a compact set:

$$y_k = x(t_k) + \epsilon_k \quad (2.11)$$

where $t_k \in \mathcal{T} \subset \mathbb{R}^d$ and ϵ_k are i.i.d errors, which are mean 0 and have a smooth density $g(\cdot)$. The unknown function is assumed to be in the Hilbert space $\mathcal{H} = L_2(\mathcal{T})$, i.e., $x \in L_2(\mathcal{T})$. We assume a centered Gaussian random field prior on the function x , $\pi_0 \sim \text{No}(0, C)$ satisfying (2.8). Clearly, the log-likelihood is given by

$$\Psi(x) = \sum_k \log g(y_k - x(t_k)).$$

By ensuring enough decay of eigenvalues, there are a large class of covariance operators C so that item 1 of Assumptions 2.1 is satisfied.

LEMMA 2.5. *If the density $g(\cdot)$ belongs to an exponential family with Gaussian or heavier than Gaussian tails, and with sufficient decay of the eigenvalues of C , items 2,3,4 of Assumptions 2.1 are satisfied.*

PROOF. Since $g(\cdot)$ has gaussian or heavier tails, the function Ψ grows at most quadratically, satisfying item 2 of Assumptions 2.1. By virtue of $g(\cdot)$ belonging to an exponential family, the functional Ψ is smooth. Furthermore imposing the condition on the growth of the function x at infinity (which is related to the eigenvalues of the prior covariance C), the required bounds on the derivatives of Ψ can be obtained. \square

2.4.2. *Statistical Inference for Stochastic Differential Equations..* Consider the following stochastic differential equation:

$$dX_t = (AX_t - BB'\nabla V(X_t, \theta)) dt + B dW_t \quad (2.12)$$

where V is a drift function, $A, B \in \mathbb{R}^{d \times d}$ and θ is an unknown parameter. The statistical goal is to estimate θ from the discrete observations $X_{t_k} = x_k$, $t_k \in [0, T]$. SDE models of the above kind have received tremendous attention in recent years (see [BRSV08] and the references therein).

From a bayesian point of view, a natural way to proceed (after carefully choosing the prior distribution for θ) is to obtain posterior samples via data augmented Gibbs sampling. This will involve two steps: sampling the conditional distribution of θ given the augmented (full) path $X_t, t \in [0, T]$ and sampling the conditional distribution of the augmented path $X_t, t \in [0, T]$ given θ , satisfying the constraint $X_{t_k} = x_k$. Sampling conditional diffusions (*i.e.*, diffusions X_t conditioned to satisfy a few values $X_{t_k} = x_k$) is a very challenging problem in general since their dynamics are quite intractable.

However for SDEs given in (2.12), there is a simple and efficient way to proceed. Let π denote the law of the diffusion bridge X_t conditioned to have $X_0 = x_0$ and $X_1 = x_1$ (more points can be easily dealt with using the Markovian property of the diffusion X_t). Notice that π is a probability measure on $\mathcal{H} = L_2[[0, 1], \mathbb{R}^d]$. If $V = 0$, then we obtain

$$dX_t = AX_t dt + B dW_t, \quad X_0 = x_0, X_1 = x_1 \quad (2.13)$$

which is a Gaussian process whose dynamics is more tractable. Let π_0 denote the law of the diffusion given in (2.13). Then it is known that ([BRSV08]) π is absolutely continuous with respect to π_0 on $\mathcal{H} = L_2[[0, 1], \mathbb{R}^d]$ with

$$\begin{aligned} \frac{d\pi}{d\pi_0}(X) &= \exp\{\Psi(X)\} \\ \Psi(X) &= -\langle 1, \Psi_1(X) \rangle, \quad \Psi_1(x) = |B^{-1}f(x)|^2 + \frac{1}{2}\text{div}f(x) + f(x)'(BB')^{-1}Ax \\ f(x) &= -BB'\nabla V(X_t, \theta). \end{aligned} \quad (2.14)$$

Thus from (2.14) we see that the target measure π satisfies our formulation. Moreover, under mild regularity conditions, it can be shown that the functional Ψ in (2.14) satisfies Assumptions 2.1 [BRSV08].

There are many more practical applications including image processing, non-linear function estimation from partial differential equations which model physical phenomena and signal processing, where the target distributions satisfy our formulation and assumptions, see [CRSW11] for a detailed account.

3. Main Theorem. This section contains a precise statement of the algorithm, statement of the main theorem showing that piecewise linear interpolant of the output of the algorithm converges weakly to a noisy gradient flow, and proof of the main theorem. The proof of various technical lemmas is deferred to section 4.

3.1. P-RWM Algorithm. We now define the Markov chain in \mathcal{H}^s which is reversible with respect to the measure π^τ given by Equation (1.13). This is the Metropolis-Hastings method introduced in [BRSV08] and referred to there as the P-RWM algorithm. Let $x \in \mathcal{H}^s$ be the current position of the Markov chain. The proposal candidate y is given by (1.10), so that

$$y = (1 - 2\delta)^{\frac{1}{2}} x + \sqrt{2\delta\tau} \xi \quad \text{where} \quad \xi = N(0, C) \quad (3.1)$$

and $\delta \in (0, \frac{1}{2})$ is a small parameter which we will send to zero in order to obtain the noisy gradient flow. In Equation (3.1), the random variable ξ is chosen *independent* of x . As described in [BRSV08] (see also [CDS11, Stu10b]), at temperature $\tau \in (0, \infty)$ the Metropolis-Hastings acceptance probability for the proposal y is given by

$$\alpha^\delta(x, \xi) = 1 \wedge \exp\left(-\frac{1}{\tau}(\Psi(y) - \Psi(x))\right). \quad (3.2)$$

The chain is then reversible with respect to π^τ . The Markov chain $x^\delta = \{x^{k,\delta}\}_{k \geq 0}$ can be written as

$$x^{k+1,\delta} = \gamma^{k,\delta} y^{k,\delta} + (1 - \gamma^{k,\delta}) x^{k,\delta} \quad \text{where} \quad y^{k,\delta} = (1 - 2\delta)^{\frac{1}{2}} x^{k,\delta} + \sqrt{2\delta\tau} \xi^k. \quad (3.3)$$

Here the ξ^k are iid Gaussian random variables $N(0, C)$ and the $\gamma^{k,\delta}$ are Bernoulli random variables which account for the accept-reject mechanism of the Metropolis-Hastings algorithm,

$$\gamma^{k,\delta} \stackrel{\text{def}}{=} \gamma^\delta(x^{k,\delta}, \xi^k) \stackrel{\mathcal{D}}{\sim} \text{Bernoulli}\left(\alpha^\delta(x^{k,\delta}, \xi^k)\right). \quad (3.4)$$

The function $\gamma^\delta(x, \xi)$ can be expressed as $\gamma^\delta(x, \xi) = \mathbb{I}_{\{U < \alpha^\delta(x, \xi)\}}$ where $U \stackrel{\mathcal{D}}{\sim} \text{Uniform}(0, 1)$ is independent from any other source of randomness. The next lemma will be repeatedly used in the sequel: it states that the size of the jump $y - x$ is of order $\sqrt{\delta}$.

LEMMA 3.1. *Under Assumptions 2.1 and for any integer $p \geq 1$ the following inequality*

$$\mathbb{E}_x[\|y - x\|_s^p]^{\frac{1}{p}} \lesssim \delta \|x\|_s + \sqrt{\delta} \lesssim \sqrt{\delta} (1 + \|x\|_s)$$

holds for any $\delta \in (0, \frac{1}{2})$.

PROOF. The definition of the proposal (3.1) shows that $\|y - x\|_s^p \lesssim \delta^p \|x\|_s^p + \delta^{\frac{p}{2}} \mathbb{E}[\|\xi\|_s^p]$. Fernique's theorem [DPZ92] shows that ξ has exponential moments and therefore $\mathbb{E}[\|\xi\|_s^p] < \infty$. This gives the conclusion. \square

For future use, we define the local mean acceptance probability at the current position x via the formula

$$\alpha^\delta(x) = \mathbb{E}_x[\alpha^\delta(x, \xi)]. \quad (3.5)$$

3.2. *Main Theorem.* Fix a time horizon $T > 0$ and a temperature $\tau \in (0, \infty)$. The piecewise linear interpolant z^δ of the Markov chain (3.3) is defined by Equation (1.6). The following is the main result of this article. Note that “weakly” refers to weak convergence of probability measures.

THEOREM 3.2. *Let Assumptions 2.1 hold. Let the Markov chain x^δ start at fixed position $x_* \in \mathcal{H}^s$. Then the sequence of processes z^δ converges weakly to z in $C([0, T]; \mathcal{H}^s)$, as $\delta \rightarrow 0$, where z solves the \mathcal{H}^s -valued stochastic differential equation*

$$\begin{aligned} dz &= -\left(z + C\nabla\Psi(z)\right) dt + \sqrt{2\tau}dW \\ z_0 &= x_* \end{aligned} \quad (3.6)$$

and W is a Brownian motion in \mathcal{H}^s with covariance operator equal to C_s .

For conceptual clarity, we derive Theorem 3.2 as a consequence of the general diffusion approximation Lemma 3.5. Consider a separable Hilbert space $(\mathcal{H}^s, \langle \cdot, \cdot \rangle_s)$ and a sequence of \mathcal{H}^s -valued Markov chains $x^\delta = \{x^{k,\delta}\}_{k \geq 0}$. The martingale-drift decomposition with time discretization δ of the Markov chain x^δ reads

$$\begin{aligned} x^{k+1,\delta} &= x^{k,\delta} + \mathbb{E}[x^{k+1,\delta} - x^{k,\delta} | x^{k,\delta}] + \left(x^{k+1,\delta} - x^{k,\delta} - \mathbb{E}[x^{k+1,\delta} - x^{k,\delta} | x^{k,\delta}]\right) \\ &= x^{k,\delta} + d^\delta(x^{k,\delta})\delta + \sqrt{2\tau\delta} \Gamma^\delta(x^{k,\delta}, \xi^k) \end{aligned} \quad (3.7)$$

where the approximate drift d^δ and volatility term $\Gamma^\delta(x, \xi^k)$ are given by

$$\begin{aligned} d^\delta(x) &= \delta^{-1} \mathbb{E}[x^{k+1,\delta} - x^{k,\delta} | x^{k,\delta} = x] \\ \Gamma^\delta(x, \xi^k) &= (2\tau\delta)^{-1/2} \left(x^{k+1,\delta} - x^{k,\delta} - \mathbb{E}[x^{k+1,\delta} - x^{k,\delta} | x^{k,\delta} = x]\right). \end{aligned} \quad (3.8)$$

Notice that $\{\Gamma^{k,\delta}\}_{k \geq 0}$, with $\Gamma^{k,\delta} \stackrel{\text{def}}{=} \Gamma^\delta(x^{k,\delta}, \xi^k)$, is a martingale difference array in the sense that $M^{k,\delta} = \sum_{j=0}^k \Gamma^{j,\delta}$ is a martingale adapted to the natural filtration $\mathcal{F}^\delta = \{\mathcal{F}^{k,\delta}\}_{k \geq 0}$ of the Markov chain x^δ . The parameter δ represents a time increment. We define the piecewise linear rescaled noise process by

$$W^\delta(t) = \sqrt{\delta} \sum_{j=0}^k \Gamma^{j,N} + \frac{t - t_k}{\sqrt{\delta}} \Gamma^{k+1,N} \quad \text{for} \quad t_k \leq t < t_{k+1}. \quad (3.9)$$

We now show that, as $\delta \rightarrow 0$, if the sequence of approximate drift functions $d^\delta(\cdot)$ converges in the appropriate norm to a limiting drift $d(\cdot)$ and the sequence of rescaled noise process W^δ converges to a Brownian motion then the sequence of piecewise linear interpolants z^δ defined by Equation (1.6) converges weakly to a diffusion process in \mathcal{H}^s . In order to state the general diffusion approximation Lemma 3.5, we introduce the following:

CONDITIONS 3.3. *There exists an integer $p \geq 1$ such that the sequence of Markov chains $x^\delta = \{x^{k,\delta}\}_{k \geq 0}$ satisfies*

1. **Convergence of the drift:** *there exists a globally Lipschitz function $d : \mathcal{H}^s \rightarrow \mathcal{H}^s$ such that*

$$\|d^\delta(x) - d(x)\|_s \lesssim \delta \cdot (1 + \|x\|_s^p) \quad (3.10)$$

2. **Invariance principle:** as δ tends to zero the sequence of processes $\{W^\delta\}_{\delta \in (0, \frac{1}{2})}$ defined by Equation (3.9) converges weakly in $C([0, T], \mathcal{H}^s)$ to a Brownian motion W in \mathcal{H}^s with covariance operator C_s .
3. **A priori bound:** the following bound holds

$$\sup_{\delta \in (0, \frac{1}{2})} \left\{ \delta \cdot \mathbb{E} \left[\sum_{k\delta \leq T} \|x^{k,\delta}\|_s^p \right] \right\} < \infty. \quad (3.11)$$

REMARK 3.4. The a-priori bound (3.11) can equivalently be stated as $\sup_{\delta \in (0, \frac{1}{2})} \left\{ \mathbb{E} \left[\int_0^T \|z^\delta(u)\|_s^p du \right] \right\} < \infty$.

