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# BAYESIAN ESTIMATION IN A MULTIDIMENSIONAL DIFFUSION MODEL WITH HIGH FREQUENCY DATA

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**ABSTRACT.** We consider nonparametric Bayesian inference in a multidimensional diffusion model with reflecting boundary conditions based on discrete high-frequency observations. We prove a general posterior contraction rate theorem in  $L^2$ -loss, which is applied to Gaussian priors. The resulting posteriors, as well as their posterior means, are shown to converge to the ground truth at the minimax optimal rate over Hölder smoothness classes in any dimension. Of independent interest and as part of our proofs, we show that certain frequentist penalized least squares estimators are also minimax optimal.

*MSC2020 subject classifications:* 62G20, 62F15, 60J60.

*Keywords:* Bayesian nonparametrics, multidimensional diffusions, high-frequency data, Gaussian processes, penalized least squares estimator.

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## 1. INTRODUCTION

Let  $\mathcal{O} \subset \mathbb{R}^d$  be a bounded convex domain with smooth boundary  $\partial\mathcal{O}$  and

$$f : \mathcal{O} \rightarrow [f_{\min}, \infty)$$

be a positive function with  $f_{\min} > 0$ . Consider the multidimensional diffusion process  $(X_t)_{t \geq 0}$  on  $\mathcal{O}$  that is reflected upon hitting the boundary  $\partial\mathcal{O}$  and arises as the solution to the SDE:

$$(1) \quad \begin{aligned} X_t &= X_0 + \int_0^t \nabla f(X_s) ds + \int_0^t \sqrt{2f(X_s)} dB_s + \ell_t, \\ \ell_t &= \int_0^t n(X_s) d|\ell|_s, \quad |\ell|_t = \int_0^t \mathbf{1}_{\{X_s \in \partial\mathcal{O}\}} d|\ell|_s, \end{aligned}$$

where  $(B_t)_{t \geq 0}$  a standard  $d$ -dimensional Brownian motion,  $(\ell_t)_{t \geq 0}$  a bounded variation process with  $\ell_0 = 0$  that accounts for the boundary reflection and  $n(x)$  denotes the unit inward normal to the boundary  $\partial\mathcal{O}$  at  $x$ . We take  $X_0$  to be uniformly distributed on  $\mathcal{O}$ , which is the invariant measure of the SDE (1), and hence  $X$  is started at stationarity. If  $\partial\mathcal{O}$  and  $\nabla f$  are continuously differentiable, existence and uniqueness of the solution to (1) follows from [37]. These conditions, together with the convexity of the domain  $\mathcal{O}$ , can be relaxed, but will be sufficient for the level of generality intended here.

Consider observations regularly collected at discrete time points, resulting in data of the form

$$(2) \quad X^N = (X_0, X_D, \dots, X_{ND})$$

with sampling interval  $D > 0$ . We consider the high-frequency and long term sampling regime, where  $D = D_N \rightarrow 0$  such that the time-horizon  $ND_N \rightarrow \infty$ . We study nonparametric Bayesian estimation of  $f$  in model (1) using Gaussian process priors. In particular, we establish minimax optimal frequentist contraction rates for the posterior for  $f$  about the ‘ground truth’  $f_0$  generating the data, thereby establishing theoretical guarantees for this method.

Diffusion models are widely used in applications, including in the physical and biological sciences, economics and finance, as well as for particle filters and emulators amongst many others purposes. Regarding the physical model underlying (1), let  $u(t, x)$  denote the intensity of a quantity that is diffusing, such as heat, in a closed system at time  $t > 0$  and location  $x \in \mathcal{O}$ . Fick’s laws of diffusion state that this is governed by the evolution equation

$$(3) \quad \frac{\partial u}{\partial t} = \nabla \cdot (f \nabla u),$$

where  $f > 0$  is the diffusivity of the possibly inhomogeneous medium  $\mathcal{O}$ , with appropriate boundary conditions. This describes the macroscopic behaviour of many particles in  $\mathcal{O}$  governed by Brownian dynamics, whose individual behaviour can then be modelled by (1). The statistical problem at hand is thus to make inference on the diffusivity  $f$  based on discrete observations of the location of a single particle.

A challenging feature of model (1) is that its generator  $\mathcal{L}_f \phi = \nabla \cdot (f \nabla \phi)$  is a divergence form operator, which implies that the invariant measure  $\mu_f$  is simply the uniform measure on the domain  $\mathcal{O}$  for all  $f$ :

$$(4) \quad \mu_f(A) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T 1_A(X_t) dt \propto \text{vol}(A),$$

for any measurable  $A \subset \mathcal{O}$ , so that the average asymptotic time spent by the process  $X$  in different regions does not provide any information about  $f$ . In particular, this contrasts with several other well-studied diffusion models where one can identify the relevant model parameters from the invariant measure  $\mu_f$ , and hence a natural statistical approach is for first estimate  $\mu_f$  and then derive plug-in estimates, see e.g. [18, 56, 30, 2]. In model (1), all information about  $f$  is thus contained in the transitions  $X_{(i-1)D} \mapsto X_{iD}$ , which motivates using a likelihood based approach, such as the Bayesian one we pursue here.

To better understand our approach, it is helpful to consider the more general diffusion model,

$$(5) \quad dX'_t = b(X'_t)dt + \sigma(X'_t)dW_t,$$

where  $b : \mathbb{R}^d \rightarrow \mathbb{R}^d$  is the drift and  $\sigma : \mathbb{R}^d \rightarrow \mathbb{R}^d \otimes \mathbb{R}^d$  is the diffusion coefficient or matrix. In the one-dimensional high frequency case where  $b$  and  $\sigma$  have the same smoothness, one can estimate the diffusivity  $\sigma$  at a faster rate than the drift  $b$  [33]. In model (1), where these parameters are coupled, the diffusivity term is similarly more informative about  $f$  than the drift, which must be exploited to obtain minimax optimal rates. While the Bayesian methodology does not explicitly make this distinction, simply placing a prior on  $f$  as usual, our proofs themselves heavily rely on this idea. One can therefore view sharp estimation of  $f$  in model (1) as qualitatively analogous to estimation of  $\sigma$  in model (5), with the added difficulty that the invariant measure is uninformative. Our work is thus relevant to the literature on estimating the diffusion coefficient [33, 15, 54] under high-frequency sampling, which is closely linked to volatility estimation, see [66, 8, 3] in econometrics or [4]. Our results indicate that Bayesian methods can correctly pick up this feature of the data via the likelihood.

We prove a general contraction rate theorem for  $f$  under approximation-theoretic conditions on the prior following the classic testing approach of Bayesian nonparametrics [26], which requires:

- (i) the integrated log-likelihood process is not too small with high probability;
- (ii) the existence of suitable tests with exponentially decaying type-II errors.

Since the present high-frequency setting involves increasingly correlated observations, establishing (i) is much more involved than in the i.i.d. setting, where the log-likelihood tensorizes [25]. In particular, we must deal with the full dependent log-likelihood ratio process as a whole. Following the intuition from the continuous observation setting [63, 41, 30], we employ martingale techniques to study an approximation of the log-likelihood which allows to deal with the dependence structure of the Markov chain. Making this approximation both precise and uniform is a key challenge, and the proof relies on refined small time expansions of the transition density or heat kernel [6, 11, 13], which can also be viewed as quantitative LAN expansions. Turning to

(ii), we construct suitable tests by establishing concentration inequalities for frequentist estimators [27]. Given the above discussion regarding model (5), our estimators must draw information from the diffusivity term to be minimax optimal. For this task, we follow the ideas of Comte et al. [15] in the scalar case of using penalized least squares estimators. As a by-product, we obtain frequentist estimators that we prove to be optimal in a minimax sense. To the best of our knowledge, these are the first minimax results for estimating the diffusion coefficient in a multidimensional setting. We finally apply our general contraction rate theorem to concrete Gaussian priors, such as the Matérn process.

Regarding related works, theoretical properties of Bayesian nonparametric methods in the scalar ( $d = 1$ ) diffusion model (5) have been well-studied, see for instance [63, 46, 62, 65, 42, 1]. Much less is known in the multivariate setting, with contraction rates recently obtained under continuous observations [41, 30] and only consistency for discrete observations [32, 40]. In particular, [40] extends the one-dimensional results of [31, 42] to establish posterior consistency in the same multidimensional model (1) in the low-frequency setting using completely different PDE techniques, showing that Bayesian methods can in principle adapt to the sampling regime, see [1] for further discussion. In the present high-frequency setup, we instead have access to refined tools from stochastic analysis, which we leverage here to obtain minimax optimal contraction rates in this regime.

Gaussian priors are widely used in practice [47] and have been applied in multiple ways to diffusion models, see for instance [46, 52, 10]. While we do not discuss computational issues here, note that posterior sampling based on discrete data is possible and is currently an active area of research, see for example [12, 43, 14, 61, 53] and the references therein.

## 2. MAIN RESULTS

**2.1. Preliminary setup for a reflected diffusion model in  $\mathbb{R}^d$ .** We now rigorously set up the statistical framework for our results in model (1). To account for the boundary behaviour, we assume that  $f$  is known to be 1 in an open neighbourhood of  $\partial\mathcal{O}$ . More precisely, for  $\mathcal{K} \subset \mathcal{O}$  a known compact set with  $\text{dist}(\mathcal{K}, \partial\mathcal{O}) > 0$ , define the parameter space

$$(6) \quad \mathcal{F}_0 = \mathcal{F}_0(\mathcal{K}, d, f_{\min}) = \left\{ f \in \mathcal{C}^\alpha(\mathcal{O}) : \inf_{x \in \mathcal{O}} f(x) \geq f_{\min} \text{ and } f(x) = 1 \text{ for all } x \in \mathcal{O} \setminus \mathcal{K} \right\},$$

where  $0 < f_{\min} < 1$  and the minimal smoothness equals

$$(7) \quad \alpha = \alpha_d = \max(4, 2 \lfloor d/4 + 1/2 \rfloor).$$

The minimal value  $\alpha_d$  scales like  $d/2$  for large dimension  $d$  and is needed to employ suitable bounds on the transition densities of the diffusion [17]. In particular, since  $\alpha \geq 4$ , this implies existence and uniqueness of the solution to (1). We consider the statistical experiment generated by the discrete observations  $X^N = (X_0, X_D, \dots, X_{ND})$  from (1) with sampling rate  $D_N = D > 0$ . We work in the high-frequency and long-term sampling regime as stated in the following assumption.

**Assumption (Sampling regime).** *Suppose that  $D = D_N \rightarrow 0$  such that  $ND \rightarrow \infty$ , but  $ND^2 \rightarrow 0$  as  $N \rightarrow \infty$ .*

This is the minimal assumption for all our results and will be assumed throughout the paper without further mention.

Let  $\mathbb{P}_f$  (simply  $\mathbb{P}$  when no confusion may arise) denote the unique law of the Markov process  $(X_t)_{t \geq 0}$  arising from (1). Consider the corresponding generator

$$(8) \quad \mathcal{L}_f(\phi) = \nabla \cdot (f \nabla \phi) = \nabla f \cdot \nabla \phi + f \Delta \phi = \sum_{j=1}^d \frac{\partial}{\partial x_j} \left( f \frac{\partial}{\partial x_j} \phi \right),$$

densely defined by its action on smooth functions  $\phi$ . For such a divergence form operator, the unique invariant probability measure can be explicitly computed as the uniform measure on  $\mathcal{O}$  as in (4), see p. 46 of [7], so that the process  $(X_t)_{t \geq 0}$  in (1) is stationary. Without loss of generality, we will assume that  $\text{vol}(\mathcal{O}) = 1$ . Let  $(P_{f,t})_{t \geq 0}$  denote the family of transition operators associated to  $(X_t)_{t \geq 0}$ , each of which admits a transition density  $p_{f,t}(x, y)$  on  $\mathcal{O} \times \mathcal{O}$ , so that for every real-valued and bounded function  $\phi : \mathcal{O} \rightarrow \mathbb{R}$ ,

$$P_{f,t}\phi(x) = \mathbb{E}_f[\phi(X_t) | X_0 = x] = \int_{\mathcal{O}} \phi(y) p_{f,t}(x, y) dy.$$

In particular  $p_{f,t}$  arises as the fundamental solution to the heat equation (3) with Neumann boundary conditions. It can be shown that there exists  $\lambda_f > 0$  such that  $\|P_{f,t}\phi\|_2 \leq e^{-\lambda_f t} \|\phi\|_2$  for every  $\phi : \mathcal{O} \rightarrow \mathbb{R}$  such that  $\int_{\mathcal{O}} \phi d\mu_f = \int_{\mathcal{O}} \phi dx = 0$ , where  $\lambda_f$  satisfies  $\lambda_f \geq f_{\min}/p_{\mathcal{O}} > 0$  with  $p_{\mathcal{O}} > 0$  the Poincaré constant for the domain  $\mathcal{O}$ , see for example Section 3.1 of [40]. This implies that the transition operator  $P_{f,D}$  of the discrete time Markov chain  $X_0, X_D, X_{2D}, \dots$  has first non-trivial eigenvalue

$$(9) \quad 1 - e^{-D\lambda_f} \geq rD > 0,$$

for some  $r = r(f_{\min}, p_{\mathcal{O}}) > 0$ , namely the Markov chain has a spectral gap decreasing linearly in the step size  $D \rightarrow 0$ .

From the above, we obtain likelihood

$$e^{\ell_N(f)} = e^{\ell(f; X_0, \dots, X_{ND})} = \prod_{i=1}^N p_{f,D}(X_{(i-1)D}, X_{iD})$$

based on observations  $X^N = (X_0, X_D, \dots, X_{ND})$ . We consider a Bayesian approach by placing on  $f$  a possibly  $N$ -dependent prior  $\Pi = \Pi_N$ , supported on some set  $\tilde{\mathcal{F}} \supseteq \mathcal{F}_0$ , leading to the posterior distribution

$$\Pi(A | X_0, X_D, \dots, X_{ND}) = \frac{\int_B \prod_{i=1}^N p_{f,D}(X_{(i-1)D}, X_{iD}) d\Pi(f)}{\int_{\tilde{\mathcal{F}}} \prod_{i=1}^N p_{f,D}(X_{(i-1)D}, X_{iD}) d\Pi(f)}, \quad A \subseteq \tilde{\mathcal{F}} \text{ measurable.}$$

In the following, we will study frequentist contraction rates for the posterior for  $f$  about the 'ground truth'  $f_0$  assumed to generate the data  $X^N$  in (1).

**Additional notation and function spaces.** Let  $|\cdot|$  denote the usual Euclidean norm on  $\mathbb{R}^d$ . For a multi-index  $j = (j_1, \dots, j_d) \in \mathbb{N}^d$ , set  $|j| = j_1 + \dots + j_d$  and consider the resulting partial differential operator  $\partial^j = \frac{\partial^{|j|}}{\partial x_1^{j_1} \dots \partial x_d^{j_d}}$ . For integer  $k \geq 0$ , let  $\mathcal{C}^k(\mathcal{O})$  denote the space of  $k$ -times differentiable functions on  $\mathcal{O}$  with uniformly continuous derivatives, while  $\mathcal{C}(\mathcal{O}) = \mathcal{C}^0(\mathcal{O})$  denotes the space of continuous function equipped with the supremum norm  $\|\cdot\|_{\infty}$ . For non-integer  $\beta > 0$ , set

$$\mathcal{C}^{\beta}(\mathcal{O}) = \left\{ f \in C^{\lfloor \beta \rfloor}(\mathcal{O}) : \sup_{x, y \in \mathcal{O}: x \neq y} \frac{|\partial^j f(x) - \partial^j f(y)|}{|x - y|^{\beta - \lfloor \beta \rfloor}} < \infty \text{ for all } |j| = \lfloor \beta \rfloor \right\},$$

where  $\lfloor \beta \rfloor$  denotes the largest integer less than or equal to  $\beta$ . For  $\beta \geq 0$ ,  $\mathcal{C}^\beta(\mathcal{O})$  is equipped with the usual norm

$$\|f\|_{\mathcal{C}^\beta} = \|f\|_{\mathcal{C}^\beta(\mathcal{O})} = \sum_{|j|=0}^{\lfloor \beta \rfloor} \sup_{x \in \mathcal{O}} |\partial^j f(x)| + \sum_{|j|=\lfloor \beta \rfloor} \sup_{x, y \in \mathcal{O}: x \neq y} \frac{|\partial^j f(x) - \partial^j f(y)|}{|x - y|^{\beta - \lfloor \beta \rfloor}},$$

where the second sum is removed for integer  $\beta$ . In particular,  $\|f\|_\infty = \|f\|_{\mathcal{C}^0}$ , and the norms  $\|\cdot\|_{\mathcal{C}^\beta}$  are non-decreasing in  $\beta$ .

Write  $\langle \cdot, \cdot \rangle_2$  for the usual inner product for  $L^2 = L^2(\mathcal{O})$ . For integer  $s \geq 0$ , define the Sobolev space on  $\mathcal{O}$  by

$$H^s(\mathcal{O}) = \{f \in L^2(\mathcal{O}) : \partial^j f \text{ exists and } \partial^j f \in L^2(\mathcal{O}) \text{ for all } |j| \leq s\}$$

equipped with the inner product

$$\langle f, g \rangle_{H^s(\mathcal{O})} = \sum_{|j| \leq s} \langle \partial^j f, \partial^j g \rangle_2.$$

For non-integer  $s \geq 0$ , one defines  $H^s(\mathcal{O})$  by interpolation [36, 59]. When no confusion may arise, we will often drop the explicit reference to the domain  $\mathcal{O}$  in the notation.

We will repeatedly use positive quantities that do depend on some parameters of the model, and that we informally call constants, and that may vary from line to line. These never depend on  $N$ , but do usually depend on the dimension  $d$  of the ambient space. Other relevant dependences may be emphasised by a subscript, such as  $C_f$ ,  $C_{\|f\|_{\mathcal{C}^k}}$  or  $C_{f, f_0}$ . The notation  $A_N \lesssim B_N$  means  $A_N \leq CB_N$  for every  $N \geq 1$ , where  $C$  is a ‘‘constant’’ according to our informal terminology. For real numbers  $a, b$ , let  $a \wedge b$  and  $a \vee b$  denote the minimum and maximum of  $a$  and  $b$ , respectively. We also sometimes write  $\mathbb{P}(A, B) = \mathbb{P}(A \cap B)$  to shorten notation.

**2.2. Gaussian process priors.** Gaussian priors are widely used in diffusion models and we investigate here their theoretical frequentist convergence rates. We assign to  $f$  a prior based on a Gaussian process, which must be modified to account for the constrained parameter space  $\mathcal{F}_0$  in (6), in particular that  $f \geq f_{\min}$  and  $f = 1$  near the boundary. We therefore employ the common approach of using a link function, which is standard for classification [47], density estimation ([26], Section 2.3.1) and inverse problems [57].

**Definition 1** (Smooth link function). *For a given lower bound  $f_{\min} \in (0, 1)$ , let  $\Phi : \mathbb{R} \rightarrow (f_{\min}, \infty)$  be an infinitely differentiable, strictly increasing bijective link function such that  $\Phi(0) = 1$ ,  $\Phi'(w) > 0$  for all  $w \in \mathbb{R}$  and  $\|\Phi^{(k)}\|_\infty < \infty$  for all  $k = 1, 2, \dots$*

It is not hard to construct such a function. Our proofs in fact permit weaker conditions on  $\Phi$ , requiring only that  $\Phi$  has ‘enough derivatives’ (roughly of the order of the prior), and that these are bounded on any compact subset of  $\mathbb{R}$ , for instance the exponential function  $t \mapsto f_{\min} + (1 - f_{\min})e^t$ . We refrain from these generalizations and consider smooth link functions for clarity of exposition. We now detail our full prior construction, starting from an underlying Gaussian process  $V$ . For definitions and background material on Gaussian processes and their associated RKHS, see Chapter 11 of [26] or [47].

**Condition 2.** *Let  $\Pi_V = \Pi_{V, N}$  be a mean-zero Gaussian Borel probability measure on the Banach space  $\mathcal{C}(\mathcal{O})$  that is supported on a separable measurable linear subspace of  $\mathcal{C}^4(\mathcal{O})$ , and assume that its reproducing kernel Hilbert space (RKHS)  $(\mathbb{H}_V, \|\cdot\|_{\mathbb{H}_V})$  embeds continuously into the Sobolev space  $H^s(\mathcal{O})$  for some  $s \geq 4$ , i.e.  $\mathbb{H}_V \hookrightarrow H^s(\mathcal{O})$ .*

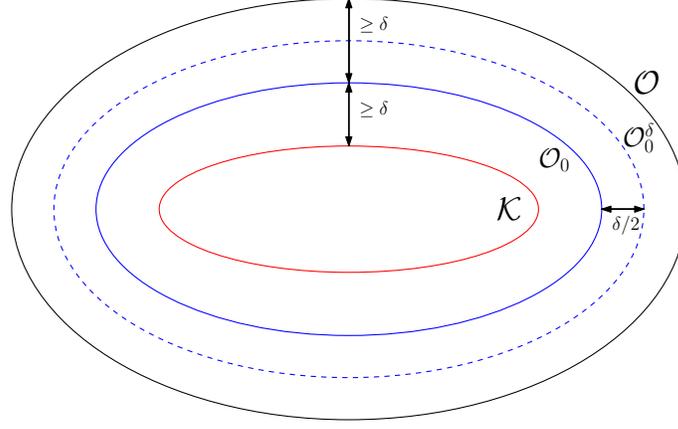


FIGURE 1. A simple example of a suitable domain  $\mathcal{O}$  (black), the region  $\mathcal{K}$  (red) where the ground truth  $f_0 \in \mathcal{F}_0$  is not equal to 1, and a set  $\mathcal{O}_0$  (blue) that  $\delta$ -separates these sets as in (10). The  $\delta/2$ -enlargement  $\mathcal{O}_0^\delta$  (dashed blue) of  $\mathcal{O}_0$  given in (19) is also plotted.

Recall that any  $f_0 \in \mathcal{F}_0$  satisfies  $\{x \in \mathcal{O} : f_0(x) \neq 1\} \subseteq \mathcal{K}$  by (6), where  $\mathcal{K} \subset \mathcal{O}$  is a known compact set with  $\text{dist}(\mathcal{K}, \partial\mathcal{O}) > 0$ . There thus exists  $\delta > 0$  and an open set  $\mathcal{O}_0$  having smooth  $\mathcal{C}^\infty$ -boundary  $\partial\mathcal{O}_0$  such that  $\mathcal{K} \subsetneq \mathcal{O}_0 \subsetneq \mathcal{O}$  and

$$(10) \quad \text{dist}(\mathcal{K}, \partial\mathcal{O}_0) \geq \delta \quad \text{and} \quad \text{dist}(\mathcal{O}_0, \partial\mathcal{O}) \geq \delta,$$

see, e.g., the proof of Proposition 8.2.1 in [19]. A simple example showing the relationship between such sets is plotted in Figure 1.

Let  $\chi \in \mathcal{C}^\infty(\mathcal{O})$  be a smooth cutoff function such that  $\chi \equiv 1$  on  $\mathcal{K}$  and  $\chi \equiv 0$  outside  $\mathcal{O}_0$ . We take as prior distribution  $\Pi = \Pi_N$  for  $f$  the law of the random function

$$(11) \quad f(x) = \Phi(\chi(x)W(x)), \quad W(x) = \frac{V(x)}{N^{d/(4s+2d)}}.$$

It follows that  $W$  is again a mean-zero Gaussian process with the same support and RKHS as  $V$ , but with rescaled covariance function. The cutoff function  $\chi$  ensures that  $f$  transitions smoothly to take value 1 near the domain boundary. Since the sample paths of  $V$  are in  $\mathcal{C}^4(\mathcal{O})$  almost surely under the prior by Condition 2, then  $\Pi(\mathcal{F}) = 1$  for

$$(12) \quad \mathcal{F} = \left\{ f \in \mathcal{C}^4(\mathcal{O}) : \inf_{x \in \mathcal{O}} f(x) \geq f_{\min} \text{ and } f(x) = 1 \text{ for all } x \in \mathcal{O} \setminus \mathcal{O}_0 \right\}.$$

Note that  $\mathcal{F}_0 \subsetneq \mathcal{F}$  since  $\mathcal{K} \subsetneq \mathcal{O}_0$ , so that the prior lives on a larger parameter space than  $\mathcal{F}_0$ , and that for any  $f_0 \in \mathcal{F}_0 \cap \mathcal{C}^s(\mathcal{O})$ , the function  $w_0 = \Phi^{-1}(f_0)$  is also in  $\mathcal{C}^s(\mathcal{O})$  with  $\text{supp}(w_0) \subseteq \mathcal{K}$ .

The following is the main result of our paper, establishing contraction rates for these rescaled Gaussian priors.

**Theorem 3.** Consider the sampling interval  $D = N^{-a}$  for some  $a \in (1/2, 1)$  and suppose  $s > s_{d,a}^*$ , where

$$(13) \quad s_{d,a}^* = \max \left( 4 + \frac{d}{2}, \frac{2-ad}{2a-1}, \frac{d(1+a)}{2(1-a)} \right).$$

Let  $\Pi = \Pi_N$  denote the prior (11) with mean-zero Gaussian process  $V \sim \Pi_V$  having RKHS  $\mathbb{H}_V$  and satisfying Condition 2 for this  $s$ . Let  $f_0 \in \mathcal{F}_0 \cap \mathcal{C}^s(\mathcal{O})$ , set  $w_0 = \Phi^{-1}(f_0)$  and suppose that there exists a sequence of functions  $v_{0,N} \in \mathbb{H}_V$  in the RKHS of  $V$  such that

- (i)  $\|v_{0,N}\|_{\mathbb{H}_V} = O(1)$ ,
- (ii)  $\|\chi v_{0,N}\|_{\mathcal{C}^\alpha} = O(1)$  for  $\alpha = \max(4, 2 \lfloor d/4 + 1/2 \rfloor)$ ,
- (iii)  $\|w_0 - \chi v_{0,N}\|_{\mathcal{C}^k} = O(N^{-\frac{s-k}{2s+d}})$  for  $k = 0, 1, 2, 3$ ,

as  $N \rightarrow \infty$ . Then for  $M > 0$  large enough, as  $N \rightarrow \infty$ ,

$$\mathbb{E}_{f_0} \Pi(f : \|f - f_0\|_2 \geq MN^{-\frac{s}{2s+d}} | X_0, X_D, \dots, X_{ND}) \rightarrow 0.$$

Since  $N^{-\frac{s}{2s+d}}$  is the minimax estimation rate in the high-frequency sampling regime (see Theorem 7 below for the corresponding lower bound), this result says that the posterior contracts about the truth at the minimax-optimal rate in any dimension  $d$ . Given the invariant measure is uninformative here, being the uniform distribution on  $\mathcal{O}$  for all  $f \in \mathcal{F}_0$ , this confirms that the Bayes method can indeed perform optimal inference by picking up sufficient information from the transitions  $X_{(i-1)D} \mapsto X_{iD}$  via the likelihood.

The minimal smoothness condition  $s_{d,a}^*$  in (13) can be rewritten as

$$s_{d,a}^* = \begin{cases} \max\left(4 + \frac{d}{2}, \frac{2-ad}{2a-1}, \frac{d(1+a)}{2(1-a)}\right) & \text{if } d = 1, 2 \text{ and } a \in (1/2, 1), \text{ or } d = 3 \text{ and } a \in (1/2, 2/3), \\ \max\left(4 + \frac{d}{2}, \frac{d(1+a)}{2(1-a)}\right) & \text{if } d = 3 \text{ and } a \in [2/3, 1), \\ \frac{d(1+a)}{2(1-a)} & \text{if } d \geq 4 \text{ and } a \in (1/2, 1). \end{cases}$$

This becomes more stringent as  $a \rightarrow 1$ , namely the frequency  $D = N^{-a} \rightarrow N^{-1}$  increases, since the time horizon  $ND = N^{1-a}$  then grows more slowly. The term  $\frac{d(1+a)}{2(1-a)}$  should be thought of as the main condition, with the extra terms for  $d = 1, 2, 3$  coming from minimal smoothness assumptions needed to use various expansions and bounds.

Theorem 3 requires that the true  $w_0 = \Phi^{-1}(f_0)$  can be very well approximated by elements  $v_{0,N}$  of the RKHS  $\mathbb{H}_V$  of  $V$ . Under Condition 2, an  $s$ -smooth truth almost lies in  $\mathbb{H}_V$  as needed, but this in turn implies that the Gaussian process  $V$  will typically have  $(s - d/2)$ -smooth sample paths (e.g. Proposition I.4 of [26] for the Matérn process), thereby undersmoothing the truth. When the prior mismatches the true smoothness, suitably rescaling the prior as in (11) has been shown to still yield optimal rates in several benchmark statistical models [64, 34]. This rescaling has also recently been used in the Bayesian inverse problems literature, where it is typically used to control stability estimates [29, 39].

We now consider two examples of Gaussian process priors satisfying the assumptions of Theorem 3. Let  $V = \{V(x) : x \in \mathcal{O}\}$  denote a Matérn process on  $\mathcal{O}$  with regularity parameter  $s - d/2 > 0$ , that is  $V$  is a mean-zero stationary Gaussian process with covariance function

$$K(x, y) = K(x - y) = \int_{\mathbb{R}^d} e^{-i(x-y) \cdot \xi} (1 + |\xi|^2)^{-s} d\xi, \quad x, y \in \mathcal{O}.$$

The covariance function can alternatively be represented in terms of special functions, see e.g. p.84 of [47]. While the Matérn process models (almost)  $(s - d/2)$ -smooth functions in a Hölder sense, its rescaled version  $W = V/N^{d/(4s+2d)}$  in (11) concentrates on  $s$ -smooth functions.

**Corollary 4.** *Let  $D = N^{-a}$  for some  $a \in (1/2, 1)$ , and let  $\Pi = \Pi_N$  denote the prior (11) with  $V$  a Matérn process of regularity  $s - d/2 > 0$  with  $s > s_{d,a}^*$  for  $s_{d,a}^*$  as in (13). If  $f_0 \in \mathcal{F}_0 \cap \mathcal{C}^s(\mathcal{O})$ , then for  $M > 0$  large enough,*

$$\mathbb{E}_{f_0} \Pi(f : \|f - f_0\|_2 \geq MN^{-\frac{s}{2s+d}} | X_0, X_D, \dots, X_{ND}) \rightarrow 0 \quad \text{as } N \rightarrow \infty.$$

As a second example, we consider a truncated Gaussian wavelet series prior. Let  $\{\psi_{lr} : l \geq J_0, r \in \mathbb{Z}^d\}$  denote an orthonormal basis of  $L^2(\mathbb{R}^d)$  composed of sufficiently regular, compactly supported Daubechies wavelets, where  $J_0 \in \mathbb{N}$  is the base resolution level of the scaling functions, which we also denote by  $\{\psi_{J_0, r}\}$  to simplify notation (see Chapter 4 of [28] for details). Let  $R_l$  denote the set of indices  $r$  for which the support of  $\psi_{lr}$  intersects  $\mathcal{O}_0$ . For  $J_0$  large enough (see Section 3), consider the Gaussian series expansion

$$(14) \quad V(x) = \sum_{l=J_0}^J \sum_{r \in R_l} 2^{-ls} g_{lr} \psi_{lr}(x), \quad g_{lr} \sim^{iid} N(0, 1),$$

where  $2^J \simeq N^{\frac{1}{2s+d}}$ . Note we could extend the second index set from  $r \in R_l$  to  $r \in \mathbb{Z}^d$  to cover all of  $\mathbb{R}^d$  since wavelet functions  $\psi_{lr}$  supported outside  $\mathcal{O}_0$  ultimately play no role in the prior (11) due to the cutoff function  $\chi$ .

**Corollary 5.** *Let  $D = N^{-a}$  for some  $a \in (1/2, 1)$ , and let  $\Pi = \Pi_N$  denote the prior (11) with  $V$  a Gaussian wavelet series as in (14) with  $s > s_{d,a}^*$  for  $s_{d,a}^*$  as in (13). If  $f_0 \in \mathcal{F}_0 \cap \mathcal{C}^s(\mathcal{O})$ , then for  $M > 0$  large enough,*

$$\mathbb{E}_{f_0} \Pi(f : \|f - f_0\|_2 \geq MN^{-\frac{s}{2s+d}} | X_0, X_D, \dots, X_{ND}) \rightarrow 0 \quad \text{as } N \rightarrow \infty.$$

Using a uniform integrability argument (e.g. Theorem 2.3.2 of [39]), this implies the same convergence rate for the posterior mean.

**Corollary 6.** *Let  $\bar{f}_N = E^\Pi[f | X_0, X_D, \dots, X_{ND}]$  denote the posterior mean based on the Matérn process or Gaussian wavelet series prior. Under the conditions of Corollary 4 (Matérn) or Corollary 5 (Gaussian wavelet series), there exists a constant  $M > 0$  such that as  $N \rightarrow \infty$ ,*

$$\mathbb{P}_{f_0}(\|\bar{f}_N - f_0\|_2 \geq MN^{-\frac{s}{2s+d}}) \rightarrow 0.$$

We thus have two concrete examples of Gaussian priors for which the posterior (means) converge to the true  $f_0 \in \mathcal{F}_0 \cap \mathcal{C}^s$  at rate  $N^{-\frac{s}{2s+d}}$ . The following lower bound shows that this is indeed the minimax rate of convergence.

