CONSISTENT INFERENCE FOR DIFFUSIONS FROM LOW FREQUENCY MEASUREMENTS

BY RICHARD NICKL

1Department of Pure Mathematics and Mathematical Statistics, University of Cambridge*; nickl@maths.cam.ac.uk

Let \((X_t)\) be a reflected diffusion process in a bounded convex domain in \(\mathbb{R}^d\), solving the stochastic differential equation
\[
dX_t = \nabla f(X_t)dt + \sqrt{2f(X_t)}dW_t, \quad t \geq 0,
\]
with \(W_t\) a \(d\)-dimensional Brownian motion. The data \(X_0, X_D, \ldots, X_{ND}\) consist of discrete measurements and the time interval \(D\) between consecutive observations is fixed so that one cannot 'zoom' into the observed path of the process. The goal is to infer the diffusivity \(f\) and the associated transition operator \(P_{t,f}\). We prove injectivity theorems and stability inequalities for the maps \(f \mapsto P_{t,f} \mapsto P_{D,f}, t < D\). Using these estimates we establish the statistical consistency of a class of Bayesian algorithms based on Gaussian process priors for the infinite-dimensional parameter \(f\), and show optimality of some of the convergence rates obtained. We discuss an underlying relationship between the degree of ill-posedness of this inverse problem and the 'hot spots' conjecture from spectral geometry.

CONTENTS

1 Introduction . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 1
2 Main results . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 5
2.1 Optimal recovery of the transition operator \(P_{D,f}\) . . . . . . . . . . . . . . 6
2.2 Injectivity of \(f \mapsto P_{t,f} \mapsto P_{D,f}, t < D\) . . . . . . . . . . . . . . 6
2.3 Bayesian inference in the diffusion model . . . . . . . . . . . . . . . . . . . . 10
2.4 Posterior consistency theorems . . . . . . . . . . . . . . . . . . . . . . . . . . 11
3 Proofs . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 13
3.1 Analytical background: reflected diffusions and their generators . . . . . . . 13
3.2 Heat equation, transition operator, and a perturbation identity . . . . . . . . 15
3.3 Information distances and small ball probabilities . . . . . . . . . . . . . . . 17
3.4 Proofs of stability estimates . . . . . . . . . . . . . . . . . . . . . . . . . . . . 18
3.5 Minimax estimation of the transition operator \(P_{D,f}\) . . . . . . . . . . . . . . 21
3.6 Bayesian contraction results . . . . . . . . . . . . . . . . . . . . . . . . . . . . 25
3.7 Neumann eigenfunctions on cylindrical domains . . . . . . . . . . . . . . . . 28
3.8 Proofs of auxiliary results . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 31
References . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 32

1. Introduction. Diffusion describes a random process for the evolution over time of phenomena such as heat flow, electric conductance, chemical reactions, or molecular dynamics, to name just a few examples. The density of a diffusing substance in an insulated medium, say a bounded convex subset \(O\) of \(\mathbb{R}^d, d \geq 1\), is described by the solutions \(u\) to the parabolic partial differential equation (PDE) known as the heat equation, \(\partial u/\partial t = L_{f,U}u\), with a divergence form elliptic second order differential operator
\[
L_{f,U} = \frac{1}{m} \nabla \cdot (mf\nabla), \quad m \equiv m_U \propto e^{-U},
\]

*I would like to thank James Norris and Gabriel Paternain for helpful discussions, three anonymous referees and the associate editor for their critical remarks, and Matteo Giordano for generating Fig.s 1-2.
and equipped with Neumann boundary conditions. Here \( f : \mathcal{O} \to [f_{\text{min}}, \infty) \), \( f_{\text{min}} > 0 \), is a positive scalar ‘diffusivity’ function and \( U : \mathcal{O} \to \mathbb{R} \) is a ‘force’ potential inducing a Gibbs measure \( \mu = \mu_U \) with (Lebesgue-) probability density \( m_U \). If \( W_t \) is a \( d \)-dimensional Brownian motion then the corresponding ‘microscopic’ statistical model for a diffusing particle is provided by solutions \( (X_t) \) to the stochastic differential equation (SDE)

\[
\begin{align*}
\mathrm{d}X_t &= \nabla f(X_t) \mathrm{d}t + f(X_t) \nabla U(X_t) \mathrm{d}t + \sqrt{2f(X_t)} \mathrm{d}W_t + \nu(X_t) \mathrm{d}L_t, \quad t \geq 0,
\end{align*}
\]

started at \( X_0 = x \in \mathcal{O} \). The process is reflected when hitting the boundary \( \partial \mathcal{O} \) of its state space: \( L_t \) is a ‘local time’ process acting only when \( X_t \in \partial \mathcal{O} \) and \( \nu(x) \) is the (inward) pointing normal vector at \( x \in \partial \mathcal{O} \). When \( f, \nabla f, \nabla U \) are Lipschitz maps on \( \mathcal{O} \), a continuous time Markov process \( (X_t : t \geq 0) \) giving a unique pathwise solution to (1) exists [69].

Real world observations of diffusion are necessarily discrete and often subject to a lower bound on the time that elapses between consecutive measurements. We denote this ‘observation distance’ by \( D > 0 \) and assume for simplicity that it is the same at each measurement. The data is \( X_0, X_D, \ldots, X_{ND} \) for some \( N \in \mathbb{N} \), that is, we are tracking the trajectory of a given particle along discrete points in time, see Fig. 1. In practice one may be observing several independent particles which essentially corresponds to (linearly) augmenting sample size \( N \) – we consider the one-particle model without loss of generality. We investigate the possibility to infer \( f, U \) and the transition operator \( P_{t,f,U} \) of the Markov process \( (X_t) \) both at \( t = D \) and at ‘unobserved’ times \( t > 0 \) by a statistical algorithm, that is, by a computable function of \( (X_{iD} : i = 1, \ldots, N) \). We are interested in the scenario where \( D > 0 \) is fixed (but known) as sample size \( N \to \infty \). This is often the most appropriate observational model: for instance the speed at which particles or molecules transverse the medium \( \mathcal{O} \) may be much faster than the frequency at which images can be taken. Following [29] we refer to this as the ‘low measurement frequency’ scenario. See [33, 34] or also Ch. 4 in [49] for such situations in the biological sciences, or [48, 62, 44] in the context of data assimilation problems.

The invariant ‘equilibrium’ distribution of the Markov process (1) is well known ([5], Sec.1.11.3) to equal \( \mu_U \) and hence identifies the potential \( U \) via its probability density \( m_U \). The infinite-dimensional parameter \( \mu_U \) (and thus \( U \)) can then be estimated from a discrete sample by standard linear density estimators \( \hat{\mu} \) that smooth the empirical measure of the \( X_{iD} \)’s near any point \( x \in \mathcal{O} \) (cf. [29] or also, with continuous data, [19, 66, 28]). Using exponentially fast mixing of ergodic averages of the Markov process towards their \( \mu_U \)-expectations (e.g., via [60] combined with Thm 4.9.3 and Sec.1.11.3 in [5], or also with [15]) one can then obtain excellent statistical guarantees for \( \| \hat{\mu} - \mu_U \| \) in relevant norms \( \| \cdot \| \).
The problem to determine diffusivity parameters \( f \) from data has a long history in mathematical inverse problems – we mention here \([13, 41, 68, 52, 73, 1]\) in the context of the Calderón problem as well as \([63, 22, 67, 38, 10, 27, 54]\) in the context of Darcy’s flow problem, and the many references therein. All these settings consider a simplified observational model where one is given a ‘steady state’ measurement of diffusion, returning the (typically ‘noisy’) solution of a time-independent elliptic PDE. The potential inferential barrier arising with low frequency measurements disappears in the reduction from a time evolution equation to the elliptic PDE and hence does not inform the statistical setting investigated here.

As the invariant measure \( \mu \) is identical for all \( f \), the information contained in low frequency discrete data from (2) is encoded in the transition operator \( P_{D,f} \) of the underlying Markov process \( (X_t) \). Little is known about how to conduct statistically valid inference in this setting, with notable exceptions being the one-dimensional case \( d = 1 \) studied in \([29, 56]\). We also mention the consistency results \([75, 32]\) as well as \([46]\) for Markovian transition operators, but these do not concern the conductivities \( f \) themselves. A first question is whether the task of identifying \( f \) from \( P_{D,f} \) for fixed observation distance \( D > 0 \) is even well-posed, that is, whether the (non-linear) map \( f \mapsto P_{D,f} \) is injective. The answer to this question is positive at least if \( f \) is prescribed near \( \partial \mathcal{O} \). Denote by \( L^2(\mathcal{O}) \) the Hilbert space of square Lebesgue integrable functions on \( \mathcal{O} \).

**Theorem 1.** Suppose positive diffusion coefficients \( f_1, f_2 \in C^2(\mathcal{O}) \) are bounded away from zero on \( \mathcal{O} \) and such that \( f_1 = f_2 \) near \( \partial \mathcal{O} \). Then if \( P_{D,f_1} = P_{D,f_2} \) coincide as bounded linear operators on \( L^2(\mathcal{O}) \) for some \( D > 0 \), we must have \( f_1 = f_2 \) on \( \partial \mathcal{O} \).

See Theorem 5 for details. That \( f \) should be known near \( \partial \mathcal{O} \) can be explained by the fact that the reflection (which is independent of \( f \)) dominates the local dynamics near \( \partial \mathcal{O} \).

Statistical algorithms are often motivated by ‘population version’ identification equations for unknown parameters, as in the one-dimensional case \( d = 1 \) considered in \([29, 56]\), who use ordinary differential equation (ODE) techniques to derive identities for \( f \) in terms of the first eigenfunction of the transition operator \( P_{D,f} \). This approach appears limited use in the present multi-dimensional context \( d > 1 \). Instead we shall maintain \( \{P_{D,f} : f \in \mathcal{F}\} \) as our statistical model for natural choices of parameter spaces \( \mathcal{F} \subset L^2(\mathcal{O}) \) of sufficiently smooth, positive, functions. This makes available the algorithmic toolbox of Bayesian statistics in infinite-dimensional parameter spaces which does not require any identification equations or inversion formulae. Instead one employs a Gaussian process prior \( \Pi \) for the function-valued parameter \( f \), see \([76, 67, 24, 54]\), and updates according to Bayes’ rule: if \( P_{D,f} \) are the transition densities of \( P_{D,f} \) (fundamental solutions), the posterior distribution is

\[
\Pi(B|X_0, X_D, \ldots, X_{ND}) = \frac{\int_B \prod_{i=1}^N P_{D,f}(X_{i-1}D, X_{i}D) d\Pi(f)}{\int_{\mathcal{F}} \prod_{i=1}^N P_{D,f}(X_{i-1}D, X_{i}D) d\Pi(f)}, \quad B \text{ measurable.}
\]
As the ‘forward map’ \( f \mapsto p_{D,f} \) can be evaluated by numerical PDE techniques for parabolic equations, one can leverage ideas from [16] (see also [30, 18, 8]) to propose computationally feasible MCMC methodology that draws approximate samples from \( \Pi(\cdot | X_0, X_D, \ldots, X_{N_D}) \), and the resulting ergodic averages approximate the posterior mean vector, which in turn gives an estimated output for \( f \). See Section 2.3, specifically Remark 3, for details.

Recent progress in Bayesian theory for non-linear inverse problems [53, 50, 59, 57], [54] has clarified that such Bayesian methods can solve non-linear problems without ‘inversion formulae’ as long as appropriate stability estimates for the forward map, here \( f \mapsto P_{D,f} \), are available. Following this strategy we prove here a first statistical consistency result in multi-dimensional diffusion models with such ‘low frequency’ measurements.

**Theorem 2.** Let \( D > 0 \) and consider data \( X_0, X_D, \ldots, X_{N_D} \) generated from the diffusion (2) in a bounded smooth convex domain \( \mathcal{O} \). Assume the ground truth \( f_0 > 1/4 \) is sufficiently regular in a Sobolev sense and equals 1/2 near \( \partial \mathcal{O} \). Assign an appropriate Gaussian process prior \( \Pi \) to \((\theta(x) : x \in \mathcal{O})\), form \( f_\theta = (1 + e^{\theta})/4 \), and consider the random field
\[
\tilde{f}_N \equiv f_{\tilde{\theta}_N}(x) \ (x \in \mathcal{O}), \quad \tilde{\theta}_N = E_{\Pi} [\theta | X_0, X_D, \ldots, X_{N_D}],
\]

arising from the posterior mean function. Then the posterior inference for the transition operators \( P_{t,f_0}, t > 0 \), as well as for \( f_0 \) is consistent, that is, as \( N \to \infty \) and in \( \mathbb{P}_{f_0} \)-probability,
\[
\| P_{t,f_N} - P_{t,f_0} \|_{L^2 \to L^2} \to 0, \quad \text{and} \quad \| \tilde{f}_N - f_0 \|_{L^2} \to 0,
\]
where \( \| \cdot \|_{L^2 \to L^2} \) denotes the operator norm on \( L^2 = L^2(\mathcal{O}) \).