It is now proved that Conditions 3.3 are sufficient to obtain a diffusion approximation for the sequence of rescaled processes z^δ defined by equation (1.6), as δ tends to zero.

LEMMA 3.5. **(General Diffusion Approximation for Markov chains)**
Consider a separable Hilbert space $(\mathcal{H}^s, \langle \cdot, \cdot \rangle_s)$ and a sequence of \mathcal{H}^s -valued Markov chains $x^\delta = \{x^{k,\delta}\}_{k \geq 0}$ starting at a fixed position $x_* \in \mathcal{H}^s$,

$$x^{0,\delta} = x_* \quad \forall \delta \in (0; 1).$$

Suppose that the drift-martingale decompositions (3.7) of x^δ satisfy Conditions 3.3. Then the sequence of rescaled interpolants $z^\delta \in C([0, T], \mathcal{H}^s)$ defined by equation (1.6) converges weakly in $C([0, T], \mathcal{H}^s)$ to $z \in C([0, T], \mathcal{H}^s)$ given by the stochastic differential equation

$$\begin{aligned} dz &= d(z) dt + \sqrt{2\tau} dW \\ z_0 &= x_* \end{aligned} \quad (3.12)$$

where W is a Brownian motion in \mathcal{H}^s with covariance C_s .

PROOF. For the sake of clarity, the proof of Lemma 3.5 is divided into several steps.

- **Integral equation representation.**

Notice that solutions of the \mathcal{H}^s -valued SDE (3.12) are nothing else than solutions of the following integral equation,

$$z(t) = x_* + \int_0^t d(z(u)) du + \sqrt{2\tau} W(t) \quad \forall t \in (0, T), \quad (3.13)$$

where W is a Brownian motion in \mathcal{H}^s with covariance operator equal to C_s . We thus introduce the Itô map $\Theta : C([0, T], \mathcal{H}^s) \rightarrow C([0, T], \mathcal{H}^s)$ that sends a function $W \in C([0, T], \mathcal{H}^s)$ to the unique solution of the integral equation (3.13): solution of (3.12) can be represented as $\Theta(W)$ where W is an \mathcal{H}^s -valued Brownian motion with covariance C_s . As is described below, the function Θ is continuous if $C([0, T], \mathcal{H}^s)$ is topologized by the uniform norm $\|w\|_{C([0, T], \mathcal{H}^s)} \stackrel{\text{def}}{=} \sup\{\|w(t)\|_s : t \in (0, T)\}$. It is crucial to notice that the rescaled process z^δ , defined in Equation (1.6), satisfies

$$z^\delta = \Theta(\widehat{W}^\delta) \quad \text{where} \quad \widehat{W}^\delta(t) := W^\delta(t) + \frac{1}{\sqrt{2\tau}} \int_0^t [d^\delta(\bar{z}^\delta(u)) - d(z^\delta(u))] du. \quad (3.14)$$

In Equation (3.14), the quantity d^δ is the approximate drift defined in Equation (3.8) and \bar{z}^δ is the rescaled piecewise constant interpolate of $\{x^{k,\delta}\}_{k \geq 0}$ defined as

$$\bar{z}^\delta(t) = x^{k,\delta} \quad \text{for} \quad t_k \leq t < t_{k+1}. \quad (3.15)$$

The proof follows from a continuous mapping argument (see below) once it is proven that \widehat{W}^δ converges weakly in $C([0, T], \mathcal{H}^s)$ to W .

- **The Itô map Θ is continuous**

It can be proved that Θ is continuous as a mapping from $(C([0, T], \mathcal{H}^s), \|\cdot\|_{C([0, T], \mathcal{H}^s)})$ to itself. The usual Picard's iteration proof of the Cauchy-Lipschitz theorem of ODEs may be employed: see [MPS11].

- **The sequence of processes \widehat{W}^δ converges weakly to W**

The process $\widehat{W}^\delta(t)$ is defined by $\widehat{W}^\delta(t) = W^\delta(t) + \frac{1}{\sqrt{2\tau}} \int_0^t [d^\delta(\bar{z}^\delta(u)) - d(z^\delta(u))] du$ and Conditions 3.3 state that W^δ converges weakly to W in $C([0, T], \mathcal{H}^s)$. Consequently, to prove that $\widehat{W}^\delta(t)$ converges weakly to W in $C([0, T], \mathcal{H}^s)$, it suffices to verify that the sequences of processes

$$(\omega, t) \mapsto \int_0^t [d^\delta(\bar{z}^\delta(u)) - d(z^\delta(u))] du \quad (3.16)$$

converges to 0 in probability with respect to the supremum norm in $C([0, T], \mathcal{H}^s)$. By Markov's inequality, it is enough to check that

$$\lim_{\delta \rightarrow 0} \mathbb{E} \left[\int_0^T \|d^\delta(\bar{z}^\delta(u)) - d(z^\delta(u))\|_s du \right] = 0.$$

Conditions 3.3 states that there exists an integer $p \geq 1$ such that $\|d^\delta(x) - d(x)\| \lesssim \delta \cdot (1 + \|x\|_s^p)$ so that for any $t_k \leq u < t_{k+1}$ we have

$$\|d^\delta(\bar{z}^\delta(u)) - d(\bar{z}^\delta(u))\|_s \lesssim \delta (1 + \|\bar{z}^\delta(u)\|_s^p) = \delta (1 + \|x^{k,\delta}\|_s^p). \quad (3.17)$$

Conditions 3.3 states that $d(\cdot)$ is globally Lipschitz on \mathcal{H}^s . Therefore, Lemma 3.1 shows that

$$\mathbb{E} \|d(\bar{z}^\delta(u)) - d(z^\delta(u))\|_s \lesssim \mathbb{E} \|x^{k+1,\delta} - x^{k,\delta}\|_s \lesssim \delta^{\frac{1}{2}} (1 + \|x^{k,\delta}\|_s). \quad (3.18)$$

From estimates (3.17) and (3.18) it follows that $\|d^\delta(\bar{z}^\delta(u)) - d(z^\delta(u))\|_s \lesssim \delta^{\frac{1}{2}} (1 + \|x^{k,\delta}\|_s^p)$. Consequently

$$\mathbb{E} \left[\int_0^T \|d^\delta(\bar{z}^\delta(u)) - d(z^\delta(u))\|_s du \right] \lesssim \delta^{\frac{3}{2}} \sum_{k \delta < T} \mathbb{E} [1 + \|x^{k,\delta}\|_s^p]. \quad (3.19)$$

The a-priori bound of Conditions 3.3 shows that this last quantity converges to 0 as δ converges to zero, which finishes the proof of Equation (3.16). This concludes the proof of $\widehat{W}^\delta(t) \Rightarrow W$.

- **Continuous mapping argument.**

It has been proved that Θ is continuous as a mapping from $(C([0, T], \mathcal{H}^s), \|\cdot\|_{C([0, T], \mathcal{H}^s)})$ to itself. The solutions of the \mathcal{H}^s -valued SDE (3.12) can be expressed as $\Theta(W)$ while the rescaled continuous interpolate z^δ also reads $z^\delta = \Theta(\widehat{W}^\delta)$. Since \widehat{W}^δ converges weakly in $(C([0, T], \mathcal{H}^s), \|\cdot\|_{C([0, T], \mathcal{H}^s)})$ to W as δ tends to 0, the continuous mapping theorem ensures that z^δ converges weakly in $(C([0, T], \mathcal{H}^s), \|\cdot\|_{C([0, T], \mathcal{H}^s)})$ to the solution $\Theta(W)$ of the \mathcal{H}^s -valued SDE (3.12). This ends the proof of Lemma 3.5.

□

In order to establish Theorem 3.2 as a consequence of the general diffusion approximation Lemma 3.5, it suffices to verify that if Assumptions 2.1 hold then Conditions 3.3 are satisfied by the Markov chain x^δ defined in section 3.1. In section 4.2 we prove the following quantitative version of the approximation $d^\delta \approx d$ where $d(x) = -\left(x + C\nabla\Psi(x)\right)$:

LEMMA 3.6. (Drift estimate)

Let Assumptions 2.1 hold and let $p \geq 1$ be an integer. Then the following estimate is satisfied,

$$\|d^\delta(x) - d(x)\|_s^p \lesssim \delta^{\frac{p}{2}}(1 + \|x\|_s^{2p}). \quad (3.20)$$

Moreover, the approximate drift d^δ is linearly bounded in the sense that

$$\|d^\delta(x)\|_s \lesssim 1 + \|x\|_s. \quad (3.21)$$

It follows from Lemma (3.6) that Equation (3.10) of Conditions 3.3 is satisfied as soon as Assumptions 2.1 hold. The invariance principle of Conditions 3.3 follows from the next lemma. It is proved in section 4.5.

LEMMA 3.7. (Invariance Principle)

Let Assumptions 2.1 hold. Then the rescaled noise process $W^\delta(t)$ defined in equation (3.9) satisfies

$$W^\delta \implies W$$

where \implies denotes weak convergence in $C([0, T]; \mathcal{H}^s)$, and W is a \mathcal{H}^s -valued Brownian motion with covariance operator C_s .

In section 4.4 it is proved that the following a priori bound is satisfied,

LEMMA 3.8. (A priori bound)

Consider a fixed time horizon $T > 0$ and an integer $p \geq 1$. Under Assumptions 2.1 the following bound holds,

$$\sup \left\{ \delta \cdot \mathbb{E} \left[\sum_{k\delta \leq T} \|x^{k,\delta}\|_s^p \right] : \delta \in (0, \frac{1}{2}) \right\} < \infty. \quad (3.22)$$

In conclusion, Lemmas 3.6 and 3.7 and 3.8 together show that Conditions 3.3 are consequences of Assumptions 2.1. Therefore, under Assumptions 2.1, the general diffusion approximation Lemma 3.5 can be applied: this concludes the proof of Theorem 3.2.

4. Key Estimates. This section assembles various results which are used in the previous section. Some of the technical proofs are deferred to the appendix.

4.1. Acceptance probability asymptotics. This section describes a first order expansion of the acceptance probability. The approximation

$$\alpha^\delta(x, \xi) \approx \bar{\alpha}^\delta(x, \xi) \quad \text{where} \quad \bar{\alpha}^\delta(x, \xi) = 1 - \sqrt{\frac{2\delta}{\tau}} \langle \nabla\Psi(x), \xi \rangle \mathbb{I}_{\{\langle \nabla\Psi(x), \xi \rangle > 0\}} \quad (4.1)$$

is valid for $\delta \ll 1$. The quantity $\bar{\alpha}^\delta$ has the advantage over α^δ of being very simple to analyse: explicit computations are available. This will be exploited in section 4.2. The quality of the approximation (4.1) is rigorously quantified in the next lemma.

LEMMA 4.1. (Acceptance probability estimate)

Let Assumptions 2.1 hold. For any integer $p \geq 1$ the quantity $\bar{\alpha}^\delta(x, \xi)$ satisfies

$$\mathbb{E}_x[|\alpha^\delta(x, \xi) - \bar{\alpha}^\delta(x, \xi)|^p] \lesssim \delta^p (1 + \|x\|_s^{2p}). \quad (4.2)$$

PROOF. See Appendix A. \square

Recall the local mean acceptance probability defined by $\alpha^\delta(x) = \mathbb{E}_x[\alpha^\delta(x, \xi)]$ in Equation (3.5). Define the approximate local mean acceptance probability by $\bar{\alpha}^\delta(x) \stackrel{\text{def}}{=} \mathbb{E}_x[\bar{\alpha}^\delta(x, \xi)]$. We now use Lemma 4.1 to approximate the local mean acceptance probability $\alpha^\delta(x)$.

COROLLARY 4.2. Let Assumptions 2.1 hold. For any integer $p \geq 1$ the following estimates hold,

$$|\alpha^\delta(x) - \bar{\alpha}^\delta(x)| \lesssim \delta (1 + \|x\|_s^2) \quad (4.3)$$

$$\mathbb{E}_x[|\alpha^\delta(x, \xi) - 1|^p] \lesssim \delta^{\frac{p}{2}} (1 + \|x\|_s^p) \quad (4.4)$$

PROOF. See Appendix A. \square

4.2. Drift Estimates. Then next lemma shows that explicit computations are available for the quantity $\bar{\alpha}^\delta$. We will use these explicit computations, together with quantification of the error committed in replacing α^δ by $\bar{\alpha}^\delta$, to estimate the mean drift (in this section) and the diffusion term (in the next section).