**Theorem 7 (Minimax lower bound).** *Let  $D = N^{-a}$  for some  $a \in (1/2, 1)$ . For any  $s > \alpha_d$  (the minimal smoothness (7)) and  $M > 0$ , the following frequentist lower bound holds:*

$$\liminf_{N \rightarrow \infty} \inf_{\hat{f}_N} \sup_{f \in \mathcal{F}_0, \|f\|_{e^s} \leq M} N^{\frac{2s}{2s+d}} \mathbb{E}_f \|\hat{f}_N - f\|_2^2 > 0,$$

where the infimum is taken among all estimators based on data (2).

In particular, we extend the univariate minimax lower bound of [33]. The proof is given in Appendix 9.1.

### 3. A GENERAL CONTRACTION THEOREM

We now state and discuss the abstract contraction rate theorem used to derive the convergence results for Gaussian process priors in Section 2.2 above. This is based on the general testing approach of Bayesian nonparametrics [26], which requires (i) that the prior puts sufficient mass on a neighbourhood of the truth and (ii) the existence of suitable tests with exponentially decaying type-II errors.

For  $0 < \varepsilon_N \leq \varepsilon_{1,N} \leq \varepsilon_{2,N} \leq \varepsilon_{3,N} \rightarrow 0$  positive sequences,  $r > 0$  and  $\alpha = \alpha_d$  as in (7), define the following neighbourhood of  $f_0$ :

$$(15) \quad \begin{aligned} \mathcal{C}_N &= \mathcal{C}_N(f_0, \varepsilon_N, \varepsilon_{1,N}, \varepsilon_{2,N}, \varepsilon_{3,N}, r) \\ &= \left\{ f \in \mathcal{F} : \|f\|_{\mathcal{C}^\alpha} \leq r, \|f - f_0\|_\infty \leq \varepsilon_N, \|f - f_0\|_{e^k} \leq \varepsilon_{k,N} \text{ for } k = 1, 2, 3 \right\}, \end{aligned}$$

which can be related to the information theoretic distance of the model induced by the log-likelihood ratio process. Further define

$$(16) \quad \begin{aligned} E_N &:= \varepsilon_N^2 \left( 1 + \frac{D}{\varepsilon_N} + \frac{D^2}{\varepsilon_N^2} + \frac{\varepsilon_{1,N}}{\varepsilon_N^2} D + \frac{\varepsilon_{2,N}}{\varepsilon_N^2} D + \frac{\varepsilon_{3,N}}{\varepsilon_N^2} D^{3/2} \right) \\ V_N &:= N\varepsilon_N^2 + N\varepsilon_{1,N}^4 D^{-1} + N^2\varepsilon_{1,N}^2 D^2 + N^2\varepsilon_{2,N}^2 D^2 + N^2\varepsilon_{3,N}^2 D^3 + N^2 D^4. \end{aligned}$$

The quantities  $NE_N$  and  $V_N$  control the expectation and variance, respectively, of the integrated log-likelihood ratio process restricted to the small-ball  $\mathcal{C}_N$ , which is used to lower bound the normalized denominator of the Bayes formula. This is the content of the next result, which is the most technically involved part of our proof.

**Theorem 8** (Evidence lower bound). *Let  $f_0 \in \mathcal{F}_0$  and  $\nu$  be a probability measure supported on  $\mathcal{C}_N$  as in (15) with  $r > 0$  and sequences  $0 < \varepsilon_N \leq \varepsilon_{1,N} \leq \varepsilon_{2,N} \leq \varepsilon_{3,N} \rightarrow 0$  satisfying  $N\varepsilon_N^2 \rightarrow \infty$  as  $N \rightarrow \infty$ . Then the integrated log-likelihood ratio process*

$$\Lambda_D^N = \int_{\mathcal{C}_N} \log \prod_{i=1}^N \frac{p_{f,D}(X_{(i-1)D}, X_{iD})}{p_{f_0,D}(X_{(i-1)D}, X_{iD})} \nu(df).$$

satisfies

$$\sup_{f \in \mathcal{C}_N} \mathbb{E}_{f_0} \left[ \log \frac{p_{f_0,D}(X_0, X_D)}{p_{f,D}(X_0, X_D)} \right] \lesssim E_N, \quad \text{Var}_{f_0}(\Lambda_D^N) \lesssim V_N,$$

where  $E_N, V_N$  are defined in (16) and the constants depend only on  $f_0, r, d, \Theta, \delta, f_{\min}$ . This implies that for every  $c > 0$ ,

$$(17) \quad \mathbb{P}_{f_0} \left( \int_{\mathcal{C}_N} \prod_{i=1}^N \frac{p_{f,D}(X_{(i-1)D}, X_{iD})}{p_{f_0,D}(X_{(i-1)D}, X_{iD})} \nu(df) \leq e^{-cN\varepsilon_N^2 - C_0NE_N} \right) \leq \frac{V_N}{c^2 N^2 \varepsilon_N^4},$$

where  $C_0 > 0$  is a fixed constant depending only on  $f_0, r, d, \Theta, \delta, f_{\min}$ .

Theorem 8 shows that the Bayesian evidence is at least  $e^{-CN\varepsilon_N^2}$  with  $\mathbb{P}_{f_0}$ -probability tending to one if

$$(18) \quad E_N \lesssim \varepsilon_N^2 \quad \text{and} \quad V_N / (N^2 \varepsilon_N^4) \rightarrow 0.$$

To help the reader understand the technical conditions, which are rather intricate in their full generality, we introduce the following concrete example with the ‘usual’ nonparametric choices of sequences for a  $\mathcal{C}^s$ -smooth truth.

**Assumption A.** *Let  $s \geq 4$ ,  $1/2 < a < 1$  and  $J \in \mathbb{N}$ . Suppose that*

$$D = N^{-a}, \quad \varepsilon_N = N^{-\frac{s}{2s+d}}, \quad \varepsilon_{k,N} = N^{-\frac{s-k}{2s+d}}, \quad k = 1, 2, 3, \quad 2^J \simeq N^{\frac{1}{2s+d}}.$$

Under Assumption A, all technical conditions reduce to conditions on  $a, s, d$ . In particular, (18) is implied by

$$s > \begin{cases} \frac{2-ad}{2a-1} & \text{if } d = 1, 2, a \in (1/2, 1), \text{ or } d = 3, a \in (1/2, 2/3], \\ 0 & \text{if } d = 3, a \in [2/3, 1), \text{ or } d \geq 4, a \in (1/2, 1). \end{cases}$$

An overview of the proof of Theorem 8 is found in Section 4.

For comparison, consider the i.i.d model  $Y_1, \dots, Y_N \sim^{iid} P$  with  $P$  having density  $p$ , so that  $(Y_1, \dots, Y_N) \sim P^N = \otimes_{i=1}^N P$ . The corresponding neighbourhood can then be expressed in terms of the Kullback-Leibler divergence and its  $2^{nd}$ -variation [25],

$$\begin{aligned} B_2(p_0, E_N, V_N) &= \left\{ p : P_0^N \log(p_0^N/p^N) \leq N E_N, \text{Var}_{P_0^N}(\log(p_0^N/p^N)) \leq V_N \right\} \\ &= \left\{ p : P_0 \log(p_0/p) \leq E_N, \text{Var}_{P_0}(\log(p_0/p)) \leq V_N/N \right\}, \end{aligned}$$

where the last equality follows from the densities tensorizing in the i.i.d. model. In this model, one can take  $E_n \simeq \varepsilon_N^2$  and  $V_N \simeq N\varepsilon_N^2$  ([26], Lemma 8.10 with  $k = 2$ ), which gives some intuition behind the roles of  $E_N$  and  $V_N$ . However, the present high-frequency diffusion model is far from i.i.d., so that we must deal with the full dependent log-likelihood ratio process  $\Lambda_D^N$  as a whole, rendering this computation much more involved.

Our strategy is to use second-order small time expansions of the transition densities [6, 11, 13], which heuristically corresponds to replacing  $p_{f,D}$  in  $\Lambda_D^N$  with the corresponding Euler scheme without drift, that is a  $N_d(x, 2Df(x)I_d)$  density. This reflects the property of model (1) that the drift is of smaller order than the diffusivity, and hence does not affect the leading order terms in  $\Lambda_D^N$  as  $D \rightarrow 0$ . Such expansions can also be viewed as a quantitative form of local asymptotic normality (LAN) with uniform remainders over  $\mathcal{C}_N$ . We then further approximate the resulting process by a martingale difference, which allows us to deal with the dependence of the process. Note that we require control of the derivatives of  $f - f_0$  up to third order in  $\mathcal{C}_N$  in (15) to ensure the higher order terms of these expansions are negligible, uniformly over  $\mathcal{C}_N$ .

Turning to the existence of tests with exponentially decreasing type-II errors, we employ plug-in tests based on estimators satisfying suitable concentration inequalities as was done for i.i.d. models in [27], see also [48, 42, 1, 38]. As estimators, we follow the ideas of Comte et al. [15] who use penalized least squares estimators in the scalar case. We therefore extend the results of [15] to the multidimensional setting with domain boundary, exploiting the structure of the  $L^2$ -loss function to obtain the required concentration inequalities.

Our proofs require certain wavelet-based approximations, which must be adapted to deal with the boundary as we now make precise. Let

$$(19) \quad \mathcal{O}_0^\delta = \{x \in \mathcal{O}, \text{dist}(x, \mathcal{O}_0) \leq \delta/2\}$$

denote the  $\delta/2$ -enlargement of  $\mathcal{O}_0$ , and note that  $\mathcal{O}_0^\delta \subsetneq \mathcal{O}$  since  $\text{dist}(\mathcal{O}_0, \partial\mathcal{O}) \geq \delta$  by assumption (10), see Figure 1 for an example. As in Section 2.2, let  $\{\psi_{lr} : l \geq J_0, r \in \mathbb{Z}^d\}$  denote an orthonormal basis of  $L^2(\mathbb{R}^d)$  composed of sufficiently regular, compactly supported Daubechies wavelets, where  $J_0 \in \mathbb{N}$  is the base resolution level of the scaling functions, which we also denote by  $\{\psi_{J_0,r}\}$  to simplify notation. Let  $R_l$  denote the set of indices  $r$  for which the support of  $\psi_{lr}$  intersects  $\mathcal{O}_0$ , in which case  $|R_l| = O(2^{ld})$  since  $\mathcal{O}_0$  is a bounded domain in  $\mathbb{R}^d$ . Since  $\text{dist}(\mathcal{O}_0^\delta, \partial\mathcal{O}) \geq \delta/2 > 0$  and  $\text{diam}(\text{supp}(\psi_{lr})) = O(2^{-l})$ , we may take  $J_0$  large enough such that no wavelet function  $\psi_{lr}$ ,  $l \geq J_0$ , has support intersecting both  $\mathcal{O}_0$  and  $(\mathcal{O}_0^\delta)^c$ . Any function  $g \in L^2(\mathcal{O})$  with  $\text{supp}(g) \subseteq \mathcal{O}_0$  can then be uniquely represented as

$$(20) \quad g = \sum_{l=J_0}^{\infty} \sum_{r \in R_l} \langle g, \psi_{lr} \rangle_2 \psi_{lr}.$$

Even though the wavelets  $\{\psi_{lr} : l \geq J_0, r \in R_l\}$  do not form an orthonormal basis of  $L^2(\mathcal{O})$  due to their behaviour on  $\mathcal{O} \setminus \mathcal{O}_0$ , any  $g$  as above can be extended to a function on  $\mathbb{R}^d$  (or any set containing  $\mathcal{O}_0$ ) by setting it to zero outside  $\mathcal{O}_0$ . In particular, the Sobolev and Holder norms on  $\mathcal{O}$  and  $\mathbb{R}^d$

coincide for such functions and we may therefore use all the usual wavelet characterizations and embeddings for Sobolev and Hölder norms. This fact will be used without mention in the proofs.

For  $J \geq J_0$ , set

$$(21) \quad V_J = V_J(\mathcal{O}_0) = \left\{ f = \sum_{l=J_0}^J \sum_{r \in R_l} f_{lr} \psi_{lr} \right\} \subset \mathcal{C}(\mathcal{O})$$

to be the linear space of all functions in the wavelet projection space of resolution level  $J$ , restricted to those wavelets with support intersecting  $\mathcal{O}_0$  but not  $(\mathcal{O}_0^\delta)^c$ . Note that

$$(22) \quad g(x) = g(x) \mathbf{1}_{x \in \mathcal{O}_0^\delta} \quad \text{for every } g \in V_J$$

since  $\text{supp}(g) \subseteq \mathcal{O}_0^\delta$  for  $g \in V_J$ . We must slightly modify the usual notion of a wavelet projection to account for the behaviour near the boundary in  $\mathcal{F}$  in (12). To that end, note that  $\text{supp}(f-1) \subseteq \mathcal{O}_0$  for any  $f \in \mathcal{F}$  and thus  $f-1$  has a wavelet expansion as in (20). Setting  $P_J : L^2(\mathcal{O}) \rightarrow V_J$  to be the  $L^2$ -projection operator onto  $V_J$ , we define the projection operator  $\bar{P}_J : \mathcal{F} \rightarrow \mathcal{F}$  by

$$(23) \quad \bar{P}_J[f](x) := 1 + P_J[f-1](x) = 1 + \sum_{l=J_0}^J \sum_{r \in R_l} \langle f-1, \psi_{lr} \rangle_2 \psi_{lr}(x), \quad x \in \mathcal{O}.$$

Since  $\text{supp}(f-1) \subseteq \mathcal{O}_0$ ,  $P_J[f-1](x) = \sum_{l=J_0}^J \sum_{r \in R_l} \langle f-1, \psi_{lr} \rangle_2 \psi_{lr}(x)$  coincides with the usual wavelet projection of  $f-1$  on all of  $\mathbb{R}^d$ .

We are now ready to define our projection estimator following Comte *et al.* [15]. Let

$$(24) \quad \hat{g}_N \in \arg \min_{g \in V_J} \sum_{i=1}^N ((Y_{i,D} - 1) \mathbf{1}_{\mathcal{A}_{i,D}} - g(X_{(i-1)D}))^2,$$

with  $\mathcal{A}_{i,D} = \{X_{(i-1)D} \in \mathcal{O}_0^\delta\}$  and

$$Y_{i,D} = \frac{1}{2dD} |X_{iD} - X_{(i-1)D}|^2.$$

Note that by (22), the sum in (24) actually spans over  $i$  such that  $X_{(i-1)D}$  lies in  $\mathcal{O}_0^\delta$ . We then consider the estimator

$$(25) \quad \hat{f}_N(x) = 1 + \hat{g}_N(x), \quad x \in \mathcal{O}.$$

The idea behind (24) is that for small  $D > 0$ , by Itô's formula, we have the signal plus noise representation

$$Y_{i,D} - 1 = f(X_{(i-1)D}) - 1 + \varepsilon_{i,D} + r_{i,D},$$

where  $\varepsilon_{i,D}$  is a martingale error term with variance of order 1 and  $r_{i,D}$  is a small remainder term combining stochastic expansions and boundary effects, see (38) in the proofs for a precise definition. Thus  $\hat{g}_N$  is an estimate of  $f-1$ , which has support contained in  $\mathcal{O}_0$  for all  $f \in \mathcal{F}$ . Indeed, one needs only estimate  $f$  on  $\mathcal{O}_0$ , since  $f \equiv 1$  is already known on  $\mathcal{O} \setminus \mathcal{O}_0$  for all  $f \in \mathcal{F}$ . This permits to separate estimation on the interior of  $\mathcal{O}$ , where the function  $f$  is unknown, with the behaviour near the boundary  $\partial\mathcal{O}$ , where the reflecting boundary conditions alter the diffusion dynamics. We next establish a concentration inequality for the estimator  $\hat{f}_N$ .

**Theorem 9** (Exponential inequality). *Let  $\hat{f}_N = \hat{f}_N(X_0, X_1, \dots, X_{ND})$  be the estimator (25). Let  $\varepsilon_N, \xi_N \rightarrow 0$ ,  $2^J = 2^{J_N} \rightarrow \infty$  and  $R_{J,4}, R_{J,\infty}$  be sequences such that  $N\varepsilon_N^2 \rightarrow \infty$  as  $N \rightarrow \infty$ . Define the sets*

$$\mathcal{F}'_N = \{f \in \mathcal{F} : \|f\|_{\mathcal{C}^1} \leq r, \|f - \bar{P}_J f\|_2 \leq C\xi_N, \|f - \bar{P}_J f\|_4 \leq R_{J,4}, \|f - \bar{P}_J f\|_\infty \leq R_{J,\infty}\},$$

where  $C, r > 0$  and  $\bar{P}_J f$  denotes the projection (23). Assume further that  $2^{Jd} = o(\sqrt{ND})$ ,

$$R_{J,4}^4 \varepsilon_N^2 + R_{J,\infty}^2 \xi_N^2 \varepsilon_N^2 \lesssim D \xi_N^4, \quad 2^{3Jd/2} N^{-1} + 2^{Jd/2} N^{-1/2} + 2^{Jd/2} \varepsilon_N^2 + \varepsilon_N \lesssim \xi_N,$$

as  $N \rightarrow \infty$ . Then there exist events  $\mathcal{B}_N$  satisfying

$$\sup_{f \in \mathcal{F}} \mathbb{P}_f(\mathcal{B}_N^c) \rightarrow 0$$

as  $N \rightarrow \infty$ , such that for every  $L > 0$ ,

$$\sup_{f \in \mathcal{F}'_N} \mathbb{P}_f(\|\hat{f}_N - \bar{P}_J f\|_2 \geq K \xi_N, \mathcal{B}_N) \leq C' e^{-LN \varepsilon_N^2},$$

where  $K$  depends on  $L$ .

The proof can be found in Section 6. Theorem 9 says that if the underlying function  $f$  can be well-enough approximated by its projection  $\bar{P}_J f$  as quantified by the conditions in  $\mathcal{F}'_N$ , then the estimator  $\hat{f}_N$  will concentrate about this projection with all but exponentially small  $\mathbb{P}_f$ -probability.

As far as we are aware, this extension of [15] in Theorem 9 is the first frequentist estimator of the diffusion function  $f$  in the multivariate setting and thus may be of independent interest. Combined with the lower bound of Theorem 7, we obtain

**Theorem 10.** *Let  $D = N^{-a}$  for some  $a \in (1/2, 1)$ ,  $s > \alpha_d$ , and let  $M > 0$ . Define  $\hat{f}_N^* = \min(\hat{f}_N, M)_+$ , where  $\hat{f}_N$  is as in (25) constructed with Daubechies wavelets with at least  $\lfloor s \rfloor - 1$  vanishing moments, and  $2^J \simeq N^{1/(2s+d)}$ . Then*

$$\sup_{f \in \mathcal{F}_0, \|f\|_{\mathcal{C}^s} \leq M} \mathbb{E}_f \|\hat{f}_N^* - f\|_2^2 \lesssim N^{-2s/(2s+d)}.$$

Combined with Theorem 7, we obtain that the (normalised) rate  $N^{-s/(2s+d)}$  is asymptotically minimax for estimating  $f$  over  $\{f \in \mathcal{F}_0 : \|f\|_{\mathcal{C}^s} \leq M\}$ .

The proof of Theorem 10 is given in Appendix 9.2. We emphasize that while this estimator plays a key role in our *proof* of minimax optimal posterior contraction rates using the Gaussian prior (11), it is not actually involved in the prior construction or Bayesian method itself. Using Theorems 8 and 9, we obtain the following general posterior contraction theorem for our setting. The proof is found in Section 7.1.

**Theorem 11 (General contraction theorem).** *Let  $\Pi = \Pi_N$  be a sequence of prior distributions supported on  $\mathcal{F}$  in (12), let  $r, K_0 > 0$  be fixed constants and  $0 < \varepsilon_N \leq \varepsilon_{1,N} \leq \varepsilon_{2,N} \leq \varepsilon_{3,N} \rightarrow 0$ ,  $\xi_N \rightarrow 0$ ,  $2^J = 2^{J_n} \rightarrow \infty$  and  $R_{J,4}, R_{J,\infty}$  be sequences satisfying  $N \varepsilon_N^2 \rightarrow \infty$ ,  $2^{Jd} = o(\sqrt{ND})$  and*

$$(26) \quad R_{J,4}^4 \varepsilon_N^2 + R_{J,\infty}^2 \xi_N^2 \varepsilon_N^2 \lesssim D \xi_N^4, \quad 2^{3Jd/2} N^{-1} + 2^{Jd/2} N^{-1/2} + 2^{Jd/2} \varepsilon_N^2 + \varepsilon_N \lesssim \xi_N,$$

as  $N \rightarrow \infty$ . Further suppose that  $E_N$  and  $V_N$  in (16) satisfy

$$E_N \leq K_0 \varepsilon_N^2, \quad \text{and} \quad V_N / (N^2 \varepsilon_N^4) \rightarrow 0.$$

Let

$$\mathcal{C}_N = \left\{ f \in \mathcal{F} : \|f\|_{\mathcal{C}^\alpha} \leq r, \|f - f_0\|_\infty \leq \varepsilon_N, \|f - f_0\|_{\mathcal{C}^k} \leq \varepsilon_{k,N} \text{ for } k = 1, 2, 3 \right\}$$

be the set defined in (15),

$$\mathcal{F}_N \subseteq \{f \in \mathcal{F} : \|f\|_{\mathcal{C}^1} \leq r, \|f - \bar{P}_J f\|_2 \lesssim \xi_N, \|f - \bar{P}_J f\|_4 \leq R_{J,4}, \|f - \bar{P}_J f\|_\infty \leq R_{J,\infty}\},$$

where  $\bar{P}_J$  denotes the projection (23), and  $C_0 > 0$  be the fixed constant in Theorem 8, which depends only on  $f_0, r, d, \Theta, \delta, f_{\min}$ . Assume the true  $f_0 \in \mathcal{F}_0$  satisfies  $\|f_0 - \bar{P}_J f_0\|_2 \lesssim \xi_N$  and  $\|f_0 - \bar{P}_J f_0\|_p \lesssim R_{J,p}$  for  $p \in \{4, \infty\}$ . Suppose that for some  $C, L > 0$ ,

- (i)  $\Pi(\mathcal{F}_N^c) \leq L e^{-(C+C_0 K_0+2)N\varepsilon_N^2}$ ,
- (ii)  $\Pi(\mathcal{C}_N) \geq e^{-CN\varepsilon_N^2}$ .

Then for  $M > 0$  large enough, as  $N \rightarrow \infty$ ,

$$\mathbb{E}_{f_0} \Pi(f : \|f - f_0\|_2 \geq M\xi_N | X_0, X_D, \dots, X_{ND}) \rightarrow 0.$$

To summarize, in order to apply Theorem 11 in examples, we must verify that the prior places most of its mass on functions  $f \in \mathcal{F}_N$  that are well-approximable by their projections  $\bar{P}_J f$ , and also that the prior places at least an exponentially small amount of mass in a neighbourhood of the truth in the sense of  $\mathcal{C}_N$ , i.e. conditions (i) and (ii) of Theorem 11, respectively.

#### 4. PROOF OF THEOREM 8: EXPECTATION AND VARIANCE OF THE INTEGRATED LOG-LIKELIHOOD RESTRICTED TO $\mathcal{C}_N$

The proof of the variance and expectation of the log-likelihood is split into several approximation steps employing different techniques. We provide here an overview of the proof, deferring the detailed technical arguments to later in the paper to aid readability. We first prove the more difficult variance bound for  $\Lambda_D^N$  in Theorem 8.

**4.1. Proof of the variance bound of Theorem 8.** For an integer  $m \geq 1$ , real-valued random variables  $(Z_{f,k} : f \in \mathcal{F}, k \geq 1)$  and a probability measure  $\nu(df)$  with support  $\mathcal{A} \subset \mathcal{F}$ , we will repeatedly use the inequalities

$$(27) \quad \text{Var}_{f_0} \left( \int_{\mathcal{F}} \sum_{k=1}^m Z_{f,k} \nu(df) \right) \leq \int_{\mathcal{F}} \text{Var}_{f_0} \left( \sum_{k=1}^m Z_{f,k} \right) \nu(df) \leq m \sum_{k=1}^m \sup_{f \in \mathcal{A}} \mathbb{E}_{f_0} [Z_{k,f}^2].$$

*Step 1: Restricting observations away from the boundary.* We first decompose the log-likelihood according to whether  $X_{(i-1)D} \in \mathcal{O}_0$  or not. On the event  $\mathcal{A}_{i,D} = \{X_{(i-1)D} \in \mathcal{O}_0^\delta\}$ , where  $\mathcal{O}_0^\delta$  is the  $\delta/2$ -enlargement of  $\mathcal{O}_0$  defined in (19) above, the process does not hit the boundary during  $[(i-1)D, iD]$  with overwhelming probability, and hence we may use analytic approximation techniques that ignore the boundary reflection. Since  $f = f_0 = 1$  near the boundary for  $f, f_0 \in \mathcal{F}$ , on  $(\mathcal{A}_{i,D})^c$  the likelihood ratio is already close to one and thus makes a negligible contribution. We quantify this last observation in the following result.

**Lemma 12.** *Let  $\mathcal{F}' = \{f \in \mathcal{F} : \|f\|_{\mathcal{C}^\alpha} \leq r\}$  for  $\alpha = \max(4, 2 \lfloor d/4 + 1/2 \rfloor)$ . Then for  $k = 1, 2$ , any  $f, f_0 \in \mathcal{F}'$  and any  $\gamma > 0$ ,*

$$\begin{aligned} & \int_{x \in \mathcal{O} \setminus \mathcal{O}_0^\delta, y \in \mathcal{O}} \left( \log \frac{p_{f_0,D}(x,y)}{p_{f,D}(x,y)} \right)^k p_{f_0}(x,y) dx dy \\ & \leq C_1 D^{-d/2} (1 + \gamma^{2k} (\log N)^k) N^{-C_2 \gamma^2} + C_3 N^{C_4 \gamma^2} \exp(-cD^{-1}), \end{aligned}$$

where the constants  $C_1 - C_4, c > 0$  are uniform over  $(\mathcal{O}, d, f_{\min}, r, \delta)$ .

The proof is based on explicit bounds for the heat kernel in small time, for instance Theorem 3.2.9 in [20] for the upper bound and Theorem 3.1 in [17] for the lower bound. It is delayed until Section 8.1. Abbreviating  $X_i^D = (X_{(i-1)D}, X_{iD})$  and applying Lemma 12 with  $k = 2$  together with

(27) yields

$$\begin{aligned} & \text{Var}_{f_0} \left( \int_{\mathcal{C}_N} \sum_{i=1}^N \log \frac{p_{f,D}}{p_{f_0,D}}(X_i^D) \mathbf{1}_{(\mathcal{A}_{i,D})^c} \nu(df) \right) \\ & \leq N^2 \int_{x \in \mathcal{O} \setminus \mathcal{O}_0^{\delta/2}, y \in \mathcal{O}} \left( \log \frac{p_{f,D}(x,y)}{p_{f_0,D}(x,y)} \right)^2 p_{f_0,D}(x,y) dx dy \\ & \lesssim D^{-d/2} (\log N)^2 N^{-C_2\mu} + N^{C_4\mu} \exp(-cD^{-1}) \end{aligned}$$

for large enough  $\mu > 0$  and constants uniform over  $\mathcal{C}_N$ . In view of the statement of Theorem 8, it remains to consider the variance of  $\int_{\mathcal{C}_N} \sum_{i=1}^N \log \frac{p_{f,D}}{p_{f_0,D}}(X_i^D) \mathbf{1}_{\mathcal{A}_{i,D}} \nu(df)$ , i.e. we may restrict to the events  $\mathcal{A}_{i,D}$ .

*Step 2: Approximation by an unbounded diffusion model on  $\mathbb{R}^d$ .* We can smoothly extend any  $f \in \mathcal{F}$  to all of  $\mathbb{R}^d$  by setting  $f = 1$  outside  $\mathcal{O}$ . Consider a diffusion process  $(\tilde{X}_t)_{t \geq 0}$  taking values on all of  $\mathbb{R}^d$  arising as the solution to the stochastic differential equation

$$(28) \quad \tilde{X}_t = x + \int_0^t \nabla f(\tilde{X}_s) ds + \int_0^t (2f(\tilde{X}_s))^{1/2} dB_s,$$

defined on the same probability space with the same driving Brownian motion  $(B_t)_{t \geq 0}$  as  $(X_t)_{t \geq 0}$ . Thus in this section,  $\mathbb{P}_f$  denotes a probability measure defined on a rich enough probability space to accommodate a Brownian motion  $(B_t)_{t \geq 0}$  (and therefore the strong solutions  $(X_t)_{t \geq 0}$  of (1) and  $(\tilde{X}_t)_{t \geq 0}$  of (28) driven by the parameter  $f$ ).

The process  $(\tilde{X}_t)_{t \geq 0}$  in turn generates a family of transition densities  $\tilde{p}_{f,D} : \mathbb{R}^d \times \mathbb{R}^d \rightarrow [0, \infty)$ . We may pick a smooth version of  $\tilde{p}_{f,D}$  so that in particular, for any  $x \in \mathcal{O}$ ,

$$(29) \quad \tilde{p}_{f,D}(x,y) dy = \mathbb{P}_f(\tilde{X}_D \in dy \mid X_0 = x).$$

Consider the decomposition

$$(30) \quad \begin{aligned} \int_{\mathcal{C}_N} \sum_{i=1}^N \log \frac{p_{f,D}}{p_{f_0,D}}(X_i^D) \mathbf{1}_{\mathcal{A}_{i,D}} \nu(df) &= \int_{\mathcal{C}_N} \sum_{i=1}^N \log \frac{\tilde{p}_{f,D}}{\tilde{p}_{f_0,D}}(X_i^D) \mathbf{1}_{\mathcal{A}_{i,D}} \nu(df) \\ &+ \int_{\mathcal{C}_N} \sum_{i=1}^N \left( \log \frac{p_{f,D}}{\tilde{p}_{f,D}} + \log \frac{\tilde{p}_{f_0,D}}{p_{f_0,D}} \right) (X_i^D) \mathbf{1}_{\mathcal{A}_{i,D}} \nu(df). \end{aligned}$$

We have an analogous result to Lemma 12 for controlling the expectation and variance of the approximation of  $\log p_{f,D}$  by  $\log \tilde{p}_{f,D}$  starting from  $x \in \mathcal{O}_0^\delta$ .

**Lemma 13.** *Let  $\mathcal{F}' = \{f \in \mathcal{F} : \|f\|_{\mathcal{C}^\alpha} \leq r\}$  for  $\alpha = \max(4, 2 \lfloor d/4 + 1/2 \rfloor)$ . Then for  $k = 1, 2$ , any  $g = f, f_0 \in \mathcal{F}'$  and any  $\gamma > 0$ ,*

$$\begin{aligned} & \int_{x \in \mathcal{O}_0^\delta, y \in \mathcal{O}} \left( \log \frac{p_{g,D}(x,y)}{\tilde{p}_{g,D}(x,y)} \right)^k p_{f_0,D}(x,y) dx dy \\ & \leq C_1 D^{-d/2} (1 + \gamma^{2k} (\log N)^k) N^{-C_2\gamma^2} + C_3 N^{C_4\gamma^2} \exp(-cD^{-1}), \end{aligned}$$

where the constants  $C_1 - C_4, c > 0$  are uniform over  $(\mathcal{O}, d, f_{\min}, r, \delta)$ . The same estimate holds replacing  $(\log \frac{p_{g,D}(x,y)}{\tilde{p}_{g,D}(x,y)})^k$  by  $(\log \frac{\tilde{p}_{g,D}(x,y)}{p_{g,D}(x,y)})^k$ .