See Theorems 9 and 10 for details. Next to the stability estimates underlying Theorem 1, a main ingredient of our proofs is an estimate (Theorem 11) on the ‘information’ (Kullback-Leibler) distance of the underlying statistical experiment in terms of a negative Sobolev norm. Our proofs provide a rate of convergence in the last limits, and the rate obtained for \( P_{t,f} \) cannot be improved (as we show) at the ‘observed time’ \( t = D \), corresponding to ‘prediction risk’. For the parameters \( f \) and \( P_{t,f}, t < D \), our inversion rates are potentially slow (i.e., only inverse logarithmic in \( N \)). The question of optimal recovery in these non-linear inverse problems is delicate as they (implicitly or explicitly) involve solving a ‘backward heat equation’ from knowledge of \( P_{D,f} \) alone. We shed some light on the issue and exhibit infinite-dimensional parameter spaces of \( f \)’s where faster than logarithmic rates (algebraic in \( 1/N \)) can be obtained. These are based on certain spectral ‘symmetry’ hypotheses on the domain \( \mathcal{O} \) and on the diffusion process. For \( d = 1 \) these hypotheses are always satisfied and our theory thus recovers the one-dimensional results from [29, 56] as a special case (but with novel proofs based on PDE theory). In multi-dimensions \( d \geq 2 \) and for \( f \) in a \( \| \cdot \|_{\infty} \)-neighbourhood of the constant function, we show that the required symmetries of \( \mathcal{O} \) can be related to the ‘hot spots conjecture’ from spectral geometry [4, 12, 36, 3, 64, 37], providing further incentives for the study of this topic. The topic of ‘fast’ rates beyond that conjecture will be investigated in future research.

In principle, the Bayesian approach can be expected to give valid inferences for any measurement regime and hence should work irrespectively of whether \( D \to 0 \) or not. In fact, a ‘high frequency’ regime is explicitly investigated in the recent contribution [35] who show posterior consistency if \( D \to 0 \) sufficiently fast compared to \( N \) (but still such that the observation horizon \( ND \to \infty \)). We also refer to Sec. 3.3 in [28] for a discussion of the hypothetical case when the entire trajectory of \((X_t)\) is observed. More generally, the recent contributions [65, 55, 28, 2] to non-parametric inference for multi-dimensional diffusions (Bayesian or not) contain many further references.
2. Main results. We are given discrete observations $X_0, X_1, \ldots, X_N$, $N \in \mathbb{N}$, of the solution $(X_t : t \geq 0)$ of the SDE (2) where $X_0 \sim \text{Unif}(O)$, that is, the diffusion is started in its (constant) invariant distribution. If $X_0 = x$ for some fixed $x$, then our proofs work as well in view of the exponentially fast mixing (36) of the process towards the uniform law $\mu$, by just discarding the ‘burn-in phase’, that is, by letting the process evolve for a while before one starts to record measurements. We emphasise again that the time interval $D > 0$ between consecutive observations remains fixed in the $N \to \infty$ asymptotics.

The domain $O$ supporting our diffusion process is a bounded convex open subset of $\mathbb{R}^d$, and to avoid technicalities we assume that the boundary of $O$ is smooth, ensuring in particular the existence of all ‘reflecting’ normal vectors $\nu$ at $\partial O$. Throughout $L^2(O)$ will denote the Hilbert space of square integrable functions for Lebesgue measure $dx$ on $O$. We also assume (solely for notational convenience) that the volume of $O$ is normalised to one, $\text{vol}(O) = 1$.

The physical model underlying (2) describes the intensity $(u(t, x) : t > 0, x \in O)$ of diffusion in an insulated medium by the equation $\partial u/\partial t = -\nabla \cdot J$ for flux $J = -f \nabla u$ (e.g., p.361f. in [70], and after (31) below). For smooth test functions $\phi$, let the elliptic operator $L_f$ be given by the action
\begin{equation}
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),
\end{equation}
where $\nabla, \nabla \cdot, \Delta$ denote the gradient, divergence and Laplace operator, respectively. Then $u$ solves the heat equation for $L_f$ with Neumann boundary conditions $\partial u/\partial \nu = 0$ on $\partial O$. Its fundamental solutions $p_{t,f}(\cdot, \cdot) : O \times O \to [0, \infty)$ describe the probabilities $\int_{O} p_{t,f}(x, y)dy$ for the position of a diffusing particle to lie in a region $U$ at time $t_0 + t$ when it was at $x \in O$ at time $t_0$. More generally the transition operator $P_{t,f}$ describes a self-adjoint action on $L^2(O)$,
\begin{equation}
P_{t,f}(\phi) = \int_{O} p_{t,f}(\cdot, y)\phi(y)dy, \quad \phi \in L^2(O).
\end{equation}
The process $(X_t : t \geq 0)$ from (2) is the unique Markov random process with these transition probabilities, infinitesimal generator $L_f$, and equilibrium (invariant) probability density $d\mu = 1$ on $O$. The generator $L_f$ with Neumann boundary condition is characterised by an infinite sequence of (orthonormal) eigen-pairs $(e_j, -\lambda_j) \in L^2(O) \times (-\infty, 0], j \geq 0$, where $e_0, f$ is the constant eigenfunction corresponding to $\lambda_0 = 0$. By ellipticity the first eigenvalue satisfies the spectral gap estimate $\lambda_1 > 0$ (see (25) below). The transition operators $P_{t,f}$ from (4) can be described in this eigen-basis via the eigenvalues $\mu_{j,f} = e^{-t\lambda_j}$, and their densities $p_{t,f}$ are uniformly bounded over $O \times O$. These well-known facts are reviewed in Sec. 3.

Some more notation: $C(O)$ denotes the space of uniformly continuous functions on $O$. The Sobolev and Hölder spaces $H^\alpha(O), C^\alpha(O)$ of maps defined on $O$ are defined as all functions that have partial derivatives up to order $\alpha \in \mathbb{N}$ defining elements of $L^2(O), C(O)$, respectively, and we set $C^\infty(O) = \cap_{\alpha > 0} C^\alpha(O), C^0(O) = C(O)$ by convention. Attaching the subscript $c$ to any of the preceding spaces denotes the linear subspaces of such functions of compact support within $O$. The Sobolev sub-spaces $H^k_0$ of $H^k$ are the completions of $C^\infty_c(O)$ for the $H^k$-norms. The symbols $\| \cdot \|_{H^k}, \| \cdot \|_{HS}$ denote the operator and Hilbert-Schmidt (HS) norm of a linear operator on a Banach space $H$, respectively. We denote by $\| \cdot \|_\infty$ the supremum norm and by $\| \cdot \|_B$ the norm of a normed space $B$, with dual space $B^*$. Throughout, $\preceq, \succeq, \asymp$ denotes inequalities in the last case two-sided) up to fixed multiplicative constants, while $Z \sim \mu$ means that a random variable $Z$ has law $\mu$. 

\[\text{INFERENCE FOR DIFFUSIONS} \quad 5\]
2.1. Optimal recovery of the transition operator $P_{D,f}$. Given our data, $P_{t,f}$ can be estimated directly at $t = D$ by evaluating a suitable set of basis functions of $L^2\left(O\right)$ at the observed ‘transition pairs’ $(X_{iD}, X_{(t+1)D})_{i=0}^{N-1}$. For instance if we take the linear span of the first $J$ eigenfunctions of the Neumann Laplacian $L_f$, $f = 1$, then a projection estimator for $P_{D,f}$ is described in (63) below. Our first theorem establishes a bound on the convergence rate for recovery of $P_{D,f}$ in operator norm $\|\cdot\|_{L^2 \rightarrow L^2}$ if the approximating space is of sufficiently high dimension $J = J_N \rightarrow \infty$ depending on the Sobolev regularity of $f$.

**Theorem 3.** Consider data $X_0, X_D, \ldots, X_{ND}$, at fixed observation distance $D > 0$, from the reflected diffusion model (2) on a bounded convex domain $O \subset \mathbb{R}^d$ with smooth boundary, started at $X_0 \sim \text{Unif}(O)$, with $f_0 \in C^2 \cap H^s, s > 2d - 1$, such that \(\inf_{x \in O} f_0(x) \geq f_{\text{min}} > 0\), $U \geq \|f_0\|_{H^s} + \|f_0\|_{C^2}$. Then the estimator $\hat{P}_J$ from (63) with choice $J_N \simeq N^{d/(2s+2+d)}$ satisfies,

$$\|\hat{P}_J - P_{D,f_0}\|_{L^2 \rightarrow L^2} = O_{P_{f_0}}\left(\frac{1}{d}N^{-\left(s+1\right)/(2s+2+d)}\right), \ N \rightarrow \infty,$$

with constants $C = C(s, D, U, d, O, f_{\text{min}}) > 0$ in the $O_{P_{f_0}}$ notation.

Our proof gives a non-asymptotic concentration inequality for the bound in (5), see Proposition 5. Moreover, as in Corollary 2 below we can deduce from (5) the convergence rate

$$\|\hat{P}_J - P_{D,f_0}\|_{H^0 \rightarrow H^0} = O_{P_{f_0}}\left(\frac{1}{d}N^{-\left(s+1-\alpha\right)/(2s+2+d)}\right), \ 0 < \alpha \leq s + 1,$$

for (stronger) operator norms on the $H^\alpha$ spaces. This rate is optimal in an information theoretic ‘minimax’ sense (cf. Ch.6 in [26]), as we now show for the case $\alpha = 2$ relevant below.

**Theorem 4.** In the setting of Theorem 3, there exists a bounded convex domain $O \subset \mathbb{R}^d$ with smooth boundary and a constant $c = c(s, D, U, d, f_{\text{min}}) > 0$ such that

$$\liminf_{N \rightarrow \infty} \inf_{P_N} \sup_{f : \|f\|_{H^\alpha(O)} \leq U, f \geq f_{\text{min}} > 0} \mathbb{P}_f\left(\|P_N - P_{D,f}\|_{H^2 \rightarrow H^2} > cN^{-\left(s-1\right)/(2s+2+d)}\right) > 1/4,$$

where the infimum extends over all estimators $\hat{P}_N$ of $P_{D,f}$ (i.e., measurable functions of the $X_0, X_D, \ldots, X_{ND}$ taking values in the space of bounded linear operators on $L^2$).

The proof relies on some results from spectral geometry that require an appropriate choice of domain, in fact $O$ is the ‘smoothed’ hyperrectangle in (15) below for $w \geq 2$ and $m$ large enough. The lower bound remains valid when restricting the supremum to $f$’s that are constant near $\partial O$. The above theorems show that the minimax rate in the class of reflected diffusion processes is faster by the power of a $\log N$-factor than the minimax rate of recovery of a general Markovian transition operator in the same regularity class, cf. Thm 2.2 in [46].

2.2. Injectivity of $f \mapsto P_{t,f} \mapsto P_{D,f}$, $t < D$.

2.2.1. Stability estimates. We now turn to the problem of guaranteeing validity of inference on $f$, and in turn also for $P_{t,f}$ for any $t > 0$. When $D \rightarrow 0$ in the asymptotics, ideas from stochastic calculus come into force and the inference problem becomes tractable either by direct techniques that identify the parameter $f$ – see [35] and references therein; or by steady state approximations to the diffusion equation (discussed in the introduction).

The ‘low frequency’ regime where $D > 0$ is fixed was studied in [29, 56] when $d = \dim(O) = 1$. The key idea of [29] is to infer $f$ from a principal component analysis (PCA) of the operator $P_{D,f}$. Following their line of work when $d > 1$ is not possible as they rely on
explicit identification equations for $f$ based on ODE techniques (see Section 3.1 in [29]), and in particular on the simplicity of the first non-zero eigenvalue $\lambda_{1,f}$ of $\mathcal{L}_f$ — both ideas do not extend to $d \geq 2$. Instead we follow the route via ‘stability estimates’ used recently in work on non-linear statistical inverse problems, see [50], [27, 1] and also [54]. We are not aware of an explicit reference that establishes the injectivity of the ‘forward’ map $f \mapsto P_{D,f}$ for arbitrary fixed $D > 0$ (and $d \geq 2$), let alone a stability estimate. Our first result achieves this when $f$ is known near the boundary of $\mathcal{O}$.

\textbf{Theorem 5.} Let $\mathcal{O}$ be a bounded convex domain in $\mathbb{R}^d, d \in \mathbb{N}$, with smooth boundary. Let $f, f_0$ be bounded from below by a constant $f_{\min} > 0$, suppose $f = f_0$ on $\mathcal{O} \setminus \mathcal{O}_0$ for some compact subset $\mathcal{O}_0$ of $\mathcal{O}$ and that $\|f\|_{C^2} + \|f_0\|_{C^2} \leq U$ for some $U$. Then there exists a positive constant depending on $D, d, \mathcal{O}_0, \mathcal{O}, U, f_{\min}$ such that

\begin{equation}
\|f - f_0\|_{L^2(\mathcal{O})} \leq C \left( \log \frac{1}{\|P_{D,f} - P_{D,f_0}\|_{L^2 \to L^2}} \right)^{-2/3}.
\end{equation}

In particular if $P_{D,f} = P_{D,f_0}$ co-incide as linear operators on $L^2(\mathcal{O})$ for some $D > 0$, we must have $f = f_0$ on $\mathcal{O}$.

The proof consists of a combination of the functional calculus identity

$P_{t,f} = \exp\{t \mathcal{L}_f\} = \exp\{t/\mathcal{L}_f^{-1}\}, \ t > 0,$

with injectivity estimates for the non-linear map $f \mapsto \mathcal{L}_f^{-1}(\phi)$ for appropriate $\phi$ (which have been developed earlier in related contexts, see, e.g., [58, 54] and therein).

It is of interest to improve the logarithmic modulus of continuity in (8). We now show that at least in some regions of the parameter space of $f_0$’s this is possible. The proof strategy is substantially different from Theorem 5 and instead of functional calculus relies on a spectral ‘pseudo-linearisation’ identity for $P_{t,f} - P_{t,f_0}$ obtained from perturbation theory for parabolic PDE. This identity simplifies when testing against eigenfunctions of $P_{t,f_0}$, and allows to identify $f_0$ if a certain transport operator (related to the stability estimates for $\mathcal{L}_f^{-1}$) is injective. Stability of this transport operator can be reduced to a hypothesis on the eigenvalues of $P_{t,f_0}$, which in turn can be tackled with techniques from spectral geometry.