LEMMA 4.3. The approximate acceptance probability $\bar{\alpha}^\delta(x, \xi)$ satisfies

$$\sqrt{\frac{2\tau}{\delta}} \mathbb{E}_x[\bar{\alpha}^\delta(x, \xi) \cdot \xi] = -C\nabla\Psi(x) \quad \forall x \in \mathcal{H}^s.$$

PROOF. Let $u = \sqrt{\frac{2\tau}{\delta}} \mathbb{E}_x[\bar{\alpha}^\delta(x, \xi) \cdot \xi] \in \mathcal{H}^s$. To prove the lemma it suffices to verify that for all $v \in \mathcal{H}^{-s}$ we have

$$\langle u, v \rangle = -\langle C\nabla\Psi(x), v \rangle.$$

To this end, use the decomposition $v = \alpha\nabla\Psi(x) + w$ where $\alpha \in \mathbb{R}$ and $w \in \mathcal{H}^{-s}$ satisfies $\langle C\nabla\Psi(x), w \rangle = 0$. Since $\xi \stackrel{\mathcal{D}}{\sim} N(0, C)$ the two Gaussian random variables

$$Z_\Psi \stackrel{\text{def}}{=} \langle \nabla\Psi(x), \xi \rangle \quad \text{and} \quad Z_w \stackrel{\text{def}}{=} \langle w, \xi \rangle$$

are independent: indeed, (Z_Ψ, Z_w) is a Gaussian vector in \mathbb{R}^2 with $\text{Cov}(Z_\Psi, Z_w) = 0$. It thus follows that

$$\begin{aligned} \langle u, v \rangle &= -2 \langle \mathbb{E}_x[\langle \nabla\Psi(x), \xi \rangle 1_{\{\langle \nabla\Psi(x), \xi \rangle > 0\}} \cdot \xi], \alpha\nabla\Psi(x) + w \rangle \\ &= -2 \mathbb{E}_x \left[\alpha Z_\Psi^2 1_{\{Z_\Psi > 0\}} + Z_w Z_\Psi 1_{\{Z_\Psi > 0\}} \right] \\ &= -2\alpha \mathbb{E}_x \left[Z_\Psi^2 1_{\{Z_\Psi > 0\}} \right] = -\alpha \mathbb{E}_x \left[Z_\Psi^2 \right] \\ &= -\alpha \langle C\nabla\Psi(x), \nabla\Psi(x) \rangle = \langle -C\nabla\Psi(x), \alpha\nabla\Psi(x) + w \rangle \\ &= -\langle C\nabla\Psi(x), v \rangle, \end{aligned}$$

which concludes the proof of Lemma 4.3. \square

We now use this explicit computation to give a proof of the drift estimate Lemma 3.6.

PROOF OF LEMMA 3.6. The function d^δ defined by Equation (3.8) can also be expressed as

$$d^\delta(x) = \left\{ \frac{(1-2\delta)^{\frac{1}{2}} - 1}{\delta} \alpha^\delta(x) x \right\} + \left\{ \sqrt{\frac{2\tau}{\delta}} \mathbb{E}_x[\alpha^\delta(x, \xi) \xi] \right\} = B_1 + B_2, \quad (4.5)$$

where the mean local acceptance probability $\alpha^\delta(x)$ has been defined in Equation (3.5) and the two terms B_1 and B_2 are studied below. To prove Equation (3.20), it suffices to establish that

$$\|B_1 + x\|_s^p \lesssim \delta^{\frac{p}{2}}(1 + \|x\|_s^{2p}) \quad \text{and} \quad \|B_2 + C\nabla\Psi(x)\|_s^p \lesssim \delta^{\frac{p}{2}}(1 + \|x\|_s^{2p}). \quad (4.6)$$

We now establish these two bounds.

- Lemma 4.1 and Corollary 4.2 show that

$$\begin{aligned} \|B_1 + x\|_s^p &= \left\{ \frac{(1-2\delta)^{\frac{1}{2}} - 1}{\delta} \alpha^\delta(x) + 1 \right\}^p \|x\|_s^p \\ &\lesssim \left\{ \left| \frac{(1-2\delta)^{\frac{1}{2}} - 1}{\delta} - 1 \right|^p + |\alpha^\delta(x) - 1|^p \right\} \|x\|_s^p \\ &\lesssim \left\{ \delta^p + \delta^{\frac{p}{2}}(1 + \|x\|_s^p) \right\} \|x\|_s^p \lesssim \delta^{\frac{p}{2}}(1 + \|x\|_s^{2p}). \end{aligned} \quad (4.7)$$

- Lemma 4.1 shows that

$$\begin{aligned} \|B_2 + C\nabla\Psi(x)\|_s^p &= \left\| \sqrt{\frac{2\tau}{\delta}} \mathbb{E}_x[\alpha^\delta(x, \xi) \xi] + C\nabla\Psi(x) \right\|_s^p \\ &\lesssim \delta^{-\frac{p}{2}} \left\| \mathbb{E}_x[\{\alpha^\delta(x, \xi) - \bar{\alpha}^\delta(x, \xi)\} \xi] \right\|_s^p + \underbrace{\left\| \sqrt{\frac{2\tau}{\delta}} \mathbb{E}_x[\bar{\alpha}^\delta(x, \xi) \xi] + C\nabla\Psi(x) \right\|_s^p}_{=0}. \end{aligned} \quad (4.8)$$

By Lemma 4.3, the second term on the right hand is equal to zero. Consequently, Cauchy Schwarz' inequality implies that

$$\begin{aligned} \|B_2 + C\nabla\Psi(x)\|_s^p &\lesssim \delta^{-\frac{p}{2}} \mathbb{E}_x[|\alpha^\delta(x, \xi) - \bar{\alpha}^\delta(x, \xi)|^2]^{\frac{p}{2}} \\ &\lesssim \delta^{-\frac{p}{2}} \left(\delta^2(1 + \|x\|_s^4) \right)^{\frac{p}{2}} \lesssim \delta^{\frac{p}{2}}(1 + \|x\|_s^{2p}). \end{aligned}$$

Estimates (4.7) and (4.8) give Equation (4.6). To complete the proof we establish the bound (3.21). The expression (4.5) shows that it suffices to verify

$$\sqrt{\frac{2\tau}{\delta}} \mathbb{E}_x[\alpha^\delta(x, \xi) \xi] \lesssim 1 + \|x\|_s.$$

To this end, we use Lemma 4.3 and Corollary 4.2. By Cauchy-Schwarz,

$$\left\| \sqrt{\frac{2\tau}{\delta}} \mathbb{E}_x[\alpha^\delta(x, \xi) \cdot \xi] \right\|_s = \left\| \sqrt{\frac{2\tau}{\delta}} \mathbb{E}_x[(\alpha^\delta(x, \xi) - 1) \cdot \xi] \right\|_s \lesssim \delta^{-\frac{1}{2}} \mathbb{E}_x[(\alpha^\delta(x, \xi) - 1)^2]^{\frac{1}{2}} \lesssim 1 + \|x\|_s,$$

which concludes the proof of Lemma 3.6. \square

4.3. *Noise Estimates.* In this section we estimate the error in the approximation $\Gamma^{k,\delta} \approx N(0, C_s)$. To this end, let us introduce the covariance operator $D^\delta(x)$ of the martingale difference Γ^δ ,

$$D^\delta(x) = \mathbb{E} \left[\Gamma^{k,\delta} \otimes_{\mathcal{H}^s} \Gamma^{k,\delta} \mid x^{k,\delta} = x \right].$$

For any $x, u, v \in \mathcal{H}^s$ the operator $D^\delta(x)$ satisfies

$$\mathbb{E} \left[\langle \Gamma^{k,\delta}, u \rangle_s \langle \Gamma^{k,\delta}, v \rangle_s \mid x^{k,\delta} = x \right] = \langle u, D^\delta(x) v \rangle_s.$$

The next lemma gives a quantitative version of the approximation $D^\delta(x) \approx C_s$.

LEMMA 4.4. (Noise estimates)

Let Assumptions 2.1 hold. For any pair of indices $i, j \geq 1$, the martingale difference term $\Gamma^\delta(x, \xi)$ satisfies

$$|\langle \hat{\varphi}_i, D^\delta(x) \hat{\varphi}_j \rangle_s - \langle \hat{\varphi}_i, C_s \hat{\varphi}_j \rangle_s| \lesssim \delta^{\frac{1}{8}} \cdot (1 + \|x\|_s) \quad (4.9)$$

$$|\text{Trace}_{\mathcal{H}^s}(D^\delta(x)) - \text{Trace}_{\mathcal{H}^s}(C_s)| \lesssim \delta^{\frac{1}{8}} \cdot (1 + \|x\|_s^2). \quad (4.10)$$

PROOF. See Appendix A. □

4.4. *A Priori bound.* Now we have all the ingredients for the proof of the a priori bound presented in Lemma 3.8 which states that the rescaled process z^δ given by Equation (1.6) does not blow up in finite time.

PROOF LEMMA 3.8. Without loss of generality, assume that $p = 2n$ for some positive integer $n \geq 1$. We now prove that there exist constants $\alpha_1, \alpha_2, \alpha_3 > 0$ satisfying

$$\mathbb{E}[\|x^{k,\delta}\|_s^{2n}] \leq (\alpha_1 + \alpha_2 k \delta) e^{\alpha_3 k \delta}. \quad (4.11)$$

Lemma 3.8 is a straightforward consequence of Equation 4.11 since this implies that

$$\delta \sum_{k\delta < T} \mathbb{E}[\|x^{k,\delta}\|_s^{2n}] \leq \delta \sum_{k\delta < T} (\alpha_1 + \alpha_2 k \delta) e^{\alpha_3 k \delta} \asymp \int_0^T (\alpha_1 + \alpha_2 t) e^{\alpha_3 t} dt < \infty.$$

For notational convenience, let us define $V^{k,\delta} = \mathbb{E}[\|x^{k,\delta}\|_s^{2n}]$. To prove Equation (4.11), it suffices to establish that

$$V^{k+1,\delta} - V^{k,\delta} \leq K \delta \cdot (1 + V^{k,\delta}), \quad (4.12)$$

where $K > 0$ is constant independent from $\delta \in (0, \frac{1}{2})$. Indeed, iterating inequality (4.12) leads to the bound (4.11), for some computable constants $\alpha_1, \alpha_2, \alpha_3 > 0$. The definition of V^k shows that

$$\begin{aligned} V^{k+1,\delta} - V^{k,\delta} &= \mathbb{E}[\|x^{k,\delta} + (x^{k+1,\delta} - x^{k,\delta})\|_s^{2n} - \|x^{k,\delta}\|_s^{2n}] \\ &= \mathbb{E} \left[\left\{ \|x^{k,\delta}\|_s^2 + \|x^{k+1,\delta} - x^{k,\delta}\|_s^2 + 2 \langle x^{k,\delta}, x^{k+1,\delta} - x^{k,\delta} \rangle_s \right\}^n - \|x^{k,\delta}\|_s^{2n} \right] \end{aligned} \quad (4.13)$$

where the increment $x^{k+1,\delta} - x^{k,\delta}$ is given by

$$x^{k+1,\delta} - x^{k,\delta} = \gamma^{k,\delta} \left((1 - 2\delta)^{\frac{1}{2}} - 1 \right) x^{k,\delta} + \sqrt{2\delta} \gamma^{k,\delta} \xi^k. \quad (4.14)$$

To bound the right-hand-side of Equation (4.13), we use a binomial expansion and control each term. To this end, we establish the following estimate: for all integers $i, j, k \geq 0$ satisfying

$$i + j + k = n \quad \text{and} \quad (i, j, k) \neq (n, 0, 0)$$

the following inequality holds,

$$\mathbb{E} \left[\left(\|x^{k,\delta}\|_s^2 \right)^i \left(\|x^{k+1,\delta} - x^{k,\delta}\|_s^2 \right)^j \left(\langle x^{k,\delta}, x^{k+1,\delta} - x^{k,\delta} \rangle_s \right)^k \right] \lesssim \delta (1 + V^{k,\delta}). \quad (4.15)$$

To prove Equation (4.15), we separate two different cases.

- Let us suppose $(i, j, k) = (n-1, 0, 1)$. Lemma 3.6 states that the approximate drift has a linearly bounded growth so that

$$\left\| \mathbb{E} [x^{k+1,\delta} - x^{k,\delta} | x^{k,\delta}] \right\|_s = \delta \|d^\delta(x^{k,\delta})\|_s \lesssim \delta (1 + \|x^{k,\delta}\|_s).$$

Consequently, we have

$$\begin{aligned} \mathbb{E} \left[\left(\|x^{k,\delta}\|_s^2 \right)^{n-1} \langle x^{k,\delta}, x^{k+1,\delta} - x^{k,\delta} \rangle_s \right] &\lesssim \mathbb{E} \left[\|x^{k,\delta}\|_s^{2(n-1)} \|x^{k,\delta}\|_s \left(\delta (1 + \|x^{k,\delta}\|_s) \right) \right] \\ &\lesssim \delta (1 + V^{k,\delta}). \end{aligned}$$

This proves Equation (4.15) in the case $(i, j, k) = (n-1, 0, 1)$.