The proof uses similar tools as for Lemma 12 and is delayed until Section 8.3. Using (27) and Lemma 13 with  $k = 2$  and  $\gamma > 0$  large enough, the  $\mathbb{P}_{f_0}$ -variance of the second term in the RHS of (30) is bounded above by

$$\begin{aligned} & N^2 \sup_{f \in \mathcal{C}_N} \mathbb{E}_{f_0} \left[ \left( \log \frac{\tilde{p}_{f,D}}{\tilde{p}_{f_0,D}}(X_0^D) + \log \frac{\tilde{p}_{f_0,D}}{\tilde{p}_{f_0,D}}(X_0^D) \right)^2 \mathbf{1}_{\mathcal{A}_{i,D}} \right] \\ & \lesssim D^{-d/2} (\log N)^2 N^{-C_2\mu} + N^{C_4\mu} \exp(-cD^{-1}), \end{aligned}$$

for large enough  $\mu > 0$  and constants uniform over  $\mathcal{C}_N$ . We have thus established that for any large enough but fixed  $\mu > 0$ ,

$$\begin{aligned} \text{Var}_{f_0}(\Lambda_D^N) & \lesssim \text{Var}_{f_0} \left( \int_{\mathcal{C}_N} \sum_{i=1}^N \log \frac{\tilde{p}_{f,D}}{\tilde{p}_{f_0,D}}(X_i^D) \mathbf{1}_{\mathcal{A}_{i,D}} \nu(df) \right) \\ & \quad + D^{-d/2} (\log N)^2 N^{-C_2\mu} + N^{C_4\mu} \exp(-cD^{-1}). \end{aligned}$$

*Step 3: Approximating  $\tilde{p}_{f,D}$  by a Gaussian transition density in small-time.* We approximate  $\tilde{p}_{f,D}$  by the transition density of the corresponding Euler scheme  $N_d(x, 2Df(x)I_d)$  without drift, namely

$$(31) \quad q_{f,D}(x, y) = \frac{1}{(4\pi Df(x))^{d/2}} \exp\left(-\frac{|y-x|^2}{4Df(x)}\right).$$

Note that while  $q_{f,D}$  is defined on  $\mathbb{R}^d \times \mathbb{R}^d$ , it will be evaluated at  $X_i^D$  which lies in  $\mathcal{O} \times \mathcal{O}$ ,  $\mathbb{P}_{f_0}$ -almost surely. Define

$$\Lambda_{q,D}^N = \int_{\mathcal{C}_N} \sum_{i=1}^N \log \frac{q_{f,D}}{q_{f_0,D}}(X_i^D) \mathbf{1}_{\mathcal{A}_{i,D}} \nu(df),$$

again writing  $X_i^D = (X_{(i-1)D}, X_{iD})$ . The key estimate to prove Theorem 8 is the following result, which quantifies this approximation.

**Proposition 14.** *For  $f_0 \in \mathcal{F}_0$  and any probability measure  $\nu$  supported on  $\mathcal{C}_N$  as in (15), it holds that*

$$\begin{aligned} & \text{Var}_{f_0} \left( \int_{\mathcal{C}_N} \sum_{i=1}^N \log \frac{\tilde{p}_{f,D}}{\tilde{p}_{f_0,D}}(X_i^D) \mathbf{1}_{\mathcal{A}_{i,D}} \nu(df) \right) \\ & \lesssim \text{Var}_{f_0}(\Lambda_{q,D}^N) + N^2 \varepsilon_N^2 D^2 + N \varepsilon_{1,N}^2 (D + ND^2) + N^2 \varepsilon_{2,N}^2 D^2 + N^2 \varepsilon_{3,N}^2 D^3 + N^2 D^4 \\ & \quad + N^2 \varepsilon_{1,N}^2 D \exp(-cD^{-1}), \end{aligned}$$

where the constants are uniform over  $(\mathcal{O}, d, f_{\min}, r, \delta)$ .

The proof of Proposition 14 relies on second-order small time expansions of the heat-kernel and is deferred to Section 5.2.

*Step 4: Variance of the proxy log-likelihood.* It remains to control the final variance term in the RHS of the last estimate. It involves the proxy density  $q_{f,D}$  but is evaluated at the points of the original diffusion  $X$  given by (1) with reflection at the boundary.

**Proposition 15.** *For  $f_0 \in \mathcal{F}$  and any probability measure  $\nu$  supported on  $\mathcal{C}_N$  as in (15), it holds that*

$$\text{Var}_{f_0}(\Lambda_{q,D}^N) \lesssim N \varepsilon_N^2 (1 + D + ND^2 + D^{-1} \varepsilon_N^2 + N e^{-C'_{f_0} D^{-1}}),$$

where the constants are uniform over  $(\mathcal{O}, d, f_{\min}, r, \delta)$ .

The proof of Proposition 15 is given in Section 5.3 and relies on martingale arguments, which are key to dealing with the dependence structure of the Markov chain. Combining the bounds from Steps 1-4 and keeping track of the leading order terms establishes the desired variance bound for  $\Lambda_D^N$  in Theorem 8.

**4.2. Proof of the expectation bound of Theorem 8.** The proof follows along similar, though easier, lines as the variance bound. The expectation bounds will be proved uniformly over  $f \in \mathcal{C}_N$ , which will sometimes be implied without explicit reference.

*Step 1: Restricting observations away from the boundary.* Applying Lemma 12 above with  $k = 1$  gives

$$\begin{aligned} \mathbb{E}_{f_0} \left[ \log \frac{p_{f_0,D}}{p_{f,D}}(X_0^D) \right] &\leq \mathbb{E}_{f_0} \left[ \log \frac{p_{f_0,D}}{p_{f,D}}(X_0^D) \mathbf{1}_{\mathcal{A}_{1,D}} \right] \\ &\quad + C_1 D^{-d/2} (\log N) N^{-C_2 \mu} + C_3 N^{C_4 \mu} \exp(-cD^{-1}) \end{aligned}$$

for large enough  $\mu > 0$ , and where the constants  $C_1 - C_4, c > 0$  are uniform over  $\mathcal{C}_N$ .

*Step 2: Local approximation by an unbounded diffusion model on  $\mathbb{R}^d$ .* Let  $\tilde{p}_{f,D} : \mathbb{R}^d \times \mathbb{R}^d \rightarrow [0, \infty)$  denote the transition density defined in (29) above, corresponding to the unbounded diffusion model over the whole space  $\mathbb{R}^d$ . Consider  $\mathbb{E}_{f_0}$ -expectation of the integrands in (minus) the decomposition (30). Using Lemma 13 above with  $k = 1$  and large enough  $\gamma > 0$ , the  $\mathbb{E}_{f_0}$ -expectation of (minus) the integrand in the second term in (30) is bounded above by

$$\sup_{f \in \mathcal{C}_N} \mathbb{E}_{f_0} \left[ \log \frac{\tilde{p}_{f,D}}{p_{f,D}}(X_0^D) \mathbf{1}_{\mathcal{A}_{1,D}} \right] \lesssim D^{-d/2} (\log N) N^{-C_2 \mu} + N^{C_4 \mu} \exp(-cD^{-1}),$$

for large enough  $\mu > 0$ . Arguing in the same way, an identical bound also holds for the  $\mathbb{E}_{f_0}$ -expectation of the integrand of minus the third term in (30). Therefore,

$$\begin{aligned} \mathbb{E}_{f_0} \left[ \log \frac{p_{f_0,D}}{p_{f,D}}(X_0^D) \mathbf{1}_{\mathcal{A}_{1,D}} \right] &\lesssim \mathbb{E}_{f_0} \left[ \log \frac{\tilde{p}_{f_0,D}}{\tilde{p}_{f,D}}(X_0^D) \mathbf{1}_{\mathcal{A}_{1,D}} \right] \\ &\quad + D^{-d/2} (\log N) N^{-C_2 \mu} + N^{C_4 \mu} \exp(-cD^{-1}). \end{aligned}$$

*Step 3: Approximating  $\tilde{p}_{f,D}$  by a Gaussian transition density in small-time.* Recalling the definition (31) of the proxy density  $q_{f,D}$  from above, we now approximate the expected log-likelihood. The proof of the following proposition is deferred to Section 5.2.

**Proposition 16.** *For  $f_0 \in \mathcal{F}_0$  and any probability measure  $\nu$  supported on  $\mathcal{C}_N$  as in (15), it holds that*

$$\begin{aligned} &\sup_{f \in \mathcal{C}_N} \mathbb{E}_{f_0} \left[ \log \frac{\tilde{p}_{f_0,D}}{\tilde{p}_{f,D}}(X_0^D) \mathbf{1}_{\mathcal{A}_{1,D}} \right] \\ &\lesssim \sup_{f \in \mathcal{C}_N} \mathbb{E}_{f_0} \left[ \log \frac{q_{f_0,D}}{q_{f,D}}(X_0^D) \mathbf{1}_{\mathcal{A}_{1,D}} \right] \\ &\quad + \varepsilon_N^2 \left( \frac{D}{\varepsilon_N} + \frac{D^2}{\varepsilon_N^2} + \frac{\varepsilon_{1,N}}{\varepsilon_N^2} D + \frac{\varepsilon_{2,N}}{\varepsilon_N^2} D + \frac{\varepsilon_{3,N}}{\varepsilon_N^2} D^{3/2} + \frac{\varepsilon_{1,N}}{\varepsilon_N^2} D^{1/2} \exp(-cD^{-1}) \right), \end{aligned}$$

where the constants are uniform over  $(\mathcal{O}, d, f_{\min}, r, \delta)$ .

*Step 4: Expectation of the proxy log-likelihood.* It finally remains to control the remaining expectation in Proposition 16 involving the proxy density  $q_{f,D}$ . The proof of the following estimate can be found in Section 5.3.

**Proposition 17.** For  $f_0 \in \mathcal{F}$  and any probability measure  $\nu$  supported on  $\mathcal{C}_N$  as in (15), it holds that

$$\sup_{f \in \mathcal{C}_N} \mathbb{E}_{f_0} \left[ \log \frac{q_{f_0, D}}{q_{f, D}}(X_0^D \mathbf{1}_{\mathcal{A}_{1, D}}) \right] \lesssim \varepsilon_N^2 + \varepsilon_N D + \varepsilon_N D^{1/2} \exp(-cD^{-1}),$$

where the constants are uniform over  $(\mathcal{O}, d, f_{\min}, r, \delta)$

Combining the bounds from Steps 1-4 and keeping track of the leading order terms establishes the expectation bound for  $\Lambda_D^N$ .

It remains to show the evidence lower bound (17). By Jensen's inequality, the desired probability in (17) is upper bounded by

$$\mathbb{P}_{f_0} \left( \int_{\mathcal{C}_N} \sum_{i=1}^N \log \frac{p_{f, D}(X_{(i-1)D}, X_{iD})}{p_{f_0, D}(X_{(i-1)D}, X_{iD})} \nu(df) \leq -cN\varepsilon_N^2 - NE_N \right).$$

Using the expectation bound just derived, the  $\mathbb{E}_{f_0}$ -expectation of the left-hand side is lower bounded by  $-NE_N$ . Using Chebychev's inequality and the variance bound just derived, the last probability is then bounded by

$$\begin{aligned} & \mathbb{P}_{f_0} \left( \int_{\mathcal{C}_N} \sum_{i=1}^N \left( \log \frac{p_{f, D}(X_{(i-1)D}, X_{iD})}{p_{f_0, D}(X_{(i-1)D}, X_{iD})} - \mathbb{E}_{f_0} \left[ \log \frac{p_{f, D}(X_{(i-1)D}, X_{iD})}{p_{f_0, D}(X_{(i-1)D}, X_{iD})} \right] \right) \nu(df) \leq -cN\varepsilon_N^2 \right) \\ & \leq \frac{1}{c^2 N^2 \varepsilon_N^4} \text{Var}_{f_0} \left( \int_{\mathcal{C}_N} \sum_{i=1}^N \log \frac{p_{f, D}(X_{(i-1)D}, X_{iD})}{p_{f_0, D}(X_{(i-1)D}, X_{iD})} \nu(df) \right) \leq \frac{V_N}{c^2 N^2 \varepsilon_N^4}, \end{aligned}$$

which completes the proof of Theorem 8.

## 5. REMAINING PROOFS FOR THEOREM 8

**5.1. Preliminary estimates.** We first gather some technical bounds. Although classical, the stochastic expansions we need require extra care due to the presence of a boundary. We start with a standard variance estimate.

**Lemma 18.** For any real-valued function  $\varphi$ ,

$$\text{Var}_{f_0} \left( \sum_{i=1}^N \varphi(X_{(i-1)D}) \right) \leq C_{f_0} N D^{-1} \text{Var}_{f_0}(\varphi(X_0)),$$

where  $C_{f_0} \leq 2/r < \infty$  with  $r = r(f_{\min}, \mathcal{O})$ .

*Proof.* Since  $(X_0, X_D, \dots, X_{ND})$  is a stationary reversible Markov chain whose spectral gap is lower bounded by  $rD$  by (9), the result follows from Theorem 3.1 in [44].  $\square$

We next need a moment bound for the increments of the diffusion.

**Lemma 19.** For every  $\tau \geq 0$  and  $p \geq 1$ , we have

$$(32) \quad \mathbb{E}_f \left[ \sup_{s \leq u \leq t} |X_u - X_s|^p \mid \mathcal{F}_s \right] \leq 2^{p-1} (\|f\|_{\mathcal{C}^1}^p (t-s)^p + c_*^{p/2} d^{p/2} p^{p/2} \|f\|_{\infty}^p (t-s)^{p/2}),$$

where  $c_*$  is a universal constant (arising in the Burkholder-Davis-Gundy inequality).

The proof is classical (see for instance Lions and Sznitman [37]) and is given in Appendix 9.3. Let

$$(33) \quad \tau_{i, D} = \inf\{t \geq 0, X_{t+(i-1)D} \in \partial\mathcal{O}\}$$

denote the hitting time of the boundary by the process  $X$  started at  $X_{(i-1)D}$ .

**Lemma 20.** Let  $f_0 \in \mathcal{F}' = \{f \in \mathcal{F} : \|f\|_{e^\alpha} \leq r\}$  for  $\alpha = \alpha_d$  as in (7). Then

$$\mathbb{P}_{f_0}(\tau_{i,D} \geq D, \mathcal{A}_{i,D}) \lesssim \exp(-cD^{-1}),$$

where the constants are uniform over  $(r, \delta)$ .

The proof is given in Appendix 9.4. We will repeatedly use the decomposition

$$(34) \quad X_{iD} - X_{(i-1)D} = b_{i,D} + \Sigma_{i,D} + L_{i,D},$$

with

$$b_{i,D} = \int_{(i-1)D}^{iD} \nabla f_0(X_s) ds, \quad \Sigma_{i,D} = \int_{(i-1)D}^{iD} \sqrt{2f_0(X_s)} dB_s, \quad L_{i,D} = \int_{(i-1)D}^{iD} n(X_s) d|\ell|_s,$$

together with the following bounds, for every  $p \geq 1$ ,

$$(35) \quad |b_{i,D}| \lesssim D, \quad \mathbb{E}_{f_0} [|\Sigma_{i,D}|^p | \mathcal{F}_{(i-1)D}] \lesssim D^{p/2}, \quad \mathbb{E}_{f_0} [|L_{i,D}|^p \mathbf{1}_{\mathcal{A}_{i,D}}] \lesssim D^{p/2} \exp(-cD^{-1}),$$

which depend only on  $\|f_0\|_{e^1}$ . The first bound is obvious, the second one stems from the Burckholder-Davis-Gundy inequality. For the third one, we rely on the following facts: first, writing  $L_{i,D} = (X_{iD} - X_{(i-1)D}) - b_{i,D} - \Sigma_{i,D}$  and using the first two bounds of (35) together with Lemma 19, we have

$$\mathbb{E}_{f_0} [|L_{i,D}|^p] \lesssim D^{p/2}.$$

Second, on  $\mathcal{A}_{i,D} \cap \{\tau_{i,D} \geq iD\}$ , we have  $L_{i,D} = 0$ . Thus, by Cauchy-Schwarz's inequality,

$$\mathbb{E}_{f_0} [|L_{i,D}|^p \mathbf{1}_{\mathcal{A}_{i,D}}] \lesssim D^{p/2} \mathbb{P}_{f_0}(\tau_{i,D} \geq D, \mathcal{A}_{i,D})^{1/2}$$

and the third estimate in (35) then follows from Lemma 20.

**5.2. Proofs of Propositions 14 and 16: approximating transition densities in small-time.** This section is devoted to the approximation of small-time transition densities for diffusions in  $\mathbb{R}^d$ . We use some Riemannian geometry to derive second-order small-time expansions of the heat kernel, following results that date back to Azencott [6]. Recall that

$$\tilde{p}_{f,D}, q_{f,D} : \mathbb{R}^d \times \mathbb{R}^d \rightarrow [0, \infty)$$

denote, respectively, (a smooth version of) the transition density of  $(\tilde{X}_t)_{t \geq 0}$  defined in (28), and the proxy transition density of an Euler scheme without drift defined in (31). The next result gives an expansion of the log-likelihood ratio of the transition densities, uniformly over the domain  $\mathcal{O}$ .

**Lemma 21.** There exist smooth functions:  $\gamma_{f,f_0} : \mathcal{O} \rightarrow \mathbb{R}^d$  with

$$\text{supp}(\gamma_{f_0,f}) \subset \mathcal{O}_0, \quad \|\gamma_{f_0,f}\|_\infty \lesssim \|f - f_0\|_{e^1},$$

where the constants in the inequality depend only on an upper bound for  $\|f\|_{e^1}$  and  $\|f_0\|_{e^1}$ , and such that the following expansion holds:

$$\begin{aligned} \log \frac{\tilde{p}_{f_0,D}(x,y)}{\tilde{p}_{f,D}(x,y)} \mathbf{1}_{\{x \in \mathcal{O}_0^\delta\}} &= \log \frac{q_{f_0,D}(x,y)}{q_{f,D}(x,y)} \mathbf{1}_{\{x \in \mathcal{O}_0^\delta\}} \\ &+ \gamma_{f_0,f}(x) \cdot (y-x) + \frac{1}{8D} |y-x|^2 \nabla(f^{-1} - f_0^{-1})(x) \cdot (y-x) \mathbf{1}_{\{x \in \mathcal{O}_0^\delta\}} \\ &+ (\|f - f_0\|_\infty D + \|f - f_0\|_{e^1} |y-x| D + |y-x|^2 D + \|f - f_0\|_{e^2} |y-x|^2 \\ &+ \|f - f_0\|_{e^3} |y-x|^3 + |y-x|^4) r_{f_0,f}(x,y), \end{aligned}$$

for a remainder term  $r_{f_0,f} : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$  satisfying

$$(36) \quad \sup_{\|f\|_{e^4} + \|f_0\|_{e^4} \leq r} \|r_{f_0,f}\|_\infty < \infty$$

for every  $r > 0$ .

While only local to  $(x, y) \in \mathcal{O} \times \mathcal{O}$ , the stability property (36) is sufficient for our purpose: the approximation is only needed for  $(x, y) = (X_{(i-1)D}, X_{iD}) \in \mathcal{O} \times \mathcal{O}$ , a property that holds  $\mathbb{P}_{f_0}$ -almost surely. The proof of Lemma 21 is deferred to Appendix 8.4.

*Proof of Proposition 14.* We apply Lemma 21, establishing suitable bounds for the remainder terms.

*Step 1:* Consider first the term  $\sum_{i=1}^N \gamma_{f_0, f}(X_{(i-1)D}) \cdot (X_{iD} - X_{(i-1)D})$  in the remainder of Lemma 21. It splits into three parts thanks to the decomposition (34) and we bound each term separately. The drift term involving  $b_{i,D}$  is of order  $D$  by (35), hence the property  $\|\gamma_{f_0, f}\|_\infty \lesssim \varepsilon_{1,N}$  yields the crude variance bound  $N^2 \varepsilon_{1,N}^2 D^2$  for the first term. For the martingale term, we have

$$\text{Var}_{f_0} \left( \sum_{i=1}^N \gamma_{f_0, f}(X_{(i-1)D}) \cdot \Sigma_{i,D} \right) \leq \sum_{i=1}^N \|\gamma_{f_0, f}\|_\infty^2 \mathbb{E}_{f_0} [|\Sigma_{i,D}|^2] \lesssim N \varepsilon_{1,N}^2 D$$

by the second estimate in (35). For the third term involving  $L_{i,D}$ , using that  $\gamma_{f_0, f}(X_{(i-1)D})$  vanishes on  $(\mathcal{A}_{i,D})^c$ , we have

$$\text{Var}_{f_0} \left( \sum_{i=1}^N \gamma_{f_0, f}(X_{(i-1)D}) \cdot L_{i,D} \right) \lesssim N \sum_{i=1}^N \|\gamma_{f_0, f}\|_\infty^2 \mathbb{E}_{f_0} [L_{i,D}^2 \mathbf{1}_{\mathcal{A}_{i,D}}] \lesssim N^2 \varepsilon_{1,N}^2 D \exp(-cD^{-1})$$

by the third estimate in (35). We have thus established

$$(37) \quad \text{Var}_{f_0} \left( \sum_{i=1}^N \gamma_{f_0, f}(X_{(i-1)D}) \cdot (X_{iD} - X_{(i-1)D}) \right) \lesssim N \varepsilon_N^2 \left( \frac{\varepsilon_{1,N}}{\varepsilon_N} \right)^2 (D + ND^2 + ND \exp(-cD^{-1})).$$

*Step 2:* We next consider the term  $\frac{1}{8D} \sum_{i=1}^N |X_{iD} - X_{(i-1)D}|^2 \zeta_{f_0, f}(X_{(i-1)D}) \cdot (X_{iD} - X_{(i-1)D}) \mathbf{1}_{\mathcal{A}_{i,D}}$ , where  $\zeta_{f_0, f} = \nabla(f^{-1} - f_0^{-1})$  satisfies  $\|\zeta_{f_0, f}\|_\infty \lesssim \varepsilon_{1,N}$  for  $f, f_0 \in \mathcal{F}'$ . Using Itô's formula, it splits into four parts according to the decomposition

$$(38) \quad |X_{iD} - X_{(i-1)D}|^2 = 2d f_0(X_{(i-1)D})D + \tilde{b}_{i,D} + \tilde{\Sigma}_{i,D} + \tilde{L}_{i,D},$$

with

$$(39) \quad \begin{aligned} \tilde{b}_{i,D} &= 2 \int_{(i-1)D}^{iD} (d(f_0(X_s) - f_0(X_{(i-1)D})) + (X_s - X_{(i-1)D}) \cdot \nabla f_0(X_s)) ds, \\ \tilde{\Sigma}_{i,D} &= 2 \int_{(i-1)D}^{iD} \sqrt{2f_0(X_s)} (X_s - X_{(i-1)D}) \cdot dB_s, \\ \tilde{L}_{i,D} &= 2 \int_{(i-1)D}^{iD} (X_s - X_{(i-1)D}) \cdot n(X_s) d|\ell|_s, \end{aligned}$$

appended with the moment estimates

$$(40) \quad \mathbb{E}_{f_0} [|\tilde{b}_{i,D}|^p] \lesssim D^{3p/2}, \quad \mathbb{E}_{f_0} [|\tilde{\Sigma}_{i,D}|^p | \mathcal{F}_{(i-1)D}] \lesssim D^p, \quad \mathbb{E}_{f_0} [|\tilde{L}_{i,D}|^p \mathbf{1}_{\mathcal{A}_{i,D}}] \lesssim D^p \exp(-cD^{-1}),$$

as for (35). More precisely,

$$\begin{aligned}\mathbb{E}_{f_0} [|\tilde{b}_{i,D}|^p] &\leq D^{p-1} \int_{(i-1)D}^{iD} \mathbb{E}_{f_0} [ |d(f_0(X_s) - f_0(X_{(i-1)D})) + (X_s - X_{(i-1)D}) \cdot \nabla f_0(X_s)|^p ] ds \\ &\leq D^p (d+1)^p \|f_0\|_{\mathcal{C}^1}^p \mathbb{E}_{f_0} \left[ \sup_{(i-1)D \leq s \leq iD} |X_s - X_{(i-1)D}|^p \right] \\ &\leq (d+1)^p \|f_0\|_{\mathcal{C}^1}^p C_{p,d,f_0} D^{3p/2}\end{aligned}$$

by Jensen's inequality and Lemma 19, with  $C_{p,f_0}$  the constant in (32). For the martingale part, the Burkholder-Davies-Gundy inequality with constant  $C_p$  yields

$$\begin{aligned}\mathbb{E}_{f_0} [|\tilde{\Sigma}_{i,D}|^p | \mathcal{F}_{(i-1)D}] &\leq C_p 2^{3p/2} \mathbb{E}_{f_0} \left[ \left( \int_{(i-1)D}^{iD} 2f_0(X_s)^{3/2} |X_s - X_{(i-1)D}|^2 ds \right)^{p/2} | \mathcal{F}_{(i-1)D} \right] \\ &\leq C_p 2^{2p} \|f_0\|_{\infty}^{3p/4} \mathbb{E}_{f_0} \left[ \sup_{(i-1)D \leq s \leq iD} |X_s - X_{(i-1)D}|^p \right] \\ &\leq C_p 2^{2p} \|f_0\|_{\infty}^{3p/4} C_{p,d,f_0} D^p,\end{aligned}$$

where we last used Lemma 19. The last bound in (40) follows exactly the same lines as the last estimate in (35), using now the bounds just established for  $\tilde{b}_{i,D}$  and  $\tilde{\Sigma}_{i,D}$  instead of those for  $b_{i,D}$  and  $\Sigma_{i,D}$ , respectively.

We are now ready to handle the term  $\sum_{i=1}^N \frac{d}{4} f_0(X_{(i-1)D}) \mathbf{1}_{\mathcal{A}_{i,D}} \zeta_{f_0,f}(X_{(i-1)D}) \cdot (X_{iD} - X_{(i-1)D})$ , exactly as in Step 1, substituting  $\zeta_{f_0,f}(X_{(i-1)D})$  by  $\frac{d}{4} f_0(X_{(i-1)D}) \zeta_{f_0,f}(X_{(i-1)D}) \mathbf{1}_{\mathcal{A}_{i,D}}$ . It has the same variance order as in (37). For the term involving the drift part  $\tilde{b}_{i,D}$  we have

$$\begin{aligned}\text{Var}_{f_0} \left( \frac{1}{8D} \sum_{i=1}^N \tilde{b}_{i,D} \zeta_{f_0,f}(X_{(i-1)D}) \cdot (X_{iD} - X_{(i-1)D}) \mathbf{1}_{\mathcal{A}_{i,D}} \right) \\ \lesssim D^{-2} N \sum_{i=1}^N \|\zeta_{f_0,f}\|_{\infty}^2 \mathbb{E}_{f_0} \left[ \tilde{b}_{i,D}^2 |X_{iD} - X_{(i-1)D}|^2 \right].\end{aligned}$$

and this yields the order  $D^{-2} N^2 \varepsilon_{1,N}^2 D^4 = N \varepsilon_N^2 \left( \frac{\varepsilon_{1,N}^2}{\varepsilon_N^2} N D^2 \right)$  by Cauchy-Schwarz's inequality combined with (40) and Lemma 19 for controlling the term within the expectation. For the third term, we use the decomposition

$$\tilde{\Sigma}_{i,D} \zeta_{f_0,f}(X_{(i-1)D}) \cdot (X_{iD} - X_{(i-1)D}) \mathbf{1}_{\mathcal{A}_{i,D}} = I + II + III,$$

with

$$\begin{aligned}I &= \tilde{\Sigma}_{i,D} \zeta_{f_0,f}(X_{(i-1)D}) \cdot b_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}}, \\ II &= \tilde{\Sigma}_{i,D} \zeta_{f_0,f}(X_{(i-1)D}) \cdot \Sigma_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}}, \\ III &= \tilde{\Sigma}_{i,D} \zeta_{f_0,f}(X_{(i-1)D}) \cdot L_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}}.\end{aligned}$$

For term  $I$ ,

$$\text{Var}_{f_0} \left( \frac{1}{8D} \sum_{i=1}^N \tilde{\Sigma}_{i,D} \zeta_{f_0,f}(X_{(i-1)D}) \cdot b_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}} \right) \lesssim D^{-2} N \sum_{i=1}^N \|\zeta_{f_0,f}\|_{\infty}^2 \mathbb{E}_{f_0} [|\tilde{\Sigma}_{i,D}|^2 |b_{i,D}|^2]$$

and this yields the order  $D^{-2}N^2\varepsilon_{1,N}^2D^4$  by Cauchy-Schwarz's inequality combined with (40) and Lemma 19 again. For term  $II$ , by Itô's formula,

$$(41) \quad \begin{aligned} \tilde{\Sigma}_{i,D}\zeta_{f_0,f}(X_{(i-1)D}) \cdot \Sigma_{i,D} &= \zeta_{f_0,f}(X_{(i-1)D}) \cdot M_{i,D} \\ &+ 2\zeta_{f_0,f}(X_{(i-1)D}) \cdot \int_{(i-1)D}^{iD} (X_s - X_{(i-1)D})f_0(X_s)ds, \end{aligned}$$

where  $M_{i,D} = \int_{(i-1)D}^{iD} \sqrt{2f_0(X_s)}(\mathbb{E}_{f_0}[\tilde{\Sigma}_{i,D}|\mathcal{F}_s] + 2\mathbb{E}_{f_0}[\Sigma_{i,D}|\mathcal{F}_s] \cdot (X_s - X_{(i-1)D}))dB_s$  is a martingale increment such that

$$\mathbb{E}_{f_0} [|\zeta_{f_0,f}(X_{(i-1)D}) \cdot M_{i,D}|^2] \lesssim \varepsilon_{1,N}^2D^3,$$

by applying repeatedly Cauchy-Schwarz's inequality together with (35), (40) and Lemma 19, hence

$$\text{Var}_{f_0} \left( \frac{1}{8D} \sum_{i=1}^N \zeta_{f_0,f}(X_{(i-1)D}) \cdot M_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}} \right) = \frac{1}{64D^2} \sum_{i=1}^N \mathbb{E}_{f_0} [|\zeta_{f_0,f}(X_{(i-1)D}) \cdot M_{i,D}|^2 \mathbf{1}_{\mathcal{A}_{i,D}}]$$

and this term is of order  $D^{-2}N\varepsilon_{1,N}^2D^3 = N\varepsilon_N^2(\frac{\varepsilon_{1,N}}{\varepsilon_N})^2D$ . Let  $G(x, y) = \zeta_{f_0,f}(x) \cdot (y - x)f_0(y)$ . For the second term in (41), by Itô's formula,

$$\int_{(i-1)D}^{iD} \zeta_{f_0,f}(X_{(i-1)D}) \cdot (X_s - X_{(i-1)D})f_0(X_s)ds = \bar{b}_{i,D}(G) + \bar{\Sigma}_{i,D}(G) + \bar{L}_{i,D}(G),$$

with

$$(42) \quad \begin{aligned} \bar{b}_{i,D}(G) &= \int_{(i-1)D}^{iD} \int_{(i-1)D}^s \mathcal{L}_{f_0}G(X_{(i-1)D}, X_u)duds, \\ \bar{\Sigma}_{i,D}(G) &= \int_{(i-1)D}^{iD} \int_{(i-1)D}^s \nabla G(X_{(i-1)D}, X_u)\sqrt{2f_0(X_u)} \cdot dB_u ds, \\ \bar{L}_{i,D}(G) &= 2 \int_{(i-1)D}^{iD} \int_{(i-1)D}^s \nabla G(X_{(i-1)D}, X_u) \cdot n(X_u)d|\ell|_u ds. \end{aligned}$$

In notation, the differential operators act on  $y \mapsto G(X_{(i-1)D}, y)$  and  $\mathcal{L}_{f_0}$  is the generator associated to the diffusion defined in (8). The expansion is appended with the moment estimates

$$\begin{aligned} \mathbb{E}_{f_0} [|\bar{b}_{i,D}(G)|^p] &\lesssim \varepsilon_{1,N}^p D^{2p}, \quad \mathbb{E}_{f_0} [|\bar{\Sigma}_{i,D}(G)|^p | \mathcal{F}_{(i-1)D}] \lesssim \varepsilon_{1,N}^p D^{3p/2}, \\ \mathbb{E}_{f_0} [|\bar{L}_{i,D}(G)|^p \mathbf{1}_{\mathcal{A}_{i,D}}] &\lesssim \varepsilon_{1,N}^p D^{3p/2} \exp(-cD^{-1}), \end{aligned}$$

in the same way as before. The variance of the term  $(4D)^{-1} \sum_{i=1}^N \bar{b}_{i,D}(G) \mathbf{1}_{\mathcal{A}_{i,D}}$  is of order  $D^{-2}N^2\varepsilon_{1,N}^2D^4$ . Also, the  $\bar{\Sigma}_{i,D}(G)$  are centred  $\mathcal{F}_{iD}$ -increments hence

$$\text{Var}_{f_0} \left( \frac{1}{4D} \sum_{i=1}^N \bar{\Sigma}_{i,D}(G) \mathbf{1}_{\mathcal{A}_{i,D}} \right) = \frac{1}{16D^2} \sum_{i=1}^N \mathbb{E}_{f_0} [(\bar{\Sigma}_{i,D}(G))^2 \mathbf{1}_{\mathcal{A}_{i,D}}] \lesssim D^{-2}N\varepsilon_{1,N}^2D^3$$

and this term is of order  $N\varepsilon_N^2(\frac{\varepsilon_{1,N}}{\varepsilon_N})^2D$ . The variance of the term  $(4D)^{-1} \sum_{i=1}^N \bar{L}_{i,D}(G) \mathbf{1}_{\mathcal{A}_{i,D}}$  is of order  $D^{-2}N^2\varepsilon_{1,N}^2D^3 \exp(-cD^{-1})$ , and the term  $II$  is controlled. For the term  $III$ , we simply have

$$\text{Var}_{f_0} \left( \frac{1}{8D} \sum_{i=1}^N \tilde{\Sigma}_{i,D}\zeta_{f_0,f}(X_{(i-1)D}) \cdot L_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}} \right) \lesssim D^{-2}N \sum_{i=1}^N \varepsilon_{1,N}^2 \mathbb{E}_{f_0} [|\tilde{\Sigma}_{i,D}|^2 |L_{i,D}|^2 \mathbf{1}_{\mathcal{A}_{i,D}}]$$

that yields the order  $N^2 \varepsilon_{1,N}^2 D^2 \exp(-cD^{-1})$ . Gathering all these estimates, we obtain that the variance of  $\frac{1}{8D} \sum_{i=1}^N |X_{iD} - X_{(i-1)D}|^2 \zeta_{f_0,f}(X_{(i-1)D}) \cdot (X_{iD} - X_{(i-1)D}) \mathbf{1}_{\mathcal{A}_{i,D}}$  is no bigger than the order established in (37).