To this end, define the first block of eigenfunctions $e_l \in H^2(\mathcal{O})$ of $-\mathcal{L}_{f_0}$ from (3) as

\begin{equation}
E_{1,f_0, t} = \sum_{l : \lambda_{l,f_0} = \lambda_{1,f_0}} e_{l,f_0} t^l,
\end{equation}

where $\lambda_{1,f_0}$ is the first (non-zero) eigenvalue. Note that the last sum is necessarily finite and $t = (t_l)$ is any vector of scalars. The following theorem shows that under certain assumptions on $E_{1,f_0, t}$ to be discussed, a Lipschitz (or Hölder) stability estimate holds true.

\textbf{Theorem 6.} In addition to the hypotheses of Theorem 5, assume also $\|f\|_{H^s} + \|f_0\|_{H^s} \leq U$ for some $s > d$ and that

\begin{equation}
\inf_{x \in \mathcal{O}_0} \frac{1}{2} \Delta E_{1,f_0, t}(x) + \mu |\nabla E_{1,f_0, t}(x)|^2_{\mathbb{R}^d} \geq c_0 > 0,
\end{equation}

for some $\mu, c_0 > 0$ and some vector $t$. Then we have

\begin{equation}
\|f - f_0\|_{L^2} \leq \bar{C}\|P_{D,f} - P_{D,f_0}\|_{H^2 \to H^2}
\end{equation}

for a constant $\bar{C} = \bar{C}(U, D, \mu, c_0, t, \mathcal{O}_0, \mathcal{O}, f_{\min}, d)$. 
By standard interpolation inequalities for Sobolev norms (p.44 in [45]) and Proposition 3 with some \( s \geq 2, k = 3 \), the bound (11) directly implies a Hölder stability estimate

\[
\|f - f_0\|_{L^2} \lesssim \|P_{D,f} - P_{D,f_0}\|_{L^2 \to L^2}^{1/2}
\]

for \( \gamma = 1/3 \). Whenever \( f, f_0 \in H^s \) we can let \( \gamma = \gamma(s) \to 1 \) as \( s \to \infty \).

As we can choose \( t \) we only need to find one linear combination of eigenfunctions in the eigenspace for \( \lambda_{1,f_0} \) that satisfies the hypothesis (10). As multiplicities of eigenvalues reflect symmetries of \( L_{f_0} \) on \( \mathcal{O} \), one could regard the added flexibility as a ‘blessing of symmetry’.

**Remark 1** (Stability for the ‘backward heat operator’). We can write \( P_{t,f} = \kappa_{t,D}(P_{D,f}) \) for the operator functional \( \kappa_{t,D} = \exp\{t(D)\log(\cdot)\} \) on the spectrum \((0, 1)\) of \( P_{D,f} \), see the identity (32). For \( t > D \) the map \( \kappa_{t,D} \) is \( C^{1+\eta}((0, 1)) \) for some \( \eta = \eta(t, D) > 0 \) and one deduces from operator-norm Lipschitz properties (e.g., Lemma 3 in [42]) that then \( \|P_{t,f} - P_{t,f_0}\|_{L^2 \to L^2} \lesssim \|P_{D,f} - P_{D,f_0}\|_{L^2 \to L^2} \). This is intuitive as the forward heat map is a smooth integral operator (the Chapman-Kolmogorov equations). In contrast in the case \( t < D \), the operator functional \( \kappa_{t,D} \) does not have a bounded Lipschitz constant on the spectrum. The last two theorems combined with Theorem 11 below (for \( D = t \) there, and via the continuous imbedding \( L^2 \to H^{-1} \)) imply the following stability estimates for the dependence of the ‘backward heat operator’ on \( f \): Under the hypotheses of Theorem 5 and assuming \( \|f\|_{H^s} + \|f_0\|_{H^s} \leq U \) for \( s > d \), we can bound the \( L^2(\mathcal{O}) \)-Hilbert Schmidt norms as

\[
\|P_{t,f} - P_{t,f_0}\|_{HS} \leq C\omega(\|P_{D,f} - P_{D,f_0}\|_{L^2 \to L^2}), \quad \text{any } 0 < t < D,
\]

where the modulus of continuity \( \omega \) can be taken to be \( \omega(z) = \log(1/z)^{-2/3} \), and with constant \( C \) now depending also on \( s, t \). In light of the exponential growth of the Lipschitz constant of \( \kappa_{t,D}, t < D \), in the tail of the spectrum of \( P_{D,f} \), one may think that such a logarithmic modulus of continuity is necessary. However, under the hypothesis (10) we can obtain a stronger Hölder modulus from our techniques. For the proof, we combine Theorem 6 (in fact (12)) and Theorem 11 below.

**Theorem 7.** Under the hypotheses of Theorem 6 we have

\[
\|P_{t,f} - P_{t,f_0}\|_{HS} \leq C'(\|P_{D,f} - P_{D,f_0}\|_{L^2 \to L^2}^\gamma), \quad \text{any } 0 < t < D,
\]

where \( 0 < \gamma < 1 \) is as in (12) and where \( C' = C(D, t, s, U, \mu, c_0, \mathcal{O}, \mathcal{O}_0, f_{\min}, d) \).

**Remark 2** (The one-dimensional case). In the one-dimensional setting \( d = 1 \), Lemma 6.1 and Proposition 6.5 in [29] prove simplicity of \( \lambda_{1,f_0} \) and the strict monotonicity in any closed subinterval \( \mathcal{O}_0 \) of \( \mathcal{O} \) of the corresponding eigenfunction \( e_{1,f_0} \) (for any \( f_0 \in H^s, s > 1 \)). This entails that the derivative \( e_{1,f_0} \) cannot vanish on \( \mathcal{O}_0 \) and verifies the key hypothesis (10) of Theorem 6 for some \( c_0 > 0 \) and all \( \mu \) large enough depending on \( \|e_{1,f_0}'\|_\infty \) (finite if \( s > 2 \)).

We next discuss an approach to verify (10) also in multi-dimensions \( d > 1 \) based on the ‘hot spots’ conjecture from spectral geometry. Ways to obtain ‘Hölder’ stability estimates that involve eigenfunctions for multiple distinct eigenvalues (rather than just the first), can be thought of too and will be investigated in future research.

2.2.2. Reflected diffusion and ‘hot spots’. While (10) is satisfied in dimension \( d = 1 \) (Remark 2), this is less clear in higher dimensions. Indeed, if the first eigenfunction \( e_{1,f} \) has a critical point in \( \mathcal{O}_0 \) with non-positive Laplacian (e.g., consider \( e_{1,f} \) near \((x_1, x_2) = 0 \) of the form \(-x_1^2 \pm x_2^2\)), the condition (10) does not hold. The hope is that eigenfunctions have special properties that exclude such situations, at least in regions \( \mathcal{O}_0 \subset \mathcal{O} \) one can identify.
Let us start with some simple examples where the condition is satisfied when \(d \geq 2\). For the Laplacian \(f = \text{const}\) on the unit cube, the first eigenfunctions of \(L_1\) corresponding to \(\lambda_{1,1}\) are cosines in one of the axial variables, constant otherwise, and \(|\nabla e_{1,1}|_{\mathbb{R}^d}\) vanishes only at the respective corners of \(\partial O\). Moreover \(|\Delta e_{1,1}|\) is bounded on any compact \(O_0 \subset O\) and so we can verify (10) for \(\mu\) large enough, appropriate \(\iota\), and such \(O_0\). The argument just given extends to cylindrical domains with base \(O_1\) equal to a convex domain in \(\mathbb{R}^{d-1}\): \[\text{PROPOSITION 1.} \quad \text{Consider a cylinder } O = O_1 \times (0, w) \text{ of height } w > 0 \text{ and with convex base } O_1 \subset \mathbb{R}^d \text{ of diameter } \text{diam}(O_1) \leq w. \text{Then (10) holds for } f_0 = 1, \text{ any compact } O_0 \subset O, \text{ some } \iota, \text{ and constants } \mu, c_0 \text{ depending on } O_0.\]

Our proof shows that when \(\text{diam}(O_1) < w\), the first eigenvalue is simple and its eigenfunction satisfies (10). When \(w = \text{diam}(O_1)\), the eigenspace of \(\lambda_{1,1}\) is possibly multi-dimensional, but there always exists one eigenfunction in that eigenspace that satisfies (10).

The proof of the last proposition is not difficult (see Section 3.7) – it draws inspiration from [40] and provides one of the few elementary examples for the validity of Rauch’s hot spots conjecture [4, 11] which is concerned precisely with domains \(O\) for which the gradient \(\nabla e_{1,1}\) of any eigenfunction of \(\Delta = L_1\) corresponding to \(\lambda_{1,1}\) has all its zeros at the boundary \(\partial O\). As the eigenfunctions are smooth in the interior of \(O\) this conjecture implies (10) for \(f = \text{const}\) and any compact \(O_0 \subset O\) as we can then choose \(\mu\) large enough depending on \(O_0\). The hot spots conjecture is believed to be true whenever \(O\) is convex but with the exception of cylinders has been proved only in special 2-dimensional cases so far, see [36, 3, 37, 64] and references therein for positive results and [12] who show that the conjecture may fail in non-convex domains. Next to convexity, symmetry properties of the domain \(O\) play a key role in these proofs – in the context of Proposition 1 the central axis play a key role in these proofs – in the context of Proposition 1 the central axis of symmetry of the cylinder ‘dominates the spectrum’ when the base \(O_1\) is small enough, providing what is necessary to verify the conjecture in this case. The case \(d = 1\) from Remark 2 can in this sense be regarded as a degenerately symmetric special case.

In this article we consider smooth domains but the preceding ‘cylinder’ is not smooth near the boundary of its base. But we can ‘round the corners’ of the cylinder without distorting the relevant spectral properties of \(L_1 = \Delta\). For example consider \(d \geq 2\) and a hyperrectangle \(O_{(w)} = (0, 1)^{d-1} \times (0, w)\) for \(w\) to be chosen, and define \[\text{(15)} \quad O_{m, w} = \{x \in \mathbb{R}^d : |x - O_{(w)}|_{\mathbb{R}^d} < 1/m\}, \ m \in \mathbb{N}.\]

Then the \(O_{m, w}\) are bounded convex domains that have smooth boundaries \(\partial O_{m, w}\) for all \(m\), and we will show that the conclusion of Proposition 1 remains valid for \(m\) large enough. Moreover, to lend more credence to (10) for \(f_0\) different from constant \(= 1\), we can extend the result to \(L_{f_0}\) for \(f_0\) in a \(L^\infty\)-neighbourhood of the constant function. This gives meaningful infinite-dimensional models for which the Hölder stability estimates from the previous subsection apply, and for which ‘fast convergence rates’ will be obtained in the next section. Incidentally they are also used to prove the lower bound in Theorem 4. For simplicity we only consider the case of simple (first) eigenvalues in the following result.

**THEOREM 8.** \(A)\) Consider domains \(O_{m, w}\) for \(w \geq 2\). Then we can choose \(m\) large enough such that the Laplacian \(-\Delta = -L_1\) on \(O_{m, w}\) has a simple eigenvalue \(0 < \lambda_{1,1,m} < \lambda_{2,1,m}\) and the corresponding eigenfunction \(e_{1,1,m}\) satisfies (10) for any compact subset \(O_0\) of \(O_{(w)}\), with constant \(\mu, c_0\) depending on \(O_0, d, w, m\).

\(B)\) The conclusions in \(A)\) remain valid if we replace \(L_1\) by \(L_{f_0}\) for any \(f_0\) that satisfies \(\|f_0\|_{L^1(\Omega_{m, w})} \leq U, s > d, \text{ as well as } \|f_0 - 1\|_{L^\infty} < \kappa\) for some \(\kappa\) small enough, with constants now depending also on \(\kappa, U\).
2.3. Bayesian inference in the diffusion model. While we have shown injectivity of the non-linear map \( f \mapsto P_{D,f} \), there is no obvious inversion formula (unless \( d = 1 \)), and so the estimate from Theorem \( 3 \) does not obviously translate into one for \( f \). The paradigm of Bayesian inversion \([67]\) can in principle overcome such issues. A natural Bayesian model for \( f \) is obtained by placing a prior probability measure \( \Pi \) on a \( \sigma \)-field \( S \) of some parameter space

\[
\mathcal{F} \subseteq C^2(0) \cap \{ f : f_{\text{min}} \leq \inf_{x \in \Omega} f(x) \}, \quad f_{\text{min}} > 0,
\]

so that unique pathwise solutions to (2) exist for all \( f \in \mathcal{F} \), with transition densities \( p_{D,f} \) as after (3). If \( B_{\Omega} \) denotes the Borel \( \sigma \)-field of \( \Omega \), and if the maps \( (f, x, y) \mapsto p_{D,f}(x, y) \) are jointly Borel measurable from \( (\mathcal{F} \times \Omega \times \Omega, S \otimes B_{\Omega} \otimes B_{\Omega}) \rightarrow \mathbb{R} \), then basic arguments (cf. \([24]\) and also \([56]\)) show that the posterior distribution is given by

\[
\Pi(B|X_0, X_D, \ldots, X_{ND}) = \int_B \prod_{i=1}^N p_{D,f}(X_{(i-1)D}, X_{iD}) d\Pi(f) \quad \text{for} \quad B \in S.
\]

This formula exposes the relationship of our setting to Bayesian non-linear inverse problems with PDEs \([67, 54]\), since the non-linear solution map \( f \mapsto p_{D,f} \) of the fundamental solution of a parabolic PDE features in the likelihood term. Even though our measurement model is much more complex than the additive Gaussian noise models considered in \([67, 54]\), we can still leverage computational ideas from this literature – see Remark 3 for details.