- Let us suppose $(i, j, k) \notin \{(n, 0, 0), (n-1, 0, 1)\}$. Because for any integer $p \geq 1$,

$$\mathbb{E}_x \left[\|x^{k+1,\delta} - x^{k,\delta}\|_s^p \right]^{\frac{1}{p}} \lesssim \delta^{\frac{1}{2}} (1 + \|x\|_s)$$

it follows from Cauchy-Schwarz inequality that

$$\mathbb{E} \left[\left(\|x^{k,\delta}\|_s^2 \right)^i \left(\|x^{k+1,\delta} - x^{k,\delta}\|_s^2 \right)^j \left(\langle x^{k,\delta}, x^{k+1,\delta} - x^{k,\delta} \rangle_s \right)^k \right] \lesssim \delta^{j+\frac{k}{2}} (1 + V^{k,\delta}).$$

Since we have supposed that $(i, j, k) \notin \{(n, 0, 0), (n-1, 0, 1)\}$ and $i + j + k = n$, it follows that $j + \frac{k}{2} \geq 1$. This concludes the proof of Equation (4.15),

The binomial expansion of Equation (4.13) and the bound (4.15) show that

$$V^{k+1,\delta} - V^{k,\delta} \lesssim \delta (1 + V^{k,\delta}).$$

This proves Equation (4.12), which concludes the proof of Lemma 3.8. \square

4.5. Invariance Principle. Combining the noise estimates of Lemma 4.4 and the a priori bound of Lemma 3.8, we show that under Assumptions 2.1 the sequence of rescaled noise processes defined in Equation 3.9 converges weakly to a Brownian motion. This is the content of Lemma 3.7 whose proof is now presented.

PROOF OF LEMMA 3.7. As described in [Ber86] [Proposition 5.1], in order to prove that W^δ converges weakly to W in $C([0, T]; \mathcal{H}^s)$ it suffices to prove that for any $t \in [0, T]$ and any pair of indices $i, j \geq 0$ the following three limits hold in probability,

$$(4.16) \quad \lim_{\delta \rightarrow 0} \delta \sum_{k\delta < t} \mathbb{E} \left[\|\Gamma^{k,\delta}\|_s^2 |x^{k,\delta} \right] = t \cdot \text{Trace}_{\mathcal{H}^s}(C_s)$$

$$(4.17) \quad \lim_{\delta \rightarrow 0} \delta \sum_{k\delta < t} \mathbb{E} \left[\langle \Gamma^{k,\delta}, \hat{\varphi}_i \rangle_s \langle \Gamma^{k,\delta}, \hat{\varphi}_j \rangle_s |x^{k,\delta} \right] = t \langle \hat{\varphi}_i, C_s \hat{\varphi}_j \rangle_s$$

$$(4.18) \quad \lim_{\delta \rightarrow 0} \delta \sum_{k\delta < T} \mathbb{E} \left[\|\Gamma^{k,\delta}\|_s^2 \mathbb{I}_{\{\|\Gamma^{k,\delta}\|_s^2 \geq \delta^{-1} \epsilon\}} |x^{k,\delta} \right] = 0 \quad \forall \epsilon > 0.$$

We now check that these three conditions are indeed satisfied.

- Condition (4.16): since $\mathbb{E} \left[\|\Gamma^{k,\delta}\|_s^2 |x^{k,\delta} \right] = \text{Trace}_{\mathcal{H}^s}(D^\delta(x^{k,\delta}))$, Lemma 4.4 shows that

$$\mathbb{E} \left[\|\Gamma^{k,\delta}\|_s^2 |x^{k,\delta} \right] = \text{Trace}_{\mathcal{H}^s}(C_s) + \mathbf{e}_1^\delta(x^{k,\delta})$$

where the error term \mathbf{e}_1^δ satisfies $|\mathbf{e}_1^\delta(x)| \lesssim \delta^{\frac{1}{8}} (1 + \|x\|_s^2)$. Consequently, to prove condition (4.16) it suffices to establish that

$$\lim_{\delta \rightarrow 0} \mathbb{E} \left[\delta \sum_{k\delta < T} \mathbf{e}_1^\delta(x^{k,\delta}) \right] = 0.$$

We have $\mathbb{E} \left[\delta \sum_{k\delta < T} \mathbf{e}_1^\delta(x^{k,\delta}) \right] \lesssim \delta^{\frac{1}{8}} \left\{ \delta \cdot \mathbb{E} \left[\sum_{k\delta < T} (1 + \|x^{k,\delta}\|_s^2) \right] \right\}$ and the apriori bound presented in Lemma 3.8 shows that

$$\sup_{\delta \in (0, \frac{1}{2})} \left\{ \delta \cdot \mathbb{E} \left[\sum_{k\delta < T} (1 + \|x^{k,\delta}\|_s^2) \right] \right\} < \infty.$$

Consequently $\lim_{\delta \rightarrow 0} \mathbb{E} \left[\delta \sum_{k\delta < T} \mathbf{e}_1^\delta(x^{k,\delta}) \right] = 0$, and the conclusion follows.

- Condition (4.17): Lemma 4.4 states that

$$\mathbb{E}_k \left[\langle \Gamma^{k,\delta}, \hat{\varphi}_i \rangle_s \langle \Gamma^{k,\delta}, \hat{\varphi}_j \rangle_s \right] = \langle \hat{\varphi}_i, C_s \hat{\varphi}_j \rangle_s + \mathbf{e}_2^\delta(x^{k,\delta})$$

where the error term \mathbf{e}_2^δ satisfies $|\mathbf{e}_2^\delta(x)| \lesssim \delta^{\frac{1}{8}} (1 + \|x\|_s)$. The exact same approach as the proof of Condition (4.16) gives the conclusion.

- Condition (4.18): from Cauchy-Schwarz and Markov's inequalities it follows that

$$\begin{aligned} \mathbb{E} \left[\|\Gamma^{k,\delta}\|_s^2 \mathbb{I}_{\{\|\Gamma^{k,\delta}\|_s^2 \geq \delta^{-1} \epsilon\}} \right] &\leq \mathbb{E} \left[\|\Gamma^{k,\delta}\|_s^4 \right]^{\frac{1}{2}} \cdot \mathbb{P} \left[\|\Gamma^{k,\delta}\|_s^2 \geq \delta^{-1} \epsilon \right]^{\frac{1}{2}} \\ &\leq \mathbb{E} \left[\|\Gamma^{k,\delta}\|_s^4 \right]^{\frac{1}{2}} \cdot \left\{ \frac{\mathbb{E} \left[\|\Gamma^{k,\delta}\|_s^4 \right]}{(\delta^{-1} \epsilon)^2} \right\}^{\frac{1}{2}} \\ &\leq \frac{1}{\epsilon^2} \delta^2 \cdot \mathbb{E} \left[\|\Gamma^{k,\delta}\|_s^4 \right]. \end{aligned}$$

Consequently we have

$$\mathbb{E} \left[\delta \sum_{k\delta < T} \mathbb{E} \left[\|\Gamma^{k,\delta}\|_s^2 \mathbb{I}_{\{\|\Gamma^{k,\delta}\|_s^2 \geq \delta^{-1} \epsilon\}} |x^{k,\delta} \right] \right] \leq \frac{1}{\epsilon^2} \delta^2 \left\{ \delta \cdot \mathbb{E} \left[\sum_{k\delta < T} \|\Gamma^{k,\delta}\|_s^4 \right] \right\}$$

and the conclusion again follows from the a priori bound Lemma 3.8.

□

5. Quadratic Variation. As discussed in the introduction, the SPDE (1.7), and the Metropolis-Hastings algorithm P-RWM which approximates it for small δ , do not satisfy the smoothing property and so almost sure properties of the limit measure π^τ are not necessarily seen at finite time. In this section we prove a limit theorem satisfied by such almost sure quantities, under P-RWM. When C is the covariance of Brownian motion or Brownian bridge then the almost sure quantity will be quadratic variation; for other covariances it will be a generalization defined precisely in the following subsection. We show that the quadratic variation of P-RWM converges as $k \rightarrow \infty$ to its value under the invariant measure. We then prove that piecewise linear interpolation of this quantity solves, in the small δ limit, a linear ODE (the “fluid limit”) whose globally attractive stable state is the almost sure quantity. This quantifies the manner in which the P-RWM method approaches statistical equilibrium.

5.1. Definition and Properties. Under Assumptions 2.1, the Karhunen-Loève expansion shows that π_0 -almost every $x \in \mathcal{H}$ satisfies

$$\lim_{N \rightarrow \infty} N^{-1} \sum_{j=1}^N \frac{\langle x, \varphi_j \rangle^2}{\lambda_j^2} = 1.$$

This motivates the definition of the quadratic variation like quantities

$$V_-(x) \stackrel{\text{def}}{=} \liminf_{N \rightarrow \infty} N^{-1} \sum_{j=1}^n \frac{\langle x, \varphi_j \rangle^2}{\lambda_j^2} \quad \text{and} \quad V_+(x) \stackrel{\text{def}}{=} \limsup_{N \rightarrow \infty} N^{-1} \sum_{j=1}^n \frac{\langle x, \varphi_j \rangle^2}{\lambda_j^2}.$$

When these two quantities are equal the vector $x \in \mathcal{H}$ is said to possess a *quadratic variation* $V(x)$ defined as $V(x) = V_-(x) = V_+(x)$. Consequently, π_0 -almost every $x \in \mathcal{H}$ possesses a quadratic variation $V(x) = 1$. It is a straightforward consequence that π_0^τ -almost every and π^τ -almost every $x \in \mathcal{H}$ possesses a quadratic variation $V(x) = \tau$. Strictly speaking this only coincides with quadratic variation when C is the covariance of a (possibly conditioned) Brownian motion; however we use the terminology more generally in this section. The next lemma proves that the quadratic variation $V(\cdot)$ behaves as it should do with respect to additivity.

LEMMA 5.1. (Quadratic Variation Additivity)

Consider a vector $x \in \mathcal{H}$ and a Gaussian random variable $\xi \stackrel{\mathcal{D}}{\sim} \pi_0$ and a real number $\alpha \in \mathbb{R}$. Suppose that the vector $x \in \mathcal{H}$ possesses a finite quadratic variation $V(x) < +\infty$. Then almost surely the vector $x + \alpha\xi \in \mathcal{H}$ possesses a quadratic variation that is equal to

$$V(x + \alpha\xi) = V(x) + \alpha^2.$$

PROOF. Let us define $V_N \stackrel{\text{def}}{=} N^{-1} \sum_{j=1}^N \frac{\langle x, \varphi_j \rangle \cdot \langle \xi, \varphi_j \rangle}{\lambda_j^2}$. To prove Lemma 5.1 it suffices to prove that almost surely the following limit holds

$$\lim_{N \rightarrow \infty} V_N = 0.$$

Borel-Cantelli Lemma shows that it suffices to prove that for every fixed $\varepsilon > 0$ we have $\sum_{N \geq 1} \mathbb{P}[|V_N| > \varepsilon] < \infty$. Notice then that V_N is a centred Gaussian random variables with variance

$$\text{Var}(V_N) = \frac{1}{N} \left(N^{-1} \sum_{j=1}^N \frac{\langle x, \varphi_j \rangle^2}{\lambda_j^2} \right) \asymp \frac{V(x)}{N}.$$

It readily follows that $\sum_{N \geq 1} \mathbb{P}[|V_N| > \varepsilon] < \infty$, finishing the proof of the Lemma. \square

5.2. *Large k Behaviour of Quadratic Variation for P-RWM.* The P-RWM algorithm at temperature $\tau > 0$ and discretization parameter $\delta > 0$ proposes a move from x to y according to the dynamics

$$y = (1 - 2\delta)^{\frac{1}{2}} x + (2\delta\tau)^{\frac{1}{2}} \xi \quad \text{with} \quad \xi \stackrel{\mathcal{D}}{\sim} \pi_0.$$

This move is accepted with probability $\alpha^\delta(x, y)$. In this case, Lemma 5.1 shows that if the quadratic variation $V(x)$ exists then the quadratic variation of the proposed move $y \in \mathcal{H}$ exists and satisfies

$$\frac{V(y) - V(x)}{\delta} = -2(V(x) - \tau). \quad (5.1)$$

Consequently, one can prove that for any finite time step $\delta > 0$ and temperature $\tau > 0$ the quadratic variation of the MCMC algorithm converges to τ .