*Step 3:* We finally control the remainder term in the expansion of Lemma 21. Define

$$\begin{aligned} \mathcal{R}_{f_0,f}^N = & \sum_{i=1}^N \left( \|f - f_0\|_{\infty} D + \|f - f_0\|_{e^1} |X_{iD} - X_{(i-1)D}| D + |X_{iD} - X_{(i-1)D}|^2 D \right. \\ & + \|f - f_0\|_{e^2} |X_{iD} - X_{(i-1)D}|^2 + \|f - f_0\|_{e^3} |X_{iD} - X_{(i-1)D}|^3 \\ & \left. + |X_{iD} - X_{(i-1)D}|^4 \right) r_{f_0,f}(X_{(i-1)D}, X_{iD}). \end{aligned}$$

By Lemma 19, the property  $f \in \mathcal{C}_N$  and the fact that  $\|r_{f_0,f}\|_{\infty} \lesssim 1$ , we readily have

$$\begin{aligned} \text{Var}_{f_0}(\mathcal{R}_{f_0,f}^N) & \lesssim N^2 (\varepsilon_N^2 D^2 + \varepsilon_{1,N}^2 D^3 + D^4 + \varepsilon_{2,N}^2 D^2 + \varepsilon_{3,N}^2 D^3 + D^4) \\ & \lesssim N \varepsilon_N^2 (ND^2 + (\frac{\varepsilon_{1,N}}{\varepsilon_N})^2 ND^3 + (\frac{\varepsilon_{2,N}}{\varepsilon_N})^2 ND^2 + (\frac{\varepsilon_{3,N}}{\varepsilon_N})^2 ND^3 + N \varepsilon_N^{-2} D^4). \end{aligned}$$

*Step 4:* Putting together the estimates established in Steps 1-3, using Lemma 21 and (27), the quantity in Proposition 14 is bounded by a multiple of

$$\begin{aligned} & \text{Var}_{f_0}(\Lambda_{q,D}^N) + \text{Var}_{f_0} \left( \int_{\mathcal{C}_N} \sum_{i=1}^N \left[ \log \frac{\tilde{p}_{f,D}(X_i^D)}{\tilde{p}_{f_0,D}(X_i^D)} - \frac{q_{f,D}(X_i^D)}{q_{f_0,D}(X_i^D)} \right] \mathbf{1}_{\mathcal{A}_{i,D}} \nu(df) \right) \\ & \lesssim \text{Var}_{f_0}(\Lambda_{q,D}^N) + \sup_{f \in \mathcal{C}_N} \text{Var}_{f_0} \left( \sum_{i=1}^N \left[ \log \frac{\tilde{p}_{f,D}(X_i^D)}{\tilde{p}_{f_0,D}(X_i^D)} - \log \frac{q_{f,D}(X_i^D)}{q_{f_0,D}(X_i^D)} \right] \right) \\ & \lesssim \text{Var}_{f_0}(\Lambda_{q,D}^N) + N \varepsilon_N^2 \left( ND^2 + (\frac{\varepsilon_{1,N}}{\varepsilon_N})^2 (D + ND^2) + (\frac{\varepsilon_{2,N}}{\varepsilon_N})^2 ND^2 + (\frac{\varepsilon_{3,N}}{\varepsilon_N})^2 ND^3 \right. \\ & \quad \left. + N \varepsilon_N^{-2} D^4 + (\frac{\varepsilon_{1,N}}{\varepsilon_N})^2 ND \exp(-cD^{-1}) \right), \end{aligned}$$

as required.  $\square$

*Proof of Proposition 16.* The proof follows similar, though easier, lines to that of Proposition 14. We thus provide only a sketch of the main bounds, matching Steps 1-4 for convenience.

*Step 1:* Consider first the term  $\gamma_{f_0,f}(X_0) \cdot (X_D - X_0)$  in the expansion provided by Lemma 21, and where we can insert the term  $\mathbf{1}_{\mathcal{A}_{1,D}}$  due to the support of  $\gamma_{f_0,f}$ . In the decomposition (34), the term  $\gamma_{f_0,f}(X_0) \Sigma_{0,D}$  has  $\mathbb{E}_{f_0}$ -expectation zero and so does not contribute. It follows that

$$\mathbb{E}_{f_0} [\gamma_{f_0,f}(X_0) \cdot (X_D - X_0)] \leq \|\gamma_{f_0,f}\|_{\infty} (\mathbb{E}_{f_0}[|b_{0,D}|] + \mathbb{E}_{f_0}[L_{0,D} \mathbf{1}_{\mathcal{A}_{1,D}}]) \lesssim \varepsilon_{1,N} (D + D^{1/2} \exp(-cD^{-1})),$$

where we used the moment bounds (35).

*Step 2:* Write  $\zeta_{f_0,f} = \nabla(f^{-1} - f_0^{-1})$  as before. In a similar way to Step 2 of the proof of Proposition 14, we have the decompositions

$$\begin{aligned} \frac{1}{8D} |X_D - X_0|^2 \mathbf{1}_{\mathcal{A}_{1,D}} & = \frac{d}{4} f_0(X_0) + \frac{1}{8D} \tilde{b}_{1,D} \mathbf{1}_{\mathcal{A}_{1,D}} + \frac{1}{8D} \tilde{\Sigma}_{1,D} \mathbf{1}_{\mathcal{A}_{1,D}} + \frac{1}{8D} \tilde{L}_{1,D} \mathbf{1}_{\mathcal{A}_{1,D}} \\ \zeta_{f_0,f}(X_0) \cdot (X_D - X_0) & = \zeta_{f_0,f}(X_0) \cdot b_{1,D} + \zeta_{f_0,f}(X_0) \cdot \Sigma_{1,D} + \zeta_{f_0,f}(X_0) \cdot L_{1,D}, \end{aligned}$$

and note the term  $\mathbb{E}_{f_0} [\frac{1}{8D} |X_D - X_0|^2 \zeta_{f_0,f}(X_0) \cdot (X_D - X_0)]$  is the sum of all expectations of cross terms in the two expansions above. Using the bounds (35) and (40) and the martingale

property of  $\Sigma_{1,D}$  that ensures  $\mathbb{E}_{f_0} \left[ \frac{d}{4} f_0(X_0) \zeta_{f_0,f}(X_0) \cdot \Sigma_{1,D} \right] = 0$ , we see by Cauchy-Schwarz's inequality for instance that all the expectations of the cross terms are of order at most  $(D + D^{1/2} \exp(cD^{-1})) \|\zeta_{f_0,f}\|_\infty = \varepsilon_{1,N}(D + D^{1/2} \exp(-cD^{-1}))$ , except maybe for the term

$$\frac{1}{8D} \mathbb{E}_{f_0} \left[ \widetilde{\Sigma}_{1,D} \zeta_{f_0,f}(X_0) \cdot \Sigma_{1,D} \right].$$

By (41), this term exactly equals

$$\frac{1}{4D} \mathbb{E}_{f_0} \left[ \zeta_{f_0,f}(X_0) \cdot \int_0^D (X_s - X_0) f_0(X_s) ds \right] = \frac{1}{4D} \mathbb{E}_{f_0} \left[ \bar{b}_{1,D}(G) + \bar{L}_{1,D}(G) \right]$$

according to (42) with  $G(x, y) = \zeta_{f_0,f}(x) \cdot (y - x) f_0(y)$ , and this term finally has the right order since  $\mathbb{E}_{f_0} [|\bar{b}_{1,D}(G)|] \lesssim \varepsilon_{1,N} D^2$  and  $\mathbb{E}_{f_0} [|\bar{L}_{1,D}(G)| \mathbf{1}_{\mathcal{A}_{1,D}}] \lesssim \varepsilon_{1,N} D^{3/2} \exp(-cD^{-1})$ .

*Step 3:* With the notation in the proof of Proposition 14, Step 3, it suffices to bound  $\mathbb{E}_{f_0} [\mathcal{R}_{f_0,f}^1]$ . By Lemma 19, the property  $f \in \mathcal{C}_N$  and the fact that  $\|r_{f_0,f}\|_\infty \lesssim 1$  again, we readily obtain

$$\mathbb{E}_{f_0} [\mathcal{R}_{f_0,f}^1] \lesssim \varepsilon_N D + \varepsilon_{1,N} D^{3/2} + D^2 + \varepsilon_{2,N} D + \varepsilon_{3,N} D^{3/2} + D^2.$$

*Step 4:* Putting together the above bounds and keeping track of the leading order terms gives

$$\begin{aligned} & \sup_{f \in \mathcal{C}_N} \mathbb{E}_{f_0} \left[ \log \frac{\tilde{p}_{f_0,D}(X_0^D)}{\tilde{p}_{f,D}(X_0^D)} \mathbf{1}_{\mathcal{A}_{1,D}} \right] \\ & \lesssim \sup_{f \in \mathcal{C}_N} \mathbb{E}_{f_0} \left[ \log \frac{q_{f_0,D}(X_0^D)}{q_{f,D}(X_0^D)} \mathbf{1}_{\mathcal{A}_{1,D}} \right] \\ & \quad + \varepsilon_N^2 \left( \frac{D}{\varepsilon_N} + \frac{D^2}{\varepsilon_N^2} + \frac{\varepsilon_{1,N}}{\varepsilon_N^2} D^{1/2} + \frac{\varepsilon_{2,N}}{\varepsilon_N^2} D + \frac{\varepsilon_{3,N}}{\varepsilon_N^2} D^{3/2} + \frac{\varepsilon_{1,N}}{\varepsilon_N} D^{1/2} \exp(-cD^{-1}) \right), \end{aligned}$$

which completes the proof of Proposition 16.  $\square$

**5.3. Proofs of Propositions 15 and 17: expectation and variance of the log-likelihood with proxy density.** Recall that the proxy  $q_{f,D}$  of the transition density  $\tilde{p}_{f,D}$  is given by

$$q_{f,D}(x, y) = \frac{1}{(4\pi D f(x))^{d/2}} \exp\left(-\frac{|y-x|^2}{4D f(x)}\right),$$

which is the density function of a  $N_d(x, 2Df(x)I_d)$  distribution, formally obtained by taking an Euler scheme without drift. Note that while  $q_{f,D}$  is defined on  $\mathbb{R}^d \times \mathbb{R}^d$ , it will be evaluated at  $(X_{(i-1)D}, X_{iD})$ , which lies in  $\mathcal{O} \times \mathcal{O}$  almost surely.

*Proof of Proposition 15. Step 1:* We look for a simple expansion of the approximate log-likelihood with the proxy. Write

$$\begin{aligned} \log \frac{q_{f,D}(x, y)}{q_{f_0,D}(x, y)} &= \frac{d}{2} \log \frac{f_0(x)}{f(x)} - \frac{1}{4D} \left( \frac{1}{f(x)} - \frac{1}{f_0(x)} \right) |y-x|^2 \\ &= \frac{d}{2} \left( \log \frac{f_0(x)}{f(x)} - \left( \frac{1}{f_0(x)} - \frac{1}{f(x)} \right) \frac{|y-x|^2}{2dD} \right). \end{aligned}$$

Recall the expansion (38) in the proof of Proposition 14 that takes the form

$$|X_{iD} - X_{(i-1)D}|^2 = 2d f_0(X_{(i-1)D}) D + \tilde{b}_{i,D} + \tilde{\Sigma}_{i,D} + \tilde{L}_{i,D}$$

for appropriate drift, diffusion and boundary remainder terms  $\tilde{b}_{i,D}$ ,  $\tilde{\Sigma}_{i,D}$  and  $\tilde{L}_{i,D}$ , respectively. Therefore, setting  $\xi_{f_0,f} = \frac{1}{f} - \frac{1}{f_0}$ , we obtain

$$(43) \quad \begin{aligned} \frac{2}{d} \log \frac{q_{f,D}(X_i^D)}{q_{f_0,D}(X_i^D)} &= \log \frac{f_0(X_{(i-1)D})}{f(X_{(i-1)D})} - \left( \frac{f_0(X_{(i-1)D})}{f(X_{(i-1)D})} - 1 \right) \\ &+ \frac{1}{2dD} \xi_{f_0,f}(X_{(i-1)D}) (\tilde{b}_{i,D} + \tilde{\Sigma}_{i,D} + \tilde{L}_{i,D}). \end{aligned}$$

Since  $|\log \kappa - (\kappa - 1)| \leq C(\kappa - 1)^2$  in a neighbourhood of  $\kappa = 1$ , the property  $\|f - f_0\|_\infty \leq \varepsilon_N$  and  $f \geq f_{\min}$  ensures

$$\left\| \log \frac{f_0}{f} - \left( \frac{f_0}{f} - 1 \right) \right\|_\infty \lesssim \varepsilon_N^2.$$

By Lemma 18, this entails

$$\text{Var}_{f_0} \left( \sum_{i=1}^N \left( \log \frac{f_0(X_{(i-1)D})}{f(X_{(i-1)D})} - \left( \frac{f_0(X_{(i-1)D})}{f(X_{(i-1)D})} - 1 \right) \right) \mathbf{1}_{\mathcal{A}_{i,D}} \right) \lesssim ND^{-1} \varepsilon_N^4.$$

*Step 2:* We next consider the term  $\sum_{i=1}^N \frac{1}{2dD} \xi_{f_0,f}(X_{(i-1)D}) \tilde{b}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}}$  and proceed similarly to Step 2 in the proof of Proposition 14 above. Define  $\tilde{G}_{i,D}(x) = df_0(x) + \nabla f_0(X_{(i-1)D}) \cdot x$  and

$$\tilde{b}_{i,D} = \int_{(i-1)D}^{iD} (\tilde{G}_{i,D}(X_s) - \tilde{G}_{i,D}(X_{(i-1)D})) ds + r_{i,D},$$

where the remainder term

$$r_{i,D} = \int_{(i-1)D}^{iD} (X_s - X_{(i-1)D}) \cdot (\nabla f_0(X_s) - \nabla f_0(X_{(i-1)D})) ds$$

satisfies  $\mathbb{E}_{f_0} [|r_{i,D}|^p] \lesssim D^{2p}$  by Jensen's and Cauchy-Schwarz's inequality together with Lemma 19, using that  $\|f_0\|_{c^2} \lesssim 1$ . By Itô's formula and (42), we obtain

$$\int_{(i-1)D}^{iD} \tilde{G}_{i,D}(X_s) ds = \bar{b}_{i,D}(\tilde{G}) + \bar{\Sigma}_{i,D}(\tilde{G}) + \bar{L}_{i,D}(\tilde{G}),$$

where

$$\begin{aligned} \mathbb{E}_{f_0} [|\bar{b}_{i,D}(\tilde{G})|^p] &\lesssim D^{2p}, \quad \mathbb{E}_{f_0} [|\bar{\Sigma}_{i,D}(\tilde{G})|^p | \mathcal{F}_{(i-1)D}] \lesssim D^{3p/2}, \\ \mathbb{E}_{f_0} [|\bar{L}_{i,D}(\tilde{G})|^p \mathbf{1}_{\mathcal{A}_{i,D}}] &\lesssim D^{3p/2} \exp(-cD^{-1}) \end{aligned}$$

in the same way as before. Then, the variance of the term  $\sum_{i=1}^N \frac{1}{2dD} \xi_{f_0,f}(X_{(i-1)D}) (\bar{b}_{i,D}(\tilde{G}) + r_{i,D}) \mathbf{1}_{\mathcal{A}_{i,D}}$  is of order  $D^{-2} N^2 \varepsilon_N^2 D^4$ . Also, the  $\bar{\Sigma}_{i,D}(\tilde{G})$  are centred  $\mathcal{F}_{iD}$ -increments hence

$$\begin{aligned} \text{Var}_{f_0} \left( \frac{1}{2dD} \sum_{i=1}^N \xi_{f_0,f}(X_{(i-1)D}) \bar{\Sigma}_{i,D}(\tilde{G}) \mathbf{1}_{\mathcal{A}_{i,D}} \right) &= \frac{1}{4d^2 D^2} \sum_{i=1}^N \mathbb{E}_{f_0} [|\xi_{f_0,f}(X_{(i-1)D}) \bar{\Sigma}_{i,D}(\tilde{G})|^2 \mathbf{1}_{\mathcal{A}_{i,D}}] \\ &\lesssim D^{-2} N \varepsilon_N^2 D^3 \end{aligned}$$

and this term is of order  $N \varepsilon_N^2 D$ . The variance of  $(2dD)^{-1} \sum_{i=1}^N \xi_{f_0,f}(X_{(i-1)D}) \cdot \bar{L}_{i,D}(\tilde{G}) \mathbf{1}_{\mathcal{A}_{i,D}}$  is of order  $D^{-2} N^2 \varepsilon_N^2 D^3 \exp(-cD^{-1})$ . Gathering all these estimates, we obtain

$$\text{Var}_{f_0} \left( \sum_{i=1}^N \frac{1}{2dD} \xi_{f_0,f}(X_{(i-1)D}) \tilde{b}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}} \right) \lesssim N \varepsilon_N^2 (ND^2 + D + ND \exp(-cD^{-1})).$$

*Step 3:* We now consider the martingale term  $\sum_{i=1}^N \frac{1}{2dD} \xi_{f_0, f}(X_{(i-1)D}) \tilde{\Sigma}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}}$ . We have

$$\begin{aligned} \text{Var}_{f_0} \left( \frac{1}{2dD} \sum_{i=1}^N \xi_{f_0, f}(X_{(i-1)D}) \tilde{\Sigma}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}} \right) &= \frac{1}{4d^2 D^2} \sum_{i=1}^N \mathbb{E}_{f_0} [(\xi_{f_0, f}(X_{(i-1)D}) \tilde{\Sigma}_{i,D})^2 \mathbf{1}_{\mathcal{A}_{i,D}}] \\ &\lesssim D^{-2} N \varepsilon_N^2 D^2 \end{aligned}$$

and this term has the right order  $N \varepsilon_N^2$ .

*Step 4:* We finally consider the remainder term  $\sum_{i=1}^N \frac{1}{2dD} \xi_{f_0, f}(X_{(i-1)D}) \tilde{L}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}}$  and conclude. We have

$$\begin{aligned} \text{Var}_{f_0} \left( \frac{1}{2dD} \sum_{i=1}^N \xi_{f_0, f}(X_{(i-1)D}) \tilde{L}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}} \right) &\lesssim D^{-2} N \sum_{i=1}^N \|\xi_{f_0, f}\|_{\infty}^2 \mathbb{E}_{f_0} [\tilde{L}_{i,D}^2 \mathbf{1}_{\mathcal{A}_{i,D}}] \\ &\lesssim N^2 \varepsilon_N^2 \exp(-cD^{-1}). \end{aligned}$$

Gathering the estimates from Steps 1-4 completes the proof of Proposition 15.  $\square$

*Proof of Proposition 17.* The proof follows similar, though easier, lines to that of the proof of Proposition 15. We thus provide only a sketch of the main bounds, matching Steps 1-4 for convenience.

*Step 1:* We again use the expansion (43) that yields

$$\begin{aligned} \frac{2}{d} \log \frac{q_{f,D}(X_i^D)}{q_{f_0,D}(X_i^D)} &= \log \frac{f_0(X_{(i-1)D})}{f(X_{(i-1)D})} - \left( \frac{f_0(X_{(i-1)D})}{f(X_{(i-1)D})} - 1 \right) \\ &\quad + \frac{1}{2dD} \xi_{f_0, f}(X_{(i-1)D}) (\tilde{b}_{i,D} + \tilde{\Sigma}_{i,D} + \tilde{L}_{i,D}). \end{aligned}$$

The main term is bounded above as before:

$$\left\| \log \frac{f_0}{f} - \left( \frac{f_0}{f} - 1 \right) \right\|_{\infty} \lesssim \varepsilon_N^2,$$

as follows from  $|\log \kappa - (\kappa - 1)| \leq C(\kappa - 1)^2$  in a neighbourhood of  $\kappa = 1$ , together with the properties  $\|f - f_0\|_{\infty} \leq \varepsilon_N$  and  $f \geq f_{\min}$ .

*Step 2:* By using the refinement of Step 2 in the proof of Proposition 15, we have

$$\tilde{b}_{i,D} = r_{i,D} + \bar{b}_{i,D}(\tilde{G}) + \bar{\Sigma}_{i,D}(\tilde{G}) + \bar{L}_{i,D}(\tilde{G}),$$

where

$$\mathbb{E}_{f_0} [ |r_{i,D} + \bar{b}_{i,D}(\tilde{G})|^p ] \lesssim D^{2p}, \quad \mathbb{E}_{f_0} [ |\bar{L}_{i,D}(\tilde{G})|^p \mathbf{1}_{\mathcal{A}_{i,D}} ] \lesssim D^{3p/2} \exp(-cD^{-1}),$$

and  $\bar{\Sigma}_{i,D}(\tilde{G})$  is a  $\mathcal{F}_{iD}$ -martingale increment. Therefore,

$$\mathbb{E}_{f_0} \left[ \frac{1}{2dD} \xi_{f_0, f}(X_{(i-1)D}) \tilde{b}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}} \right] \lesssim \varepsilon_N (D + D^{1/2} \exp(-cD^{-1})).$$

*Step 3:* Since  $\tilde{\Sigma}_{i,D}$  is a  $\mathcal{F}_{iD}$ -increment, we simply have

$$\mathbb{E}_{f_0} \left[ \frac{1}{2dD} \xi_{f_0, f}(X_{(i-1)D}) \tilde{\Sigma}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}} \right] = 0.$$

*Step 4:* We finally have

$$\mathbb{E}_{f_0} \left[ \left| \frac{1}{2dD} \xi_{f_0, f}(X_{(i-1)D}) \tilde{L}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}} \right| \right] \lesssim \varepsilon_N D^{1/2} \exp(cD^{-1}).$$

Gathering the estimates from Steps 1-4 completes the proof of Proposition 17.  $\square$

## 6. PROOF OF THEOREM 9: AN EXPONENTIAL INEQUALITY FOR A LEAST SQUARES TYPE ESTIMATOR

**6.1. Risk decomposition.** Recall from (23) that  $\bar{P}_J f = 1 + P_J[f - 1]$  for  $f \in \mathcal{F}$ , where  $P_J$  is the wavelet projection onto the space  $V_J$  in (21) used to reconstruct functions with support in  $\mathcal{O}_0$ , such as  $f - 1$  when  $f \in \mathcal{F}$ . We will decompose  $\|\hat{f}_N - \bar{P}_J f\|_2$  into martingale, bias and remainder terms that we control on the event

$$(44) \quad \mathcal{B}_N = \left\{ (1 - \kappa)\|g\|_2^2 \leq |g|_N^2 \leq (1 + \kappa)\|g\|_2^2 \text{ for all } g \in V_J \right\},$$

for some fixed  $0 < \kappa < 1$ , and where

$$|g|_N^2 = \frac{1}{N} \sum_{i=1}^N g(X_{(i-1)D})^2 \mathbf{1}_{\mathcal{A}_{i,D}}, \quad \mathcal{A}_{i,D} = \{X_{(i-1)D} \in \mathcal{O}_0^\delta\},$$

denotes a random empirical semi-norm for every continuous function on the  $\delta/2$ -enlargement  $\mathcal{O}_0^\delta$  of  $\mathcal{O}_0$ . By classical concentration techniques, we prove in Appendix 9.6 the following result.

**Lemma 22.** *Suppose that  $2^J \rightarrow \infty$  and  $2^{Jd} = o(\sqrt{ND})$  as  $N \rightarrow \infty$ . Then for every  $0 < \kappa < 1$ , as  $N \rightarrow \infty$ ,*

$$\sup_{f \in \mathcal{F}} \mathbb{P}_f(\mathcal{B}_N^c) \rightarrow 0.$$

By Lemma 22 we have  $\sup_{f \in \mathcal{F}} \mathbb{P}_f(\mathcal{B}_N^c) \rightarrow 0$  as  $N \rightarrow \infty$  for every  $0 < \kappa < 1$  under the theorem hypotheses, so that we may further restrict to working on  $\mathcal{B}_N$ . We have under  $\mathbb{P}_f$

$$(45) \quad Y_{i,D} = (2d)^{-1} D^{-1} |X_{iD} - X_{(i-1)D}|^2 = f(X_{(i-1)D}) + \mathcal{R}_{i,D},$$

with

$$(46) \quad \mathcal{R}_{i,D} = (2d)^{-1} D^{-1} (\tilde{b}_{i,D} + \tilde{\Sigma}_{i,D} + \tilde{L}_{i,D}),$$

where we recall the above decomposition from (38)-(39) but with  $f_0$  replaced by  $f$ . Let

$$\Gamma_N(g) = \frac{1}{N} \sum_{i=1}^N (Y_{i,D} - 1 - g(X_{(i-1)D}))^2 \mathbf{1}_{\mathcal{A}_{i,D}}$$

denote the normalized objective function defining our least squares estimator (24), using in particular that  $g(X_{(i-1)D}) = 0$  on  $(\mathcal{A}_{i,D})^c$  for all  $g \in V_J$ . By (45), for any function  $g$ ,

$$(47) \quad \Gamma_N(g) - \Gamma_N(f - 1) = |1 + g - f|_N^2 + \frac{2}{N} \sum_{i=1}^N (f - 1 - g)(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}}.$$

Since  $\Gamma_N(\hat{g}_N) = \inf_{g \in V_J} \Gamma_N(g)$  by construction, we have  $\Gamma_N(\hat{g}_N) - \Gamma_N(f - 1) \leq \Gamma_N(P_J[f - 1]) - \Gamma_N(f - 1)$ . Substituting (47) into both sides of this inequality with  $g = \hat{g}_N$  and  $g = P_J[f - 1]$ , respectively, then yields (with  $\hat{f}_N = \hat{g}_N + 1$ )

$$\begin{aligned} & |\hat{f}_N - f|_N^2 + 2N^{-1} \sum_{i=1}^N (f - \hat{f}_N)(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}} \\ & \leq |1 + P_J[f - 1] - f|_N^2 + 2N^{-1} \sum_{i=1}^N (f - 1 - P_J[f - 1])(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}}, \end{aligned}$$

or equivalently

$$(48) \quad |\widehat{f}_N - f|_N^2 \leq |P_J[f - 1] - (f - 1)|_N^2 + 2N^{-1} \sum_{i=1}^N (\widehat{f}_N - 1 - P_J[f - 1])(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}}.$$

Using that  $\widehat{f}_N - 1 - P_J[f - 1] \in V_J$  and  $2ab \leq \rho a^2 + \rho^{-1}b^2$  for any  $a, b, \rho > 0$ , on the event  $\mathcal{B}_N$ , the second term in the last display equals

$$\begin{aligned} & \frac{2}{N} \sum_{i=1}^N (\widehat{g}_N - P_J[f - 1])(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}} \\ & \leq 2 \|\widehat{g}_N - P_J[f - 1]\|_2 \sup_{g \in V_J: \|g\|_2=1} \frac{1}{N} \sum_{i=1}^N g(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}} \\ & \leq \rho \|\widehat{g}_N - P_J[f - 1]\|_2^2 + \rho^{-1} \left( \sup_{g \in V_J: \|g\|_2 \leq 1} \frac{1}{N} \sum_{i=1}^N g(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}} \right)^2 \\ & \leq (1 - \kappa)^{-1} \rho \|\widehat{g}_N - P_J[f - 1]\|_N^2 + \rho^{-1} \left( \sup_{g \in V_J: \|g\|_2 \leq 1} \frac{1}{N} \sum_{i=1}^N g(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}} \right)^2. \end{aligned}$$

Substituting this last display into (48) then gives

$$\begin{aligned} |\widehat{f}_N - f|_N^2 & \leq |P_J[f - 1] - (f - 1)|_N^2 + (1 - \kappa)^{-1} \rho \|\widehat{g}_N - P_J[f - 1]\|_N^2 \\ & \quad + \rho^{-1} \left( \sup_{g \in V_J: \|g\|_2 \leq 1} \frac{1}{N} \sum_{i=1}^N g(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}} \right)^2. \end{aligned}$$

Using that  $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$  for  $a, b > 0$ , this implies

$$\begin{aligned} |\widehat{f}_N - 1 - P_J[f - 1]|_N & \leq |\widehat{f}_N - f|_N + |f - 1 - P_J[f - 1]|_N \\ & \leq 2|f - 1 - P_J[f - 1]|_N + (1 - \kappa)^{-1/2} \rho^{1/2} |\widehat{f}_N - 1 - P_J[f - 1]|_N \\ & \quad + \rho^{-1/2} \left| \sup_{g \in V_J: \|g\|_2 \leq 1} \frac{1}{N} \sum_{i=1}^N g(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}} \right|. \end{aligned}$$

Collecting the  $|\widehat{f}_N - 1 - P_J[f - 1]|_N$  terms on the left-hand side thus yields the risk decomposition

$$\begin{aligned} & \left(1 - \sqrt{\frac{\rho}{1-\kappa}}\right) |\widehat{f}_N - 1 - P_J[f - 1]|_N \\ & \leq 2|f - 1 - P_J[f - 1]|_N + \rho^{-1/2} \left| \sup_{g \in V_J: \|g\|_2 \leq 1} \frac{1}{N} \sum_{i=1}^N g(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}} \right|. \end{aligned}$$

Taking  $\rho > 0$  small enough that  $\rho/(1 - \kappa) < 1$  and using that  $|\widehat{f}_N - 1 - P_J[f - 1]|_N \geq \sqrt{1 - \kappa} \|\widehat{f}_N - 1 - P_J[f - 1]\|_2$  on  $\mathcal{B}_N$ , we then obtain that on  $\mathcal{B}_N$ ,

$$C^{-1} \|\widehat{f}_N - 1 - P_J[f - 1]\|_2 \leq 2|f - 1 - P_J[f - 1]|_N + \rho^{-1/2} \left| \sup_{g \in V_J: \|g\|_2 \leq 1} \frac{1}{N} \sum_{i=1}^N g(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}} \right|,$$

where  $C^{-1} = \sqrt{1 - \kappa}(1 - \sqrt{\rho/(1 - \kappa)}) = \sqrt{1 - \kappa} - \sqrt{\rho} > 0$ . Recalling that  $\bar{P}_J f = 1 + P_J[f - 1]$ , we finally obtain the following risk decomposition:

$$(49) \quad \mathbb{P}_f(\|\widehat{f}_N - \bar{P}_J f\|_2 \geq K\xi_N, \mathcal{B}_N) \leq \mathbb{P}_f(\|f - 1 - P_J[f - 1]\|_N \geq K_1\xi_N, \mathcal{B}_N) \\ + \mathbb{P}_f\left(\sup_{g \in \mathcal{V}_J: \|g\|_2 \leq 1} \sum_{i=1}^N g(X_{(i-1)D}) \mathcal{R}_{i,D} \mathbf{1}_{A_{i,D}} \geq K_2 N \xi_N, \mathcal{B}_N\right)$$

where the constants  $K_i = C_i K$  for constants  $C_i$  depending only on  $\kappa$  and  $\rho$ , which are henceforth considered fixed. It therefore suffices to prove that each term on the right-hand side of (49) is bounded by a multiple of  $e^{-LN\varepsilon_N^2}$  for arbitrary fixed  $L > 0$  and large enough  $K = K(L)$ .