The priors \( \Pi \) we consider will be of Gaussian process type. With an eye on obtaining sharp results in some cases we give a concrete construction of a prior, but the proofs below can be applied to general classes of high- or infinite-dimensional priors (commonly used in the literature \([24, 50, 51, 54]\)) replacing the truncated Gaussian series in the next display. Take the first \( K \) eigenfunctions \( \{e_k : 0 \leq k \leq K\} \) of the Neumann-Laplacian \( -\Delta = -\mathcal{L}_1 \) for eigenvalues \( 0 = \lambda_0 < \lambda_1 \leq \lambda_2 < \ldots \), and for \( s \geq 0 \) define a Gaussian random field

\[
\theta(x) = \frac{\zeta(x)}{N^{d/(4s+4+2d)}} \left( g_0 + \sum_{1 \leq k \leq K} \lambda_k^{-s/2} g_k e_k(x) \right), \quad x \in \Omega, \quad g_k \sim \text{iid} N(0, 1), \quad K \in \mathbb{N},
\]

where for some compact subset \( \Omega_0 \subset \Omega \), the map \( \zeta \in C^\infty(\Omega) \) is a non-negative cut-off function vanishing on \( \Omega \setminus \Omega_0 \) and equal 1 on some further compact subset \( \Omega_{00} \) of the interior of \( \Omega_0 \). As in \([50, 54]\), the \( N \)-dependent rescaling provides extra regularisation required in the proofs – it also allows us to remove the strong prior restrictions from \([56]\) in the case \( d = 1 \).

For fixed \( K \), the Law \( \theta \) of \( \theta \) is a probability measure supported in the space \( \mathbb{R}^{K+1} \simeq \{ \zeta g : g \in E_K \} \) where \( E_K \subset C^\infty \) is the finite-dimensional linear span of the \( \{e_k : 0 \leq k \leq K\} \). As \( K \rightarrow \infty \) the Law \( \theta \) models a \( s \)-smooth Gaussian random field on \( \Omega \) that is supported in a strict subset of \( \Omega \). The prior for the diffusivity \( f \in \mathcal{F} = C^2 \cap \{ f \geq 1/4 \} \) (equipped with the trace Borel \( \sigma \)-algebra \( S \) of the separable Banach space \( C(\Omega) \)) is then

\[
f = f_\theta = \frac{1}{4} + e^{\theta} \frac{1}{4}, \quad \Pi = \text{Law}(f)
\]

which equals 1/2 on \( \Omega \setminus \Omega_0 \). Note that the ‘base case’ \( \theta = 0 \) corresponds to \( f = 1/2 \) and hence to the case where the diffusion in (2) is a standard reflected Brownian motion with generator \( \mathcal{L}_{1/2} = \Delta/2 \). The construction can be adapted to any fixed \( f_{\text{min}} > 0 \) replacing 1/4.

**Remark 3.** The numerical computation of the posterior measure (16) is possible via MCMC methods. For instance, since our priors are Gaussian, we can use the standard pCN proposal (see \([16]\) or Section 1.2.4 in \([54]\)) to set up a Markov chain \( (\theta_m)_{m=1}^M \in \mathbb{R}^{K+1} \) that has \( \Pi(\theta|X_0, X_D, \ldots, X_{ND}) \) as invariant distribution. Posterior functionals

\[
E\Pi[H(\theta)|X_0, X_D, \ldots, X_{ND}], \quad H : \mathbb{R}^{K+1} \rightarrow \mathbb{R}^k, \quad k \in \mathbb{N},
\]
The posterior mean estimate $f_{\bar{\theta}}$ with $\bar{\theta} = M^{-1} \sum_{m=1}^{M} \vartheta_m$ after $M = 10000$ pCN iterates, for sample sizes $N = 2500$ (left) and $N = 25000$ (center), at sampling frequency $D = 0.05$; the true field $f_0$ (right).

can be approximated by ergodic averages $M^{-1} \sum_{m=1}^{M} H(\vartheta_m)$, see Fig. 2 for an illustration with $H = id$. The computation of each iterate $\vartheta_m$ of this chain requires the draw of a $(K+1)$-dimensional Gaussian (from the prior) and the evaluation of the log-likelihood function

$$\ell_N(\vartheta_m) \equiv \sum_{i=1}^{N} \log p_{D,f_{\vartheta_m}}(X_{(i-1)D}, X_{iD}).$$

In light of the representation (33), the latter can be evaluated by standard numerical methods for elliptic PDEs that compute the first few eigen-pairs $(e_j,f_{\vartheta_m},\lambda_j,f_{\vartheta_m})$ of the differential operator $-L_{f_{\vartheta_m}}$ with Neumann boundary conditions. Explicit error bounds for the approximation of the transition densities can be obtained from the exponential decay of the tail of the series in (33) via Corollary 1, and since $D > 0$ is fixed in our setting. Moreover, taking limits in the pseudo-linearisation identity (42) below allows to check the gradient stability condition from [59, 9], which is a key to give computational guarantees for MCMC.

**Remark 4 (Adding a drift).** The above Bayesian methodology extends to more general diffusion models (1) by proceeding as in [56], Sec. 2.3.2. One employs a hierarchical prior construction that first specifies a prior for the diffusivity $f$ and then models the ‘remaining’ drift $\nabla U$ conditionally on $f$, for instance by priors as in [28]. One can employ MCMC samplers for hierarchical priors, and proceed similar to [74] in the ‘drift step’. Alternatively one can simply plug in an empirical estimate for $U$ (e.g., via an estimate $\hat{\mu}$ as after (30) in [56]), avoiding hierarchical methods. When $d > 1$, the case of drift vector fields in (1) that are not in gradient form $\nabla U$ is innately more challenging as one loses self-adjointness of the infinitesimal generator. Some ideas for how to deal with such non-reversible processes can be found in [55, 2], but for many applications, gradients of ‘force’ potentials $U$ provide natural non-parametric models with relevant physical interpretation [28, 33, 34].

**Remark 5 (Different boundary conditions).** The reflected diffusion model (2) – which corresponds to Neumann boundary conditions – is essential to obtain a Markov process that does not ‘terminate’ at a finite time (as would be the case for Dirichlet boundary conditions). Processes that are periodic on a $d$-dimensional cube, or that reflect along directions different from the inward normal vector at $\partial \mathcal{O}$, can be accommodated as well (but, at least in the latter case, introduce further tedious technicalities).

2.4. Posterior consistency theorems. We now obtain mathematical guarantees for the inference provided by $\Pi(\cdot|X_0, X_D, \ldots, X_{N_D})$, following the programme of Bayesian Non-parametrics [24] in the context of non-linear inverse problems [54].
2.4.1. Posterior reconstruction of $P_{D,f}$. We show that the Bayesian approach attains the optimal convergence rate for inference on the transition operator at the ‘observed’ times $D$. 

**Theorem 9.** Consider discrete data $X_0, X_D, \ldots, X_{ND}$, at fixed observation distance $D > 0$, from the reflected diffusion model (2) on a bounded convex domain $\mathcal{O} \subset \mathbb{R}^d$ with smooth boundary, started at $X_0 \sim \mathcal{U}nif(O)$. Assume $f_0 \in H^s$, $s > \max(2 + d/2, 2d - 1)$, satisfies $\inf_{x \in \partial \mathcal{O}} f_0(x) > 1/4$ and $f_0 = 1/2$ on $\mathcal{O} \setminus \partial \mathcal{O}$. Let $\Pi(\cdot | X_0, X_D, \ldots, X_{ND})$ be the posterior distribution (16) resulting from the prior $\Pi$ for $f$ from (17) with $K \simeq N^{d/(2s+2+d)}$ and the given $s$. Then there exists $M$ depending on $D, \mathcal{O}, \mathcal{O}_0, s, d$ and $U \geq ||f_0||_{H^s}$ such that

$$\Pi(f : \|P_{D,f} - P_{D,f_0}\|_{L^2(\mathcal{O})} \geq MN^{-(s+1)/(2s+2+d)} | X_0, X_D, \ldots, X_{ND}) \rightarrow P_{f_0} 0.$$ 

Inspection of our proofs shows that one obtains convergence rates also in $\| \cdot \|_{H^s} \rightarrow H^s$ norms as in (6). When the first non-zero eigenvalue $\lambda_{1,f_0}$ of $L_{f_0}$ is simple, the previous theorem implies consistency of the PCA provided by $P_{D,f}$. Since draws $P_{D,f} X_0, X_D, \ldots, X_{ND}$ are self-adjoint Markov transition operators, we can extract their ‘principal component’, or second eigenfunction, $e_{1,f}$. By the operator norm convergence of $P_{D,f}$ to $P_{D,f_0}$, the simplicity of the eigenvalue $\lambda_{1,f_0}$ eventually translates into simplicity of $\lambda_{1,f}$ with probability approaching one, and a unique $e_{1,f}$ then exists (up to choice of sign), cf. Proposition 9. Using quantitative perturbation arguments (e.g., Proposition 4.2 in [29]) one obtains

$$\Pi(f : ||e_{1,f} - e_{1,f_0}||_{L^2(\mathcal{O}} ) \geq MN^{-(s+1)/(2s+2+d)} | X_0, X_D, \ldots, X_{ND}) \rightarrow P_{f_0} 0.$$ 

In dimension $d = 1$, the top eigenfunction fully identifies $f$ with an explicit reconstruction formula [29, 56], but in multi-dimensions this approach is not feasible, also because $\lambda_{1,f_0}$ is not simple in general, in which case the PCA for the eigenfunction will not be consistent.

2.4.2. Consistency and convergence rates for the non-linear inverse problem. We now state the main statistical result of this article.

**Theorem 10.** Consider the setting of Theorem 9. Then there exists a sequence $\eta_N \rightarrow 0$ such that as $N \rightarrow \infty$,

$$\Pi(f : ||f - f_0||_{L^2(\mathcal{O})} \geq \eta_N | X_0, X_D, \ldots, X_{ND}) \rightarrow P_{f_0} 0,$$

as well as, for any $t > 0$,

$$\Pi(f : ||P_{t,f} - P_{t,f_0}||_{L^2(\mathcal{O})} \geq \eta_N | X_0, X_D, \ldots, X_{ND}) \rightarrow P_{f_0} 0.$$ 

Specifically we can take $\eta_N = O((\log N)^{-d'})$ for some $d' > 0$. Moreover, if in addition (10) holds for $f_0$, then we can take $\eta_N = O(N^{-(s+1)/(2s+2+d)}).$

When $t \geq D$ we could obtain directly the convergence rate $\eta_N = N^{-(s+1)/(2s+2+d)}$ for operator norms $\|P_{t,f} - P_{t,f_0}\|_{L^2(\mathcal{O})}$ from Theorem 9 and the argument sketched at the beginning of Remark 1. But for $t < D$ we are solving a genuine inverse problem. Note further that the $HS$-norms equivalently bound the $L^2(\mathcal{O} \times \mathcal{O}, dx \otimes dx)$ norms of the difference between the transition densities $p_{t,f} - p_{t,f_0}$ from (33).

In order to obtain faster rates $\eta_N$, the hypothesis (10) needs to hold only at the ground truth $f_0$ and not throughout the parameter space of prior diffusivities $f$. Next to the one-dimensional case discussed in Remark 2, Theorem 8 describes an infinite-dimensional class of $f_0$’s for which such faster rates can indeed be attained also when $d \geq 2$.

Using uniform integrability type arguments as in [50, 54], a similar convergence rate can be proved for the posterior mean vector $\theta = E[|\theta| X_0, X_D, \ldots, X_{ND}]$ and the induced conductivity $f_\theta$ and transition operators $P_{t,f_\theta}$, yielding Theorem 2. See Subsection 3.6.3.
3. Proofs.

3.1. Analytical background: reflected diffusions and their generators.

3.1.1. Divergence form operators. Let $\mathcal{O}$ be a bounded convex domain in $\mathbb{R}^d$ with smooth boundary and such that $\text{vol}(\mathcal{O}) = 1$. Consider the divergence form elliptic operator $\mathcal{L}_f \phi = \nabla \cdot (f \nabla \phi)$ from (3). The Sobolev space $H^1(\mathcal{O})$ can be endowed both with the usual norm $\|\phi\|_{H^1} = \|\phi\|_{L^2} + \|\nabla \phi\|_{L^2}$ or with the equivalent norm $\|\phi\|_{H^1} := \|\phi\|_{L^2} + \|\sqrt{f} \nabla \phi\|_{L^2}$ with equivalence constants depending only on $f_{\text{min}}, \|f\|_{\infty}$. Moreover the elements of $H^1$ satisfying zero Neumann-boundary conditions (in the usual trace sense) are defined as

$$H^1_\nu(\mathcal{O}) := \{ \phi \in H^1(\mathcal{O}), \frac{\partial \phi}{\partial \nu} = 0 \text{ on } \partial \mathcal{O} \},$$

with $\nu$ the unit normal vector. By the divergence theorem (e.g., p.143 in [71])

$$\langle \mathcal{L}_f \phi_1, \phi_2 \rangle_{L^2} = -\langle f \nabla \phi_1, \nabla \phi_2 \rangle_{L^2} = \langle \phi_1, \mathcal{L}_f \phi_2 \rangle_{L^2}, \ \forall \phi_i \in H^1_\nu(\mathcal{O}),$$

so $\mathcal{L}_f$ is self-adjoint for the $L^2$-inner product on $H^1_\nu$. This operator can be closed to give an operator $E_f$ on the domain $H^1(\mathcal{O})$ that coincides with $-\mathcal{L}_f$ on $H^1_\nu$ ([21], Theorem 7.2.1), and which corresponds to the bi-linear symmetric (Dirichlet) form

$$\mathcal{E}_f(\phi_1, \phi_2) = \langle \sqrt{f} \nabla \phi_1, \sqrt{f} \nabla \phi_2 \rangle_{L^2}, \ \phi_i \in H^1(\mathcal{O}),$$

which in turn defines a Markov process $(X_t : t \geq 0)$ arising from a semi-group with infinitesimal generator $\mathcal{L}_f$ and $d\mu(x) = dx$ as invariant probability measure. An application of Ito’s formula shows that this Markov process describes solutions of the SDE (2) with ‘reflection’ of the process at the boundary’ provided by the (inward) normal vector $\nu$ and the ‘local time’ process $L_t$ that is non-zero only when $X_t \in \partial \mathcal{O}$. Details can be found in [69], [7] (ch. 37, 38), [6] (Sec. I.12. and p.52) and also [5].