PROPOSITION 5.2. (Limiting Quadratic Variation) *Let Assumptions 2.1 hold and $\{x^{k,\delta}\}_{k \geq 0}$ be the Markov chain of section 3.1. Then almost surely the quadratic variation of the Markov chain converges to τ ,*

$$\lim_{k \rightarrow \infty} V(x^{k,\delta}) = \tau.$$

PROOF. Let us first show that the number of accepted moves is infinite. If this were not the case, the Markov chain would eventually reach a position $x^{k,\delta} = x \in \mathcal{H}$ such that all subsequent proposals $y^{k+l} = (1 - 2\delta)^{\frac{1}{2}} x^k + (2\delta\tau)^{\frac{1}{2}} \xi^{k+l}$ would be refused. This means that the i.i.d. Bernoulli random variables $\gamma^{k+l} = \text{Bernoulli}(\alpha^\delta(x^k, y^{k+l}))$ satisfy $\gamma^{k+l} = 0$ for all $l \geq 0$. This can only happen with probability 0. Indeed, since $\mathbb{P}[\gamma^{k+l} = 1] > 0$, one can use Borel-Cantelli Lemma to show that almost surely there exists $l \geq 0$ such that $\gamma^{k+l} = 1$. To conclude the proof of the Proposition, notice then that the sequence $\{u_k\}_{k \geq 0}$ defined by $u_{k+1} - u_k = -2\delta(u_k - \tau)$ converges to τ . \square

5.3. *Fluid Limit for Quadratic Variation of P-RWM.* To gain further insight into the rate at which the limiting behaviour of the quadratic variation is observed for P-RWM we derive an ODE “fluid limit” for the Metropolis-Hastings algorithm. We introduce the continuous time process $t \mapsto v^\delta(t)$ defined as continuous piecewise linear interpolation of the process $k \mapsto V(x^{k,\delta})$ as follows:

$$v^\delta(t) = \frac{1}{\delta} (t - t_k) V(x^{k+1,\delta}) + \frac{1}{\delta} (t_{k+1} - t) V(x^{k,\delta}) \quad \text{for} \quad t_k \leq t < t_{k+1}. \quad (5.2)$$

Since the acceptance probability of P-RWM approaches 1 as $\delta \rightarrow 0$ (see Corollary 4.2) Equation (5.1) shows heuristically that the trajectories of the process $t \mapsto v^\delta(t)$ should be well approximated by the solution of the (non stochastic) differential equation

$$\dot{v} = -2(v - \tau) \quad (5.3)$$

We prove such a result, in the sense of convergence in probability in $C([0, T]; \mathbb{R})$:

THEOREM 5.3. (Fluid Limit For Quadratic Variation) *Let Assumptions 2.1 hold. Let the Markov chain x^δ start at fixed position $x_* \in \mathcal{H}^s$. Assume that $x_* \in \mathcal{H}$ possesses a finite quadratic variation, $V(x_*) < \infty$. Then the function $v^\delta(t)$ converges in probability in $C([0, T], \mathbb{R})$, as δ goes to 0, to the solution of the differential equation (5.3) with initial condition $v_0 = V(x_*)$.*

As already indicated, the heart of the proof of the result consists in showing that the acceptance probability of the algorithm converges to 1 as δ goes to 0. We prove such a result as Lemma 5.4 below, and then proceed to prove Theorem 5.3. To this end we introduce $t^\delta(k)$, the number of accepted moves:

$$t^\delta(k) \stackrel{\text{def}}{=} \sum_{l \leq k} \gamma^{l,\delta},$$

where $\gamma^{l,\delta} = \text{Bernoulli}(\alpha^\delta(x, y))$ is the Bernoulli random variable defined in Equation (3.4). Since the acceptance probability of the algorithm converges to 1 as $\delta \rightarrow 0$, the approximation $t^\delta(k) \approx k$ holds. In order to prove a fluid limit result on the interval $[0, T]$ one needs to prove that the quantity $|t^\delta(k) - k|$ is small when compared to δ^{-1} . The next Lemma shows that such a bounds holds uniformly on the interval $[0, T]$.

LEMMA 5.4. (Number of Accepted Moves) *Let Assumptions 2.1 hold. The number of accepted moves $t^\delta(\cdot)$ verifies*

$$\lim_{\delta \rightarrow 0} \sup \{ \delta \cdot |t^\delta(k) - k| : 0 \leq k \leq T\delta^{-1} \} = 0$$

where the convergence holds in probability.

PROOF. The proof is given in Appendix B. □

We now complete the proof of Theorem 5.3 using the key Lemma 5.4.

PROOF OF THEOREM 5.3. The proof consists in proving that the trajectory of the quadratic variation process behaves as if all the move were accepted. The main ingredient is the uniform lower bound on the acceptance probability given by Lemma 5.4.

Recall that $v^\delta(k\delta) = V(x^{k,\delta})$. Consider the piecewise linear function $\hat{v}^\delta(\cdot) \in C([0, T], \mathbb{R})$ defined by linear interpolation of the values $\hat{v}^\delta(k\delta) = u^\delta(k)$ and where the sequence $\{u^\delta(k)\}_{k \geq 0}$ satisfies $u^\delta(0) = V(x_*)$ and

$$u^\delta(k+1) - u^\delta(k) = -2\delta(u^\delta(k) - \tau).$$

The value $u^\delta(k) \in \mathbb{R}$ represents the quadratic variation of $x^{k,\delta}$ if the k first moves of the MCMC algorithm had been accepted. One can readily check that as δ goes to zero the sequence of continuous functions $\hat{v}^\delta(\cdot)$ converges in $C([0, T], \mathbb{R})$ to the solution $v(\cdot)$ of the differential equation (5.3). Consequently, to prove Theorem 5.3 it suffices to show that for any $\varepsilon > 0$ we have

$$\lim_{\delta \rightarrow 0} \mathbb{P} \left[\sup \left\{ |V(x^{k,\delta}) - u^\delta(k)| : k \leq \delta^{-1}T \right\} > \varepsilon \right] = 0. \quad (5.4)$$

The definition of the number of accepted moves $t^\delta(k)$ is such that $V(x^{k,\delta}) = u^\delta(t^\delta(k))$. Note that

$$(5.5) \quad u^\delta(k) = (1 - 2\delta)^k u_0 + (1 - (1 - 2\delta)^k) \tau.$$

Hence, for any integers $t_1, t_2 \geq 0$, we have $|u^\delta(t_2) - u^\delta(t_1)| \leq |u^\delta(|t_2 - t_1|) - u^\delta(0)|$ so that

$$|V(x^{k,\delta}) - u^\delta(k)| = |u^\delta(t^\delta(k)) - u^\delta(k)| \leq |u^\delta(k - t^\delta(k)) - u^\delta(0)|.$$

Equation (5.5) shows that $|u^\delta(k) - u^\delta(0)| \lesssim (1 - (1 - 2\delta)^k)$. This implies that

$$|V(x^{k,\delta}) - u^\delta(k)| \lesssim 1 - (1 - 2\delta)^{k-t^\delta(k)} \lesssim 1 - (1 - 2\delta)^{\delta^{-1}S}$$

where $S = \sup \{ \delta \cdot |t^\delta(k) - k| : 0 \leq k \leq T\delta^{-1} \}$. Since for any $a > 0$ we have $1 - (1 - 2\delta)^{a\delta^{-1}} \rightarrow 1 - e^{-2a}$, Equation (5.4) follows if one can prove that as δ goes to 0 the supremum S converges to 0 in probability: this is precisely the content of Lemma 5.4. This concludes the proof of Theorem 5.3. \square

6. Numerical results. The numerical results comparing the efficiency of the S-RWM and P-RWM are clearly explained in a companion paper [CRSW11] and we refer the interested reader to that paper. In this section, we present some numerical simulations demonstrating our results in the context of simulated annealing. We consider the minimisation of a functional $J(\cdot)$ defined on the Sobolev space $H_0^1(\mathbb{R}) \subset C^0([0, 1]) \subset L^2(0, 1)$. Functions $x \in H_0^1([0, 1])$ are continuous and satisfy $x(0) = x(1) = 0$. For a given real parameter $\lambda > 0$, the functional $J : H_0^1([0, 1]) \rightarrow \mathbb{R}$ is composed of two competitive terms, as follows:

$$J(x) = \frac{1}{2} \int_0^1 |\dot{x}(s)|^2 ds + \frac{\lambda}{4} \int_0^1 (x(s)^2 - 1)^2 ds. \quad (6.1)$$

The first term penalises functions that deviate from being flat, whilst the second term penalises functions that deviate from one in absolute value. Critical points of the functional $J(\cdot)$ solve the following Euler-Lagrange equation:

$$\begin{aligned} \ddot{x} + \lambda x(1 - x^2) &= 0 \\ x(0) &= x(1) = 0. \end{aligned} \quad (6.2)$$

Clearly $x \equiv 0$ is a solution for all $\lambda \in \mathbb{R}^+$. If $\lambda \in (0, \pi^2)$ then this is the unique solution of the Euler-Lagrange equation and is the global minimizer of J . For each integer k there is a supercritical bifurcation at parameter value $\lambda = k^2\pi^2$. For $\lambda > \pi^2$ there are two minimizers, both of one sign and one being minus the other. The three different solutions of (6.2) which exist for $\lambda = 2\pi^2$ are displayed in Figure 1, at which value the zero (blue dotted) solution is a saddle point, and the two green solutions are the global minimizers of J . These properties of J are overviewed in, for example, [Hen81]. We will show how these global minimizers can emerge from an algorithm whose only ingredients are an ability to evaluate Ψ and to sample from the Gaussian measure with Cameron-Martin norm $\int_0^1 |\dot{x}(s)|^2 ds$. We emphasize that we are not advocating this as the optimal method for solving the Euler-Lagrange equations (6.2). We have chosen this example for its simplicity, in order to illustrate the key ingredients of the theory developed in this paper.

The P-RWM algorithm to minimize J given by (6.1) is implemented on $L^2([0, 1])$. Recall from section 1 that the Gaussian measure $N(0, C)$ may be identified by finding the covariance operator for which the $H_0^1([0, 1])$ norm $\|x\|_C^2 \stackrel{\text{def}}{=} \int_0^1 |\dot{x}(s)|^2 ds$ is the Cameron-Martin norm. In [HAVW05] it is shown that the Wiener bridge measure $\mathbb{W}_{0 \rightarrow 0}$ on $L^2([0, 1])$ has precisely this Cameron-Martin norm; indeed it is demonstrated that C^{-1} is the densely defined operator $-\frac{d^2}{ds^2}$ with $D(C^{-1}) = H^2([0, 1]) \cap H_0^1([0, 1])$. In this regard it is also instructive to adopt the physicists viewpoint that

$$\mathbb{W}_{0 \rightarrow 0}(dx) \propto \exp \left(-\frac{1}{2} \int_0^1 |\dot{x}(s)|^2 ds \right) dx$$

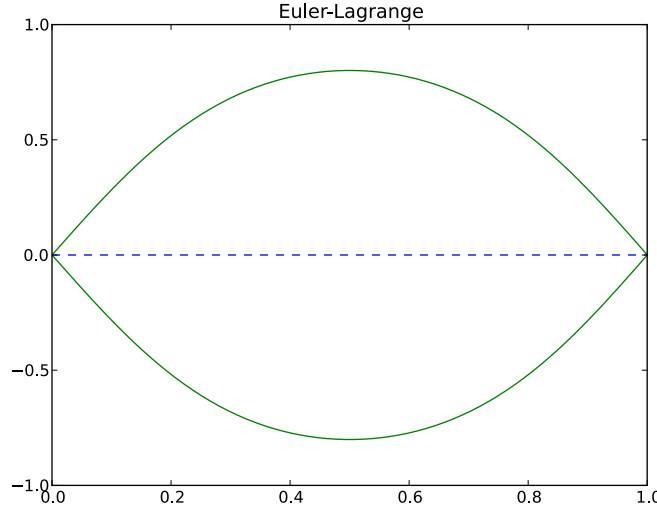


FIG 1. The three solutions of the Euler-Lagrange Equation (6.2) for $\lambda = 2\pi^2$. Only the two non-zero solutions are global minimum of the functional $J(\cdot)$. The dotted solution is a local maximum of $J(\cdot)$.

although, of course, there is no Lebesgue measure in infinite dimensions. Using an integration by parts, together with the boundary conditions on $H_0^1([0, 1])$, then gives

$$\mathbb{W}_{0 \rightarrow 0}(dx) \propto \exp\left(\frac{1}{2} \int_0^1 x(s) \frac{d^2 x}{ds^2}(s) ds\right) dx$$

and the inverse of C is clearly identified as the differential operator above. See [CH06] for basic discussion of the physicists viewpoint on Wiener measure. For a given temperature parameter τ the Wiener bridge measure $\mathbb{W}_{0 \rightarrow 0}^\tau$ on $L^2([0, 1])$ is defined as the law of $\{\sqrt{\tau} W(t)\}_{t \in [0, 1]}$ where $\{W(t)\}_{t \in [0, 1]}$ is a standard Brownian bridge on $[0, 1]$ drawn from $\mathbb{W}_{0 \rightarrow 0}$.

The posterior distribution $\pi^\tau(dx)$ is defined by the change of probability formula

$$\frac{d\pi^\tau}{d\mathbb{W}_{0 \rightarrow 0}^\tau}(x) \propto e^{-\Psi(x)} \quad \text{with} \quad \Psi(x) = \frac{\lambda}{4} \int_0^1 (x(s)^2 - 1)^2 ds.$$

Notice that $\pi_0^\tau(H_0^1([0, 1])) = \pi^\tau(H_0^1([0, 1])) = 0$ since a Brownian bridge is almost surely not differentiable anywhere on $[0, 1]$. It is for this reason that the algorithm is implemented on $L^2([0, 1])$ even though the functional $J(\cdot)$ is defined on the Sobolev space $H_0^1([0, 1])$. In terms of Assumptions 2.1(1) we have $\kappa = 1$ and the measure π_0^τ is supported on \mathcal{H}^r if and only if $r < \frac{1}{2}$, see Remark 2.2; note also that $H_0^1([0, 1]) = \mathcal{H}^1$. Assumption 2.1(2) is satisfied for any choice $s \in [\frac{1}{4}, \frac{1}{2})$ because \mathcal{H}^s is embedded into $L^4([0, 1])$ for $s \geq \frac{1}{4}$. We add here that Assumptions 2.1(3-4) do not hold globally, but only locally on bounded sets, but the numerical results below will indicate that the theory developed in this paper is still relevant and could be extended to nonlocal versions of Assumptions 2.1(3-4), with considerable further work.