**6.2. Bias term.** We consider here the first term in (49), which is a bias term with the randomness only entering from the design in the random empirical semi-norm  $|\cdot|_N$ . Write  $g_J = f - 1 - P_J[f - 1]$  and

$$Z_N(g_J) = |g_J|_N^2 - \|g_J\|_2^2 = \frac{1}{N} \sum_{i=1}^N (g_J(X_{(i-1)D})^2 - \mathbb{E}_f[g_J(X_{(i-1)D})^2]),$$

since  $\mathbb{E}_f[g_J(X_{(i-1)D})^2] = \|g_J\|_2^2$ . The variance satisfies

$$\text{Var}_f(g_J(X_{(i-1)D})^2) \leq \mathbb{E}_f[g_J(X_{(i-1)D})^4] = \|g_J\|_{L^4}^4,$$

while  $|g_J(x)^2 - \mathbb{E}_f[g_J(X_{(i-1)D})^2]| \leq 2\|g_J\|_\infty^2$ . Since  $(X_0, X_D, \dots, X_{ND})$  is a stationary reversible Markov chain whose spectral gap is lower bounded by  $rD$  by (9), Theorem of 3.3 of [44] (cf. (3.21)) yields

$$\mathbb{P}_f(N|Z_N(g_J)| \geq t) \leq 2 \exp\left(-\frac{rDt^2}{4N\|g_J\|_{L^4}^4 + 20\|g_J\|_\infty^2 t}\right)$$

for all  $t > 0$ . Setting  $t = MN\xi_N^2$  then gives

$$\mathbb{P}_f(|Z_N(g_J)| \geq M\xi_N^2) \leq 2 \exp\left(-\frac{rDM^2N\xi_N^4}{4\|g_J\|_{L^4}^4 + 20M\|g_J\|_\infty^2 \xi_N^2}\right).$$

By rearranging, one gets that the right-hand side is smaller than  $2e^{-LN\varepsilon_N^2}$  if and only if

$$4L\|g_J\|_{L^4}^4 \varepsilon_N^2 + 20LM\|g_J\|_\infty^2 \xi_N^2 \varepsilon_N^2 \leq rDM^2 \xi_N^4.$$

Since  $r = r(f_{\min}, \mathcal{O})$  by (9), we have shown that for any  $L > 0$ , there exists  $M = M(L, r) > 0$  large enough such that

$$\sup_{\substack{f \in \mathcal{F}: \|f - P_J f\|_\infty \leq R_{J,\infty}, \\ \|f - P_J f\|_{L^4} \leq R_{J,4}}} \mathbb{P}_f(\|f - 1 - P_J[f - 1]\|_N^2 \geq \|f - 1 - P_J[f - 1]\|_2^2 + M\xi_N^2) \leq 2e^{-LN\varepsilon_N^2}$$

for any  $\varepsilon_N, \xi_N, R_{J,4}, R_{J,\infty}$  such that  $R_{J,4}^4 \varepsilon_N^2 + R_{J,\infty}^2 \xi_N^2 \varepsilon_N^2 \lesssim D\xi_N^4$ , as assumed by the theorem hypotheses.

**6.3. Deviation of the remainder term.** We now consider the second term in (49) involving  $\mathcal{R}_{i,D}$ . By a union bound, up to a modification of the constants, it suffices to prove the deviation for each term in the decomposition (46).

*Step 1:* We postpone the term involving the drift  $\tilde{b}_{i,D}$  to Step 3 and rather first control the term involving  $\tilde{\Sigma}_{i,D}$  in (46). We will prove

$$(50) \quad \mathbb{P}_f \left( \sup_{g \in V_J : \|g\|_2 \leq 1} |\tilde{Z}_N(g)| \geq MN\xi_N, \mathcal{B}_N \right) \leq e^{-LN\varepsilon_N^2},$$

for sufficiently large  $M$ , where

$$\tilde{Z}_N(g) = D^{-1} \sum_{i=1}^N g(X_{(i-1)D}) \tilde{\Sigma}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}}.$$

Define

$$\mathbb{P}_{\mathcal{B}_N, f} = \mathbb{P}_f(\cdot | \mathcal{B}_N) = \mathbb{P}_f(\mathcal{B}_N)^{-1} \mathbb{P}_f(\cdot \cap \mathcal{B}_N).$$

Since  $\mathbb{P}_f(\mathcal{B}_N) \rightarrow 1$  uniformly in  $f \in \mathcal{F}$  by Lemma 22, we have  $\frac{1}{2}\mathbb{P}_{\mathcal{B}_N, f} \leq \mathbb{P}_f(\cdot \cap \mathcal{B}_N) \leq \mathbb{P}_{\mathcal{B}_N, f}$  for  $N$  large enough. It thus suffices to establish (50) with  $\mathbb{P}_{\mathcal{B}_N, f}$  instead of  $\mathbb{P}_f$ . We prove a Bernstein inequality for the increments of the process  $(\tilde{Z}_N(g) : g \in V_J)$  and conclude using a chaining argument under  $\mathbb{P}_{\mathcal{B}_N, f}$ . To that end, we need the following result, see e.g. [45, 22].

**Lemma 23.** *Let  $(\mathcal{M}_n)_{n \geq 0}$  be a  $(\mathcal{G}_n)_{n \geq 0}$ -martingale with  $\mathcal{M}_0 = 0$  and let  $\langle \mathcal{M} \rangle_n = \sum_{i=1}^n \mathbb{E}[|\mathcal{M}_i - \mathcal{M}_{i-1}|^2 | \mathcal{G}_{i-1}]$  denotes its predictable quadratic variation. If for some  $c > 0$ ,*

$$\sum_{i=1}^n \mathbb{E}[|\mathcal{M}_i - \mathcal{M}_{i-1}|^p | \mathcal{G}_{i-1}] \leq \frac{c^{p-2} p!}{2} \langle \mathcal{M} \rangle_n \quad \text{for every } p \geq 2,$$

then for every  $t, y > 0$ ,

$$\mathbb{P}(\mathcal{M}_n \geq t, \langle \mathcal{M} \rangle_n \leq y) \leq \exp\left(-\frac{t^2}{2(y+ct)}\right).$$

We will apply Lemma 23 to the  $\mathcal{G}_n$ -martingale  $\mathcal{M}_n = \tilde{Z}_N(g) = D^{-1} \sum_{i=1}^n g(X_{(i-1)D}) \tilde{\Sigma}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}}$ , with  $\mathcal{G}_n = \sigma(X_{iD} : 0 \leq i \leq n)$ . First, applying the Burkholder-Davis-Gundy inequality with best constant  $c_*^{p/2} p^{p/2}$  (see e.g. [9]), we have for all  $p \geq 1$ :

$$\begin{aligned} & \mathbb{E}_f \left[ |D^{-1} \tilde{\Sigma}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}}|^p | \mathcal{F}_{(i-1)D} \right] \\ &= D^{-p} \mathbb{E}_f \left[ \left| \int_{(i-1)D}^{iD} \sqrt{2f(X_s)} (X_s - X_{(i-1)D}) \cdot dB_s \right|^p | \mathcal{F}_{(i-1)D} \right] \mathbf{1}_{\mathcal{A}_{i,D}} \\ &\leq D^{-p} (2\|f\|_\infty c_* p)^{p/2} \mathbb{E}_f \left[ \left| \int_{(i-1)D}^{iD} |X_s - X_{(i-1)D}|^2 ds \right|^{p/2} | \mathcal{F}_{(i-1)D} \right] \\ &\leq (D^{-1} 2\|f\|_\infty c_* p)^{p/2} \max_{1 \leq j \leq d} \mathbb{E}_f \left[ \sup_{(i-1)D \leq s \leq iD} |X_s - X_{(i-1)D}|^p | \mathcal{F}_{(i-1)D} \right] \\ &\leq (2\|f\|_\infty c_* p)^{p/2} 2^{p-1} (\|f\|_{\mathfrak{e}_1}^p D^{p/2} + (c_* p)^{p/2} \|f\|_\infty^p) \\ &\leq (C\|f\|_{\mathfrak{e}_1}^{3/2})^p p!, \end{aligned}$$

for some  $C > 0$  that only depends on  $d$ , since  $D \rightarrow 0$  and where we used Lemma 19 to obtain the second last inequality together with  $p^p \leq (C')^p p!$  for some universal constant  $C' \geq 1$ . Next, we claim that the following lower bound holds

$$(51) \quad \mathbb{E}_f \left[ (D^{-1} \tilde{\Sigma}_{i,D})^2 \mathbf{1}_{\mathcal{A}_{i,D}} | \mathcal{F}_{(i-1)D} \right] \geq df_{\min}^2 - O(D^{1/2}).$$

Assuming for now that (51) is true, for  $D \rightarrow 0$  small enough,

$$\begin{aligned} \sum_{i=1}^n |g(X_{(i-1)D})|^p &\leq \|g\|_\infty^{p-2} \sum_{i=1}^n |g(X_{(i-1)D})|^2 \frac{2}{f_{\min}^2 d} \mathbb{E}_f \left[ \left( \frac{1}{D} \tilde{\Sigma}_{i,D} \right)^2 \mathbf{1}_{\mathcal{A}_{i,D}} \mid \mathcal{F}_{(i-1)D} \right] \\ &= \frac{2}{f_{\min}^2 d} \|g\|_\infty^{p-2} \langle \mathcal{M} \rangle_n. \end{aligned}$$

It follows that

$$\begin{aligned} \sum_{i=1}^n \mathbb{E} \left[ |\mathcal{M}_i - \mathcal{M}_{i-1}|^p \mid \mathcal{F}_{(i-1)D} \right] &= \sum_{i=1}^n |g(X_{(i-1)D})|^p \mathbb{E}_f \left[ |D^{-1} \tilde{\Sigma}_{i,D} \mathbf{1}_{\mathcal{A}_{i,D}}|^p \mid \mathcal{F}_{(i-1)D} \right] \\ &\leq (C \|f\|_{\mathcal{C}^1}^{3/2})^p p! \sum_{i=1}^n |g(X_{(i-1)D})|^p \\ &\leq \frac{2}{f_{\min}^2 d} (C \|f\|_{\mathcal{C}^1}^{3/2})^p p! \|g\|_\infty^{p-2} \langle \mathcal{M} \rangle_n \end{aligned}$$

for small enough  $D$ . The condition of Lemma 23 therefore holds with

$$c = C_{f_{\min}, \|f\|_{\mathcal{C}^1}} = \max(1, 4C^2 \|f\|_{\mathcal{C}^1}^2 d^{-1} f_{\min}^{-2}) C \|f\|_{\mathcal{C}^1}^{3/2} \|g\|_\infty.$$

Moreover, recalling that  $g \in V_J$  in (49) and using the bound (40), on the event  $\mathcal{B}_N$ ,

$$\langle \mathcal{M} \rangle_N = \frac{1}{D^2} \sum_{i=1}^N g(X_{(i-1)D})^2 \mathbb{E}_f \left[ \tilde{\Sigma}_{i,D}^2 \mid \mathcal{F}_{(i-1)D} \right] \mathbf{1}_{\mathcal{A}_{i,D}} \leq C_{\|f\|_{\mathcal{C}^1}} N |g|_N^2 \leq C_{\|f\|_{\mathcal{C}^1}} (1 + \kappa) N \|g\|_2^2.$$

Applying Lemma 23 at  $n = N$  with  $y = C_{\|f\|_{\mathcal{C}^1}} (1 + \kappa) N \|g\|_2^2$ , we finally obtain for all  $t > 0$ ,

$$\begin{aligned} \mathbb{P}_{\mathcal{B}_N, f} \left( |\tilde{Z}_N(g)| \geq t \right) &\leq 2\mathbb{P}_f \left( |\mathcal{M}_N| \geq t, \mathcal{B}_N \right) \\ &\leq 2\mathbb{P}_f \left( |\mathcal{M}_N| \geq t, \langle \mathcal{M} \rangle_N \leq C_{\|f\|_{\mathcal{C}^1}} N \|g\|_2^2 \right) \\ &\leq 4 \exp \left( - \frac{t^2}{2(C_{\|f\|_{\mathcal{C}^1}} N \|g\|_2^2 + C_{\|f\|_{\mathcal{C}^1}, f_{\min}} \|g\|_\infty t)} \right). \end{aligned}$$

Using that  $\|g\|_\infty \leq C 2^{Jd/2} \|g\|_2$  for  $g \in V_J$ , we have that for all  $g, g' \in V_J$  and  $t > 0$ ,

$$\mathbb{P}_{\mathcal{B}_N, f} \left( |\tilde{Z}_N(g) - \tilde{Z}_N(g')| \geq t \right) \leq 4 \exp \left( - \frac{Ct^2}{N \|g - g'\|_2^2 + 2^{Jd/2} \|g - g'\|_2 t} \right).$$

We may therefore apply the generic chaining bound in Lemma 31 in Section 9.5 below with  $m = \dim(V_J) = O(2^{Jd})$ ,  $\|\mathcal{G}_J\|_2 = \sup_{g, h \in \mathcal{G}_J} \|g - h\|_2 \leq 2$ ,  $\alpha^2 = N$ ,  $\beta = 2^{Jd/2}$  to obtain that for all  $u \geq 1$ ,

$$\mathbb{P}_{\mathcal{B}_N, f} \left( \sup_{g \in V_J: \|g\|_2 \leq 1} |\tilde{Z}_N(g)| \geq C_{\|f\|_{\mathcal{C}^1}, f_{\min}} (2^{3Jd/2} + 2^{Jd/2} N^{1/2} + 2^{Jd/2} u + N^{1/2} \sqrt{u}) \right) \leq e^{-u}.$$

Setting  $u = LN\varepsilon_N^2$  with  $L > 0$  then gives

$$\mathbb{P}_{\mathcal{B}_N, f} \left( \sup_{g \in V_J: \|g\|_2 \leq 1} |\tilde{Z}_N(g)| \geq MN\xi_N \right) \leq e^{-LN\varepsilon_N^2}$$

for any  $\varepsilon_N, \xi_N, 2^J$  satisfying

$$(52) \quad 2^{3Jd/2} N^{-1} + 2^{Jd/2} N^{-1/2} + 2^{Jd/2} \varepsilon_N^2 + \varepsilon_N \lesssim \xi_N$$

upon taking  $M = M(L, \|f\|_{\mathcal{C}^1}, f_{\min})$  large enough. This establishes (50), so that we have the required exponential inequality in (49) for the term  $(dD)^{-1} \tilde{\Sigma}_{i,D}$  in  $\mathcal{R}_{i,D}$ .

It remains to prove (51). By Itô's isometry,

$$\begin{aligned}\mathbb{E}_f[(D^{-1}\tilde{\Sigma}_{i,D})^2\mathbf{1}_{\mathcal{A}_{i,D}}|\mathcal{F}_{(i-1)D}] &= \frac{8}{D^2}\mathbb{E}_f\left[\int_{(i-1)D}^{iD}|X_s - X_{(i-1)D}|^2 f(X_s)ds|\mathcal{F}_{(i-1)D}\right]\mathbf{1}_{\mathcal{A}_{i,D}} \\ &\geq \frac{8f_{\min}}{D^2}\mathbb{E}_f\left[\int_{(i-1)D}^{(i-1)D+\tau_{i,D}\wedge D}|X_s - X_{(i-1)D}|^2 ds|\mathcal{F}_{(i-1)D}\right]\mathbf{1}_{\mathcal{A}_{i,D}},\end{aligned}$$

where  $\tau_{i,D}$  defined in (33) is the hitting time of the boundary  $\partial\mathcal{O}$  by the process  $X$  started at time  $(i-1)D$ . Furthermore,

$$\begin{aligned}(53) \quad &\mathbb{E}_f\left[\int_{(i-1)D}^{(i-1)D+\tau_{i,D}\wedge D}|X_s - X_{(i-1)D}|^2 ds|\mathcal{F}_{(i-1)D}\right] \\ &= \mathbb{E}_f\left[\int_{(i-1)D}^{(i-1)D+\tau_{i,D}\wedge D}\int_{(i-1)D}^s df(X_u)duds|\mathcal{F}_{(i-1)D}\right] \\ &+ 2\mathbb{E}_f\left[\int_{(i-1)D}^{(i-1)D+\tau_{i,D}\wedge D}\int_{(i-1)D}^s (X_s - X_{(i-1)D}) \cdot \nabla f(X_u)duds|\mathcal{F}_{(i-1)D}\right].\end{aligned}$$

Lemma 19 applied to the second term of the right-hand side of (53) yields

$$\left|2\mathbb{E}_f\left[\int_{(i-1)D}^{(i-1)D+\tau_{i,D}\wedge D}\int_{(i-1)D}^s (X_s - X_{(i-1)D}) \cdot \nabla f(X_u)duds|\mathcal{F}_{(i-1)D}\right]\right| \lesssim D^{2+1/2}$$

up to a (deterministic) constant that depends only on  $\|f\|_{C^1}$ , while the first term of the right-hand side of (53) times  $\mathbf{1}_{\mathcal{A}_{i,D}}$  can be bounded below by  $df_{\min}$  times

$$\begin{aligned}\mathbb{E}_f[(\tau_{i,D} \wedge D)^2\mathbf{1}_{\{\tau_{i,D} \geq D\}}|\mathcal{F}_{(i-1)D}]\mathbf{1}_{\mathcal{A}_{i,D}} &= D^2\mathbb{P}_f(\tau_{i,D} \geq D|\mathcal{F}_{(i-1)D})\mathbf{1}_{\mathcal{A}_{i,D}} \\ &\geq D^2(1 - C\exp(-cD^{-1}))\mathbf{1}_{\mathcal{A}_{i,D}}\end{aligned}$$

thanks to Lemma 20. We thus have

$$\mathbb{E}_f\left[\int_{(i-1)D}^{(i-1)D+\tau_{i,D}\wedge D}|X_s - X_{(i-1)D}|^2 ds|\mathcal{F}_{(i-1)D}\right] \geq dD^2f_{\min} - O(D^{5/2})$$

and (51) readily follows.

*Step 2:* We next turn to the boundary term in (46). Set  $\tilde{L}_N(g) = D^{-1}\sum_{i=1}^N g(X_{(i-1)D})\tilde{L}_{i,D}\mathbf{1}_{\mathcal{A}_{i,D}}$ . Since  $\sup_{g \in V_J, \|g\|_2 \leq 1} |g|_N^2 \leq (1 + \kappa)$  on  $\mathcal{B}_N$ , by Cauchy-Schwarz's inequality,

$$\begin{aligned}\mathbb{P}_f\left(\sup_{g \in V_J, \|g\|_2 \leq 1} |\tilde{L}_N(g)| \geq CN\xi_N, \mathcal{B}_N\right) &\leq \mathbb{P}_f\left((1 + \kappa)D^{-2}N^{-1}\sum_{i=1}^N \tilde{L}_{i,D}^2\mathbf{1}_{\mathcal{A}_{i,D}} \geq C\xi_N^2\right) \\ &\leq \sum_{i=1}^N \mathbb{P}_f(\tau_{i,D} \geq D, \mathcal{A}_{i,D}) \lesssim N\exp(-cD^{-1})\end{aligned}$$

using that  $\tilde{L}_{i,D}$  vanishes on  $\{\tau_{i,D} < D\} \cap \mathcal{A}_{i,D}$  and Lemma 20.

*Step 3:* We finally consider the drift term in (46). Setting  $\tilde{b}_N(g) = D^{-1}\sum_{i=1}^N g(X_{(i-1)D})\tilde{b}_{i,D}\mathbf{1}_{\mathcal{A}_{i,D}}$ , we will prove

$$(54) \quad \mathbb{P}_f\left(\sup_{g \in V_J, \|g\|_2 \leq 1} |\tilde{b}_N(g)| \geq MN\xi_N, \mathcal{B}_N\right) \leq C\exp(-LN\varepsilon_N^2)$$

for arbitrary fixed  $L > 0$  and  $M = M(L)$  large enough, under the assumption  $ND^2 \rightarrow 0$ . By Itô's formula, with  $H(x, y) = d(f(y) - f(x)) + (y - x) \cdot \nabla f(y)$ , similarly to (42) in Step 2 of the proof of Proposition 14, we can decompose

$$\tilde{b}_{i,D} = \int_{(i-1)D}^{iD} H(X_{(i-1)D}, X_s) ds = \bar{b}_{i,D}(H) + \bar{\Sigma}_{i,D}(H) + \bar{L}_{i,D}(H),$$

with

$$\begin{aligned} \bar{b}_{i,D}(H) &= \int_{(i-1)D}^{iD} \int_{(i-1)D}^s \mathcal{L}_f H(X_{(i-1)D}, X_u) du ds \\ \bar{\Sigma}_{i,D}(H) &= \int_{(i-1)D}^{iD} \int_{(i-1)D}^s \nabla H(X_{(i-1)D}, X_u) \sqrt{2f(X_u)} \cdot dB_u ds \\ \bar{L}_{i,D}(H) &= \int_{(i-1)D}^{iD} \int_{(i-1)D}^s \nabla H(X_{(i-1)D}, X_u) \cdot n(X_u) d|\ell|_u. \end{aligned}$$

We bound the deviation probability each contribution in the expansion of  $\tilde{b}_N(g)$  via a union bound. Using Cauchy-Schwarz's inequality and the bound

$$\left| \int_{(i-1)D}^{iD} \int_{(i-1)D}^s \mathcal{L}_f H(X_{(i-1)D}, X_u) du ds \right| \leq \frac{1}{2} D^2 \|\mathcal{L}_f H\|_\infty \leq C_{\mathcal{O}, \|f\|_{e^3}} D^2,$$

where the supremum is taken over  $(x, y) \in \mathcal{O} \times \mathcal{O}$ , we derive

$$\begin{aligned} &\mathbb{P}_f \left( \sup_{g \in V_J, \|g\|_2 \leq 1} D^{-1} \left| \sum_{i=1}^N g(X_{(i-1)D}) \bar{b}_{i,D}(H) \mathbf{1}_{\mathcal{A}_{i,D}} \right| \geq CN \xi_N, \mathcal{B}_N \right) \\ &\leq \mathbb{P}_f \left( N^{-1} \sum_{i=1}^N (\bar{b}_{i,D}(H))^2 \geq C^2 D^2 \xi_N^2 \right) \leq N \mathbf{1}_{\{C_{\mathcal{O}, \|f\|_{e^3}}^2 D^2 \geq C \xi_N\}} \end{aligned}$$

where we used that  $\sup_{g \in V_J, \|g\|_2 \leq 1} |g|_N^2 \leq (1 + \kappa)$  on  $\mathcal{B}_N$ . The assumptions  $ND^2 \rightarrow 0$  and  $N\xi_N^2 \rightarrow \infty$  together imply that for sufficiently large  $N$ , we necessarily have  $C_{\mathcal{O}, \|f\|_{e^3}}^2 D^2 < C \xi_N^2$  and the above probability is thus zero. For the martingale term associated to  $\bar{\Sigma}_{i,D}(H)$ , we proceed exactly as in Step 1: define

$$\bar{\mathcal{M}}_n = D^{-1} \sum_{i=1}^n g(X_{(i-1)D}) \bar{\Sigma}_{i,D}(H) \mathbf{1}_{\mathcal{A}_{i,D}}.$$

By Fubini's theorem and the Burkholder-Davis-Gundy inequality:

$$\begin{aligned} &\mathbb{E}_f \left[ |D^{-1} \bar{\Sigma}_{i,D}(H) \mathbf{1}_{\mathcal{A}_{i,D}}|^p \mid \mathcal{F}_{(i-1)D} \right] \\ &= D^{-p} \mathbb{E}_f \left[ \left| \int_{(i-1)D}^{iD} (u - (i-1)D) \nabla H(X_{(i-1)D}, X_u) \sqrt{2f(X_u)} \cdot dB_u \right|^p \mid \mathcal{F}_{(i-1)D} \right] \mathbf{1}_{\mathcal{A}_{i,D}} ds \\ &\leq D^{-p} (c_* p)^{p/2} \mathbb{E}_f \left[ \left| \int_{(i-1)D}^{iD} (u - (i-1)D)^2 |\nabla H(X_{(i-1)D}, X_u)|^2 2f(X_u) ds \right|^{p/2} \mid \mathcal{F}_{(i-1)D} \right] \mathbf{1}_{\mathcal{A}_{i,D}} ds \\ &\leq D^{p/2-1} (c_* p)^{p/2} \|\nabla H\|_\infty^{p/2-1} \mathbb{E}_f \left[ (D^{-1} \bar{\Sigma}_{i,D}(H) \mathbf{1}_{\mathcal{A}_{i,D}})^2 \mid \mathcal{F}_{(i-1)D} \right] \\ &\leq (D^{1/2} C_{\|f\|_{e^2}})^{p-2} p! \mathbb{E}_f \left[ (D^{-1} \bar{\Sigma}_{i,D}(H) \mathbf{1}_{\mathcal{A}_{i,D}})^2 \mid \mathcal{F}_{(i-1)D} \right] \end{aligned}$$

with  $C_{\|f\|_{e^3}} \geq C' \max(1, (2c_* \|f\|_\infty)^{1/2} \|\nabla H\|_\infty)$  and  $C'$  a universal constant such that  $p^p \leq C' p!$ . It follows that

$$\begin{aligned} \sum_{i=1}^n \mathbb{E}[|\mathcal{M}_i - \mathcal{M}_{i-1}|^p | \mathcal{F}_{(i-1)D}] &= \sum_{i=1}^n |g(X_{(i-1)D})|^p \mathbb{E}_f[|D^{-1} \bar{\Sigma}_{i,D}(H) \mathbf{1}_{\mathcal{A}_{i,D}}|^p | \mathcal{F}_{(i-1)D}] \\ &\leq (D^{1/2} C_{\|f\|_{e^2}} \|g\|_\infty)^{p-2} p! \langle \bar{\mathcal{M}} \rangle_n, \end{aligned}$$

so that the condition of Lemma 23 holds with  $c = D^{1/2} C'_{\|f\|_{e^2}} \|g\|_\infty$  for instance. Moreover,

$$\langle \bar{\mathcal{M}} \rangle_N = \sum_{i=1}^N g(X_{(i-1)D})^2 \mathbb{E}_f[(D^{-1} \bar{\Sigma}_{i,D}(H) \mathbf{1}_{\mathcal{A}_{i,D}})^2 | \mathcal{F}_{(i-1)D}] \leq CN |g|_N^2 D \leq C(1 + \kappa) \|g\|_2^2 ND$$

on the event  $\mathcal{B}_N$ , so that applying Lemma 23 with  $n = N$  and  $y = C(1 + \kappa) \|g\|_2^2 ND$  yields

$$\begin{aligned} \mathbb{P}_{\mathcal{B}_N, f} \left( D^{-1} \sum_{i=1}^n g(X_{(i-1)D}) \bar{\Sigma}_{i,D}(H) \mathbf{1}_{\mathcal{A}_{i,D}} \geq t \right) &\leq C \mathbb{P}_f(\bar{\mathcal{M}}_N \geq t, \langle \bar{\mathcal{M}} \rangle_N \leq C' ND \|g\|_2^2) \\ &\leq 2C \exp\left(-C \frac{t^2}{ND \|g\|_2^2 + D^{1/2} \|g\|_\infty}\right) \end{aligned}$$

for all  $t > 0$ . Setting  $\bar{Z}_N(g) = D^{-1} \sum_{i=1}^n g(X_{(i-1)D}) \bar{\Sigma}_{i,D}(H) \mathbf{1}_{\mathcal{A}_{i,D}}$ , the process  $\bar{Z}_N = (\bar{Z}_N(g) : g \in \{V_J : \|g\|_2 \leq 1\})$  therefore satisfies the conditions of Lemma 31 with  $m = \dim(V_J) = O(2^{Jd})$ ,  $\|g\|_2 \leq 2$ ,  $\alpha^2 = ND$ ,  $\beta = D^{1/2} 2^{Jd/2}$ , where we have also used the linearity of  $g \mapsto \bar{Z}_N(g)$  and that  $\|g\|_\infty \leq C 2^{Jd/2} \|g\|_2$  for  $g \in V_J$ . Lemma 31 thus implies that for all  $u \geq 1$ ,

$$\mathbb{P}_{\mathcal{B}_N, f} \left( \sup_{g \in V_J, \|g\|_2 \leq 1} |\bar{Z}_N(g)| \geq CD^{1/2} (2^{3Jd/2} + 2^{Jd/2} N^{1/2} + \sqrt{u} N^{1/2} + u 2^{Jd/2}) \right) \leq e^{-u}.$$

Returning to (54), we want a bound of the form

$$\mathbb{P}_{\mathcal{B}_N, f} \left( \sup_{g \in V_J, \|g\|_2 \leq 1} |\bar{Z}_N(g)| \geq CN \xi_N \right) \leq e^{-LN \varepsilon_N^2}.$$

Setting  $u = LN \varepsilon_N^2$  in the second last display, this follows as soon as

$$D^{1/2} (2^{3Jd/2} N^{-1} + 2^{Jd/2} N^{-1/2} + \varepsilon_N + 2^{Jd/2} \varepsilon_N^2) \lesssim \xi_N.$$

But this is exactly condition (52) above with the left-side multiplied by the superoptimal factor  $D^{1/2}$ , and hence this condition is implied by (52). For the boundary term associated to  $\bar{L}_{i,D}(H)$ , we proceed exactly as in Step 2, replacing  $\tilde{L}_{i,D}$  by  $\bar{L}_{i,D}$ . The conclusion is the same.

## 7. PROOFS OF POSTERIOR CONTRACTION RESULTS

**7.1. Proof of Theorem 11: a general contraction theorem.** The proof follows the general testing approach of [26] and the idea of using plug-in tests based on frequentist estimators satisfying concentration inequalities [27], adapted to the present high-frequency multidimensional diffusion setting. The next result follows by combining the proof of Theorem 8.9 in [26] for the i.i.d. case with our evidence lower bound in Theorem 8.

**Lemma 24.** *Suppose  $f_0 \in \mathcal{F}_0$  and let  $\Pi = \Pi_N$  be a sequence of prior distributions supported on  $\mathcal{F}$  in (12). Further let  $0 < \varepsilon_N \leq \varepsilon_{1,N} \leq \varepsilon_{2,N} \leq \varepsilon_{3,N} \rightarrow 0$ ,  $\xi_N \rightarrow 0$  be positive sequences such that  $N \varepsilon_N^2 \rightarrow \infty$ , let  $E_N$  and  $V_N$  be the corresponding quantities defined in (16), and let  $r > 0$  be fixed. Set*

$$\mathcal{C}_N = \left\{ f \in \mathcal{F} : \|f\|_{e^\alpha} \leq r, \|f - f_0\|_\infty \leq \varepsilon_N, \|f - f_0\|_{e^k} \leq \varepsilon_{k,N} \text{ for } k = 1, 2, 3 \right\}$$

to be the set defined in (15) and  $C_0 > 0$  to be the fixed constant in Theorem 8, which depends only on  $f_0, r, d, \mathcal{O}, \delta, f_{\min}$ . Suppose that for some  $K_0 > 0$ ,

$$E_N \leq K_0 \varepsilon_N^2, \quad V_N / (N^2 \varepsilon_N^4) \rightarrow 0,$$

as  $N \rightarrow \infty$ . Further suppose that for some  $C, L, M > 0$ , the prior  $\Pi$  satisfies  $\Pi(\mathcal{C}_N) \geq e^{-CN\varepsilon_N^2}$ , and there exist sets  $\mathcal{F}_N \subseteq \mathcal{F}$  satisfying  $\Pi(\mathcal{F}_N^c) \leq Le^{-(C+C_0K_0+2)N\varepsilon_N^2}$ , events  $B_N$  satisfying  $\mathbb{P}_{f_0}(B_N) \rightarrow 1$  and a sequence of test functions  $\Psi_N = \Psi_N(X_0, X_D, \dots, X_{ND})$  such that

$$\mathbb{E}_{f_0}[\Psi_N 1_{B_N}] \rightarrow 0, \quad \sup_{f \in \mathcal{F}_N: \|f - f_0\|_2 \geq M\xi_N} \mathbb{E}_f[(1 - \Psi_N) 1_{B_N}] \leq Le^{-(C+C_0K_0+2)N\varepsilon_N^2}.$$

Then as  $N \rightarrow \infty$ ,

$$\mathbb{E}_{f_0} \Pi(f : \|f - f_0\|_2 \geq M\xi_N | X_0, X_D, \dots, X_{ND}) \rightarrow 0.$$

*Proof.* Writing  $A_N = \{f : \|f - f_0\|_2 \geq M\xi_N\}$  and  $X^N = (X_0, X_D, \dots, X_{ND})$ , we have

$$\mathbb{E}_{f_0} \Pi(A_N | X^N) \leq \mathbb{E}_{f_0} [\Pi(A_N | X^N) (1 - \Psi_N) 1_{B_N}] + \mathbb{E}_{f_0} [\Psi_N 1_{B_N}] + \mathbb{P}_{f_0}(B_N^c).$$

Since the last two terms tend to zero by assumption, it remains to control the first term. We thus need only prove convergence in  $\mathbb{P}_{f_0}$ -probability to zero of

$$\Pi(A_N | X^N) (1 - \Psi_N) 1_{B_N} = \frac{\int_{A_N} \prod_{i=1}^N \frac{p_{f,D}(X_{(i-1)D}, X_{iD})}{p_{f_0,D}(X_{(i-1)D}, X_{iD})} d\Pi(f)}{\int_{\mathcal{F}} \prod_{i=1}^N \frac{p_{f,D}(X_{(i-1)D}, X_{iD})}{p_{f_0,D}(X_{(i-1)D}, X_{iD})} d\Pi(f)} (1 - \Psi_N) 1_{B_N}.$$

By Theorem 8, we have for any  $c > 0$  and any probability measure  $\nu$  supported on  $\mathcal{C}_N$ ,

$$\mathbb{P}_{f_0} \left( \int_{\mathcal{C}_N} \prod_{i=1}^N \frac{p_{f,D}(X_{(i-1)D}, X_{iD})}{p_{f_0,D}(X_{(i-1)D}, X_{iD})} \nu(df) \leq e^{-cN\varepsilon_N^2 - C_0NE_N} \right) \leq \frac{V_N}{c^2 N^2 \varepsilon_N^4}.$$

Let  $\nu = \Pi(\cdot \cap \mathcal{C}_N) / \Pi(\mathcal{C}_N)$  be the prior distribution conditioned to the set  $\mathcal{C}_N$ , and define the events

$$\Omega_N = \left\{ \int_{\mathcal{C}_N} \prod_{i=1}^N \frac{p_{f,D}(X_{(i-1)D}, X_{iD})}{p_{f_0,D}(X_{(i-1)D}, X_{iD})} d\Pi(f) \geq \Pi(\mathcal{C}_N) e^{-(C_0K_0+1)N\varepsilon_N^2} \geq e^{-(C+C_0K_0+1)N\varepsilon_N^2} \right\},$$

where we used  $\Pi(\mathcal{C}_N) \geq e^{-CN\varepsilon_N^2}$  in the last inequality. Setting  $c = 1$  and since  $E_N \leq K_0\varepsilon_N^2$  by assumption, the second last display implies  $\mathbb{P}_{f_0}(\Omega_N^c) \leq V_N / (N^2 \varepsilon_N^4) \rightarrow 0$  as  $N \rightarrow \infty$ . Thus for any  $\eta > 0$ ,

$$\begin{aligned} & \mathbb{P}_{f_0} (\Pi(A_N | X^N) (1 - \Psi_N) 1_{B_N} > \eta) \\ & \leq \mathbb{P}_{f_0} \left( e^{(C+C_0K_0+1)N\varepsilon_N^2} \int_{A_N} \prod_{i=1}^N \frac{p_{f,D}(X_{(i-1)D}, X_{iD})}{p_{f_0,D}(X_{(i-1)D}, X_{iD})} d\Pi(f) (1 - \Psi_N) 1_{B_N} > \eta \right) + \mathbb{P}_{f_0}(\Omega_N^c). \end{aligned}$$

By Fubini's theorem and since  $0 \leq 1 - \Psi_N \leq 1$ ,

$$\begin{aligned} & \mathbb{E}_{f_0} \int_{A_N} \prod_{i=1}^N \frac{p_{f,D}(X_{(i-1)D}, X_{iD})}{p_{f_0,D}(X_{(i-1)D}, X_{iD})} d\Pi(f) (1 - \Psi_N) 1_{B_N} \\ & = \int_{A_N} \mathbb{E}_f [(1 - \Psi_N) 1_{B_N}] d\Pi(f) \\ & \leq \Pi(\mathcal{F}_N^c) + \sup_{f \in \mathcal{F}_N: \|f - f_0\|_2 \geq M\xi_N} \mathbb{E}_f [(1 - \Psi_N) 1_{B_N}] \leq 2Le^{-(C+C_0K_0+2)N\varepsilon_N^2} \end{aligned}$$

using the assumptions on the tests  $\Psi_N$  and on  $\mathcal{F}_N$ . Combining the last two displays and using Markov's inequality gives for any  $\eta > 0$ ,

$$\mathbb{P}_{f_0}(\Pi(A_N|X^N)(1 - \Psi_N)1_{\mathcal{B}_N} > \eta) \leq 2\eta^{-1}Le^{-N\varepsilon_N^2} + \mathbb{P}_{f_0}(\Omega_N^c) \rightarrow 0$$

since  $N\varepsilon_N^2 \rightarrow \infty$  as  $N \rightarrow \infty$ .  $\square$

It therefore remains to show that the required tests in Lemma 24 exist under the conditions of Theorem 11. Setting  $\widehat{f}_N$  to be the projection estimator in (25), consider tests of the form

$$(55) \quad \Psi_N = \Psi_N(X_0, X_D, \dots, X_{ND}) = \{\|\widehat{f}_N - f_0\|_2 \geq \widetilde{M}\xi_N\},$$

where  $\widetilde{M} > 0$  is a large enough constant. The required properties then follow from Theorem 9.