3.1.2. Spectral resolution of the generator. We recall here some standard facts on the spectral theory of the generator $\mathcal{L}_f$ with Neumann boundary conditions. The arguments follow closely the treatment of the standard Laplacian $f = 1$ on p.403 in [71] (see also Ch.7.2 in [21]), and extend straightforwardly to $\mathcal{L}_f$ as long as $0 < f_{\text{min}} \leq f \leq \|f\|_{\infty} \leq U < \infty$.

Denote by $E_f$ the operator mapping $H^1$ into $L^2$ defined before (23). By (23) the linear operator $id + E_f$ satisfies

$$\langle (id + E_f) \phi, \phi \rangle_{L^2} = \|\phi\|_{L^2}^2 + \|\sqrt{f} \nabla \phi\|_{L^2}^2 = \|\phi\|_{H^1}^2 = \|\phi\|_{H^1}^2, \ \phi \in H^1,$$

from which one deduces that the linear operator $id + E_f$ defines a bijection between $H^1$ and $(H^1)^*$ with operator norms depending only on $f_{\text{min}}, U$. If we restrict its inverse $T_{1,f}$ to the Hilbert space $L^2(\mathcal{O})$ then it defines a self-adjoint operator which is also compact as it maps $L^2$ into $H^1$ which embeds compactly into $L^2$. By the spectral theorem there exist $L^2$-orthonormal eigenfunctions $e_0 = 1$ and $e_{1,f}, \ldots, e_{j,f}, \ldots, \in H^1_\nu \cap L^2$ corresponding to eigenvalues $\lambda_0 = 0 \leq \lambda_{1,f}, \ldots, \lambda_{j,f} \uparrow \infty$ such that

$$\mathcal{L}_f e_{j,f} = -\lambda_{j,f} e_{j,f}, \ \ j \in \mathbb{N} \cup \{0\}.$$

We denote by

$$\mathcal{L}^{-1}_{f} = -\sum_{j \geq 1} \lambda_{j,f}^{-1} e_{j,f} \langle e_{j,f}, \cdot \rangle_{L^2}.$$
the corresponding inverse operator acting on the Hilbert space

$$L^2_0 := L^2 \cap \left\{ \phi : \int_\mathcal{O} \phi(x) dx = \langle \phi, e_0 \rangle_{L^2} = 0 \right\},$$

for which the \( \{e_j : j \geq 1\} \) form an orthonormal basis. Clearly \( L^2 = L^2_0 \oplus \{\text{constants}\} \).

We next record the following "uniform in \( f \)" spectral gap estimate: the first (nontrivial) eigenvalue \( \lambda_{1,f} \) has variational characterisation (see Sec. 4.5 in [21])

$$\lambda_{1,f} = -\sup_{u \in H^1_0; \langle u, 1 \rangle_{L^2} = 0} \frac{\langle L_f u, u \rangle_{L^2}}{\|u\|^2_{L^2}} = \inf_{u \in H^1_0; \langle u, 1 \rangle_{L^2} = 0} \frac{\langle f \nabla u, \nabla u \rangle_{L^2}}{\|u\|^2_{L^2}} \geq \frac{f_{\min}}{p_\mathcal{O}} > 0$$

where we have used the Poincaré-inequality (Theorem 1 on p.292 in [23]): \( \|u\|^2_{L^2} \leq p_\mathcal{O} \|\nabla u\|^2_{L^2} \) for \( u \in L^2_0 \) and Poincaré constant \( p_\mathcal{O} > 0 \) depending only on \( \mathcal{O} \). For subsequent eigenvalues we know that they can have at most finite multiplicities (e.g., Theorem 4.2.2 in [21]), and in fact that they obey Weyl’s law (e.g., using p.111 in [70]),

$$\lambda_{j,1} \asymp j^{2/d} \text{ as } j \to \infty.$$  

The preceding asymptotics hold initially for the standard Laplacian (\( f = 1 \)), with the constants involved depending only on \( \text{vol}(\mathcal{O}), d \). By the variational characterisation of the \( \lambda_j \)'s (Sec. 4.5 in [21]) and since

$$\|f \nabla u, \nabla u\|_{L^2} \simeq \|\nabla u\|^2_{L^2}, \quad f_{\min} \leq f \leq \|f\|_{\infty},$$

holds for the quadratic form featuring in (25), the \( \lambda_{j,f} \) corresponding to conductivities \( f \) differ by at most a fixed constant that depends only on \( f_{\min}, \|f\|_{\infty} \).

Taking the eigenpairs \( (e_{j,f}, \lambda_{j,f}) \) of \( L_f \) one can define Hilbert spaces

$$\mathcal{H}^k_0(\mathcal{O}) = \left\{ \phi \in L^2_0(\mathcal{O}) : \sum_{j \geq 1} \lambda_{j,f}^k \langle \phi, e_{j,f} \rangle^2_{L^2} \equiv \|\phi\|_{\mathcal{H}^k_0} < \infty \right\}, \quad k \in \mathbb{N}.$$

Any \( \phi \in L^2_0 \) can be written as \( \sum_{j \geq 1} e_{j,f} \langle \phi, e_{j,f} \rangle_{L^2} \) and hence \( \mathcal{H}^0_0 = L^2_0 \) by Parseval’s identity. The following proposition (proved in Section 3.8) summarises some basic properties.

**Proposition 2.** Let \( \mathcal{O} \) be a bounded convex domain in \( \mathbb{R}^d \) with smooth boundary and let \( f \in C^1(\mathcal{O}) \) be s.t. \( \inf_{x \in \partial \mathcal{O}} f(x) \geq f_{\min} > 0 \). Then \( \mathcal{H}^1_0(\mathcal{O}) = H^1(\mathcal{O}) \cap L^2_0 \) and

$$\mathcal{H}^2_f = H^2 \cap H^1_0 \cap L^2 = \{ h \in L^2_0 : L_f h \in L^2_0, (\partial h / \partial \nu) = 0 \text{ on } \partial \mathcal{O} \}.$$

If we assume in addition that for some integer \( k \geq 2 \) either \( A \|f\|_{C^{k-1}} \leq U \) or \( B \|f\|_{H^{s}} \leq U \) for some \( s > d \) s.t. \( k \leq s + 1 \), then we have

$$H^k_f(\mathcal{O}) \subset H^k(\mathcal{O}) \text{ and } \|\phi\|_{H^k} \asymp \|\phi\|_{H^k_f} \text{ for } \phi \in H^k_f.$$  

We further have the embedding \( H^k_f \cap L^2 \subset H^k \) and also if \( H^k_f \) is replaced by \( H^k_c / \mathbb{R} \) (modulo constants). Finally we have \( H^k_f = H^k_{f'} \) for any pair \( f, f' \) satisfying \( A \) or \( B \), with equivalent norms. All embedding/equivalence constants depend only on \( f_{\min}, U, d, k, \mathcal{O} \).

**Corollary 1.** Under the hypotheses of Proposition 2B), the eigenfunctions \( e_{j,f} \) corresponding to eigenvalues \( \lambda_{j,f} \) of \(-L_f \) satisfy for some \( C < \infty \) depending only on \( \mathcal{O}, d, k, U, f_{\min} \),

$$\|e_{j,f}\|_{H^k} \lesssim \lambda_{j,f}^{k/2} \leq C j^{k/d}, \quad j \geq 0,$$

which whenever \( k > d/2 \) implies as well

$$e_{j,f}\|_{\infty} \lesssim j^{\tau} \quad \forall \tau > 1/2, \quad j \geq 0.$$
PROOF. By definition (27) and (26), the result is true for the $H^k$-norm replacing the $H^k_f$-norm, and since $e_{j,f} \in \bar{H}^k_f$, Proposition 2 implies (29), and (30) then follows from the Sobolev imbedding. \qed

3.2. Heat equation, transition operator, and a perturbation identity. For fixed $T > 0$ let us consider solutions $v = v_{f,\phi} : (0, T] \times O \to \mathbb{R}$ in $L^2$ to the heat equation

$$\frac{\partial}{\partial t} v - \nabla \cdot (f \nabla v) = 0 \text{ on } (0, T] \times O,$$

$$\frac{\partial v}{\partial \nu} = 0 \text{ on } (0, T] \times \partial O,$$

$$v(0, \cdot) = \phi \text{ on } O,$$

for any initial condition satisfying $\int_O \phi = 0$. The unique solution of this PDE is given by

$$v_{f,\phi}(t, \cdot) = P_t, f(\phi) = \sum_{j \geq 1} e^{-t\lambda_j} e_{j,f}(\phi)_{L^2}, \quad t > 0, \quad \phi \in L^2_0(O),$$

which also lie in $L^2_0$. We can add any fixed constant $c$ to both the initial condition $\phi$ and solution $v$, by extending the above series to include $j = 0$ for $e_0 = 1, \lambda_0 = 0$. The symmetric non-negative (Prop. 4) fundamental solutions of the heat equation are then

$$p_{t,f}(x, y) = \sum_{j \geq 0} e^{-t\lambda_j} e_{j,f}(x)e_{j,f}(y), \quad x, y \in O.$$

These are precisely the kernels of the transition operator $P_{t, f}$ in (4) and also the transition probability densities of the Markov process $(X_t : t \geq 0)$ arising from the Dirichlet form (23), cf., e.g., Sec.1.14 in [5].

3.2.1. Heat kernel estimates. By the bounds on eigenfunctions and eigenvalues from (26), (30), the series in (33) defining $p_{t, f}$ converge in $H^k_f$, and by the Sobolev imbedding with $k > d/2$ then also uniformly on $O$.

**Proposition 3.** Under the hypotheses of Proposition 2B, we have for any fixed $t > 0$

$$\sup_{x \in \partial O} \|p_{t,f}(x, \cdot)\|_{H^k} \leq c_{ub} < \infty,$$

where $c_{ub} = c_{ub}(k, t, f_{min}, U, \partial O, d) < \infty$.

**Proof.** Using the representation (33) and Corollary 1 we obtain

$$\|p_{t,f}(x, \cdot)\|_{H^k} \leq \sum_{j \geq 0} e^{-t\lambda_j} \|e_j\|_{H^k} \|e_j\|_{\infty} \leq \sum_{j \geq 0} j^{t+(k/d)} e^{-ctj^{2/d}} \leq c_{ub}.$$

A further key fact is that the transition densities are bounded from below on a convex domain $O$. See Section 3.8 for the proof.

**Proposition 4.** Let $O$ be a bounded convex domain with smooth boundary and suppose $f \geq f_{min} > 0$ satisfies $\|f\|_{C^\alpha} \leq B$ for some even integer $\alpha > (d/2) - 1$. Then we have for every $t > 0$ and some positive constant $c_{lb}(t, O, d, f_{min}, B, \alpha) > 0$ that

$$\inf_{x,y \in O} p_{t,f}(x, y) \geq c_{lb}.$$
Using Proposition 6.3.4 in [5] and (25), (95) (or by estimating the tail of the series in (33) and integrating the result \(dx\) one also obtains geometric ergodicity of the diffusion process,

\[
\sup_{x \in \mathcal{O}} \|p_{t,f}(x, \cdot) - \mu\|_{TV} \leq Ce^{-\lambda_1 t}, \quad \forall t \geq t_0 > 0, \quad d\mu(x) = e_0(x) = 1, \quad x \in \mathcal{O}.
\]

3.2.2. Perturbation and pseudo-linearisation identity. In this subsection we consider two conductivities \(f, f' \geq f_{\min} > 0\) whose \(C^2(\mathcal{O})\)-norms are bounded by a fixed constant \(U\) and study the resulting difference of the action of the transition operators \(P_{t,f} - P_{t,f'}\) on the eigen-functions \((e_{j,f} : j \geq 1) \subset H^2(\mathcal{O})\) of \(L_f\). We will use the factorisation of space and time variables in the identity \(P_{t,f}(e_{j,f}) = e^{-t\lambda_j} e_{j,f}\) which holds as well for the eigenblocks (with \(t = (t_i)\) any finite sequence)

\[
P_{t,f}(E_{j,f,u}) = \sum_{k=1}^{\lambda_{j,f}} e_{i,f,t}
\]

corresponding to the eigenvalue \(\lambda_{j,f}\), that is, we have

\[
P_{t,f}(E_{j,f,u}) = e^{-t\lambda_j} E_{j,f,u}, \quad j \geq 0.
\]

By (31), (32), the functions

\[
v_j(\cdot,t) = P_{t,f'}(E_{j,f,u}) - P_{t,f}(E_{j,f,u}), \quad t \in (0,T], \quad j \geq 1,
\]

solve the inhomogeneous PDE

\[
\frac{\partial}{\partial t} v - \nabla \cdot (f' \nabla v) = \tilde{G}_j \quad \text{on} \quad (0,T] \times \mathcal{O}
\]

\[
\frac{\partial v}{\partial t} = 0 \quad \text{on} \quad (0,T] \times \partial\mathcal{O}
\]

\[
v(0,\cdot) = 0 \quad \text{on} \quad \mathcal{O}
\]

where

\[
\tilde{G}_j(t) = -\nabla \cdot [(f - f') \nabla P_{t,f}(E_{j,f,u})] = e^{-t\lambda_j} G_j, \quad G_j := -\nabla \cdot [(f - f') \nabla E_{j,f,u}],
\]

with eigenvalues \(\lambda_{j,f}\) of \(-L_f\). Standard semi-group arguments (Proposition 4.1.2 in [47]) imply that the solution \(v\) of (39) can be represented by the ‘variation of constants’ formula

\[
v_j(\cdot,t) = \int_0^t e^{(t-s)L_f} \tilde{G}_j(s) ds.
\]