Following section 3.1, the P-RWM Markov chain at temperature $\tau > 0$ and time discretization $\delta > 0$ proposes moves from x to y according to

$$y = (1 - 2\delta)^{\frac{1}{2}} x + (2\delta\tau)^{\frac{1}{2}} \xi$$

where $\xi \in C([0, 1], \mathbb{R})$ is a standard Brownian bridge on $[0, 1]$. The move $x \rightarrow y$ is accepted with probability $\alpha^\delta(x, \xi) = 1 \wedge \exp(-\tau^{-1}[\Psi(y) - \Psi(x)])$. Figure 2 displays the convergence of the Markov chain $\{x^{k, \delta}\}_{k \geq 0}$ to a minimiser of the functional $J(\cdot)$. Note that this convergence is not shown with respect to the space $H_0^1([0, 1])$ on which J is defined, but rather in $L^2([0, 1])$; indeed $J(\cdot)$ is almost surely infinite when evaluated at samples of the P-RWM algorithm, precisely because $\pi_0^\tau(H_0^1([0, 1])) = 0$, as discussed above.

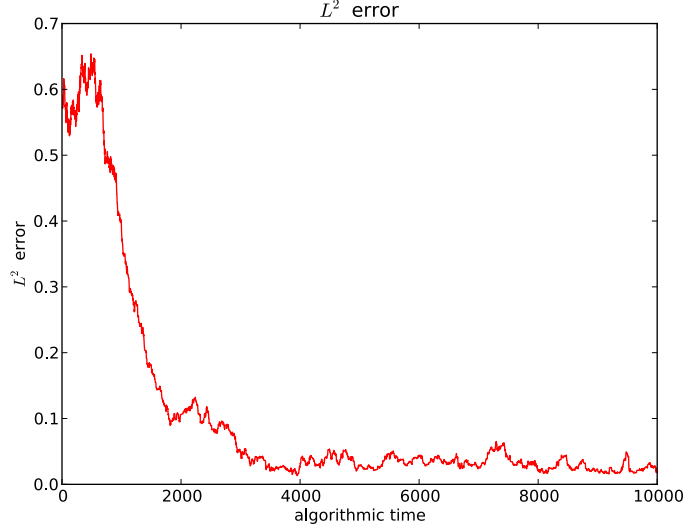


FIG 2. *P-RWM parameters: $\lambda = 2\pi^2$, $\delta = 1.10^{-2}$, $\tau = 1.10^{-2}$. The algorithm is started at the zero function, $x^{0, \delta}(t) = 0$ for $t \in [0, 1]$. After a transient phase, the algorithm fluctuates around a global minimiser of functional $J(\cdot)$. The L^2 error $\|x^{k, \delta} - (\text{minimiser})\|_{L^2}$ is plotted as a function of the algorithmic time k .*

Of course the algorithm does not converge *exactly* to a minimiser of $J(\cdot)$, but fluctuates in a neighbourhood of it. As described in the introduction of this article, in a finite dimensional setting the target probability distribution π^τ has Lebesgue density proportional to $\exp(-\tau^{-1} J(x))$. This intuitively shows that the size of the fluctuations around the minimum of the functional $J(\cdot)$ are of size proportional to $\sqrt{\tau}$. Figure 3 shows this phenomenon on log-log scales: the asymptotic mean error $\mathbb{E}[\|x - (\text{minimiser})\|_2]$ is displayed as a function of the temperature τ . Figure 4 illustrates Theorem 5.3. One can observe the path $\{v^\delta(t)\}_{t \in [0, T]}$ for a finite time step discretization parameter δ as well as the limiting path $\{v(t)\}_{t \in [0, T]}$ that is solution of the differential equation (5.3).

7. Conclusion. We have studied random walk algorithms for Bayesian nonparametric problems with Gaussian priors and proved two main results. In the following we briefly summarize our results, their implications and scope for future work.

- Our main emphasis is on the fact that it is very important to pay attention to the infinite dimensional structure of the prior distribution and the likelihood while designing MCMC algorithms. We illustrate this point by showing that the two near-identical looking variants of RWM, the standard random walk (S-RWM) and the preconditioned random walk (P-RWM) behave entirely differently in high dimensions. Although the proposal for S-RWM differs only through a multiplicative factor in the systematic component, and thus implementation of either is practically identical, the S-RWM method is not defined on infinite dimensional

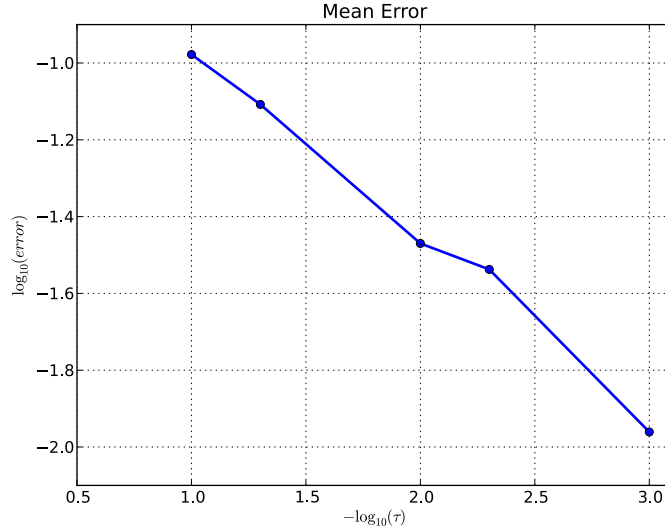


FIG 3.

Mean error $\mathbb{E}[\|x - (\text{minimiser})\|_2]$ as a function of the temperature τ .

Hilbert space as mentioned in the introduction. On the contrary, the P-RWM proposal is just the time discretization of the Ornstein-Uhlenbeck process on the function space \mathcal{H} and thus is defined on the infinite dimensional Hilbert space. This turns out to matter if we compare both methods when applied in \mathbb{R}^N for $N \gg 1$, as would occur if approximating a problem in infinite dimensional Hilbert space: in this setting the S-RWM method requires the choice $\delta = \mathcal{O}(N^{-1})$ to see the diffusion (SDE) limit [MPS11] and so requires $\mathcal{O}(N)$ steps to see $\mathcal{O}(1)$ decrease in the objective function, or to draw independent samples from the target measure; in contrast the P-RWM produces a diffusion limit for $\delta \rightarrow 0$ independently of N and so requires $\mathcal{O}(1)$ steps to see $\mathcal{O}(1)$ decrease in the objective function, or to draw independent samples from the target measure. Mathematically this last point is manifest in the fact that we may take the limit $N \rightarrow \infty$ (and work on the infinite dimensional Hilbert space) followed by the limit $\delta \rightarrow 0$.

- The practical consequence of our main result is that, while implementing RWM algorithms for simulating posterior distribution with Gaussian random field priors, P-RWM should be used instead of S-RWM or its variants. The P-RWM may be viewed as a natural analogue of a random walk Metropolis-Hastings method for posterior measures which have a likelihood ratio with respect to a Gaussian random field.
- More generally, we emphasize the fact that designing MCMC algorithms for nonparametric problems needs more study since it is extremely useful for applied researchers to have guidelines regarding implementation of algorithms. For nonparametric problems, construction of prior distributions and likelihood modeling must be integrated with designing proposals and vice versa. This synthesis will have a beneficial impact on both the statistical inference and the efficiency of the algorithm. In this regard, we also advocate that in bayesian nonparametric problems, the primary focus should be on optimal design of algorithms (which inherit the structure of prior and the likelihood) as compared to optimal scaling.
- There are a host of tools known outside the statistics literature which are extremely useful

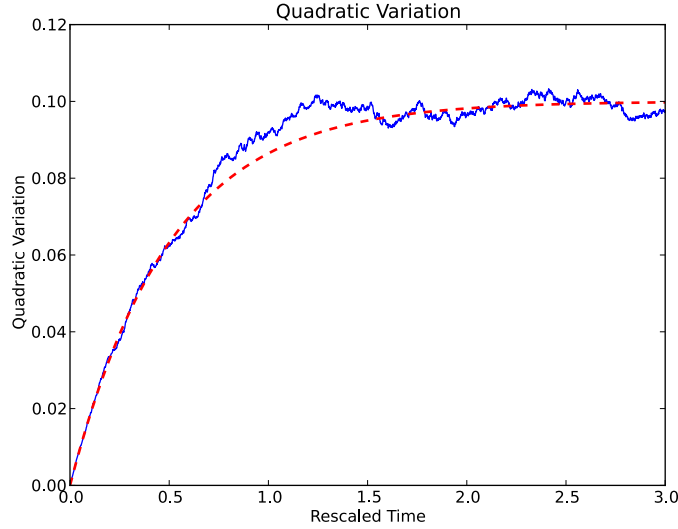


FIG 4. *P*-RWM parameters: $\lambda = 2\pi^2$, $\tau = 1.10^{-1}$, $\delta = 1.10^{-3}$ and the algorithm starts at $x^{k,\delta} = 0$. The rescaled quadratic variation process (full line) behaves as the solution of the differential equation (dotted line), as predicted by Theorem 5.3. The quadratic variation converges to τ , as described by Proposition 5.2.

for obtaining useful guidelines for implementation of algorithms. For instance, the *P*-RWM adheres to the “optimize then discretize” perspective whereas the *S*-RWM sticks to the “discretize then optimize” view point. In numerical analysis, it is known that in some problems, the former performs better than the latter (see [HPUU08], Chapter 3). We illustrate this point in statistical examples.

- We have demonstrated a class of algorithms to minimize the functional J given by (1.11). The Assumptions 2.1 encode the intuition that the quadratic part of J dominates. Under these assumptions we study the properties of an algorithm which requires only the evaluation of Ψ and the ability to draw samples from Gaussian measures with (Cameron-Martin) norm given by the quadratic part of J . We demonstrate that, in a certain parameter limit, the algorithm behaves like a noisy gradient flow for the functional J and that, furthermore, the size of the noise can be controlled systematically. Thus we have constructed a simulated annealing algorithm on Hilbert space, and connected this to a diffusion process (SDE), a connection made in finite dimensions in [GH86]. The applications we are interested in are mainly on Bayesian nonparametrics; but of course, there are many more problems to which our techniques and results are applicable, *e.g.*, optimization, control theory, etc.
- The methods that we employ for the derivation of the diffusion (SDE) limit use a combination of ideas from numerical analysis and the weak convergence of probability measures. This approach is encapsulated in Lemma 3.5 which is structured in such a way that it, or variants of it, may be used to prove diffusion limits for a variety of problems, especially when there is an underlying Gaussian structure.
- The diffusion limits proved in our results might not hold for discrete priors such as the Dirichlet processes or more generally Lévy random field priors [WCT11] because there is no underlying Gaussian measure. In these cases, one might expect a pure jump process as a limit instead of a diffusion process. These class of models are very important in applications used

in varied fields including computer science, machine learning and engineering. Thus it is of great importance to understand and quantify their efficiency; to achieve this will need new techniques and will be pursued elsewhere.

APPENDIX A: PROOFS OF SOME LEMMAS FROM SECTION 4

PROOF OF LEMMA 4.1. Let us introduce the two 1-Lipschitz functions $h, h_* : \mathbb{R} \rightarrow \mathbb{R}$ defined by

$$h(x) = 1 \wedge e^x \quad \text{and} \quad h_*(x) = 1 + x 1_{\{x < 0\}}. \quad (\text{A.1})$$

The function h_* is a first order approximation of h in a neighbourhood of zero and we have

$$\alpha^\delta(x, \xi) = h\left(-\frac{1}{\tau}\{\Psi(y) - \Psi(x)\}\right) \quad \text{and} \quad \bar{\alpha}^\delta(x, \xi) = h_*\left(-\sqrt{\frac{2\delta}{\tau}} \langle \nabla \Psi(x), \xi \rangle\right)$$

where the proposal y is a function of x and ξ , as described in Equation (3.1). Since $h_*(\cdot)$ is close to $h(\cdot)$ in a neighbourhood of zero, the proof is finished once it is proved that $-\frac{1}{\tau}\{\Psi(y) - \Psi(x)\}$ is close to $-\sqrt{\frac{2\delta}{\tau}} \langle \nabla \Psi(x), \xi \rangle$. We have $\mathbb{E}_x[|\alpha^\delta(x, \xi) - \bar{\alpha}^\delta(x, \xi)|^p] \lesssim A_1 + A_2$ where the quantities A_1 and A_2 are given by

$$\begin{aligned} A_1 &= \mathbb{E}_x \left[\left| h\left(-\frac{1}{\tau}\{\Psi(y) - \Psi(x)\}\right) - h\left(-\sqrt{\frac{2\delta}{\tau}} \langle \nabla \Psi(x), \xi \rangle\right) \right|^p \right] \\ A_2 &= \mathbb{E}_x \left[\left| h\left(-\sqrt{\frac{2\delta}{\tau}} \langle \nabla \Psi(x), \xi \rangle\right) - h_*\left(-\sqrt{\frac{2\delta}{\tau}} \langle \nabla \Psi(x), \xi \rangle\right) \right|^p \right]. \end{aligned}$$