**Lemma 25.** *Let  $\varepsilon_N, \xi_N \rightarrow 0$ ,  $2^J = 2^{J_N} \rightarrow \infty$  and  $R_{J,4}, R_{J,\infty}$  satisfy the conditions of of Theorem 9 and define the sets*

$$\mathcal{F}'_N = \{f \in \mathcal{F} : \|f\|_{\mathcal{C}^1} \leq r, \|f - \overline{P}_J f\|_2 \leq C\xi_N, \|f - \overline{P}_J f\|_4 \leq R_{J,4}, \|f - \overline{P}_J f\|_\infty \leq R_{J,\infty}\},$$

where  $C, r > 0$  and  $\overline{P}_J$  denotes the projection (23). Assume the true  $f_0 \in \mathcal{F}_0$  satisfies the same conditions as  $\mathcal{F}'_N$ , possibly up to different constants (e.g.  $\|f_0 - \overline{P}_J f_0\|_2 \leq M_0\xi_N$  for some  $M_0 > 0$ ). Then for any  $R > 0$ , one can take  $M, \widetilde{M} > 0$  large enough (depending also on  $R$ ) such that the tests  $\Psi_N$  in (55) satisfy

$$\mathbb{E}_{f_0}[\Psi_N 1_{\mathcal{B}_N}] \rightarrow 0, \quad \sup_{f \in \mathcal{F}'_N : \|f - f_0\|_2 \geq M\xi_N} \mathbb{E}_f[(1 - \Psi_N)1_{\mathcal{B}_N}] \leq C'e^{-RN\varepsilon_N^2},$$

where the event  $\mathcal{B}_N$  satisfies  $\sup_{f \in \mathcal{F}} \mathbb{P}_f(\mathcal{B}_N^c) \rightarrow 0$  as  $N \rightarrow \infty$ .

*Proof.* Consider the event  $\mathcal{B}_N$  in (44) and used in Theorem 9, which by Lemma 22 satisfies  $\mathbb{P}_{f_0}(\mathcal{B}_N) \rightarrow 1$  as  $N \rightarrow \infty$  since  $f_0 \in \mathcal{F}_0 \subset \mathcal{F}$ . Using the definition (55) of the test  $\Psi_N$ , that  $\|f_0 - \overline{P}_J f_0\|_2 \leq M_0\xi_N$  and the triangle inequality,

$$\mathbb{E}_{f_0}[\Psi_N 1_{\mathcal{B}_N}] \leq \mathbb{P}_{f_0}(\|\widehat{f}_N - \overline{P}_J f_0\|_2 \geq (\widetilde{M} - M_0)\xi_N, \mathcal{B}_N).$$

Since the conditions of Theorem 9 are satisfied, applying that theorem with  $\widetilde{M} > 0$  large enough bounds the right-hand side by  $C'e^{-N\varepsilon_N^2} \rightarrow 0$ , giving the first part of the lemma.

For the type-II errors, let  $f \in \mathcal{F}'_N$  satisfy  $\|f - f_0\|_2 \geq M\xi_N$  for some  $M > 0$  to be specified below. Then, since  $\|f - \overline{P}_J f\|_2 \leq C\xi_N$ ,

$$\begin{aligned} \mathbb{E}_f[(1 - \Psi_N)1_{\mathcal{B}_N}] &= \mathbb{P}_f(\|\widehat{f}_N - f_0\|_2 \leq \widetilde{M}\xi_N, \mathcal{B}_N) \\ &\leq \mathbb{P}_f(\|f_0 - f\|_2 - \|\widehat{f}_N - \overline{P}_J f\|_2 - \|f - \overline{P}_J f\|_2 \leq \widetilde{M}\xi_N, \mathcal{B}_N) \\ &\leq \mathbb{P}_f((M - \widetilde{M} - C)\xi_N \leq \|\widehat{f}_N - \overline{P}_J f\|_2, \mathcal{B}_N) \leq C'e^{-RN\varepsilon_N^2}, \end{aligned}$$

uniformly over such  $f$ , where the last inequality follows from Theorem 9 upon taking  $M = M(R, \widetilde{M}, C) > 0$  large enough.  $\square$

Theorem 11 then follows from using the tests in Lemma 25 together with Lemma 24.

**7.2. Proof of Theorem 3: contraction rates for Gaussian priors.** Let  $\|\cdot\|_{\mathbb{H}_W}$  denote the RKHS of  $W$ . Then  $\chi W$  in (11) is a mean-zero Gaussian process with RKHS  $\mathbb{H}_{\chi W} = \{\chi w : w \in \mathbb{H}_W\}$  and whose RKHS norm satisfies that for every  $w \in \mathbb{H}_W$ , there exists some  $w^* \in \mathbb{H}_W$  such that  $\chi w = \chi w^*$  and

$$\|\chi w\|_{\mathbb{H}_{\chi W}} = \|w^*\|_{\mathbb{H}_W}$$

(Exercise 2.6.5 of [28]). Furthermore, we have that  $\mathbb{H}_W = \mathbb{H}_V$  with RKHS norm  $\|\cdot\|_{\mathbb{H}_W} = \sqrt{N}\varepsilon_N\|\cdot\|_{\mathbb{H}_V}$ .

We require the following lemma about the concentration of Gaussian measures on suitable sieve sets. The proof is similar to Theorem 2.2.2 of [39] (see also Lemma 5.2(i) in [30]) and is hence omitted.

**Lemma 26.** For  $s, M > 0$  and the sequence  $\varepsilon_N = N^{-\frac{s}{2s+d}}$ , define the sets

$$(56) \quad \mathcal{W}_N = \{W = W_1 + W_2 : \|W_1\|_\infty \leq \varepsilon_N, \|W_2\|_{H^s} \leq M, \|W\|_{\mathcal{C}^4} \leq M\}.$$

Let  $W = V/(\sqrt{N}\varepsilon_N)$  for  $V \sim \Pi_V$  a mean-zero Gaussian process satisfying Condition 2. Then for every  $K > 0$ , there exists  $M > 0$  large enough such that  $\Pi_W(\mathcal{W}_N^c) \leq e^{-KN\varepsilon_N^2}$ .

*Proof of Theorem 3.* We verify the assumptions of Theorem 11 with  $\varepsilon_N = N^{-\frac{s}{2s+d}}$ ,  $\varepsilon_{k,N} = N^{-\frac{s-k}{2s+d}}$ ,  $k = 1, 2, 3$ , and  $2^J \simeq N^{\frac{1}{2s+d}}$  as in Assumption A.

*Small-ball probability:* consider the ‘‘small-ball condition’’ (ii) in Theorem 11. Recall that under the prior  $\Pi$  in (11),  $f = \Phi(\chi W)$  with  $W = V/(\sqrt{N}\varepsilon_N)$  for  $V$  a mean-zero Gaussian process and a strictly increasing link function  $\Phi$  satisfying  $\|\Phi^{(k)}\|_\infty < \infty$  for  $k = 1, 2, \dots$ . We first state some useful inequalities regarding the smoothness of compositions of functions. By Theorem 4.3(ii)(3) in [21], for any  $r \geq 1$ ,

$$(57) \quad \|\Phi(g)\|_{\mathcal{C}^r} \leq C_{r,d}\|\Phi\|_{\mathcal{C}^r}(1 + \|g\|_{\mathcal{C}^r}^r).$$

Using the multivariate version of Faà di Bruno’s formula [16], one can show that for any  $g, g_0 \in \mathcal{C}^k$  and integer  $k \geq 1$ ,

$$(58) \quad \|\Phi(g) - \Phi(g_0)\|_{\mathcal{C}^k} \leq C_{k,d} \max_{1 \leq j \leq k+1} \|\Phi^{(j)}\|_\infty (1 + \|g\|_{\mathcal{C}^k}^k + \|g_0\|_{\mathcal{C}^k}^k) \|g - g_0\|_{\mathcal{C}^k}$$

(see e.g. Lemma 2 in [49] for the proof of a similar argument).

Since  $f_0 \in \mathcal{C}^s$ , we have  $w_0 = \Phi^{-1}(f_0) \in \mathcal{C}^s$  by (57) [applied with  $\Phi^{-1}$  instead of  $\Phi$ ]. Similarly, since  $f_0 \in \mathcal{F}_0 \subseteq \mathcal{C}^\alpha(\mathcal{O})$  for  $\alpha = 4 \vee (2 \lfloor d/4 + 1/2 \rfloor)$  in (7), we may find  $r > 0$  large enough that  $\|w_0\|_{\mathcal{C}^\alpha} \leq r$ . Writing  $\Pi_W$  for the law of  $W$  under the prior, (57) and (58) together imply that

$$\begin{aligned} \Pi(\mathcal{C}_N) &= \Pi(f \in \mathcal{F} : \|f\|_{\mathcal{C}^\alpha} \leq r, \|f - f_0\|_\infty \leq \varepsilon_N, \|f - f_0\|_{\mathcal{C}^k} \leq \varepsilon_{k,N} \text{ for } k = 1, 2, 3) \\ &\geq \Pi_W(W \in \mathcal{C}^4(\mathcal{O}) : 1 + \|\chi W\|_{\mathcal{C}^\alpha}^\alpha \lesssim r, \|\chi W - w_0\|_\infty \lesssim \varepsilon_N, \\ &\quad (1 + r^{k/\alpha})\|\chi W - w_0\|_{\mathcal{C}^k} \lesssim \varepsilon_{k,N} \text{ for } k = 1, 2, 3), \end{aligned}$$

where the  $\lesssim$  above depend only on  $\Phi, d, \alpha$ . Under the theorem hypotheses, the last probability is lower bounded by

$$\begin{aligned} \Pi_W(W \in \mathcal{C}^4(\mathcal{O}) : \|\chi W - \chi v_{0,N}\|_{\mathcal{C}^\alpha} \lesssim r^{1/\alpha}, \|\chi W - \chi v_{0,N}\|_\infty \lesssim \varepsilon_N, \\ \|\chi W - \chi v_{0,N}\|_{\mathcal{C}^k} \lesssim r^{-k/\alpha} \varepsilon_{k,N} \text{ for } k = 1, 2, 3), \end{aligned}$$

possibly after replacing  $r > 0$  by a larger constant and then  $\varepsilon_{k,N}$  by a multiple of itself. Since  $\chi W$  is a mean-zero Gaussian process under the prior, and  $\chi v_{0,N} \in \mathbb{H}_{\chi W}$  is in its RKHS, Lemma I.27 of

[26] lower bounds the last display by

$$e^{-\frac{1}{2}\|\chi v_{0,N}\|_{\mathbb{H}_{\chi W}}^2} \Pi_W(W \in \mathcal{C}^4(\mathcal{O}) : \|\chi W\|_{\mathcal{C}^\alpha} \lesssim r^{1/\alpha}, \|\chi W\|_\infty \lesssim \varepsilon_N, \|\chi W\|_{\mathcal{C}^k} \lesssim r^{-k/\alpha} \varepsilon_{k,N} \text{ for } k = 1, 2, 3).$$

Note that  $\|\chi v_{0,N}\|_{\mathbb{H}_{\chi W}}^2 \leq N\varepsilon_N^2 \|v_{0,N}\|_{\mathbb{H}_V}^2 = O(N\varepsilon_N^2)$  using Exercise 2.6.5 of [28] and the assumption on  $v_{0,N}$ . Using the last display, that  $\chi \in \mathcal{C}^\infty$ ,  $W = V/\sqrt{N}\varepsilon_N$  and the Gaussian correlation inequality [51] (see Lemma A.2 in [30] for the exact formulation we use), we have

$$(59) \quad \begin{aligned} \Pi(\mathcal{C}_N) &\geq e^{-CN\varepsilon_N^2} \Pi_V(V \in \mathcal{C}^4(\mathcal{O}) : \|V\|_{\mathcal{C}^\alpha} \lesssim r^{1/\alpha} \sqrt{N}\varepsilon_N) \\ &\times \prod_{k=0}^3 \Pi_V(V \in \mathcal{C}^4(\mathcal{O}) : \|V\|_{\mathcal{C}^k} \lesssim r^{-k/\alpha} \sqrt{N}\varepsilon_N \varepsilon_{k,N}), \end{aligned}$$

for some  $C > 0$  and where above we have written  $\varepsilon_{0,N} = \varepsilon_N$ . It therefore suffices to lower bound each of the prior probabilities in (59).

For  $\mathbb{H}_{V,1}$  and  $H_1^s$  the unit balls of the RKHS  $\mathbb{H}_V$  and  $H^s$ , respectively, we have under Condition 2 that for integer  $k \geq 0$ ,

$$\log N(\mathbb{H}_{V,1}, \|\cdot\|_{\mathcal{C}^k}, \tau) \leq \log N(cH_1^s, \|\cdot\|_{\mathcal{C}^k}, \tau) \lesssim \tau^{-\frac{d}{s-k}}.$$

where the last inequality follows by arguing as in the proof of Theorem 4.3.36 in [28] as soon as  $s - k > d/2$ . Applying the small ball estimate in Theorem 1.2 of [35] (in particular, (1.3) in [35] with exponents  $\alpha = \frac{2d}{2(s-k)-d}$  and  $\beta = 0$ ), we have for  $s - k > d/2$ ,

$$\Pi_V(\|V\|_{\mathcal{C}^k} \leq \eta) \geq \exp\left(-c\eta^{-\frac{2d}{2(s-k)-d}}\right) \quad \text{as } \eta \rightarrow 0.$$

Using the last display with  $\eta_N = 1/(\log N)$  and  $k = \alpha$  shows that the first prior probability in (59) is greater than or equal to  $e^{-c(\log)^{\kappa}} \geq e^{-CN\varepsilon_N^2}$  for  $s > \alpha + d/2$ , any fixed  $r > 0$  and some  $\kappa > 0$ . In particular, it can be checked that the minimal smoothness  $s_{d,\alpha}^*$  in (13) assumed in the present theorem satisfies  $s_{d,\alpha}^* \geq \alpha + d/2$  for any dimension  $d \in \mathbb{N}$ , and hence this last condition is satisfied.

For the choice  $\varepsilon_{k,N} = N^{-\frac{s-k}{2s+d}}$ , we have  $\sqrt{N}\varepsilon_{0,N}\varepsilon_{k,N} = N^{-\frac{s-k-d/2}{2s+d}} \rightarrow 0$  for  $s > k + d/2$ . Using the last display with  $\eta = \eta_{k,N} = cr^{-k/\alpha} \sqrt{N}\varepsilon_{0,N}\varepsilon_{k,N}$  then yields

$$\prod_{k=0}^3 \Pi_V(\|V\|_{\mathcal{C}^k} \lesssim r^{-k/\alpha} \sqrt{N}\varepsilon_N \varepsilon_{k,N}) \geq \prod_{k=0}^3 \exp\left(-c\eta_{k,N}^{-\frac{2d}{2(s-k)-d}}\right) \geq \exp\left(-cr^{\frac{6d}{(2s-6-d)\alpha}} N\varepsilon_N^2\right)$$

taking  $r > 1$  and using that  $(\sqrt{N}\varepsilon_{0,N}\varepsilon_{k,N})^{-\frac{2d}{2(s-k)-d}} = N^{\frac{d}{2s+d}} = N\varepsilon_N^2$ . In particular, taking  $\varepsilon_N$  a large multiple of itself if necessary, the last display is lower bounded by  $e^{-CN\varepsilon_N^2}$  for any fixed  $r > 1$  and  $s > k + d/2$ . Together with (59), this gives the required lower bound  $\Pi(\mathcal{C}_N) \geq e^{-CN\varepsilon_N^2}$ , which verifies the small-ball condition (ii) in Theorem 11.

*Sieve sets:* consider the condition (i) in Theorem 11. For  $s$  as in this theorem and  $M > 0$ , let  $\mathcal{W}_N$  be the set defined in (56). For any  $K > 0$ , we can find  $M = M(K) > 0$  sufficiently large that  $\Pi_W(\mathcal{W}_N^c) \leq e^{-KN\varepsilon_N^2}$  by Lemma 26. In particular, let  $K > C + C_0K_0 + 2$  for  $C$  the constant in Theorem 11 coming from the small-ball condition (ii) just proved. Define

$$\mathcal{F}_n = \{f = \Phi(\chi w) : w \in \mathcal{W}_N\},$$

so that  $\Pi(\mathcal{F}_N^c) \leq e^{-KN\varepsilon_N^2}$  as required. Since  $w \in \mathcal{W}_N$  satisfies  $\|w\|_{\mathcal{C}^4} \leq M$ , we have  $\|\Phi(\chi w)\|_{\mathcal{C}^1} \leq C_d \|\Phi\|_{\mathcal{C}^1} (1 + \|\chi\|_{\mathcal{C}^1} \|w\|_{\mathcal{C}^1}) \leq C_{d,\Phi,\chi} (1 + M)$  using (57). To verify the bias conditions, we invoke Lemma 27 below with  $p = 2, 4, \infty$  to get that for all  $f \in \mathcal{F}_n$ ,

$$\|f - \bar{P}_J f\|_p \lesssim \varepsilon_N + C2^{-J(s-d/2+d/p-n)}(M + M^s) \lesssim 2^{-J(s-d/2+d/p-n)}$$

for any  $\eta > 0$  when  $p = 4$  or  $\infty$ , and  $\eta = 0$  when  $p = 2$ . Therefore, since  $2^{-Js} \simeq \varepsilon_N$ ,  $\mathcal{F}_N$  satisfies

$$\mathcal{F}_N \subseteq \{f \in \mathcal{F} : \|f\|_{\mathcal{C}^1} \lesssim 1, \|f - \overline{P}_J f\|_2 \lesssim \varepsilon_N, \|f - \overline{P}_J f\|_4 \lesssim R_{J,4}, \|f - \overline{P}_J f\|_\infty \lesssim R_{J,\infty}\}$$

for  $R_{J,4} \simeq 2^{-J(s-d/4-\eta)} \simeq N^{-\frac{s-d/4-\eta}{2s+d}}$  and  $R_{J,\infty} \simeq 2^{-J(s-d/2-\eta)} \simeq N^{-\frac{s-d/2-\eta}{2s+d}}$ , i.e. condition (i) in Theorem 11.

We lastly verify the numeric constraints on the sequence choices with also  $D = N^{-a}$ ,  $a \in (1/2, 1)$ . Since  $f_0 \in \mathcal{F}_0 \cap \mathcal{C}^s(\mathcal{O})$ , we have by similar arguments to the above that  $\|f_0 - \overline{P}_J f_0\|_2 \lesssim \varepsilon_N$  and  $\|f_0 - \overline{P}_J f_0\|_p \lesssim R_{J,p}$  for  $p \in \{4, \infty\}$ . The condition  $2^{Jd} \simeq N^{\frac{d}{2s+d}} = o(\sqrt{ND}) = o(N^{(1-a)/2})$  is equivalent to  $\frac{d(1+a)}{2(1-a)} < s$ . Turning to the quantitative conditions (26), for our sequence choices these reduce to

$$\begin{aligned} R_{J,4}^4 \varepsilon_N^2 &\lesssim D \xi_N^4 &\iff N^{\frac{a}{4} - \frac{3s/2-d/4-\eta}{2s+d}} &\lesssim \xi_N \\ R_{J,\infty}^2 \xi_N^2 \varepsilon_N^2 &\lesssim D \xi_N^4 &\iff N^{\frac{a}{2} - \frac{2s-d/2-\eta}{2s+d}} &\lesssim \xi_N \\ 2^{3Jd/2} N^{-1} + 2^{Jd/2} N^{-1/2} + 2^{Jd/2} \varepsilon_N^2 + \varepsilon_N &\lesssim \xi_N &\iff N^{-\frac{2s-d/2}{2s+d}} + N^{-\frac{s}{2s+d}} &\lesssim \xi_N \end{aligned}$$

Since  $s > d/2$  by assumption, we finally get rate

$$\xi_N \simeq N^{-\frac{s}{2s+d}} + N^{\frac{a}{4} - \frac{3s/2-d/4-\eta}{2s+d}} + N^{\frac{a}{2} - \frac{2s-d/2-\eta}{2s+d}},$$

i.e. the largest of the three conditions above. One can check that  $N^{-\frac{s}{2s+d}}$  is the largest term for  $s > \frac{d(1+a)}{2(1-a)}$ ,  $a \in (1/2, 1)$  and  $\eta > 0$  small enough.  $\square$

**Lemma 27.** For  $s > d/2 \vee 1$  and  $M > 0$ , let  $\mathcal{W}_N$  be the set (56). Let  $\Phi \in \mathcal{C}^\infty(\mathbb{R})$  be a link function,  $\chi \in \mathcal{C}^\infty(\mathcal{O})$  a smooth cutoff function such that  $\chi \equiv 1$  on  $K$  and  $\chi \equiv 0$  outside  $\mathcal{O}_0$ ,  $w \in \mathcal{W}_N$  and  $\overline{P}_J$  be the projection operator (23). Then for  $p \in [2, \infty]$ , any  $\eta > 0$  and  $w \in \mathcal{W}_N$ ,

$$\|\Phi \circ (\chi w) - \overline{P}_J[\Phi \circ (\chi w)]\|_p \leq C \varepsilon_N + C 2^{-J(s-d/2+d/p-\eta)} (M + M^s),$$

where  $C$  depends only on  $\Phi, \chi, p, s, d, \text{vol}(\mathcal{O}), \eta$  and the wavelet basis. If  $p = 2$ , we may further take  $\eta = 0$ .

*Proof.* Let  $w \in \mathcal{W}_N$  and write  $w = w_1 + w_2$  as in (56). Then for any  $x \in \mathcal{O}$ ,

$$\begin{aligned} (60) \quad |\Phi \circ (\chi w)(x) - 1 - P_J[\Phi \circ (\chi w) - 1](x)| &\leq |\Phi \circ (\chi w_1 + \chi w_2)(x) - \Phi \circ (\chi w_2)(x)| \\ &\quad + |\Phi \circ (\chi w_2)(x) - 1 - P_J[\Phi \circ (\chi w_2) - 1](x)| \\ &\quad + |P_J[\Phi \circ (\chi w_2) - 1](x) - P_J[\Phi \circ (\chi w_1 + \chi w_2) - 1](x)|. \end{aligned}$$

By the mean-value theorem, the first term in (60) is bounded by  $\|\Phi'\|_\infty \|\chi\|_\infty \|w_1\|_\infty$ . Let  $K_J(x, y) = 2^{Jd} \sum_{k \in \mathbb{Z}} \phi(2^J x - k) \phi(2^J y - k)$  denote the wavelet projection kernel on all of  $\mathbb{R}^d$ , where  $\phi$  is the Daubechies father wavelet. By the localization property of wavelets,  $\int_{\mathbb{R}^d} |K_J(x, y)| dy \lesssim 1$  for all  $x \in \mathbb{R}^d$ . Since the full  $L^2$ -projection operator  $\tilde{P}_J : L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$  onto  $\{\psi_{l,r} : l \leq J, r \in \mathbb{Z}^d\}$  satisfies  $\tilde{P}_J[g](x) = \int_{\mathbb{R}^d} K_J(x, y) g(y) dy$ , and  $P_J$  and  $\tilde{P}_J$  coincide for functions whose support is contained in  $\mathcal{O}_0$ , the third term in (60) can be expanded as

$$\begin{aligned} &|P_J[\Phi \circ (\chi w_2) - 1](x) - P_J[\Phi \circ (\chi w_1 + \chi w_2) - 1](x)| \\ &= \left| \int_{\mathbb{R}^d} K_J(x, y) (\Phi(\chi(y)w_2(y)) - \Phi(\chi(y)w_1(y) + \chi(y)w_2(y))) dy \right| \\ &\lesssim \|\Phi'\|_\infty \|\chi\|_\infty \|w_1\|_\infty \int_{\mathbb{R}^d} |K_J(x, y)| dy \lesssim \|w_1\|_\infty. \end{aligned}$$

Combining the bounds for (60), taking  $p^{th}$ -powers of everything and integrating over the bounded domain  $\mathcal{O}$  then yields

$$\|\Phi \circ (\chi w) - 1 - P_J[\Phi \circ (\chi w) - 1]\|_p^p \lesssim \|w_1\|_\infty^p + \|\Phi \circ (\chi w_2) - 1 - P_J[\Phi \circ (\chi w_2) - 1]\|_p^p.$$

Note that (60) equals zero for  $x \notin \mathcal{O}$ , and hence the  $L^p$ -norms in the last display can equivalently be considered over either  $\mathcal{O}$  or  $\mathbb{R}^d$ . Consider the latter, and let  $B_{pq}^t$  denote the usual Besov spaces over  $\mathbb{R}^d$ . Using the wavelet characterization of Besov spaces ([28], Chapter 4.3), the embedding  $B_{p1}^0(\mathbb{R}^d) \hookrightarrow L^p(\mathbb{R}^d)$  ((4.93) in [28]) and the usual decay bounds for wavelet projections, the second term in the last equation is bounded by a constant times

$$\|\Phi \circ (\chi w_2) - 1 - P_J[\Phi \circ (\chi w_2) - 1]\|_{B_{p1}^0}^p \lesssim 2^{-Jtp} \|\Phi \circ (\chi w_2) - 1\|_{B_{p1}^t}^p$$

for  $t > 0$ , with the obvious modifications if  $p = \infty$ . Using the embedding  $H^s(\mathbb{R}^d) = B_{22}^s(\mathbb{R}^d) \hookrightarrow B_{p1}^{s-d/2+d/p-\eta}$  for any  $p > 2$  and  $\eta > 0$  ([28], Proposition 4.3.10), we may set  $t = s - d/2 + d/p - \eta$  in the last display and replace the  $B_{p1}^t$ -norm by an  $H^s$ -norm. Since  $\Phi \in \mathcal{C}^\infty(\mathbb{R})$  and  $s > d/2 \vee 1$ , Theorem 4(i) of [55] yields  $\|\Phi \circ (\chi w_2) - 1\|_{H^s} \lesssim \|\chi w_2\|_{H^s} + \|\chi w_2\|_{H^s}^s \lesssim \|w_2\|_{H^s} + \|w_2\|_{H^s}^s$ . In summary, for  $p > 2$  we have

$$\|\Phi \circ (\chi w) - 1 - P_J[\Phi \circ (\chi w) - 1]\|_p \lesssim \|w_1\|_\infty + 2^{-J(s-d/2+d/p-\eta)} (\|w_2\|_{H^s} + \|w_2\|_{H^s}^s)$$

for any  $\eta > 0$ . The case  $p = 2$  follows similarly, but more easily. In particular, since  $H^t = B_{22}^t$  for  $t \in \mathbb{R}$ , we may avoid the use of embeddings and thus can obtain the same result with  $\eta = 0$ . Substituting in the bounds for  $w_1$  and  $w_2$  coming from the definition (56) of  $\mathcal{W}_N$  then gives the result.  $\square$

### 7.3. Proof of Corollaries 4 and 5: examples of Gaussian process priors.

*Proof of Corollary 4.* The Matérn process on all of  $\mathbb{R}^d$  has RKHS norm equal to  $\|\cdot\|_{\mathbb{H}_V} = \|\cdot\|_{H^s(\mathbb{R}^d)}$  ([26], Chapter 11), and hence its restriction to  $\mathcal{O}$  has RKHS norm equal to  $H^s(\mathcal{O})$  by Exercise 2.6.5 of [28]. Moreover, by Proposition I.4 of [26],  $V$  has a version whose sample paths are in  $\mathcal{C}^r(\mathcal{O})$   $\Pi$ -almost surely for any  $r < s - d/2$ . In particular,  $\mathcal{C}^r(\mathcal{O})$  is a separable linear subspace of  $\mathcal{C}^4(\mathcal{O})$  for any  $r > 4$ , a suitable choice of which exists as soon as  $s > d/2 + 4$ . The Matérn process thus satisfies Condition 2 for  $s > d/2 + 4$  since its RKHS norm equals the  $H^s(\mathcal{O})$ -norm.

We may therefore apply Theorem 3 to the Matérn process when  $f_0 \in \mathcal{C}^s(\mathcal{O})$ . Indeed, since  $w_0 = \Phi^{-1}(f_0) \in \mathcal{C}^s(\mathcal{O})$  by (57) (which applies also to  $\Phi^{-1}$ ) and  $\text{supp}(w_0) \subseteq K$ , we may take the constant sequence  $v_{0,N} = w_0 \in H^s(\mathcal{O}) = \mathbb{H}_V$ , which trivially satisfies the conditions (i)-(iii) in Theorem 3.  $\square$

*Proof of Corollary 5.* The Gaussian wavelet series prior (14) has RKHS equal to

$$\mathbb{H}_V = \left\{ h = \sum_{l=J_0}^J \sum_{r \in R_l} h_{lr} \psi_{lr} : \|h\|_{\mathbb{H}_V}^2 = \sum_{l=J_0}^J \sum_{r \in R_l} 2^{2ls} h_{lr}^2 < \infty \right\},$$

with  $\|h\|_{\mathbb{H}_V} = \infty$  if  $h$  is not a truncated sum up to level  $J$ . Hence  $\mathbb{H}_V \hookrightarrow H^s(\mathcal{O})$  by the wavelet characterization of  $L^2$ -Sobolev norms. Draws from the prior (14) are finite sums of wavelets  $(\psi_{lr})$ , hence  $V$  will almost surely have the same Hölder smoothness as  $(\psi_{lr})$ . Thus taking a smooth enough wavelet basis, we have that  $V$  is supported on a separable linear subspace of  $\mathcal{C}^4(\mathcal{O})$ , thereby satisfying Condition 2.