For \((e_k,f',\lambda_{k,f'})\) the eigen-pairs of \(-L_f\) we thus arrive at

\[
P_{t,f'}(E_{j,f,u}) - P_{t,f}(E_{j,f,u}) = v_j(\cdot,t) = \sum_{k \geq 1} \int_0^t e^{-s\lambda_j} e^{-(t-s)\lambda_{k,f'}} (e_{k,f'}, G_j)_{L^2 e_{k,f'}} ds
\]

\[
\equiv \sum_k b_{k,j} (e_{k,f'}, G_j)_{L^2 e_{k,f'}}, \quad j \geq 1,
\]

for coefficients

\[
b_{k,j} = b_{k,j}(t) = \int_0^t e^{-s\lambda_j} e^{-(t-s)\lambda_{k,f'}} ds.
\]

We can regard (42) as a spectral ‘pseudo-linearisation’ identity for \(P_{t,f'} - P_{t,f}\), similar to analogous results employed to prove stability estimates in other inverse problems, e.g., [50]. It could also be the starting point to prove LAN-type expansions in our model as in [77].
3.3. Information distances and small ball probabilities. For \((X_t : t \geq 0)\) the diffusion process (2) with transition densities from (33), the Kullback-Leibler (KL-) divergence in our discrete measurement model with observation distance \(D > 0\) is defined as

\[
KL(f, f_0) = E_{f_0} \left[ \log \frac{p_{D,f_0}(X_0, X_D)}{p_{D,f}(X_0, X_D)} \right], \quad f, f_0 \in \mathcal{F},
\]

where we regard the \(p_{D,f}\) from (33) as joint probability densities on \(O \times O\) (as \(\text{vol}(O) = 1\)).

In the following theorem \(\| \cdot \|_{HS}\) denotes the HS norm for operators on the Hilbert space \(L^2(O)\) (or just \(L^2_v(O)\)). Note further that \(H^1_c \subset H^2_0\) implies \((H^1_0)^* = H^{-1} \subset (H^1_c)^*\) so the r.h.s. in (45) can be bounded by \(\| f - f_0 \|^2_{H^{-1}}\) and then also by \(\| f - f_0 \|_{L^2}\).

**Theorem 11.** Let \(f, f_0\) satisfy the conditions of Proposition 2B) for some \(s > d\). Suppose \(f = f_0\) outside of a compact subset \(O_0 \subset O\). Then for any \(D > 0\) there exist positive constants \(C_0, C_1\) depending on \(D, O, O_0, s, d, U, f_0\) such that

\[
KL(f, f_0) \leq C_0\| p_{D,f_0} - p_{D,f} \|_{H^s}^2 \leq C_1\| f - f_0 \|_{L^2}. \tag{45}
\]

**Proof.** Using Propositions 3, 4 (noting also \(H^s \subset C^\alpha\) by the Sobolev imbedding) and standard inequalities from information theory (as at the beginning of the proof of Lemma 14 in [56], or see Appendix B in [24]) one shows

\[
KL(f, f_0) \lesssim c(\alpha)\| p_{D,f_0} - p_{D,f} \|_{L^2(O \times O)}^2 \lesssim \| p_{D,f_0} - p_{D,f} \|_{HS}^2. \tag{46}
\]

The HS-norm of an operator \(A\) on any Hilbert space \(H\) can be represented as \(\| A \|_{HS}^2 = \sum_j \| A e_j \|_{L^2}^2\) where the \((e_j)\) are any orthonormal basis of \(H\). In what follows we take the basis \((e_j) \equiv (e_{j,f})\) arising from the spectral decomposition of \(L_f\), and hence need to bound

\[
\sum_{j \geq 1} \| p_{D,f_0}(e_{j,f}) - p_{D,f}(e_{j,f}) \|_{L^2}^2, \tag{47}
\]

where the HS-norms can be taken over the Hilbert space \(L^2_v(O, dx)\) as both operators have identical first eigenfunction \(e_{0,f_0} = 1 = e_{0,f}\). For each summand \(p_{D,f_0}(e_{j,f}) - p_{D,f}(e_{j,f})\) we apply the representation (42) with \(f' = f_0, f = f\) and \(\tau_t\) selecting the relevant \(j\)-th eigenfunction if there are multiplicities. We then write shorthand

\[
g_j = -\nabla \cdot [(f - f_0)\nabla e_{j,f}]
\]

for \(G_j\) from (40) with these choices. We can bound the coefficients (43) as

\[
|b_{k,j}| = e^{-t\lambda_{k,f_0}} \left( \int_0^{t/2} e^{-s\lambda_{j,f}} e^{s\lambda_{k,f_0}} ds + \int_{t/2}^t e^{-s\lambda_{j,f}} e^{s\lambda_{k,f_0}} ds \right)
\leq e^{-t\lambda_{k,f_0}/2} \lambda_{j,f}^{-1} + e^{-t\lambda_{j,f}/2} \lambda_{k,f_0}^{-1},
\]

so that by Parseval’s identity, for \(0 < t \leq T\), and writing \((e_k, \lambda_k) = (e_{k,f_0}, \lambda_{k,f_0})\) for the remainder of the proof,

\[
\| P_t f_0(e_{j,f}) - P_t f(e_{j,f}) \|_{L^2}^2 = \sum_k b_{k,j}^2 \langle e_k, g_j \rangle^2 \lesssim \sum_{k \geq 1} e^{-t\lambda_k} \lambda_{j,f}^{-2} \langle e_k, g_j \rangle^2 + \sum_{k \geq 1} e^{-t\lambda_{j,f}} \lambda_k^{-2} \langle e_k, g_j \rangle^2.
\]

Returning to (47) we are thus left with bounding the double sum

\[
\sum_{j \geq 1} \| p_{D,f_0}(e_j) - p_{D,f}(e_j) \|_{L^2}^2 \lesssim \sum_{j,k} e^{-D\lambda_k} \lambda_{j,f}^{-2} \langle e_k, g_j \rangle^2 + \sum_{j,k} e^{-D\lambda_{j,f}} \lambda_k^{-2} \langle e_k, g_j \rangle^2. \tag{48}
\]
By the divergence theorem
\[ \langle e_k, g_j \rangle_{L^2} = \langle e_k, \nabla \cdot [(f - f_0)\nabla e_{j,f}] \rangle_{L^2} = \langle e_{j,f}, \nabla \cdot [(f - f_0)\nabla e_k] \rangle \]
so by Parseval’s identity and (27) (with norm there well-defined also for negative \( k \)), the r.h.s. in (48) is bounded by
\[ \sum_k e^{-D\lambda_k} \| \nabla \cdot [(f - f_0)\nabla e_k] \|^2_{\tilde{H}^{-2}_f} + \sum_j e^{-D\lambda_j} \| \nabla \cdot [(f - f_0)\nabla e_{j,f}] \|^2_{H^{-2}_f}. \]
In the next step we use the basic sequence space duality relationship \( \tilde{H}^{-2}_f = (H^2_f)^* \). Moreover, noting \( f = f_0 \) outside of \( \mathcal{O}_0 \), we take a suitable smooth cut-off function \( \zeta \) that equals one on \( \mathcal{O}_0 \) and is compactly supported in \( \mathcal{O} \). Then we apply the divergence theorem in conjunction with Proposition 2 to obtain
\[ \| \nabla \cdot [(f - f_0)\nabla e_{j,f}] \|^2_{H^{-2}_f} = \sup_{\|\psi\|_{H^2_0} \leq 1} \left| \int_{\mathcal{O}} \psi \nabla \cdot [(f - f_0)\nabla e_{j,f}] \right| \]
\[ \leq \sup_{\|\psi\|_{H^2_0} \leq 1} \| \nabla e_{j,f} \cdot \nabla \tilde{\psi} \|_{H^1} \| f - f_0 \|_{(H^1_f)^*} \]
\[ \lesssim \| f - f_0 \|_{(H^1_f)^*} \sup_{\|\tilde{\psi}\|_{H^2} \leq c} \| \tilde{\psi} \|_{H^2} \| e_{j,f} \|_{B^2}. \]
with spaces \( B^2 \) as after (92). For \( d \leq 3 \) we have \( B^2 = H^2 \) and then \( \| e_{j,f} \|_{B^2} \lesssim j^{2/d} \) in view of Corollary 1 with \( k = 2 \leq s + 1 \). For \( d > 3 \) and \( k = 2 + d/2 + \eta \leq s + 1, \eta > 0 \), we use the Sobolev embedding \( H^k \subset C^2 = B^2 \) and again Corollary 1 to bound \( \| e_{j,f} \|_{C^2} \). In both cases the r.h.s. in the last display is bounded by a constant multiple of \( j^{c(d)} \| f - f_0 \|_{(H^1_f)} \), for some constant \( c(d) > 0 \). Inserting these bounds into the second summand in (49) and using (26), the series
\[ \sum_j j^{2c(d)} e^{-cDj^{2/d}} < \infty \]
is convergent (for \( D > 0 \) fixed). The same estimate holds for \( e_{j,f}, \lambda_{j,f}, \tilde{H}^{-2}_f \) replaced by \( e_k, \lambda_k, \tilde{H}^{-2}_f \), summing the first term in (49) – completing the proof of the theorem.

3.4. Proofs of stability estimates.

3.4.1. Proof of Theorem 5. Take \( \phi \in C_c^\infty(\mathcal{O}) \) such that \( \phi = 1 \) on \( \mathcal{O}_0 \) and \( \int_{\mathcal{O}} \phi = 0 \) (as \( \mathcal{O}_0 \) is a compact subset of \( \mathcal{O} \), such \( \phi \) exists). By the results from Section 3.1.2, the inhomogeneous elliptic PDE (58) in Lemma 2 below has unique solution
\[ u_{f,\phi} = L^{-1}_f \phi = -\sum_{j=1}^{\infty} \lambda_{j,f}^{-1} e_{j,f} \langle e_{j,f}, \phi \rangle_{L^2(\mathcal{O})}. \]
In particular Proposition 2 implies that \( \phi \in \tilde{H}^2_f \) and that \( u_{f,\phi} \) is bounded in \( \tilde{H}^4_f \subset H^3 \). The same arguments apply to \( f_0 \) replacing \( f \). Now Lemma 2 implies
\[ \| f - f_0 \|_{L^2(\mathcal{O})} \lesssim \| f_0 \|_{C^1} \| u_{f,\phi} - u_{f_0,\phi} \|_{H^2(\mathcal{O})} \leq C \| u_{f,\phi} - u_{f_0,\phi} \|_{L^2}^{1/3}. \]
for finite constant \( C = C(\|u,\phi\|_{H^2}, \|u_{f,0},\phi\|_{H^2}) \leq C(U) \), where we have also used the standard interpolation for \( H^2 \)-norms (p.44 in [45]). We now estimate the right hand side in the last display. As \( \phi \in L^2 \) we have for any \( J \in \mathbb{N} \) that
\[
\|u_{f,\phi} - \sum_{j \leq J} (-\lambda_j^{-1} f) e_{j,f} \langle e_{j,f}, \phi \rangle_{L^2} \|_{L^2}^2 \leq \sum_{j > J} \lambda_j^{-2} \langle e_{j,f}, \phi \rangle_{L^2}^2 \leq C_{\phi, f_{min}, U} J^{-c(d)},
\]
for \( c(d) = 4/d \), using also (26), and similarly for \( f = f_0 \). By the triangle inequality (52)
\[
\|u_{f,\phi} - u_{f_0,\phi}\|_{L^2} \leq \left\| \sum_{j \leq J} \lambda_j^{-1} f e_{j,f} \langle e_{j,f}, \phi \rangle_{L^2} - \sum_{j \leq J} \lambda_j^{-1} f_0 e_{j,f_0} \langle e_{j,f_0}, \phi \rangle_{L^2} \right\|_{L^2} + 2C_{\phi, f_{min}, U} J^{-c(d)}.
\]
Let us further define ‘truncated’ transition operators
\[
P_{D,f,J}(\phi) = \sum_{j \leq J} e^{-D\lambda_j t} e_{j,f} \langle e_{j,f}, \phi \rangle_{L^2}, \quad \mu_{j,f} = e^{-D\lambda_j t}, \quad \phi \in L^2_0,
\]
which, just as in the display above (52) and in view of (26), satisfy the estimate
\[
\|P_{D,f} - P_{D,f,J}\|_{L^2 \to L^2} \leq e^{-cJ^{2/d}}, \quad \bar{c} = \bar{c}(D, U, f_{min}) > 0,
\]
and the same is true for \( f_0 \) replacing \( f \). The operators \( P_{D,f,J} \) are self-adjoint on \( L^2_0(O) \) and by what precedes and (26), (25), the union of their spectra is contained in
\[
[\min_{f_0} \mu_{J,f}, \max_{f_0} \mu_{J,f}] \subset [e^{-cJ^{2/d}}, e^{-Df_{min}/p\alpha}], \quad c' = c'(D, U, f_{min}) > 0.
\]
We can employ a cut-off function and construct smooth \( \kappa_J \) compactly supported on \( (e^{-cJ^{2/d}}/2, 1) \) such that
\[
\kappa_J(z) = \frac{D}{\log z}, \quad \text{on} \quad \left[ \min_{f_0} \mu_{J,f}, \max_{f_0} \mu_{J,f} \right].
\]
Then since \( \lambda_j^{-1} = \kappa_J(e^{-D\lambda_j}) = \kappa_J(\mu_j) \) on the last interval, we can write, using the notation of functional calculus,
\[
\left\| \sum_{j \leq J} \lambda_j^{-1} e_{j,f} \langle e_{j,f}, \phi \rangle_{L^2} - \sum_{j \leq J} \lambda_j^{-1} e_{j,f_0} \langle e_{j,f_0}, \phi \rangle_{L^2} \right\|_{L^2} \\
\leq \|\kappa_J(P_{D,f,J}) - \kappa_J(P_{D,f_0,J})\|_{L^2 \to L^2} \\
\leq \|\kappa_J\|_{B_{1,1}^1(\mathbb{R})} \|P_{D,f,J} - P_{D,f_0,J}\|_{L^2 \to L^2} \lesssim e^{cJ^{2/d}} \|P_{D,f} - P_{D,f_0}\|_{L^2 \to L^2} + e^{-cJ^{2/d}}
\]
where we have used Lemma 3 in [42] for the self-adjoint operators \( P_{D,f,J}, P_{D,f_0,J} \) on \( L^2_0 \) and the bound \( \|\kappa_J\|_{B_{1,1}^1(\mathbb{R})} \lesssim e^{cJ^{2/d}} \) (using results in Sec. 4.3 in [26]). Combining all that precedes, we obtain the overall estimate
\[
\|f - f_0\|^3_{L^2(O)} \lesssim e^{cJ^{2/d}} \|P_{D,f} - P_{D,f_0}\|_{L^2 \to L^2} + e^{-cJ^{2/d}} + J^{-c(d)}
\]
where \( J \in \mathbb{N} \) was arbitrary. Choosing \( J \) such that
\[
J^{2/d} = \frac{1}{2c} \log \left( \frac{1}{\|P_{D,f} - P_{D,f_0}\|_{L^2 \to L^2}} \right) \\
(we can increase \( 2c \) if necessary to ensure \( J \in \mathbb{N} \)) implies for some \( \delta' = \delta'(c, \bar{c}) > 0 \) that
\[
\|f - f_0\|^3_{L^2(O)} \lesssim \log \left( \frac{1}{\|P_{D,f} - P_{D,f_0}\|_{L^2 \to L^2}} \right)^{-\delta} + \|P_{D,f} - P_{D,f_0}\|^\delta_{L^2 \to L^2}, \quad \delta = c(d)/2.
\]
As the \( \|f - f_0\|_{L^2} \leq 2U \) are uniformly bounded, we can absorb the second term into the first after adjusting constants, so the stability estimate is proved, and the injectivity assertion of the theorem follows directly from it.
3.4.2. Proof of Theorem 6. For eigenblocks $E_{1,f_0,t} \in H^2_{f_0}$ from (37), Proposition 2 gives