By Lemma 2.4, the first order Taylor approximation of Ψ is controled, $|\Psi(y) - \Psi(x) - \langle \nabla \Psi(x), y - x \rangle| \lesssim \|y - x\|_s^2$. The definition of the proposal y given in Equation (3.1) shows that $\|(y - x) - \sqrt{2\delta\tau}\xi\|_s \lesssim \delta\|x\|_s$. Assumptions 2.1 state that for $z \in \mathcal{H}^s$ we have $\langle \nabla \Psi(x), z \rangle \lesssim (1 + \|x\|_s) \cdot \|z\|_s$. Since the function $h(\cdot)$ is 1-Lipschitz it follows that

$$\begin{aligned} A_1 &= \mathbb{E}_x \left[\left| h\left(-\frac{1}{\tau}\{\Psi(y) - \Psi(x)\}\right) - h\left(-\sqrt{\frac{2\delta}{\tau}} \langle \nabla \Psi(x), \xi \rangle\right) \right|^p \right] \\ &\lesssim \mathbb{E}_x \left[|\Psi(y) - \Psi(x) - \langle \nabla \Psi(x), y - x \rangle|^p + |\langle \nabla \Psi(x), y - x - \sqrt{2\delta\tau}\xi \rangle|^p \right] \\ &\lesssim \mathbb{E}_x \left[\|y - x\|_s^{2p} + (1 + \|x\|_s^p) \cdot (\delta \|x\|_s)^p \right] \lesssim \delta^p (1 + \|x\|_s^{2p}). \end{aligned} \quad (\text{A.2})$$

Lemma 3.1 has been used to control the size of $\mathbb{E}_x[\|y - x\|^p]$. To bound A_2 , notice that for $z \in \mathbb{R}$ we have $|h(z) - h_*(z)| \leq \frac{1}{2}z^2$. Therefore the quantity A_2 can be bounded by

$$A_2 \lesssim \mathbb{E}_x \left[|\sqrt{\delta} \langle \nabla \Psi(x), \xi \rangle|^{2p} \right] \lesssim \delta^p \mathbb{E}_x \left[(1 + \|x\|_s^{2p}) \|\xi\|_s^{2p} \right] \lesssim \delta^p (1 + \|x\|_s^{2p}). \quad (\text{A.3})$$

Estimates (A.2) and (A.3) together give Equation (4.2). \square

PROOF OF COROLLARY 4.2. Let us prove Equations (4.3) and (4.4).

- Lemma 4.1 and Jensen's inequality give Equation (4.3).

- To prove (4.4), one can suppose $\delta^{\frac{p}{2}} \|x\|_s^p \leq 1$. Indeed, if $\delta^{\frac{p}{2}} \|x\|_s^p \geq 1$, we have

$$\mathbb{E}_x \left[|\alpha^\delta(x, \xi) - 1|^p \right] \lesssim 1 \leq \delta^{\frac{p}{2}} \|x\|_s^p \leq \delta^{\frac{p}{2}} (1 + \|x\|_s^p),$$

which gives the result. We thus suppose from now on that $\delta^{\frac{p}{2}} \|x\|_s \leq 1$. Under Assumptions 2.1 we have $\|\nabla \Psi(x)\|_{-s} \lesssim 1 + \|x\|_s$. Lemma 2.4 shows that for all $x, y \in \mathcal{H}^s$ we have $|\Psi(y) - \Psi(x) - \langle \nabla \Psi(x), y - x \rangle| \lesssim \|y - x\|_s^2$. The function $h(x) = 1 \wedge e^x$ is 1-Lipschitz, $\alpha^\delta(x, \xi) = h(-\frac{1}{\tau}[\Psi(y) - \Psi(x)])$ and $h(0) = 1$. Consequently,

$$\begin{aligned} \mathbb{E}_x \left[|\alpha^\delta(x, \xi) - 1|^p \right] &= \mathbb{E}_x \left[\left| h\left(-\frac{1}{\tau}[\Psi(y) - \Psi(x)]\right) - h(0) \right|^p \right] \\ &\lesssim \mathbb{E}_x \left[|\Psi(y) - \Psi(x)|^p \right] \lesssim \mathbb{E}_x \left[|\langle \nabla \Psi(x), y - x \rangle|^p + \|y - x\|_s^{2p} \right] \\ &\lesssim (1 + \|x\|_s^p) \cdot \mathbb{E}_x \left[\|y - x\|_s^p \right] + \mathbb{E}_x \left[\|y - x\|_s^{2p} \right]. \end{aligned}$$

By Lemma 3.1, for any integer $\beta \geq 1$ we have $\mathbb{E}_x \left[\|y - x\|_s^\beta \right] \lesssim \delta^\beta \|x\|_s^\beta + \delta^{\frac{\beta}{2}}$ so that the assumption $\delta^{\frac{p}{2}} \|x\|_s^p \leq 1$ leads to

$$\begin{aligned} \mathbb{E}_x \left[|\alpha^\delta(x) - 1|^p \right] &\lesssim (1 + \|x\|_s^p) \cdot (\delta^p \|x\|_s^p + \delta^{\frac{p}{2}}) + (\delta^{2p} \|x\|_s^{2p} + \delta^p) \\ &\lesssim (1 + \|x\|_s^p) \cdot (\delta^{\frac{p}{2}} + \delta^{\frac{p}{2}}) + (\delta^p + \delta^p) \\ &\lesssim \delta^{\frac{p}{2}} (1 + \|x\|_s^p). \end{aligned}$$

This finishes the proof of Corollary 4.2. □

PROOF OF LEMMA 4.4. The martingale difference $\Gamma^\delta(x, \xi)$ defined in Equation (3.8) can also be expressed as

$$\Gamma^\delta(x, \xi) = \xi + F(x, \xi)$$

where the error term $F(x, \xi) = F_1(x, \xi) + F_2(x, \xi)$ is given by

$$\begin{aligned} F_1(x, \xi) &= (2\tau\delta)^{-\frac{1}{2}} \left((1 - 2\delta)^{\frac{1}{2}} - 1 \right) (\gamma^\delta(x, \xi) - \mathbb{E}_x[\gamma^\delta(x, \xi)])x \\ F_2(x, \xi) &= (\gamma^\delta(x, \xi) - 1) \cdot \xi - \mathbb{E}_x[\gamma^\delta(x, \xi) \cdot \xi]. \end{aligned}$$

We now prove that the quantity $F(x, \xi)$ satisfies

$$\mathbb{E}_x \left[\|F(x, \xi)\|_s^2 \right] \lesssim \delta^{\frac{1}{4}} (1 + \|x\|_s^2) \quad (\text{A.4})$$

- We have $\delta^{-\frac{1}{2}} \left((1 - 2\delta)^{\frac{1}{2}} - 1 \right) \lesssim \delta^{\frac{1}{2}}$ and $|\gamma^\delta(x, \xi)| \leq 1$. Consequently,

$$\mathbb{E}_x \left[\|F_1(x, \xi)\|_s^2 \right] \lesssim \delta \|x\|_s^2 \quad (\text{A.5})$$

- Let us now prove that F_2 satisfies

$$\mathbb{E}_x \left[\|F_2(x, \xi)\|_s^2 \right] \lesssim \delta^{\frac{1}{4}} (1 + \|x\|_s^{\frac{1}{2}}). \quad (\text{A.6})$$

To this end, use the decomposition

$$\begin{aligned}\mathbb{E}_x \left[\|F_2(x, \xi)\|_s^2 \right] &\lesssim \mathbb{E}_x \left[|\gamma^\delta(x, \xi) - 1|^2 \cdot \|\xi\|_s^2 \right] + \|\mathbb{E}_x[\gamma^\delta(x, \xi) \cdot \xi]\|_s^2 \\ &= I_1 + I_2.\end{aligned}$$

Cauchy-Schwarz inequality shows that $I_1 \lesssim \mathbb{E}_x \left[|\gamma^\delta(x, \xi) - 1|^4 \right]^{\frac{1}{2}}$ where the Bernoulli random variable $\gamma^\delta(x, \xi)$ can be expressed as $\gamma^\delta(x, \xi) = \mathbb{1}_{\{U < \alpha^\delta(x, \xi)\}}$ where $U \stackrel{\mathcal{D}}{\sim} \text{Uniform}(0, 1)$ is independent from any other source of randomness. Consequently

$$\mathbb{E}_x \left[|\gamma^\delta(x, \xi) - 1|^4 \right] = \mathbb{E}_x \left[\mathbb{1}_{\{\gamma^\delta(x, \xi) \neq 1\}} \right] = 1 - \alpha^\delta(x)$$

where the mean local acceptance probability $\alpha^\delta(x)$ is defined by $\alpha^\delta(x) = \mathbb{E}_x[\alpha^\delta(x, \xi)] \in [0, 1]$. The convexity of the function $x \rightarrow |1 - x|$ ensures that

$$|1 - \alpha^\delta(x)| = |1 - \mathbb{E}_x[\alpha^\delta(x, \xi)]| \leq \mathbb{E}_x[|1 - \alpha^\delta(x, \xi)|] \lesssim \delta^{\frac{1}{2}} (1 + \|x\|)$$

where the last inequality follows from Corollary 4.2. This proves that $I_1 \lesssim \delta^{\frac{1}{4}} (1 + \|x\|^{\frac{1}{2}})$. To bound I_2 , it suffices to notice

$$\begin{aligned}I_2 &= \|\mathbb{E}_x[\gamma^\delta(x, \xi) \cdot \xi]\|_s^2 = \|\mathbb{E}_x[(\gamma^\delta(x, \xi) - 1) \cdot \xi]\|_s^2 \\ &\lesssim \mathbb{E}_x \left[|\gamma^\delta(x, \xi) - 1|^2 \cdot \|\xi\|_s^2 \right] = I_1\end{aligned}$$

so that $I_2 \lesssim I_1 \lesssim \delta^{\frac{1}{4}} (1 + \|x\|^{\frac{1}{2}})$ and $\mathbb{E}_x \left[\|F_2(x, \xi)\|_s^2 \right] \lesssim \delta^{\frac{1}{4}} (1 + \|x\|^{\frac{1}{2}})$.

Combining Equation (A.5) and (A.6) gives Equation (A.4).

Let us now describe how Equations (4.7) and (4.8) follow from the estimate (A.4).

- We have $\mathbb{E}[\langle \hat{\varphi}_i, \xi \rangle_s \langle \hat{\varphi}_j, \xi \rangle_s] = \langle \hat{\varphi}_i, C_s \hat{\varphi}_j \rangle_s$ and $\mathbb{E}_x[\langle \hat{\varphi}_i, \Gamma^\delta(x, \xi) \rangle_s \langle \hat{\varphi}_j, \Gamma^\delta(x, \xi) \rangle_s] = \langle \hat{\varphi}_i, D^\delta(x) \hat{\varphi}_j \rangle_s$ with $\Gamma^\delta(x, \xi) = \xi + F(x, \xi)$. Consequently,

$$\begin{aligned}\langle \hat{\varphi}_i, D^\delta(x) \hat{\varphi}_j \rangle_s - \langle \hat{\varphi}_i, C_s \hat{\varphi}_j \rangle_s &= \mathbb{E}_x[\langle \hat{\varphi}_i, F(x, \xi) \rangle_s \langle \hat{\varphi}_j, F(x, \xi) \rangle_s] \\ &\quad + \mathbb{E}_x[\langle \hat{\varphi}_i, \xi \rangle_s \langle \hat{\varphi}_j, F(x, \xi) \rangle_s] \\ &\quad + \mathbb{E}_x[\langle \hat{\varphi}_i, F(x, \xi) \rangle_s \langle \hat{\varphi}_j, \xi \rangle_s].\end{aligned}$$

We have $|\langle \hat{\varphi}_i, F(x, \xi) \rangle_s| \leq \|F(x, \xi)\|_s$ and Cauchy Schwarz's inequality proves that

$$\begin{aligned}\mathbb{E}_x[\langle \hat{\varphi}_i, F(x, \xi) \rangle_s \langle \hat{\varphi}_j, \xi \rangle_s]^2 &\leq \mathbb{E}_x[\|F(x, \xi)\|_s \|\xi\|_s]^2 \\ &\lesssim \mathbb{E}_x[\|F(x, \xi)\|_s^2].\end{aligned}$$

It thus follows from Equation (A.4) that

$$\begin{aligned}|\langle \hat{\varphi}_i, D^\delta(x) \hat{\varphi}_j \rangle_s - \langle \hat{\varphi}_i, C_s \hat{\varphi}_j \rangle_s| &\lesssim \mathbb{E}_x[\|F(x, \xi)\|_s^2] + \mathbb{E}_x[\|F(x, \xi)\|_s^2]^{\frac{1}{2}} \\ &\lesssim \delta^{\frac{1}{8}} (1 + \|x\|_s),\end{aligned}$$

finishing the proof of (4.7).