We may therefore apply Theorem 3. For  $f_0 \in \mathcal{C}^s(\mathcal{O})$ ,  $w_0 = \Phi^{-1}(f_0) \in \mathcal{C}^s(\mathcal{O})$  by (57) (which applies also to  $\Phi^{-1}$ ) and  $\text{supp}(w_0) \subseteq K \subseteq \mathcal{O}_0$ . Set

$$v_{0,N}(x) = \sum_{l=J_0}^J \sum_{r \in R_l} \langle w_0, \psi_{lr} \rangle_2 \psi_{lr}(x),$$

the wavelet projection at resolution level  $J$ . In particular,  $\|v_{0,N}\|_{\mathbb{H}_V} \simeq \|v_{0,N}\|_{H^s} \leq \|w_0\|_{H^s} < \infty$ . Moreover, using that  $w_0 = \chi w_0$  and the standard Besov space embeddings  $B_{\infty\infty}^r \hookrightarrow \mathcal{C}^r \hookrightarrow B_{\infty 1}^r$  for all  $r \geq 0$ , we have

$$\begin{aligned} \|w_0 - \chi v_{0,N}\|_{\mathcal{C}^k} &\lesssim \|w_0 - v_{0,N}\|_{\mathcal{C}^k} \lesssim \sum_{l=J+1}^{\infty} 2^{l(k+d/2)} \max_{r \in R_l} |\langle w_0, \psi_{lr} \rangle_2| \\ &\lesssim \|w_0\|_{B_{\infty\infty}^s} \sum_{j=J+1}^{\infty} 2^{-l(s-k)} \lesssim \|w_0\|_{\mathcal{C}^s} 2^{-J(s-k)} \lesssim N^{-\frac{s-k}{2s+d}} \end{aligned}$$

since  $2^J \simeq N^{\frac{1}{2s+d}}$ . Together these verify conditions (i)-(iii) of Theorem 3, thereby giving the desired result.  $\square$

## 8. HEAT KERNEL ESTIMATES IN SMALL TIME

In this section, we use various estimates for the transition densities of diffusions to study the expectation and variance of the integrated log-likelihood process  $\Lambda_{p,D}^N$  in Theorem 8. For terms near the boundary (the events  $(\mathcal{A}_{i,D})^c$ ), it suffices to use upper and lower bounds of the same order. Combining the upper bound from Theorem 3.2.9 of [20] with the lower bound from Theorem 3.1 of [17], one has that for  $x, y \in \mathcal{O}$ , the transition densities of  $(X_t)$  generated by (1) satisfy:

$$(61) \quad c_f^- D^{-d/2} \exp\left(-C_f^- \frac{|y-x|^2}{D}\right) \leq p_{f,D}(x, y) \leq c_f^+ D^{-d/2} \exp\left(-C_f^+ \frac{|y-x|^2}{D}\right),$$

where these estimates are *uniform* over  $f \in \mathcal{C}_N \subset \{f : f \geq f_{\min}, \|f\|_{\mathcal{C}^\alpha} \leq r\}$  for any positive even integer  $\alpha > d/2 - 1$ , see also the proof of Proposition 4 of [40]. In particular, the smallest such integer is  $2 \lfloor d/4 + 1/2 \rfloor$ , which is exactly the minimal smoothness assumption used to define  $\alpha = \alpha_d$  in (7). For the main terms in the interior of  $\mathcal{O}$  (the events  $\mathcal{A}_{i,D}$ ), we will require more precise estimates, which are developed in Section 8.4 below.

**8.1. Proof of Lemma 12.** Using (61), we have

$$\log \frac{c_{f_0}^-}{c_f^+} - (C_{f_0}^- - C_f^+) \frac{|y-x|^2}{D} \leq \log \frac{p_{f_0,D}(x, y)}{p_{f,D}(x, y)} \leq \log \frac{c_{f_0}^+}{c_f^-} - (C_{f_0}^+ - C_f^-) \frac{|y-x|^2}{D},$$

which implies for  $k = 1, 2$ ,

$$\left( \log \frac{p_{f_0,D}(x, y)}{p_{f,D}(x, y)} \right)^k p_{f_0,D}(x, y) \leq (c_{f_0,f} + C_{f_0,f} \frac{|y-x|^{2k}}{D^k}) D^{-d/2} \exp\left(-C_{f_0}^+ \frac{|y-x|^2}{D}\right)$$

for all  $x, y \in \mathcal{O}$ . Since all constants above are uniform over  $\mathcal{F}^l$  by (61), so too are all constants below, which will not be explicitly mentioned. For  $\gamma > 0$ , the region of the integral such that

$|y - x| \geq \gamma\sqrt{D \log N}$  thus satisfies

$$(62) \quad \int_{x \in \mathcal{O} \setminus \mathcal{O}_0^{\delta/2}, |y-x| \geq \gamma\sqrt{D \log N}} \left( \log \frac{p_{f_0, D}(x, y)}{p_{f, D}(x, y)} \right)^k p_{f_0, D}(x, y) dx dy \leq C_{f, f_0} D^{-d/2} (1 + \gamma^{2k} (\log N)^k) N^{-C_{f_0}^+ \gamma^2}.$$

Using that  $\log(1+z) \leq |z|$  for  $z \geq -1$  and (61), for  $k = 1$ ,

$$\log \frac{p_{f_0, D}(x, y)}{p_{f, D}(x, y)} p_{f_0, D}(x, y) \leq |p_{f, D}(x, y) - p_{f_0, D}(x, y)| \frac{p_{f_0, D}(x, y)}{p_{f, D}(x, y)} \leq \frac{c_{f_0}^+}{c_f} |p_{f, D}(x, y) - p_{f_0, D}(x, y)| \exp \left( (C_f^- - C_{f_0}^+) \frac{|y-x|^2}{D} \right).$$

Similarly for  $k = 2$ ,

$$\begin{aligned} & \left( \log \frac{p_{f_0, D}(x, y)}{p_{f, D}(x, y)} \right)^2 \\ & \leq \frac{(p_{f, D}(x, y) - p_{f_0, D}(x, y))^2}{\min(p_{f, D}(x, y), p_{f_0, D}(x, y))^2} \\ & \leq (p_{f, D}(x, y) - p_{f_0, D}(x, y))^2 \min(c_f^-, c_{f_0}^-)^{-2} D^d \exp \left( 2 \max(C_f^+, C_{f_0}^+) \frac{|y-x|^2}{D} \right) \\ & \leq C'_{f, f_0} |p_{f, D}(x, y) - p_{f_0, D}(x, y)| D^{d/2} \exp \left( C_{f, f_0} \frac{|y-x|^2}{D} \right) \end{aligned}$$

using the rough bound

$$(p_{f, D}(x, y) - p_{f_0, D}(x, y))^2 \leq |p_{f, D}(x, y) - p_{f_0, D}(x, y)| (p_{f, D}(x, y) + p_{f_0, D}(x, y))$$

with (61). Therefore, for  $y$  such that  $|y - x| \leq \gamma\sqrt{D \log N}$ , we obtain

$$(63) \quad \int_{x \in \mathcal{O} \setminus \mathcal{O}_0^{\delta/2}, |y-x| \leq \gamma\sqrt{D \log N}} \left( \log \frac{p_{f_0, D}(x, y)}{p_{f, D}(x, y)} \right)^k p_{f_0, D}(x, y) dx dy \leq C_{f, f_0} N^{C'_{f, f_0} \gamma^2} \int_{x \in \mathcal{O} \setminus \mathcal{O}_0^{\delta/2}} \|p_{f, D}(x, \cdot) - p_{f_0, D}(x, \cdot)\|_{TV} dx,$$

where  $\|\cdot\|$  denote total variation norm and  $p_{f, D}(x, \mathcal{A}) = \int_{\mathcal{A}} p_{f, D}(x, y) dy$  for any Borel  $\mathcal{A} \subset \mathcal{O}$  with a slight abuse of notation. Thanks to Lemma 28 right below, the last display is then bounded by  $C_{f, f_0, \delta} N^{C'_{f, f_0} \gamma^2} \exp(-c_\delta D^{-1})$ , which completes the proof.

**8.2. The behaviour of the transition density near the boundary.** The following lemma shows that the transition densities for different functions in  $\mathcal{F}$  are similar for points near the boundary.

**Lemma 28.** *For  $x \in \mathcal{O} \setminus \mathcal{O}_0^\delta$  and  $f, f_0 \in \mathcal{F}$ , it holds that*

$$\|p_{f, D}(x, \cdot) - p_{f_0, D}(x, \cdot)\|_{TV} \leq \frac{16}{\sqrt{\pi\delta}} e^{-\delta^2/(16D)}.$$

*Proof.* Write  $\mathbb{P}_x^f$  for the law of the solution  $X$  to (1) with conductivity  $f$  conditional on  $X_0 = x$ . Let  $\tau = \inf\{t \geq 0, X_t \in \partial\mathcal{O}_0\}$  denote the hitting time of the boundary of  $\mathcal{O}_0$ . For a Borel set  $\mathcal{A} \subset \mathcal{O}$ , by the strong Markov property,

$$p_{f, D}(x, \mathcal{A}) = \mathbb{E}_x^f[\mathbf{1}_{\{X_D \in \mathcal{A}\}} \mathbf{1}_{\{\tau > D\}}] + \mathbb{E}_x^f[p_{f, D-\tau}(X_\tau, \mathcal{A}) \mathbf{1}_{\{\tau \leq D\}}].$$

Since  $x \in \mathcal{O} \setminus \mathcal{O}_0^\delta$ , we have

$$\mathbb{E}_x^f[\mathbf{1}_{\{X_D \in \mathcal{A}\}} \mathbf{1}_{\{\tau > D\}}] = \mathbb{E}_x^{f_0}[\mathbf{1}_{\{X_D \in \mathcal{A}\}} \mathbf{1}_{\{\tau > D\}}]$$

since the functions  $f$  and  $f_0$  coincide on  $\mathcal{O} \setminus \mathcal{O}_0$ . It follows that

$$(64) \quad \|p_{f,D}(x, \cdot) - p_{f_0,D}(x, \cdot)\|_{TV} \leq 2\mathbb{P}_x(\tau \leq D).$$

Here, for  $x \in \mathcal{O} \setminus \mathcal{O}_0^\delta$ , the hitting time  $\tau$  of the boundary of  $\mathcal{O}_0$  by the process  $(x + \sqrt{2}B_t + \ell_t)_{t \geq 0}$  has law that does not depend on  $f$  nor  $f_0$ . Introduce now the two stopping times  $0 \leq S \leq T$ :

$$S = \inf\{t \geq 0, X_t \in \partial\mathcal{O}_0^\delta\}, \quad T = \inf\{t \geq S, |X_t - X_S| \geq \delta\},$$

the first hitting time of the boundary  $\partial\mathcal{O}_0^\delta$  and the first exit time of the ball of center  $X_S$  and radius  $\delta/2$ , respectively. Necessarily,

$$\{\tau \leq D\} \subset \left\{ \sup_{0 \leq t \leq D} |X_{(t+S) \wedge T} - X_S| = \delta/2 \right\}.$$

Moreover, the process  $(X_{(t+S) \wedge T} - X_S)_{t \geq 0}$  has the same law as  $(\sqrt{2}B_{t \wedge T})_{t \geq 0}$ . It follows that

$$\begin{aligned} \mathbb{P}_x(\tau \leq D) &\leq \mathbb{P}_x \left( \sup_{0 \leq t \leq D} |B_{t \wedge T}| \geq \delta/2^{3/2} \right) \leq \mathbb{P}_x \left( \sup_{0 \leq t \leq D} |B_t| \geq \delta/2^{3/2} \right) \\ &\leq 4\mathbb{P}_x \left( B_D \geq \delta/2^{3/2} \right) \leq \frac{4}{\sqrt{2\pi}} \frac{2^{3/2}}{\delta} \exp \left( -\frac{\delta^2}{16D} \right), \end{aligned}$$

where the third inequality follow from the reflection principle for Brownian motion and the last inequality from the standard Gaussian tail bound. Combining (64) with the last display proves the lemma.  $\square$

**8.3. Proof of Lemma 13.** Let  $g = f$  or  $f_0$  in the notation below. For  $\tilde{p}_{g,D}(x, y)$ , an estimate of the kind (61) is classical (see e.g. [5, 24] for diffusion processes over the whole space  $\mathbb{R}^d$ ). Using the analogous estimate to (61), one can then argue exactly as in the proof of Lemma 12, again splitting the integral according to whether  $|y - x| \leq \gamma\sqrt{D \log N}$  or not. In particular, using the analogues of (62) and (63), one gets for  $k = 1, 2$  and any  $\gamma > 0$ ,

$$\begin{aligned} &\int_{x \in \mathcal{O}_0^\delta, y \in \mathcal{O}} \left( \log \frac{p_{g,D}(x, y)}{\tilde{p}_{g,D}(x, y)} \right)^k p_{f_0,D}(x, y) dx dy \\ &\leq C_{g,f_0} D^{-d/2} (1 + \gamma^{2k} (\log N)^k) N^{-C_{f_0}^+ \gamma^2} + C_{g,f_0} N^{C'_{g,f_0} \gamma^2} \int_{x \in \mathcal{O}_0^\delta} \|p_{g,D}(x, \cdot) - \tilde{p}_{g,D}(x, \cdot)\|_{TV} dx, \end{aligned}$$

where the constants are uniform over  $\mathcal{F}$ ,  $\|\cdot\|_{TV}$  denotes total variation distance on  $\mathbb{R}^d$ , and we implicitly extend  $p_{g,D}(x, \cdot)$  into a probability measure on  $\mathbb{R}^d$  by setting  $p_{g,D}(x, \mathcal{A}) = p_{g,D}(x, \mathcal{A} \cap \mathcal{O})$  for any Borel set  $\mathcal{A}$  in  $\mathbb{R}^d$ . We claim that

$$(65) \quad \|p_{g,D}(x, \cdot) - \tilde{p}_{g,D}(x, \cdot)\|_{TV} \leq 4d \exp \left( -\frac{\delta^2}{20d \|g\|_\infty D} \right)$$

for  $x \in \mathcal{O}_0^\delta$  and any  $g \in \mathcal{F}$  with  $D < D_0(\delta, \|g\|_{e^1})$  small enough. By (65) the second last display is then bounded by

$$C_{g,f_0} D^{-d/2} (1 + \gamma^{2k} (\log N)^k) N^{-C_{f_0}^+ \gamma^2} + C_{g,f_0} N^{C'_{g,f_0} \gamma^2} \exp(-c_{|g|_\infty, \delta} D^{-1}),$$

which completes the proof. It thus remains to prove (65). Let  $x \in \mathcal{O}_0^\delta$  and  $\tilde{\tau} = \inf\{t \geq 0, \tilde{X}_t \in \partial\mathcal{O}\}$  be the hitting time of the boundary  $\partial\mathcal{O}$ . For any Borel set  $\mathcal{A}$  in  $\mathbb{R}^d$ , by the strong Markov property,

$$\begin{aligned} p_{g,D}(x, \mathcal{A}) &= \mathbb{E}_g[\mathbf{1}_{\{X_D \in \mathcal{A}\}} \mathbf{1}_{\{\tilde{\tau} > D\}} | X_0 = x] + \mathbb{E}_g[p_{g,D-\tilde{\tau}}(X_{\tilde{\tau}}, \mathcal{A} \cap \mathcal{O}) \mathbf{1}_{\{\tilde{\tau} \leq D\}} | X_0 = x] \\ &= \tilde{p}_{g,D}(x, \mathcal{A}) - \mathbb{E}_g[\mathbf{1}_{\{\tilde{X}_D \in \mathcal{A}\}} \mathbf{1}_{\{\tilde{\tau} \leq D\}} | X_0 = x] + \mathbb{E}_g[p_{g,D-\tilde{\tau}}(X_{\tilde{\tau}}, \mathcal{A} \cap \mathcal{O}) \mathbf{1}_{\{\tilde{\tau} \leq D\}} | X_0 = x], \end{aligned}$$

since  $X_t$  and  $\tilde{X}_t$  both started at  $x \in \mathcal{O}_0^\delta$  at  $t = 0$  coincide until they hit the boundary  $\partial\mathcal{O}$ . It follows that

$$\|p_{g,D}(x, \cdot) - \tilde{p}_{g,D}(x, \cdot)\|_{TV} \leq 2\mathbb{P}_g(\tilde{\tau} \leq D | X_0 = x).$$

We conclude thanks to Lemma 20.

**8.4. Proof of Lemma 21: approximating transition densities for small-time.** We rely on a key second-order estimate of the heat kernel in small time, associated to the metric tensor  $g_{ij}(x) = f(x)^{-1} \delta_{ij}$  induced by the diffusion matrix  $f(x)^{-1} \text{Id}$  on  $\mathbb{R}^d$ , viewed as a Riemannian manifold. For  $x, y \in \mathbb{R}^d$ , let

$$\ell_f(x, y) = \inf \left\{ \int_0^1 \frac{|\dot{\gamma}_t|}{f(\gamma_t)^{1/2}} dt, \gamma_0 = x, \gamma_1 = y \right\}$$

denote the Riemannian geodesic distance between  $x$  and  $y$ , where the infimum is taken over all smooth paths  $\gamma : [0, 1] \rightarrow \mathbb{R}^d$  connecting  $x$  and  $y$  at times 0 and 1, and  $\dot{\gamma}_t$  is the time derivative of  $\gamma_t$ .

**Lemma 29.** *The following small time expansion holds:*

$$\tilde{p}_{f,D}(x, y) = \frac{1}{(4\pi D)^{d/2}} \exp\left(-\frac{1}{4D} \ell_f(x, y)^2\right) (\alpha_f(x, y) + \beta_f(x, y)D + D^2 \Gamma_{f,D}(x, y)),$$

where

$$(66) \quad \|\alpha_f\|_\infty + \|\beta_f\|_\infty + \sup_{D>0} \|\Gamma_{f,D}\|_\infty \lesssim 1,$$

and the  $\|\cdot\|_\infty$ -norm is taken for  $(x, y) \in \mathcal{O}$  and the estimates are uniform over  $f \in \mathcal{C}_N$ . Moreover, there exist smooth functions

$$\alpha, \beta : \mathbb{R} \rightarrow \mathbb{R}, \quad \alpha^i, \beta^i : \mathbb{R}^2 \rightarrow \mathbb{R}, \quad \alpha^{ij}, \beta^{ij} : \mathbb{R}^3 \rightarrow \mathbb{R}, \quad \alpha^{ijk}, \beta^{ijk} : \mathbb{R}^4 \rightarrow \mathbb{R},$$

for  $1 \leq i, j, k \leq d$ , independent of  $f$ , such that

$$\begin{aligned} \alpha_f(x, y) &= \alpha(f(x)) + \sum_{i=1}^d \alpha^i(f(x), \partial_i f(x)) (x^i - y^i) \\ &\quad + \sum_{i,j=1}^d \alpha^{ij}(f(x), \partial_i f(x), \partial_j^2 f(x)) (x^i - y^i)(x^j - y^j) \\ &\quad + \sum_{i,j,k=1}^d \alpha^{ijk}(f(x), \partial_i f(x), \partial_j^2 f(x), \partial_{ijk}^3 f(x)) (x^i - y^i)(x^j - y^j)(x^k - y^k) \\ (67) \quad &\quad + |x - y|^4 r_f(x, y), \end{aligned}$$

where  $x = (x^1, \dots, x^d), y = (y^1, \dots, y^d)$  and the remainder term satisfies  $\|r_f\|_\infty \lesssim 1$ , uniformly in  $f \in \mathcal{C}_N$  with the supremum taken over  $(x, y) \in \mathcal{O} \times \mathcal{O}$ . Moreover,

$$(68) \quad \alpha(f(x)) = f(x)^{-d/2}.$$

The same expansion holds for  $\beta_f$  (except for (68)) with functions  $\beta, \beta^i, \beta^{ij}, \beta^{ijk}$  and a remainder term  $\tilde{r}_f$  satisfying the same property as  $r_f$ .

The existence of a small time expansion of the heat kernel in the first part of the lemma is classical, see e.g. [11]. The robust estimates (66) follows from the main result of Azencott [6]. The second part uses the strategy of Bilal [13] in order to mix small time and space expansions, which is the key idea to control the density near the diagonal in small time.

*Proof.* Consider the Fokker-Planck equation

$$\partial_t \rho_t + \operatorname{div}(b_f \rho_t) = \frac{1}{2} \sum_{i,j=1}^d \partial_{ij}^2 ((\sigma_f \sigma_f^\top)_{ij} \rho_t)$$

with initial value  $\rho_0(dy)$  as a probability distribution. In our case,  $b_f = \nabla f$  and  $(\sigma_f \sigma_f^\top)_{ij} = 2f \delta_{ij}$ , yielding

$$\partial_t \rho_t = \Delta(f \rho_t) - \operatorname{div}(\nabla f \rho_t) =: \mathcal{D}_f \rho_t,$$

where

$$\mathcal{D}_f \phi = \Delta(f \phi) - \sum_{i=1}^d \partial_i (\partial_i f \phi) = f \Delta \phi + \nabla f \cdot \nabla \phi.$$

Whenever existence and uniqueness hold, the solution is given by  $\rho_t(y) = \int_{\mathcal{O}} \tilde{p}_{f,t}(x, y) \rho_0(dx)$ , where  $\tilde{p}_{f,t}(x, y)$  is the Markov transition density we are looking to expand. Rewriting  $\tilde{p}_{f,t}(x, y)$  as  $f(x)^{-d/2} K_t(x, y)$ , this satisfies the Fokker-Planck equation if

$$\partial_t K_t(x, \cdot) = \mathcal{D}_f K_t(x, \cdot)$$

with  $K_t(x, y) \rightarrow f(x)^{d/2} \delta_x(dy)$  weakly as  $t \rightarrow 0$ . Our ansatz for the heat kernel takes the form  $K_t(x, y) \sim K_t^0(x, y) \sum_{r=0}^{\infty} F_r(x, y) t^r$ , where

$$K_t^0(x, y) = \frac{1}{(4\pi t)^{d/2}} \exp\left(-\frac{\ell_f(x, y)^2}{4t}\right)$$

and  $a_t \sim \sum_{r \geq 0} b_r t^r$  means  $a_t = \sum_{r=0}^k b_r t^r + O(t^{k+1})$ . It remains to find a formula for the so-called De Witt coefficients  $F_r(x, y)$  for  $r = 0, 1$  that is compatible with the expansion (67) via the representation  $\alpha_f(x, y) = f(x)^{-d/2} F_0(x, y)$  and  $\beta_f(x, y) = f(x)^{-d/2} F_1(x, y)$ , and we can then conclude with Azencott's result. Define now the operators

$$(69) \quad \mathcal{A}_f \phi = (2f \nabla \ell_f^2) \cdot \nabla \phi + (f \Delta \ell_f^2 - 2d + \nabla f \cdot \nabla \ell_f^2) \phi,$$

$$(70) \quad \mathcal{B}_f \phi = 4\Delta \phi + 2d \nabla f \nabla \phi.$$

Following Bilal [13], we have a recursion formula that gives  $F_0$  and  $F_1$  as solutions of the following system of differential equations (in the  $y$  variable)

$$\mathcal{A}_f F_0 = 0, \quad (\mathcal{A}_f + 8) F_1 = \mathcal{B}_f F_0, \quad F_0(x, x) = 1.$$

We further expand  $F_r(x, y)$ ,  $r = 0, 1$ , via

$$\begin{aligned} F_r(x, y) &= a_r(x) + \sum_{i=1}^d b_{i,r}(x)(x^i - y^i) + \sum_{i,j=1}^d c_{ij,r}(x)(x^i - y^i)(x^j - y^j) \\ &\quad + \sum_{i,j,k=1}^d d_{ijk,r}(x)(x^i - y^i)(x^j - y^j)(x^k - y^k) + O(|x - y|^4), \end{aligned}$$

for smooth functions  $a_r, b_r, c_r$  and  $d_r$ . An inspection of (69) and (70) shows that after a suitable asymptotic expansion of  $\nabla \ell_f^2$  and  $\Delta \ell_f^2$  around  $x$  in the  $y$  variable, the symbols of  $\mathcal{A}_f$  and  $\mathcal{B}_f$  only involve smooth local functions of  $f(x), \partial_i f(x), \partial_{ij}^2 f(x)$  and  $\partial_{ijk}^3 f(x)$  with increasing differentiation order. This implies

$$\begin{aligned} a_r(x) &= \tilde{a}_r(f(x)), b_{i,r}(x) = \tilde{b}_{i,r}(f(x), \partial_i f(x)), \\ c_{ij,r}(x) &= \tilde{c}_r(f(x), \partial_i f(x), \partial_{ij}^2 f(x)), d_{ijk,r}(x) = \tilde{d}_{r,ijk}(f(x), \partial_i f(x), \partial_{ij}^2 f(x), \partial_{ijk}^3 f(x)) \end{aligned}$$

for smooth functions  $\tilde{a}_r, \tilde{b}_r, \tilde{c}_r$  and  $\tilde{d}_r$  and proves the lemma.  $\square$

*Completion of the proof of Lemma 21.* Using Lemma 29, and a first-order Taylor's expansion, write

$$(71) \quad \begin{aligned} \log \frac{\tilde{p}_{f_0,D}(x,y)}{\tilde{p}_{f,D}(x,y)} &= -\frac{1}{4D}(\ell_{f_0}(x,y)^2 - \ell_f(x,y)^2) + \log \frac{\alpha_{f_0}(x,y)}{\alpha_f(x,y)} \\ &+ \left( \frac{\beta_{f_0}(x,y)}{\alpha_{f_0}(x,y)} - \frac{\beta_f(x,y)}{\alpha_f(x,y)} \right) D + D^2 \Gamma'_{f_0,f,D}(x,y), \end{aligned}$$

where  $\sup_{f \in \mathcal{C}_N} \sup_{D > 0} \|\Gamma'_{f_0,f,D}\|_\infty \lesssim 1$ , thanks to (66), (68) and  $f(y) \geq f_{\min} > 0$  on  $\mathcal{O}$ . The linear term in  $D$  can be rewritten as

$$\frac{\beta_{f_0}(x,y)}{\alpha_{f_0}(x,y)} - \frac{\beta_f(x,y)}{\alpha_f(x,y)} = \frac{\beta_{f_0}(x,y) - \beta_f(x,y)}{\alpha_{f_0}(x,y)} + (\alpha_f(x,y) - \alpha_{f_0}(x,y)) \frac{\beta_f(x,y)}{\alpha_{f_0}(x,y)\alpha_f(x,y)}.$$

Using (67),

$$\begin{aligned} \alpha_f(x,y) - \alpha_{f_0}(x,y) &= \alpha(f(x)) - \alpha(f_0(x)) \\ &+ \sum_{i=1}^d \left( \alpha^i(f(x), \partial_i f(x)) - \alpha^i(f_0(x), \partial_i f_0(x)) \right) (x^i - y^i) \\ &+ |x - y|^2 r'_{f_0,f}(x,y), \end{aligned}$$

with  $\|r'_{f_0,f}\|_\infty \leq C(\|f\|_{\mathcal{C}^3}, \|f_0\|_{\mathcal{C}^3})$ . Using the same inequality for  $\beta_f(x,y) - \beta_{f_0}(x,y)$  and that  $\alpha, \beta, \alpha^i, \beta^i$  and  $\alpha^{ij}, \beta^{ij}$  are smooth,

$$|\alpha_f(x,y) - \alpha_{f_0}(x,y)| + |\beta_f(x,y) - \beta_{f_0}(x,y)| \lesssim \|f - f_0\|_\infty + \|f - f_0\|_{\mathcal{C}^1} |x - y| + |x - y|^2,$$

with the constant depending only on an upper bound for  $\|f\|_{\mathcal{C}^3}$  and  $\|f_0\|_{\mathcal{C}^3}$ . Using the expansion for  $\alpha_f(x,y)$  in Lemma 29, (68) and that  $f \geq f_{\min}$ , we have that  $\alpha_f(x,y), \alpha_{f_0}(x,y) \geq c > 0$ , uniformly over  $\mathcal{C}_N$ . It follows that

$$(72) \quad \left| \frac{\beta_{f_0}(x,y)}{\alpha_{f_0}(x,y)} - \frac{\beta_f(x,y)}{\alpha_f(x,y)} \right| \leq (\|f - f_0\|_\infty + \|f - f_0\|_{\mathcal{C}^1} |x - y| + |x - y|^2) r''_{f,f_0}(x,y),$$

with  $\sup_{f \in \mathcal{C}_N} \|r''_{f,f_0}\|_\infty \lesssim 1$ .