$$
\|E_{1,f_0,t}\|_{H^2} \lesssim \|E_{1,f_0,0}\|_{H^2_{f_0}} = |t|\lambda_{1,f_0} < \infty, \text{ where } |t|^2 = \sum_k t_k^2.
$$

Then, using the representation (42) with choices $\bar{f} = f_0, f' = f$ and Proposition 2,

$$
\|P_{D,f} - P_{D,f_0}\|_{H^2 \to H^2} \gtrsim \|P_{D,f}(E_{1,f_0,t}) - P_{D,f_0}(E_{1,f_0,t})\|_{H^2_{f_0}}
$$

(53)

$$
= \sum_k \lambda_{k,f}^2 |b_{k,1}|^2 |\langle G, e_{k,f} \rangle|^2,
$$

where $G = \nabla \cdot [(f - f_0)\nabla E_{1,f_0,t}]$ and $b_{k,1} = \int_0^t e^{-s\lambda_{1,f_0}} e^{-(t-s)\lambda_{k,f}} ds$. We can write

$$
b_{k,1} = e^{-t\lambda_{k,f}} e^{-t(\lambda_{1,f_0} - \lambda_{k,f}) - 1} t^{-t\lambda_{1,f_0}} e^{-(t-s)\lambda_{k,f}} ds.
$$

for some mean values $\xi(\lambda_{1,f_0}, \lambda_{k,f})$ in the interval $[-t\lambda_{1,f_0}, -t\lambda_{k,f}]$ arising from the mean value theorem applied to the exponential map. This remains true in the degenerate case where $\lambda_{1,f_0} = \lambda_{k,f}$ as then $b_{1,k} = e^{-t\lambda_{1,f_0}}$.

Now recalling the distribution of the eigenvalues from (26) we see that for $k \leq K$ with $K$ fixed, the last displayed exponential is bounded below by a fixed constant depending on $K, d$, while for large values of $k$, the last but one term in the last display is of order $1/\lambda_{k,f}$ for $t$ fixed. Hence we have for all $k$, and some $C = C(t, d, \mathcal{O}, f_{\min}, U)$,

(54)

$$
|b_{k,1}| \geq C\lambda_{k,f}^{-1}.
$$

Combining this estimate with (53) and Parseval’s identity gives

(55)

$$
\|P_{D,f} - P_{D,f_0}\|_{H^2 \to H^2} \gtrsim \|G\|_{L^2} = \|\nabla \cdot [(f - f_0)\nabla E_{1,f_0,t}]\|_{L^2}.
$$

The theorem then follows from Lemma 1 with $u_0 = E_{1,f_0,t}$ which satisfies (56) by hypothesis (10) and is supremum-norm bounded by (30).

3.4.3. Stability of a transport operator. We now give a stability lemma for the operator

$$
T(h) = \nabla \cdot (h \nabla u_0), h \in C^1,
$$

for appropriate choices of $u_0$. It features regularly in stability estimates for elliptic PDEs, see Chapter 2 in [54] for references.

**Condition 1.** Let $u_0 \in H^2(\mathcal{O})$ be a function such that $\sup_{x \in \mathcal{O}_0} |u_0(x)| \leq u < \infty$ and

(56)

$$
\frac{1}{2} \Delta u_0(x) + \mu |\nabla u_0(x)|^2 \geq c_0 > 0, \text{ a.e. } x \in \mathcal{O}_0,
$$

for some compact subset $\mathcal{O}_0$ of $\mathcal{O}$.

**Lemma 1.** For $u_0$ as in Condition 1 and any $h \in C^1$ that vanishes on $\mathcal{O} \setminus \mathcal{O}_0$, the operator $T(h)$ satisfies $\|\nabla \cdot (h \nabla u_0)\|_{L^2(\mathcal{O})} \geq \|h\|_{L^2(\mathcal{O})}$ for a constant $c = c(u, c_0, \mu) > 0$.

**Proof.** The divergence theorem applied to any $v \in H^2(\mathcal{O})$ vanishing at $\partial \mathcal{O}$ gives

$$
\langle \Delta u_0, v^2 \rangle_{L^2} + \frac{1}{2} \langle \nabla u_0, \nabla (v^2) \rangle_{L^2} = \frac{1}{2} \langle \Delta u_0, v^2 \rangle_{L^2}.
$$

For $v = e^{-\mu u_0}h$ with $\mu > 0$ from (56)

$$
\frac{1}{2} \int_\mathcal{O} \nabla (v^2) \cdot \nabla u_0 = - \int_\mathcal{O} \mu |\nabla u_0|^2 v^2 + \int_\mathcal{O} v e^{-\mu u_0} \nabla h \cdot \nabla u_0,
$$

where
so that by the Cauchy-Schwarz inequality
\[ \left| \int_{\mathcal{O}} \left( \frac{1}{2} \Delta u_0 + \mu |\nabla u_0|^2 \right) v^2 \right|^2 = \left| \langle \Delta u_0 + \mu |\nabla u_0|^2, v^2 \rangle_{L^2} + \frac{1}{2} \langle \nabla u_0, \nabla (v^2) \rangle_{L^2} \right|^2 \]
(57)
\[ = \left| \langle h \Delta u_0 + \nabla h \cdot \nabla u_0, h e^{-2\mu u_0} \rangle_{L^2} \right| \leq \tilde{\mu} \| \nabla \cdot (h \nabla u_0) \|_{L^2} \| h \|_{L^2} \]
for \( \tilde{\mu} = \exp(2\|u_0\|_{\infty}) \). Now by (56) and since \( h = 0 = v \) on \( \mathcal{O} \setminus \mathcal{O}_0 \) by hypothesis we have
\[ \left| \int_{\mathcal{O}} \left( \frac{1}{2} \Delta u_0 + \mu |\nabla u_0|^2 \right) v^2 \right|^2 = \left| \int_{\mathcal{O}_0} \left( \frac{1}{2} \Delta u_0 + \mu |\nabla u_0|^2 \right) v^2 \right|^2 \geq c_0 \int_{\mathcal{O}_0} v^2 \]
and fusing also (57) we deduce \( \| \nabla \cdot (h \nabla u_0) \|_{L^2} \| h \|_{L^2} \geq c' \| v \|_{L^2(\mathcal{O}_0)}^2 \geq \varepsilon \| h \|_{L^2(\mathcal{O})}^2 \). □

**Lemma 2.** Let \( \mathcal{O}_0 \) be any compact subset of a bounded smooth domain \( \mathcal{O} \) and suppose that \( f_1, f_2 \) are two \( C^2 \)-diffusivities \( f_i \geq f_{\text{min}} > 0, i = 1, 2 \), such that \( f_1 = f_2 \) on \( \mathcal{O} \setminus \mathcal{O}_0 \). Suppose for some \( \phi \in C^\infty(\mathcal{O}) \cap L^2(\mathcal{O}) \) s.t. \( \phi \geq 1 \) on \( \mathcal{O}_0 \), functions \( u_{f_i}, i = 1, 2 \), solve
\[ \Delta u_i(x) = f_i \phi \]
(58)
Then we have for some constant \( C = C(\| \phi \|_{\infty}, \| f_1 \|_{C^1}) > 0 \) that
\[ \| f_1 - f_2 \|_{L^2(\mathcal{O})} \leq C \| f_2 \|_{C^1} \| u_{f_1} - u_{f_2} \|_{H^2}. \]
(59)

**Proof.** Let us write \( h = f_1 - f_2 \). By (58), we have on \( \mathcal{O} \)
\[ \Delta u_i(x) = f_i \phi \]
(60)
We can upper bound the \( \| \cdot \|_{L^2} \)-norm of r.h.s. by
\[ \| \nabla \cdot (f_2 \nabla (u_{f_2} - u_{f_1})) \|_{L^2} \leq \| \nabla f_2 \|_{\infty} \| u_{f_2} - u_{f_1} \|_{H^1} + \| f_2 \|_{\infty} \| u_{f_2} - u_{f_1} \|_{H^2} \]
(61)
To lower bound the left hand side of (61) we apply Lemma 1 with \( u_0 = u_{f_1} \) to \( \| \nabla \cdot (h \nabla u_{f_1}) \|_{L^2} \). The hypothesis on \( \phi \) implies \( 1 \leq f_1 \Delta u_{f_1} + \nabla f_1 \cdot \nabla u_{f_1} \) on \( \mathcal{O}_0 \), so that either \( \Delta u_{f_1}(x) \geq 1/2 \| f_1 \|_{\infty} \) or \( |\nabla u_{f_1}(x)|^2 \geq (1/2) \| f_1 \|_{C^1}^2 \) for \( x \in \mathcal{O}_0 \). Since \( \| u_{f_1} \|_{\infty} + \| \Delta u_{f_1} \|_{\infty} \lesssim \| u_{f_1} \|_{C^2} \lesssim \varepsilon \| f_1 \|_{C^1} \) by a \( C^0 \)-regularity estimate (e.g., Thm 4.3.4 in [72]) for solutions of (58) with \( f_1 \in C^1 \) this implies (56) and by Lemma 1 this result. □

**3.5. Minimax estimation of the transition operator \( P_{D,f} \).**

**3.5.1. Operator norm convergence.** In this subsection we construct explicit estimator \( \hat{P}_D \) for the transition operator \( P_{D,f} \) and prove Theorem 3. While it is possible to take \( \hat{P}_D \) self-adjoint, this will not be required here.