- We have $\text{Trace}_{\mathcal{H}^s}(C_s) = \mathbb{E}[\|\xi\|_s^2]$ and $\text{Trace}_{\mathcal{H}^s}(D^\delta(x)) = \mathbb{E}[\|\Gamma^\delta(x, \xi)\|_s^2]$. Estimate (A.4) thus shows that

$$\begin{aligned}
|\text{Trace}_{\mathcal{H}^s}(D^\delta(x)) - \text{Trace}_{\mathcal{H}^s}(C_s)| &= |\mathbb{E}[\|\Gamma^\delta(x, \xi)\|_s^2 - \|\xi\|_s^2]| = |\mathbb{E}[\|\xi + F(x, \xi)\|_s^2 - \|\xi\|_s^2]| \\
&\lesssim |\mathbb{E}[\langle 2\xi + F(x, \xi), F(x, \xi) \rangle_s]| \lesssim \mathbb{E}[\|2\xi + F(x, \xi)\|_s \|F(x, \xi)\|_s] \\
&\lesssim \mathbb{E}[4\|\xi\|_s^2 + \|F(x, \xi)\|_s^2]^{\frac{1}{2}} \cdot \mathbb{E}[\|F(x, \xi)\|_s^2]^{\frac{1}{2}} \\
&\lesssim \left(1 + \delta^{\frac{1}{4}} (1 + \|x\|_s^2)\right)^{\frac{1}{2}} \cdot \left(\delta^{\frac{1}{8}} (1 + \|x\|_s)\right) \lesssim \delta^{\frac{1}{8}} (1 + \|x\|_s^2),
\end{aligned}$$

finishing the proof of (4.8). □

APPENDIX B: PROOF OF LEMMA 5.4

Before proceeding to give the proof, let us give a brief proof sketch. The proof of Lemma 5.4 consists in showing first that for any $\varepsilon > 0$ one can find a ball of radius $R(\varepsilon)$ around 0 in \mathcal{H}^s ,

$$B_0(R(\varepsilon)) = \{x \in \mathcal{H}_s : \|x\|_s \leq R(\varepsilon)\},$$

such that with probability $1 - 2\varepsilon$ we have $x^{k,\delta} \in B_0(R(\varepsilon))$ and $y^{k,\delta} \in B_0(R(\varepsilon))$ for all $0 \leq k \leq T\delta^{-1}$. As is described below, the existence of such a ball follows from the bound

$$\mathbb{E}[\sup_{t \in [0, T]} \|x(t)\|_s] < +\infty \tag{B.1}$$

where $t \mapsto x(t)$ is the solution of the stochastic differential equation (3.6). For the sake of completeness, we include a proof of Equation (B.1). The solution $t \mapsto x(t)$ of the stochastic differential equation (3.6) satisfies $x(t) = \int_0^t d(x(u)) du + \sqrt{2\tau} W(t)$ for all $t \in [0, T]$ where the drift function $d(x) = -(x + C\nabla\Psi(x))$ is globally Lipschitz on \mathcal{H}^s , as described in Lemma 2.4. Consequently $\|d(x)\|_s \leq A(1 + \|x\|_s)$ for some positive constant $A > 0$. The triangle inequality then shows that

$$(B.2) \quad \|x(t)\|_s \leq A \int_0^t (1 + \|x(u)\|_s) du + \sqrt{2\tau} \|W(t)\|_s.$$

By Gronwall's inequality we obtain

$$(B.3) \quad \sup_{[0, T]} \|x(t)\|_s \leq (AT + \sup_{[0, T]} \|W(t)\|_s) [1 + ATe^{AT}].$$

Since $\mathbb{E}[\sup_{[0, T]} \|W(t)\|_s] < \infty$, the bound (B.1) is proved.

PROOF OF LEMMA 5.4. The proof consists in showing that the acceptance probability of the algorithm is sufficiently close to 1 so that approximation $t^\delta(k) \approx k$ holds. The argument can be divided into 3 main steps. In the first part, we show that we can find a finite ball $B(0, R(\varepsilon))$ such that the trajectory of the Markov chain $\{x^{k,\delta}\}_{k \leq T\delta^{-1}}$ remains in this ball with probability at least $1 - 2\varepsilon$. This observation is useful since the function Ψ is Lipschitz on any ball of finite radius in \mathcal{H}^s . In the second part, using the fact that Ψ is Lipschitz on $B(0, R(\varepsilon))$, we find a lower bound for the acceptance probability α^δ . Then, in the last step, we use a moment estimate to prove that one can make the lower bound uniform on the interval $0 \leq k \leq T\delta^{-1}$.

- **Restriction to a Ball of Finite Radius**

First, we show that with high probability the trajectory of the MCMC algorithm stays in a ball of finite radius. The functional $x \mapsto \sup_{t \in [0, T]} \|x(t)\|_s$ is continuous on $C([0, T], \mathcal{H}_s)$ and $\mathbb{E}[\sup_{t \in [0, T]} \|x(t)\|_s] < \infty$ for $t \mapsto x(t)$ following the stochastic differential equation (3.6), as proved in Equation (B.1). Consequently, the weak convergence of z^δ to the solution of (3.6) encapsulated in Theorem 3.2 shows that $\mathbb{E}[\sup_{k < T\delta^{-1}} \|x^{k, \delta}\|_s]$ can be bounded by a finite universal constant independent from δ . Given $\varepsilon > 0$, Markov inequality thus shows that one can find a radius $R_1 = R_1(\varepsilon)$ large enough so that the inequality

$$\mathbb{P}[\|x^{k, \delta}\|_s < R_1 \quad \text{for all } 0 \leq k \leq T\delta^{-1}] > 1 - \varepsilon \quad (\text{B.4})$$

for any $\delta \in (0, \frac{1}{2})$. By Fernique's Theorem there exists $\alpha > 0$ such that $\mathbb{E}[e^{\alpha \|\xi\|_s^2}] < \infty$. This implies that $\mathbb{P}[\|\xi\|_s > r] \lesssim e^{-\alpha r^2}$. Therefore, if $\{\xi_k\}_{k \geq 0}$ are i.i.d. Gaussian random variables distributed as $\xi \stackrel{\mathcal{D}}{\sim} \pi_0$, the union bound shows that

$$\mathbb{P}[\|\sqrt{\delta}\xi_k\|_s \leq r \quad \text{for all } 0 \leq k \leq T\delta^{-1}] \gtrsim 1 - T\delta^{-1} \exp(-\alpha \delta^{-1} r^2).$$

This proves that one can choose $R_2 = R_2(\varepsilon)$ large enough in such a manner that

$$\mathbb{P}[\|\sqrt{\delta}\xi_k\|_s < R_2 \quad \text{for all } 0 \leq k \leq T\delta^{-1}] > 1 - \varepsilon \quad (\text{B.5})$$

for any $\delta \in (0, \frac{1}{2})$. At temperature $\tau > 0$ the MCMC proposals are given by $y^{k, \delta} = (1 - 2\delta)^{\frac{1}{2}} x^{k, \delta} + (2\delta\tau)^{\frac{1}{2}} \xi_k$. It thus follows from the bounds (B.4) and (B.5) that with probability at least $(1 - 2\varepsilon)$ the vectors $x^{k, \delta}$ and $y^{k, \delta}$ belong to the ball $B_0(R(\varepsilon)) = \{x \in \mathcal{H}_s : \|x\|_s < R(\varepsilon)\}$ for $0 \leq k \leq T\delta^{-1}$ where radius $R(\varepsilon)$ is given by $R(\varepsilon) = R_1(\varepsilon) + R_2(\varepsilon)$.

- **Lower Bound for Acceptance Probability**

We now give a lower bound for the acceptance probability $\alpha^\delta(x^{k, \delta}, \xi^k)$ that the move $x^{k, \delta} \rightarrow y^{k, \delta}$ is accepted. Assumptions 2.1 state that $\|\nabla \Psi(x)\|_{-s} \lesssim 1 + \|x\|_s$. Therefore, the function $\Psi : \mathcal{H}^s \rightarrow \mathbb{R}$ is Lipschitz on $B_0(R(\varepsilon))$,

$$\|\Psi\|_{\text{lip}, \varepsilon} \stackrel{\text{def}}{=} \sup \left\{ \frac{|\Psi(y) - \Psi(x)|}{\|y - x\|_s} : x, y \in B_0(R(\varepsilon)) \right\} < \infty.$$

One can thus bound the acceptance probability $\alpha^\delta(x^{k, \delta}, \xi^k) = 1 \wedge \exp(-\tau^{-1}[\Psi(y^{k, \delta}) - \Psi(x^{k, \delta})])$ for $x^{k, \delta}, y^{k, \delta} \in B_0(R(\varepsilon))$. Since the function $z \mapsto 1 \wedge e^{-\tau^{-1}z}$ is Lipschitz with constant τ^{-1} , the definition of $\|\Psi\|_{\text{lip}, \varepsilon}$ shows that the bound

$$\begin{aligned} 1 - \alpha^\delta(x^{k, \delta}, \xi^k) &\leq \tau^{-1} \|\Psi\|_{\text{lip}, \varepsilon} \|y^{k, \delta} - x^{k, \delta}\|_s \\ &\leq \tau^{-1} \|\Psi\|_{\text{lip}, \varepsilon} \left\{ [(1 - 2\delta)^{\frac{1}{2}} - 1] \|x^{k, \delta}\|_s + (2\delta\tau)^{\frac{1}{2}} \|\xi^k\|_s \right\} \\ &\lesssim \sqrt{\delta} (1 + \|\xi^k\|_s) \end{aligned}$$

holds for every $x^{k, \delta}, y^{k, \delta} \in B_0(R(\varepsilon))$. Hence, there exists a constant $K = K(\varepsilon)$ such that $\hat{\alpha}^\delta(\xi^k) = 1 - K\sqrt{\delta} (1 + \|\xi^k\|_s)$ satisfies $\alpha^\delta(x^{k, \delta}, \xi^k) > \hat{\alpha}^\delta(\xi^k)$ for every $x^{k, \delta}, y^{k, \delta} \in B_0(R(\varepsilon))$. Since the trajectory of the MCMC algorithm stays in the ball $B_0(R(\varepsilon))$ with probability at least $1 - 2\varepsilon$ the inequality

$$\mathbb{P}[\alpha^\delta(x^{k, \delta}, \xi^k) > \hat{\alpha}^\delta(\xi^k) \quad \text{for all } 0 \leq k \leq T\delta^{-1}] > 1 - 2\varepsilon.$$

holds for every $\delta \in (0, \frac{1}{2})$.

- **Second Moment Method**

To prove that $t^\delta(k)$ does not deviate too much from k , we show that its expectation satisfies $\mathbb{E}[t^\delta(k)] \approx k$ and we then control the error by bounding the variance. Since the Bernoulli random variable $\gamma^{k,\delta} = \text{Bernoulli}(\alpha^\delta(x^{k,\delta}\xi^k))$ are not independent, the variance of $t^\delta(k) = \sum_{l \leq k} \gamma^{l,\delta}$ is not easily computable. We thus introduce i.i.d. auxiliary random variables $\hat{\gamma}^{k,\delta}$ such that

$$\sum_{l \leq k} \hat{\gamma}^{l,\delta} = \hat{t}^\delta(k) \approx t^\delta(k) = \sum_{l \leq k} \gamma^{l,\delta}.$$

As described below, the behaviour of $\hat{t}^\delta(k)$ is readily controlled since it is a sum of i.i.d. random variables. The proof then exploits the fact that $\hat{t}^\delta(k)$ is a good approximation of $t^\delta(k)$.

The Bernoulli random variables $\gamma^{k,\delta}$ can be described as $\gamma^{k,\delta} = \mathbb{I}(U_k < \alpha^\delta(x^{k,\delta}\xi^k))$ where $\{U_k\}_{k \geq 0}$ are i.i.d. random variables uniformly distributed on $(0, 1)$. As a consequence, with probability at least $1 - 2\varepsilon$, the random variables $\hat{\gamma}^{k,\delta} = \mathbb{I}(U_k < \hat{\alpha}^\delta)$ satisfy $\gamma^{k,\delta} \geq \hat{\gamma}^{k,\delta}$ for all $0 \leq k \leq T\delta^{-1}$. Therefore, with probability at least $1 - 2\varepsilon$, we have $t^\delta(k) \geq \hat{t}^\delta(k)$ for all $0 \leq k \leq T\delta^{-1}$ where $\hat{t}^\delta(k) = \sum_{l \leq k} \hat{\gamma}^{l,\delta}$. Consequently, since $t^\delta(k) \leq k$, to prove Lemma 5.4 it suffices to show instead that the following limit in probability holds,

$$\lim_{\delta \rightarrow 0} \sup \{ \delta \cdot |\hat{t}^\delta(k) - k| : 0 \leq k \leq T\delta^{-1} \} = 0. \quad (\text{B.6})$$

Contrary to the random variables $\{\gamma^{k,\delta}\}_{k \geq 0}$, the random variables $\{\hat{\gamma}^{k,\delta}\}_{k \geq 0}$ are i.i.d. and are thus easily controlled. By Doob's inequality we have

$$\mathbb{P} \left[\sup \{ \delta \cdot |\hat{t}^\delta(k) - \mathbb{E}[\hat{t}^\delta(k)]| : 0 \leq k \leq T\delta^{-1} \} > \eta \right] \leq 2 \frac{\text{Var}(\hat{t}^\delta(T\delta^{-1}))}{(\delta^{-1}\eta)^2} \leq 2 \frac{\delta T}{\eta^2}.$$

Since $\mathbb{E}[\hat{t}^\delta(k)] = k \cdot \{1 - K\sqrt{\delta} (1 + \mathbb{E}[\|\xi^k\|_s])\}$, Equation (B.6) follows. This finishes the proof of Lemma 5.4. □

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