Next, writing  $\tilde{\alpha}_f(x,y) = f(y)^{d/2} \alpha_f(x,y)$  and  $\tilde{\alpha}_{f_0}(x,y) = f_0(y)^{d/2} \alpha_{f_0}(x,y)$ ,

$$(73) \quad \log \frac{\alpha_{f_0}(x,y)}{\alpha_f(x,y)} = \frac{d}{2} \log \frac{f(x)}{f_0(x)} + \log \tilde{\alpha}_{f_0}(x,y) - \log \tilde{\alpha}_f(x,y).$$

Using the expansion (67),

$$\begin{aligned}\tilde{\alpha}_f(x, y) &= 1 + \sum_{i=1}^d \tilde{\alpha}^i(f(x), \partial_i f(x))(x^i - y^i) \\ &\quad + \sum_{i,j=1}^d \tilde{\alpha}^{ij}(f(x), \partial_i f(x), \partial_{ij}^2 f(x))(x^i - y^i)(x^j - y^j) \\ &\quad + \sum_{i,j,k=1}^d \tilde{\alpha}^{ijk}(f(x), \partial_i f(x), \partial_{ij}^2 f(x), \partial_{ijk}^3 f(x))(x^i - y^i)(x^j - y^j)(x^k - y^k) \\ &\quad + |x - y|^4 r'_f(x, y)\end{aligned}$$

where similarly  $\tilde{\alpha}_f^\lambda(y) = f(y)^{d/2} \alpha^\lambda(y)$  for  $\lambda = i, ij, ijk$  and  $\alpha^\lambda(y)$  are the smooth functions given in (67) that do not depend on  $f$  or  $f_0$ . For notational simplicity, using only a subscript to indicate the dependence on  $f$  and setting  $z = x - y$ , the above expansion can be concisely written as

$$\tilde{\alpha}_f = 1 + \sum_i \tilde{\alpha}_f^i z^i + \sum_{ij} \tilde{\alpha}_f^{ij} z^i z^j + \sum_{ijk} \tilde{\alpha}_f^{ijk} z^i z^j z^k + O(|z|^4).$$

Expanding the logarithm around  $z = 0$  to order 3,

$$\begin{aligned}\log \tilde{\alpha}_f &= \sum_i \tilde{\alpha}_f^i z^i + \sum_{ij} \tilde{\alpha}_f^{ij} z^i z^j + \sum_{ijk} \tilde{\alpha}_f^{ijk} z^i z^j z^k + O(|z|^4) \\ &\quad - \frac{1}{2} \left( \sum_i \tilde{\alpha}_f^i z^i + \sum_{ij} \tilde{\alpha}_f^{ij} z^i z^j + \sum_{ijk} \tilde{\alpha}_f^{ijk} z^i z^j z^k + O(|z|^4) \right)^2 \\ &\quad + \frac{1}{3} \left( \sum_i \tilde{\alpha}_f^i z^i + \sum_{ij} \tilde{\alpha}_f^{ij} z^i z^j + \sum_{ijk} \tilde{\alpha}_f^{ijk} z^i z^j z^k + O(|z|^4) \right)^3 + O(|z|^4)\end{aligned}$$

Keeping track of only the leading order terms, the quadratic term in the last display equals

$$\sum_{ij} (\alpha'_f)^{ij} z^i z^j + \sum_{ijk} (\alpha''_f)^{ijk} z^i z^j z^k + O(|z|^4),$$

with  $(\alpha'_f)^{ij} = \tilde{\alpha}_f^i \tilde{\alpha}_f^j$  and  $(\alpha''_f)^{ijk} = \tilde{\alpha}_f^i \tilde{\alpha}_f^j \tilde{\alpha}_f^k$ . Likewise, the cubic term equals  $\sum_{ijk} (\alpha''_f)^{ijk} z^i z^j z^k + O(|z|^4)$  with  $(\alpha''_f)^{ijk} = \tilde{\alpha}_f^i \tilde{\alpha}_f^j \tilde{\alpha}_f^k$ . Therefore,

$$\log \tilde{\alpha}_f = \sum_i \bar{\alpha}_f^i z^i + \sum_{ij} \bar{\alpha}_f^{ij} z^i z^j + \sum_{ijk} \bar{\alpha}_f^{ijk} z^i z^j z^k + O(|z|^4),$$

with  $\bar{\alpha}_f^i = \tilde{\alpha}_f^i$ ,  $\bar{\alpha}_f^{ij} = \tilde{\alpha}_f^i \tilde{\alpha}_f^j - \frac{1}{2} \tilde{\alpha}_f^i \tilde{\alpha}_f^j$  and  $\bar{\alpha}_f^{ijk} = \tilde{\alpha}_f^i \tilde{\alpha}_f^j \tilde{\alpha}_f^k - \frac{1}{2} \tilde{\alpha}_f^i \tilde{\alpha}_f^j \tilde{\alpha}_f^k + \frac{1}{3} \tilde{\alpha}_f^i \tilde{\alpha}_f^j \tilde{\alpha}_f^k$ . Set now

$$\begin{aligned}\gamma_{f_0, f}^i(x) &= \bar{\alpha}_f^i(f(x), \partial_i f(x)) - \bar{\alpha}_{f_0}^i(f_0(x), \partial_i f_0(x)), \\ \gamma_{f_0, f}^{ij}(x) &= \bar{\alpha}_f^{ij}(f(x), \partial_i f(x), \partial_{ij}^2 f(x)) - \bar{\alpha}_{f_0}^{ij}(f_0(x), \partial_i f_0(x), \partial_{ij}^2 f_0(x)), \\ \gamma_{f_0, f}^{ijk}(x) &= \bar{\alpha}_f^{ijk}(f(x), \partial_i f(x), \partial_{ij}^2 f(x), \partial_{ijk}^3 f(x)) - \bar{\alpha}_{f_0}^{ijk}(f_0(x), \partial_i f_0(x), \partial_{ij}^2 f_0(x), \partial_{ijk}^3 f_0(x)),\end{aligned}$$

where we recall  $\tilde{\alpha}_f^\lambda(y) = f(y)^{d/2} \alpha^\lambda(y)$ . This gives the expansion

$$(74) \quad \begin{aligned} \log \frac{\tilde{\alpha}_{f_0}(x, y)}{\tilde{\alpha}_f(x, y)} &= \sum_{i=1}^d \gamma_{f_0, f}^i(x) (x^i - y^i) + \sum_{i, j=1}^d \gamma_{f_0, f}^{ij}(x) (x^i - y^i) (x^j - y^j) \\ &+ \sum_{i, j, k=1}^d \gamma_{f_0, f}^{ijk}(x) (x^i - y^i) (x^j - y^j) (x^k - y^k) + |x - y|^{4d} \tilde{r}_{f_0, f}(x, y), \end{aligned}$$

where  $\|\tilde{r}_{f_0, f}\|_\infty \lesssim 1$  is uniform over an upper bound for  $\|f\|_{e^4}$  and  $\|f_0\|_{e^4}$ . By triangle inequality,

$$\|\gamma_{f_0, f}^i\|_\infty \lesssim \|f^{d/2} - f_0^{d/2}\|_\infty + \|f - f_0\|_{e^1} \lesssim \|f - f_0\|_{e^1},$$

since  $f, f_0 \geq f_{\min}$  and where the constants in the inequality depend only on  $f_{\min}$  and an upper bound for  $\|f\|_{e^1}$  and  $\|f_0\|_{e^1}$ . Using similar expressions for  $\|\gamma_{f_0, f}^{ij}\|_\infty$  and  $\|\gamma_{f_0, f}^{ijk}\|_\infty$ , we infer

$$(75) \quad \begin{aligned} &\left| \sum_{i, j=1}^d \gamma_{f_0, f}^{ij}(x) (x^i - y^i) (x^j - y^j) + \sum_{i, j, k=1}^d \gamma_{f_0, f}^{ijk}(x) (x^i - y^i) (x^j - y^j) (x^k - y^k) \right| \\ &\lesssim \|f - f_0\|_{e^2} |x - y|^2 + \|f - f_0\|_{e^3} |x - y|^3, \end{aligned}$$

again uniformly over  $|f|_{e^4}$  and  $|f_0|_{e^4}$ . Hence, combining (71), (72), (73), (74) and (75), we obtain

$$\begin{aligned} &\log \frac{\tilde{p}_{f_0, D}(x, y)}{\tilde{p}_{f, D}(x, y)} \mathbf{1}_{\{x \in \mathcal{O}_\delta^\dagger\}} \\ &= \left( -\frac{1}{4D} (\ell_{f_0}(x, y)^2 - \ell_f(x, y)^2) - \frac{d}{2} \log \frac{f_0(x)}{f(x)} \right) \mathbf{1}_{\{x \in \mathcal{O}_\delta^\dagger\}} \\ &\quad + \gamma_{f_0, f}(x) \cdot (y - x) \mathbf{1}_{\{x \in \mathcal{O}_{\delta/2}^\dagger\}} \\ &\quad + (\|f - f_0\|_\infty D + \|f - f_0\|_{e^1} |y - x| D + |y - x|^2 D + \|f - f_0\|_{e^2} |y - x|^2 \\ &\quad \quad + \|f - f_0\|_{e^3} |y - x|^3 + |y - x|^4) r_{f_0, f}(x, y), \end{aligned}$$

with  $\sup_{f \in \mathcal{C}_N} \|r_{f_0, f}\|_\infty \lesssim 1$ . With a slight abuse of notation, we may incorporate the term  $\mathbf{1}_{\{x \in \mathcal{O}_\delta^\dagger\}}$  into the definition of  $\gamma_{f_0, f}(x)$ . The final step is to expand the Riemannian metric  $\ell_f$ .

**Lemma 30.** *We have*

$$\ell_f(x, y)^2 = \frac{|x - y|^2}{f(x)} + \frac{1}{2} |x - y|^2 \nabla f^{-1}(x) \cdot (x - y) + |x - y|^4 r_f(x, y),$$

where  $\sup_{f \in \mathcal{C}_N} \|r_f\|_\infty \lesssim 1$ .

*Proof.* This is textbook Riemannian geometry, see for instance in Appendix B in Bilal [13], the uniformity in  $f \in \mathcal{C}_N$  being straightforward.  $\square$

Combining Lemma 30 with the expansion just derived completes the proof of Lemma 21.

## 9. APPENDIX

**9.1. Proof of Theorem 7: minimax lower bound.** We go along a classical scheme via the usual Assouad cube technique, see for instance Tsybakov [60].

*Step 1:* Pick a cube  $[c_1, c_2]^d \subset \mathcal{K}$  and a smooth wavelet  $\psi$  with compact support on  $\mathbb{R}$ . Set  $\psi_{J, k} = 2^{J/2} \psi(2^J \cdot - k)$  and denote by  $K_J \subset \mathbb{Z}$  a maximal set of indices  $k$  such that  $\text{supp}(\psi_{J, k}) \subset [c_1, c_2]$  for

all  $k \in K_J$ , and  $\text{supp}(\psi_{Jk}) \cap \text{supp}(\psi_{Jk'}) = \emptyset$  for every  $k, k' \in K_J$  with  $k \neq k'$ . For  $\ell = (\ell_1, \dots, \ell_d) \in (K_J)^d$ , set

$$\psi_{J,(\ell_1, \dots, \ell_d)}(x) = \prod_{i=1}^d \psi_{J\ell_i}(x^i), \quad x = (x^1, \dots, x^d) \in \mathcal{O},$$

so that  $\text{supp}(\psi_{J,(\ell_1, \dots, \ell_d)}) \subset [c_1, c_2]^d$  and  $\text{supp}(\psi_{J,(\ell_1, \dots, \ell_d)}) \cap \text{supp}(\psi_{J,(\ell'_1, \dots, \ell'_d)}) = \emptyset$  for  $(\ell_1, \dots, \ell_d) \neq (\ell'_1, \dots, \ell'_d)$  in  $(K_J)^d$ . For  $\varepsilon = (\varepsilon_{(\ell_1, \dots, \ell_d)} : \ell_1, \dots, \ell_d \in K_J) \in \{-1, 1\}^{|K_J|^d}$ , we set

$$f_\varepsilon(x) = 1 + \gamma \sum_{(\ell_1, \dots, \ell_d) \in (K_J)^d} \varepsilon_{(\ell_1, \dots, \ell_d)} \psi_{J,(\ell_1, \dots, \ell_d)}(x), \quad \varepsilon_{(\ell_1, \dots, \ell_d)} \in \{-1, 1\}.$$

Taking  $\gamma \simeq N^{-1/2}$  and  $2^J \simeq N^{1/(2s+d)}$ , we have  $f_\varepsilon \in \mathcal{F}_0 \cap \{f : \|f\|_{C^s} \leq M\}$  by choosing prefactors sufficiently small to accomodate constants.

*Step 2:* For an arbitrary estimator  $\widehat{f}_N$ , we repeat the classical argument to bound the maximal  $L^2$  risk. We have

$$\begin{aligned} \sup_{f \in \mathcal{F}_0 \cap \{f : \|f\|_{C^s} \leq M\}} \mathbb{E}_f \|\widehat{f}_N - f\|_2^2 &\geq \max_{\varepsilon \in \{-1, 1\}^{|K_J|^d}} \mathbb{E}_{f_\varepsilon} \|\widehat{f}_N - f_\varepsilon\|_2^2 \\ &\geq \frac{1}{2^{|K_J|^d}} \sum_{(\ell_1, \dots, \ell_d) \in (K_J)^d} \sum_{\varepsilon \in \{-1, 1\}^{|K_J|^d}} \int_{\text{supp}(\psi_{J,(\ell_1, \dots, \ell_d)})} \mathbb{E}_{f_\varepsilon} |\widehat{f}_N(x) - f_\varepsilon(x)|^2 dx. \end{aligned}$$

For a given configuration  $(\ell_1, \dots, \ell_d)$ , we write  $\varepsilon = (\tilde{\varepsilon}_{(\ell_1, \dots, \ell_d)}, \varepsilon_{(\ell_1, \dots, \ell_d)}) \in \{-1, 1\}^{|K_J|^d}$  with  $\tilde{\varepsilon}_{(\ell_1, \dots, \ell_d)} \in \{-1, 1\}^{|K_J|^{d-1}}$  and  $\varepsilon_{(\ell_1, \dots, \ell_d)} \in \{-1, 1\}$ , possibly after reordering. It follows that

$$\begin{aligned} &\sum_{\varepsilon \in \{-1, 1\}^{|K_J|^d}} \int_{\text{supp}(\psi_{J,(\ell_1, \dots, \ell_d)})} \mathbb{E}_{f_\varepsilon} |\widehat{f}_N(x) - f_\varepsilon(x)|^2 dx \\ &= \sum_{\tilde{\varepsilon}_{(\ell_1, \dots, \ell_d)} \in \{-1, 1\}^{|K_J|^{d-1}}} \int_{\text{supp}(\psi_{J,(\ell_1, \dots, \ell_d)})} \left( \mathbb{E}_{f_{(\tilde{\varepsilon}_{(\ell_1, \dots, \ell_d)}, +1)}} |\widehat{f}_N(x) - f_{(\tilde{\varepsilon}_{(\ell_1, \dots, \ell_d)}, +1)}(x)|^2 \right. \\ &\quad \left. + \mathbb{E}_{f_{(\tilde{\varepsilon}_{(\ell_1, \dots, \ell_d)}, -1)}} |\widehat{f}_N(x) - f_{(\tilde{\varepsilon}_{(\ell_1, \dots, \ell_d)}, -1)}(x)|^2 \right) dx \\ &\geq \frac{1}{2} \sum_{\tilde{\varepsilon}_{(\ell_1, \dots, \ell_d)} \in \{-1, 1\}^{|K_J|^{d-1}}} \int_{\text{supp}(\psi_{J,(\ell_1, \dots, \ell_d)})} |f_{(\tilde{\varepsilon}_{(\ell_1, \dots, \ell_d)}, +1)}(x) - f_{(\tilde{\varepsilon}_{(\ell_1, \dots, \ell_d)}, -1)}(x)|^2 dx \\ &\quad \times e^{-\rho} \left( 1 - (1 - e^{-\rho})^{-1} \|\mathbb{P}_{f_{(\tilde{\varepsilon}_{(\ell_1, \dots, \ell_d)}, +1)}} - \mathbb{P}_{f_{(\tilde{\varepsilon}_{(\ell_1, \dots, \ell_d)}, -1)}}\|_{TV} \right) \end{aligned}$$

for any  $\rho > 0$ , as follows by triangle inequality and classical information bounds, see e.g. [31] Section 5. From

$$\int_{\text{supp}(\psi_{J,(\ell_1, \dots, \ell_d)})} |f_{(\tilde{\varepsilon}_{(\ell_1, \dots, \ell_d)}, +1)}(x) - f_{(\tilde{\varepsilon}_{(\ell_1, \dots, \ell_d)}, -1)}(x)|^2 dx = 4\gamma^2 \|\psi_{J,(\ell_1, \dots, \ell_d)}\|_2^2 \simeq \gamma^2,$$

we infer

$$\sup_{f \in \mathcal{F}_0 \cap \{f : \|f\|_{C^s} \leq M\}} \mathbb{E}_f \|\widehat{f}_N - f\|_2^2 \gtrsim 2^J \gamma^2 \simeq N^{-2s/(2s+d)}$$

by taking  $\rho$  sufficiently large and using  $|K_J| \gtrsim 2^J$ , provided the total variation is bounded away from 1 uniformly in  $\varepsilon$ .

*Step 3:* Write  $g_\varepsilon = f_{(\tilde{\varepsilon}_{(\ell_1, \dots, \ell_d)}, 1)}$  and  $h_\varepsilon = f_{(\tilde{\varepsilon}_{(\ell_1, \dots, \ell_d)}, -1)}$ . It remains to bound

$$\|\mathbb{P}_{g_\varepsilon} - \mathbb{P}_{h_\varepsilon}\|_{TV}^2 \leq 2\mathbb{E}_{g_\varepsilon} \left[ \log \frac{d\mathbb{P}_{g_\varepsilon}}{d\mathbb{P}_{h_\varepsilon}} \right] = 2N\mathbb{E}_{g_\varepsilon} \left[ \log \frac{p_{g_\varepsilon, D}(X_0, X_D)}{p_{h_\varepsilon, D}(X_0, X_D)} \right]$$

by Pinsker's inequality and the fact that the diffusion is stationary for the last equality. We plan to apply a slight modification of Theorem 8 having  $\varepsilon_N = N^{-1/2}$  for subsets  $\mathcal{C}_N$  of the form  $\|f - f_0\|_2 \leq \varepsilon_N$  and  $\|f - f_0\|_\infty \rightarrow 0$ , the rest being unchanged. This is simply done by revisiting Step 1 in the proof of Proposition 17. Indeed, it suffices to notice that

$$\mathbb{E}_{f_0} \left[ \log \frac{f_0(X_{(i-1)D})}{f(X_{(i-1)D})} - \left( \frac{f_0(X_{(i-1)D})}{f(X_{(i-1)D})} - 1 \right) \right] \lesssim \|f_0 - f\|_2^2$$

for  $\|f - f_0\|_\infty$  sufficiently small, using that  $X_{(i-1)D}$  is uniformly distributed. This is the case for  $f_0 = g_\varepsilon$  and  $f = h_\varepsilon$ . In turn, we check that under the sampling assumption  $D = N^{-a}$  with  $1/2 < a < 1$ , we have  $E_N \lesssim N^{-1}$ . The result follows.

**9.2. Proof of Theorem 10.** If  $f \in \mathcal{F}_0$  and  $\|f\|_{\mathcal{C}^s} \leq M$ , we have  $0 \leq f(x) \leq M$  for every  $x \in \mathcal{O}$ . By construction, we also have  $0 \leq \widehat{f}_N^*(x) \leq M$  for every  $x \in \mathcal{O}$ . It follows that

$$\mathbb{E}_f \|\widehat{f}_N^* - f\|_2^2 \leq \mathbb{E}_f [\|\widehat{f}_N^* - f\|_2^2 \mathbf{1}_{\mathcal{B}_N}] + 2M^2 \mathbb{P}_f(\mathcal{B}_N^c),$$

where  $\mathcal{B}_N$  is the event in (44). A glance at the proof of Lemma 22 shows that we in fact have the rate

$$\sup_{f \in \mathcal{F}} \mathbb{P}_f(\mathcal{B}_N^c) \lesssim e^{-2Jd} \lesssim N^{-1},$$

hence the second term has a negligible order. Next,  $|\widehat{f}_N^*(x) - f(x)| = |\min(\widehat{f}_N(x), M)_+ - f(x)| \leq |\widehat{f}_N(x) - f(x)|$  since  $0 \leq f(x) \leq M$ . Therefore,

$$\mathbb{E}_f [\|\widehat{f}_N^* - f\|_2^2 \mathbf{1}_{\mathcal{B}_N}] \leq \mathbb{E}_f [\|\widehat{f}_N - f\|_2^2 \mathbf{1}_{\mathcal{B}_N}] \lesssim \|f - \overline{P}_J f\|_{L^2}^2 + \mathbb{E}_f [\|\widehat{f}_N - \overline{P}_J f\|_{L^2}^2 \mathbf{1}_{\mathcal{B}_N}],$$

where  $\overline{P}_J f$  denotes the projection (23). The first term is of order  $2^{-2Js} \simeq N^{-2s/(2s+d)}$  by wavelet approximation since the Daubechies wavelet has at least  $\lfloor s \rfloor - 1$  vanishing moments, and thus has the right order. The second term also has the right order as a direct consequence of Theorem 9.

**9.3. Proof of Lemma 19.** Set

$$Y_t = X_0 + \int_0^t \nabla f(X_s) ds + \int_0^t \sqrt{2f(X_s)} dB_s.$$

Then  $(X, \ell)$  is solution of the Skorokhod problem for  $(\mathcal{O}, n, Y)$  since

$$X_t = Y_t + \int_0^t n(X_s) d\ell_s,$$

and the Skorokhod mapping:  $\Gamma : Y \mapsto X = \Gamma Y$  is uniquely defined see e.g. Lions and Sznitman [37]. Moreover, we have  $\Omega_\delta(\Gamma Y) \leq \Omega_\delta(Y)$ , where

$$\Omega_\delta(\psi) = \sup_{0 \leq s, t \leq T, |t-s| \leq \delta} |\psi(t) - \psi(s)|$$

denotes the modulus of continuity of  $\psi : [0, T] \rightarrow \mathbb{R}^d$ , so that it suffices to prove (32) for  $Y$  instead of  $X$ . We bound the first term by

$$\sup_{s \leq u \leq t} \left| \int_s^u \nabla f(X_v) dv \right|^p \leq \|f\|_{\mathcal{C}^1}^p (t-s)^p.$$

For the second term, we apply the Burkholder-Davis-Gundy inequality to obtain

$$\begin{aligned} \mathbb{E}_f \left[ \sup_{s \leq u \leq t} \left| \int_s^u \sqrt{2f(X_v)} dB_v \right|^p \middle| \mathcal{F}_s \right] &\leq C_p d^{p/2} \mathbb{E}_f \left[ \left| \int_s^t f(X_u) du \right|^{p/2} \middle| \mathcal{F}_s \right] \\ &\leq C_{p,d} \|f\|_\infty^{p/2} (t-s)^{p/2}. \end{aligned}$$

**9.4. Proof of Lemma 20.** Consider the process  $(\tilde{X}_t)_{t \geq 0}$  defined in (28). On  $\mathcal{A}_{i,D}$ , the two paths  $(X_t - X_{(i-1)D})_{t \geq (i-1)D}$  and  $(\tilde{X}_t - X_{(i-1)D})_{t \geq (i-1)D}$  coincide for  $t - (i-1)D \leq \tau_{i,D}$ . Using that  $\text{dist}(\mathcal{O}_0^\delta, \partial \mathcal{O}) \geq \delta/2$ , it follows that

$$\begin{aligned} \mathbb{P}_{f_0}(\tau_{i,D} \geq D, \mathcal{A}_{i,D}) &\leq \mathbb{P}_{f_0} \left( \sup_{0 \leq t \leq D} |\tilde{X}_{(i-1)D+t} - X_{(i-1)D}|^2 > \frac{\delta}{2}, X_{(i-1)D} \in \mathcal{O}_0^\delta \right) \\ &\leq \sup_{x \in \mathcal{O}_0^\delta} \mathbb{P}_{f_0} \left( \sup_{0 \leq t \leq D} |\tilde{X}_t - x|^2 > \frac{\delta}{2} \middle| X_0 = x \right), \end{aligned}$$

by the Markov property. By Itô's formula, we further have

$$\sup_{0 \leq t \leq D} |\tilde{X}_t - x|^2 \leq 2D^2 \sum_{i=1}^d \|f_0\|_{\mathcal{C}^1}^2 + 2 \sup_{0 \leq t \leq D} \left| \int_0^t (2f_0(\tilde{X}_s))^{1/2} dB_s \right|^2,$$

and hence

$$\begin{aligned} \mathbb{P}_{f_0} \left( \sup_{0 \leq t \leq D} |\tilde{X}_t - x|^2 \geq \frac{1}{4} \delta^2 \middle| X_0 = x \right) &\leq \mathbb{P}_{f_0} \left( \sup_{0 \leq t \leq D} |\mathcal{M}_t(g)|^2 \geq \frac{1}{4} \delta^2 - C_f D^2 \middle| X_0 = x \right) \\ &\leq \mathbb{P}_{f_0} \left( \sup_{0 \leq t \leq D} |\mathcal{M}_t(f_0)|^2 \geq \frac{1}{5} \delta^2 \middle| X_0 = x \right) \end{aligned}$$

for small enough  $D$ , where  $\mathcal{M}_t(f_0) = \int_0^t (2f_0(\tilde{X}_s))^{1/2} dB_s$  is a  $d$ -dimensional martingale with predictable bracket  $\langle \mathcal{M}^i f_0, \mathcal{M}^j f_0 \rangle_t = 2 \int_0^t f_0(\tilde{X}_s) ds \delta_{ij} \leq 2 \|f_0\|_\infty t \delta_{ij}$ . It follows that for any  $x \in \mathcal{O}_0^\delta$ :

$$\begin{aligned} \mathbb{P}_{f_0} \left( \sup_{0 \leq t \leq D} |\tilde{X}_t - x|^2 \geq \frac{1}{4} \delta^2 \middle| X_0 = x \right) &\leq \sum_{i=1}^d \mathbb{P}_{f_0} \left( \sup_{0 \leq t \leq D} |\mathcal{M}_t^i(f_0)| \geq \frac{1}{\sqrt{5d}} \delta \middle| X_0 = x \right) \\ &\leq 2d \exp \left( - \frac{\delta^2}{20d \|f_0\|_\infty D} \right), \end{aligned}$$

where we have used Bernstein's inequality for continuous local martingale  $(\mathcal{M}_t)_{t \geq 0}$ :

$$\mathbb{P} \left( \sup_{0 \leq s \leq t} \mathcal{M}_s \geq x, \langle \mathcal{M} \rangle_t \leq y \right) \leq e^{-x^2/(2y)}$$

(see e.g. [50] p.154).

**9.5. A generic chaining inequality and the event  $\mathcal{B}_N$ .** In several places, we require the following concentration inequality, which is based on a chaining argument for stochastic processes with mixed tails, see Theorem 2.2.28 in [58] or Theorem 3.5 in [23].

**Lemma 31.** *Let  $S \subset L^2(\mathcal{O})$  be a finite-dimensional linear space with dimension  $\dim(S) = m < \infty$ . Let  $Z = (Z(g) : g \in \mathcal{G})$  be a stochastic process with index set  $\mathcal{G} \subset S$  satisfying  $\|\mathcal{G}\|_2 = \sup_{g,h \in \mathcal{G}} \|g - h\|_2 < \infty$ . Suppose that  $Z$  satisfies for all  $g, h \in \mathcal{G}$  and  $t \geq 0$ ,*

$$\mathbb{P}(|Z(g) - Z(h)| \geq t) \leq C \exp \left( - \frac{ct^2}{\alpha^2 \|g - h\|_2^2 + \beta \|g - h\|_2 t} \right),$$

where  $C, c, \alpha, \beta > 0$ . Then for any  $g_0 \in \mathcal{G}$  and all  $u \geq 1$ ,

$$\mathbb{P} \left( \sup_{g \in \mathcal{G}} |Z(g) - Z(g_0)| \geq K(m\beta + \sqrt{m}\alpha + \beta u + \alpha\sqrt{u}) \|\mathcal{G}\|_2 \right) \leq e^{-u},$$

where  $K$  depends only on  $C$  and  $c$ .

*Proof.* Let  $(e_k : 1 \leq k \leq m)$  be an  $L^2$ -orthonormal basis for  $S$ . After rearranging, the Bernstein inequality implies that for  $C_1, C_2 > 0$  large enough, depending only on  $C$  and  $c$ ,

$$\mathbb{P} (|Z(g) - Z(h)| \geq C_1\beta u \|g - h\|_2 + C_2\alpha\sqrt{u} \|g - h\|_2) \leq 2e^{-u}$$

holds for all  $u \geq 0$ . The process  $Z$  therefore has a *mixed tail* as in (3.8) of Dirksen [23] with respect to the metrics

$$\begin{aligned} d_1(g, h) &= C_1\beta \|g - h\|_2 = C_1\beta |\langle g - h, e_k \rangle_{\mathbb{R}^m}|, \\ d_2(g, h) &= C_2\alpha \|g - h\|_2 = C_2\alpha |\langle g - h, e_k \rangle_{\mathbb{R}^m}|, \end{aligned}$$

where the last equalities follow from Parseval's theorem and  $|\cdot|_{\mathbb{R}^m}$  is the Euclidean norm on  $\mathbb{R}^m$ . The  $d_1$ - and  $d_2$ -diameters of  $\mathcal{G}$  are therefore bounded by  $\Delta_{d_1}(\mathcal{G}) \leq C_1\beta \|\mathcal{G}\|_2$  and  $\Delta_{d_2}(\mathcal{G}) \leq C_2\alpha \|\mathcal{G}\|_2$ , respectively. Theorem 3.5 of [23] thus yields that for absolute constants  $C', c' > 0$  and any  $u \geq 1$ ,

$$\mathbb{P} \left( \sup_{g \in \mathcal{G}} |Z(g) - Z(g_0)| \geq C'\gamma_1(\mathcal{G}, d_1) + C'\gamma_2(\mathcal{G}, d_2) + c'C_1\beta \|\mathcal{G}\|_2 u + c'C_2\alpha \|\mathcal{G}\|_2 \sqrt{u} \right) \leq e^{-u},$$

where  $\gamma_1, \gamma_2$  are the 'generic chaining functionals' defined in [23]. In particular, (2.3) of [23] gives the estimate  $\gamma_\alpha(\mathcal{G}, d_i) \leq C(\alpha) \int_0^\infty (\log N(\mathcal{G}, d_i, \varepsilon))^{1/\alpha} d\varepsilon$ , where  $N(\mathcal{G}, d_i, \varepsilon)$  denotes the covering number of the set  $\mathcal{G}$ , i.e. the smallest number of  $d_i$ -balls of radius  $\varepsilon$  needed to cover  $\mathcal{G}$ . Since  $\mathcal{G} \subset S$  and  $S$  is a finite-dimensional linear space, the second-last display implies that

$$N(\mathcal{G}, d_1, \varepsilon) \leq N(\{x \in \mathbb{R}^m : |x|_{\mathbb{R}^m} \leq \|\mathcal{G}\|_2\}, C_1\beta |\cdot|_{\mathbb{R}^m}, \varepsilon),$$

and likewise for  $d_2$ . Using for instance Proposition 4.3.34 in the textbook [28] to bound the log-covering number of a ball in finite-dimensional Euclidean space,

$$\begin{aligned} \gamma_1(\mathcal{G}, d_1) &\lesssim \int_0^\infty \log N(\{x \in \mathbb{R}^m : |x|_{\mathbb{R}^m} \leq \|\mathcal{G}\|_2\}, C_1\beta |\cdot|_{\mathbb{R}^m}, \varepsilon) d\varepsilon \\ &\leq \int_0^{\Delta_{d_1}(\mathcal{G})} m \log \left( \frac{3\Delta_{d_1}(\mathcal{G})}{\varepsilon} \right) d\varepsilon = m\Delta_{d_1}(\mathcal{G}) \int_0^1 \log(3/u) du \lesssim mC_1\beta \|\mathcal{G}\|_2. \end{aligned}$$

Similarly,

$$\gamma_2(\mathcal{G}, d_2) \lesssim \int_0^{\Delta_{d_2}(\mathcal{G})} \sqrt{m \log \left( \frac{3\Delta_{d_2}(\mathcal{G})}{\varepsilon} \right)} d\varepsilon = \sqrt{m}\Delta_{d_2}(\mathcal{G}) \int_0^1 \sqrt{\log(3/u)} du \lesssim \sqrt{m}C_2\alpha \|\mathcal{G}\|_2.$$

Substituting these bounds into the exponential inequality derived above then gives the result.  $\square$

9.6. **Proof of Lemma 22.** We have

$$\begin{aligned}
\mathbb{P}_f(\mathcal{B}_N^c) &\leq \mathbb{P}_f(\exists g \in V_J : (1 - \kappa)\|g\|_2^2 > |g|_N^2) + \mathbb{P}_f(\exists g \in V_J : |g|_N^2 > (1 + \kappa)\|g\|_2^2) \\
&= \mathbb{P}_f(\exists g \in V_J : \|g\|_2 = 1, 1 - \kappa > |g|_N^2) + \mathbb{P}_f(\exists g \in V_J : \|g\|_2 = 1, |g|_N^2 > 1 + \kappa) \\
(76) \quad &\leq 2\mathbb{P}_f\left(\sup_{g \in V_J: \|g\|_2=1} \left| |g|_N^2 - 1 \right| > \kappa\right) \\
&= 2\mathbb{P}_f\left(\sup_{g \in V_J: \|g\|_2=1} \left| \sum_{i=1}^N (g(X_{iD})^2 - \mathbb{E}_f[g(X_{iD})^2]) \right| > \kappa N\right)
\end{aligned}$$

since  $\mathbb{E}_f[g(X_{iD})^2] = \int_{\mathcal{O}} g(x)^2 dx = 1$  by stationarity. Write  $\mathcal{G}_J = \{g \in V_J : \|g\|_2 = 1\}$  and define the process  $Z_N = (Z_N(g) : g \in \mathcal{G}_J)$  by

$$Z_N(g) = \sum_{i=1}^N (g(X_{iD})^2 - \mathbb{E}_f[g(X_{iD})^2]).$$

For  $g, h \in \mathcal{G}_J$ , we have  $\mathbb{E}_f[g(X_{iD})^2 - h(X_{iD})^2] = 0$  and  $\text{Var}_f(g(X_{iD})^2 - h(X_{iD})^2) = \|g^2 - h^2\|_2^2$ . Since  $(X_0, X_D, \dots, X_{ND})$  is a stationary reversible Markov chain whose spectral gap is lower bounded by  $rD$  by (9), Theorem 3.3 of [44] (cf. (3.21)) yields yields

$$\begin{aligned}
\mathbb{P}_f(|Z_N(g) - Z_N(h)| \geq t) &= \mathbb{P}_f\left(\left|\sum_{i=1}^N g(X_{iD})^2 - h(X_{iD})^2\right| \geq t\right) \\
&\leq 2 \exp\left(-\frac{\lambda_f D t^2}{4N\|g^2 - h^2\|_2^2 + 10\|g^2 - h^2\|_\infty t}\right) \\
&\leq 2 \exp\left(-\frac{\lambda_f D t^2}{4N\|g + h\|_\infty^2 \|g - h\|_2^2 + 10\|g + h\|_\infty \|g - h\|_\infty t}\right) \\
&\leq 2 \exp\left(-\frac{C t^2}{N 2^{Jd} D^{-1} \|g - h\|_2^2 + 2^{Jd} D^{-1} \|g - h\|_2 t}\right)
\end{aligned}$$

using that  $\|g\|_\infty \leq C 2^{Jd/2} \|g\|_2 = C 2^{Jd/2}$  for  $g \in \mathcal{G}_J$ , and where  $C$  depends on  $r$ , and hence  $f_{\min}$  and  $\mathcal{O}$  by (9). Applying Lemma 31 with  $m = \dim(V_J) = O(2^{Jd})$ ,  $\|\mathcal{G}_J\|_2 = \sup_{g, h \in \mathcal{G}_J} \|g - h\|_2 \leq 2$ ,  $\alpha^2 = N 2^{Jd} D^{-1}$ ,  $\beta = 2^{Jd} D^{-1}$  and  $u = 2^{Jd}$  thus gives

$$\mathbb{P}_f\left(\sup_{g \in \mathcal{G}_J} |Z_N(g)| \geq C \left(2^{2Jd} D^{-1} + 2^{Jd} N^{1/2} D^{-1/2}\right)\right) \leq e^{-2^{Jd}} \rightarrow 0$$

since  $2^J \rightarrow \infty$  as  $N \rightarrow \infty$ . Since  $2^{Jd} =$  by assumption, the right-hand side within the last probability is  $o(N)$  as  $N \rightarrow \infty$ . Together with (76) this gives the result.

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