For \( J \in \mathbb{N} \) take \( E_J \equiv \{ e_{j,i} : 0 \leq j \leq J - 1 \} \) the eigenfunctions of the Neumann Laplacian \( \mathcal{L}_1 \) on \( \mathcal{O} \) (including \( e_0 = 1 \)) and regard \( E_J \simeq \mathbb{R}^J \) as a normed space equipped with the Euclidean norm via Parseval’s identity for \( L^2(\mathcal{O}) \). Given the observations \( X_0, X_D, \ldots, X_{ND} \) define a \( J \times J \) matrix by
\[ \hat{P}_{j,j'} = \frac{1}{N} \sum_{i=1}^{N} e_{j,i}(X_{(i-1)D}) e_{j',i}(X_{iD}), \quad 0 \leq j, j' \leq J - 1. \]
(62)
Via the injection of $E_J \simeq \mathbb{R}^J$ into $L^2(O)$ we can regard $\hat{P}_J$ as a bounded linear operator $\hat{P}_J$ on $L^2$ described by the action
\[ \langle \hat{P}_J e_{j,1}, e_{j',1} \rangle_{L^2} \equiv \hat{P}_{j,j'}, \quad 0 \leq j, j' \leq J - 1 \]
(63)
\[ = 0 \quad \text{otherwise}. \]
Similarly the transition operator $P_{D,f}$ induces a matrix $P_{D,f,j,j'}$ via
\[ P_{D,f,j,j'} = \langle P_{D,f} e_{j,1}, e_{j',1} \rangle_{L^2} = \mathbb{E}_f e_{j,1}(X_0) e_{j',1}(X_D), \quad 0 \leq j, j' \leq J - 1, \]
\[ = 0 \quad \text{otherwise}, \]
which equals the expectation $\mathbb{E}_f \hat{P}_{D,J} = P_{D,f,J}$ under the law $\mathbb{P}_f$ of $(X_t: t \geq 0)$ started in stationarity $X_0 \sim \text{Unif}(O)$. The latter matrix corresponds to the operator on $L^2$ arising from the composition $\pi_E P_{D,J}$ where $\pi_E$ describes the projection onto $E_J$—note that $E_J$ are not the eigen-spaces of $P_{D,J}$ unless $f = 1$. To obtain an estimate for the approximation error from $E_J$, note first that by Proposition 2 and (27), (26), for any $\phi \in L^2_0$ s.t. $\|\phi\|_{L^2} \leq 1$,
\[ \|P_{D,f}(\phi)\|_{H^{s+1}}^2 \lesssim \|P_{D,f}(\phi)\|_{H^{s+1}}^2 = \sum_{j \geq 1} e^{-2D\lambda_{j+1}} \|\phi, e_{j,1} \|^2_{L^2} \leq B' \]
(64)
for some $B' = B'(U) < \infty$ since $\|f\|_{H^{s}} \leq U$ by hypothesis. Therefore, using again (27), (26) and Parseval’s identity
\[ \|\pi_E P_{D,J} - P_{D,f}(\phi)\|_{L^2 \to L^2} = \sup_{\phi \in L^2_0, \|\phi\|_{L^2} = 1} \|\pi_E P_{D,J} - P_{D,f}(\phi)\|_{L^2} \]
(65)
\[ \leq \sup_{\|\phi\|_{H^{s+1}} \leq B'} \|\pi_E \psi - \psi\|_{L^2} \leq \sup_{\|\phi\|_{H^{s+1}} \leq B'} \sqrt{\sum_{j \geq 1} \lambda_{j+1}^{-s} \lambda_{j+1}^{s+1} \|\psi, e_{j,1} \|^2_{L^2}} \lesssim J^{-(s+1)/d}. \]
To bound the operator norms on approximation spaces $E_J \simeq \mathbb{R}^J$ we use a standard covering argument in finite dimensional spaces (e.g., the proof of Lemma 1.1 in [14]) to the effect that
\[ \|\hat{P}_J - \pi_E P_{D,J}\|_{L^2 \to L^2} = \|\hat{P}_J - \pi_E P_{D,J}\|_{E_J \to E_J} \leq 2 \max_{u,v \in D_J(1/4)} |u^T (\hat{P}_J - P_{D,J}) v| \]
where $D_J(1/4)$ is a discrete 1/4-net of unit vectors (i.e., $\|u\|_{\mathbb{R}^J} = 1$) covering the unit sphere of $\mathbb{R}^J$ of cardinality at most $\text{card}(D_J(1/4)) \leq A^J$ for some $A > 0$, see, e.g., [26], p.373. By a union bound and for $g(x,y) = u(x) v(y)$ with $u = \sum_j u_j e_j$, $v = \sum_j v_j e_j$, we obtain
\[ \mathbb{P}_f \left( \|\hat{P}_J - \pi_E P_{D,J}\|_{L^2 \to L^2} > \varepsilon \sqrt{\frac{J}{N}} \right) \]
\[ \leq A^J \max_{u,v \in D_J(1/4)} \mathbb{P}_f \left( |u^T (\hat{P}_J - P_{D,J}) v| > \varepsilon \sqrt{\frac{J}{4N}} \right) \]
\[ = A^J \max_{g} \mathbb{P}_f \left( \left| \sum_{i=1}^N g(X_{(i-1)D}, X_i) - \mathbb{E}_f g(X_{(i-1)D}, X_i) \right| > \varepsilon \sqrt{JN/4} \right) \]
We can apply the concentration inequality Proposition 6 below with $h = g - \int_D g dP_{D,J}$ an element of the Hilbert space $L^2_0(P_{D_J})$ from (69) below. We have, using also Proposition 3,
\[ \|h\|_{L^2(P_{D,J})} \lesssim \|h\|_{L^2(O \times O, dx \otimes dx)} \leq C \]
as well as $\|h\|_{\infty} \leq H \lesssim J^{2\tau+1}$ in view of the estimate
\[ \|u\|_{\infty} \leq \|u\|_{E_J} \sqrt{\sum_{j \leq J} \|e_j\|^2_{\infty}} \lesssim J^{\tau+1/2}, \quad \tau > 1/2, \]
where we have used (30). In this way we obtain overall:

**Proposition 5.** Let \( D > 0 \) and suppose \( X_0, X_D, \ldots, X_{ND} \) arise from the diffusion (2) started at \( X_0 \sim \text{Unif}(\mathcal{O}) \) on a bounded smooth convex domain \( \mathcal{O} \) with \( f : \mathcal{O} \rightarrow [f_{\min}, \infty), f_{\min} > 0 \) s.t. \( \|f\|_{H^s} + \|f\|_{C^2} \leq U, s > d \). Let \( J > 0 \) be s.t. \( \bar{J} \leq \sqrt{N} \) for some \( \bar{\tau} > 5/2 \). Then for all \( c > 0 \) we can choose \( C = C(U, D) > 0 \) such that

\[
\mathbb{P}_f \left( \|\hat{P}_f - P_{D,f}\|_{L^2 \rightarrow L^2} \geq C \left( \sqrt{J/N} + J^{-(s+1)/d} \right) \right) \leq e^{-cJ}.
\]

In particular for \( s > 2d - 1 \) we can choose \( J \simeq N^{d/(2s+2+d)} \) to prove Theorem 3. A bound on the \( H^2 \rightarrow H^2 \)-operator norms follows as well: Since the imbedding \( H^2 \subset L^2 \) is continuous and since \( \|v\|_{H^2} \simeq \|v\|_{H^2} \leq J^{2/d} \|v\|_{L^2} \) whenever \( v \in E_f \), we have

\[
\|\hat{P}_D - \pi_{E_f} P_{D,f}\|_{H^2 \rightarrow H^2} \lesssim J^{2/d} \|\hat{P}_D - \pi_{E_f} P_{D,f}\|_{L^2 \rightarrow L^2}
\]

and as in (65) and by Proposition 2 the approximation errors scale like

\[
\|\pi_{E_f} P_{D,f} - P_{D,f}\|_{H^2 \rightarrow H^2} \lesssim \sup_{\|\psi\|_{H^2} \leq J} \|\pi_{E_f} \psi - \psi\|_{H^2} \lesssim J^{(s-1)/d}.
\]

**Corollary 2.** In the setting of Proposition 5 we also have

\[
\mathbb{P}_f \left( \|\hat{P}_D - P_{D,f}\|_{H^2 \rightarrow H^2} \geq C \left( \sqrt{J/N} + J^{-(s+1)/d} \right) \right) \leq e^{-cJ},
\]

3.5.2. A concentration inequality for ergodic averages. Consider the discrete Markov chain \( X_D, \ldots, X_{ND} \) arising from sampling the diffusion (2) started in stationarity \( X_0 \sim \text{Unif}(\mathcal{O}) \). The transition operator of this chain is \( P_{D,f} \) from (32), with spectrum \( 1 > e^{-D\lambda_{1,f}} \geq e^{-D\lambda_{2,f}} \geq \ldots \) and the first spectral gap is bounded as

\[
1 - e^{-D\lambda_{1,f}} \geq r_D
\]
in view of (25) for some \( r_D = r(D, f_{\min}, \mathcal{O}, U) > 0 \). We initially establish concentration bounds for additive functionals

\[
\sum_{i=1, i \text{ odd}}^N h(X_{(i-1)D}, X_{iD}), \quad \text{and} \quad \sum_{i=1, i \text{ even}}^N h(X_{(i-1)D}, X_{iD}), \quad h : \mathcal{O} \times \mathcal{O} \rightarrow \mathbb{R},
\]

of bivariate Markov chains in \( \mathcal{O} \times \mathcal{O} \) arising from

\((X_0, X_D), (X_{2D}, X_{3D}), (X_{4D}, X_{5D}), \ldots, \) and \((X_D, X_{2D}), (X_{3D}, X_{4D}), (X_{5D}, X_{6D}), \ldots, \)

respectively. By a union bound this will give concentration inequalities for ergodic averages \( \sum_{i=1}^N h(X_{(i-1)D}, X_{iD}) \) along all indices \( i \), see (74) below.

The transition operators \( P_{D,f}' \) of the new bivariate Markov chains have invariant measure \( p_{D,f}(x, y) \) on \( \mathcal{O} \times \mathcal{O} \). If we define

\[
L^2_0(P_{D,f}) := \left\{ h : \int_{\mathcal{O}} \int_{\mathcal{O}} h(x, y)p_{D,f}(x, y)dydx = 0 \right\}
\]

then one shows

\[
\sup_{h : \int \int_{\mathcal{O} \times \mathcal{O}} h} \frac{\|P_{D,f}'[h]\|_{L^2(P_{D,f})}}{\|h\|_{L^2(P_{D,f})}} \leq \sup_{h : \int \int_{\mathcal{O} \times \mathcal{O}} h} \frac{\|P_{D,f}[h]\|_{L^2}}{\|h\|_{L^2}} \leq e^{-D\lambda_{1,f}}
\]
by a basic application of Jensen’s inequality (cf. Lemma 24 in [56]), and by (68). By the variational characterisation of eigenvalues and (68) this implies that the first spectral gap \( \rho_D \) of \( P'_{D,f} \) is also bounded as

\[
\rho_D = 1 - e^{-D\lambda_1} \geq r_D.
\]

We deduce from Theorem 3.1 in [60] that for any \( h \in L^2_0(P_{D,f}) \) we have the variance bound

\[
\text{Var}_f \left( \frac{1}{N} \sum_{i=1, \text{i odd}}^N h(X_{(i-1)D}, X_{iD}) \right) \leq \frac{2}{N \rho_D} \|h\|_{L^2(P_{D,f})}^2 \leq \frac{1}{N r_D} \|h\|_{L^2(P_{D,f})}^2
\]

where we have also used (71). Similarly, requiring in addition \( \|h\|_\infty \leq H \), Theorem 3.3 and eq. (3.21) in [60] imply the concentration inequality.

\[
P_f \left( \sum_{i=1, \text{i odd}}^N h(X_{(i-1)D}, X_{iD}) \geq x \right) \leq 2 \exp \left\{ -\frac{x^2 r_D}{4N \|h\|_{L^2(P_{D,f})}^2} + 10xH \right\}, \quad x > 0.
\]

The same inequality applies to the even indices \( i \), so that by a union bound we obtain:

**Proposition 6.** Let \( h \in L^2_0(P_{D,f}) \) be s.t. \( \|h\|_\infty \leq H \), and let \( X_0, X_D, \ldots, X_{ND} \) be sampled discretely at observation distance \( D > 0 \) from the diffusion \( (X_t : t \geq 0) \) from (2) with \( f_{\min} \leq f \leq U < \infty \). Then for some constant \( c = c(r, D) \) and all \( x > 0 \) we have

\[
P_f \left( \sum_{i=1}^N h(X_{(i-1)D}, X_{iD}) \geq x \right) \leq 4 \exp \left\{ -\frac{c x^2}{N \|h\|_{L^2(P_{D,f})}^2} + xH \right\}.
\]

3.5.3. **Proof of the minimax lower bound Theorem 4.** Given the analytical estimates obtained so far, the proof follows ideas of the lower bound Theorem 10 of [58] and we sketch here only the necessary modifications. Let us take the same set of functions \( \{f_m : m = 1, \ldots, M\}, f_0 = 1 \) from (4.17) in [58] and consider only \( j \) large enough in that construction such that all the wavelets featuring there are contained inside of the compact subset \( \mathcal{O}_0 \) of the ‘smoothed’ \( d \)-dimensional hypercube \( \mathcal{O} \equiv \mathcal{O}_{m,w} \) from (15) for \( m, w \) from Theorem 8B). In particular we can choose \( j \) so large that \( \|f_m - 1\|_\infty < \kappa \) for the \( \kappa \) from Theorem 8B). We apply Theorem 6.3.2 in [26] (taking also note of (6.99) there to obtain an ‘in probability version’ of the lower bound) as in Step VII of the proof of Theorem 10 in [58], noting that in our setting we can control the KL-divergences \( KL(f_m, f_0) \leq 2 \|f_m - f_0\|_{H^{-1}} \) via Theorem 11 and the imbedding \( (H^1(\mathcal{O}))^* \subset H^{-1}(\mathcal{O}) \), the result will thus follow if we can show that the transition operators induced by the \( P_{D,f,m} \)’s are appropriately separated for the \( H^2 \)-operator norms. Using the inequality (55) we have

\[
\|P_{D,f,m} - P_{D,f,m'}\|_{H^2 \rightarrow H^2} \geq \|\nabla \cdot [(f_m - f_{m'})\nabla e_{1,f,m'}]\|_{L^2}, \quad 1 \leq m, m' \leq M,
\]

where we note that on our ‘smoothed’ cylinder, the eigenfunctions \( e_{1,f,m'} \) are all simple thanks to Theorem 8B). To proceed we need to lower bound the \( L^2 \)-norms of the r.h.s. of (4.19) in [58], with \( u_{f,m} \) there replaced by our \( e_{1,f,m} \). As will be shown in the proof of Proposition 8, the first eigenfunction \( e_{1,1} \) of \( \Delta \) on \([0,1]^d \times (0, w)\) has all partial derivatives equal to zero except with respect to one, say the first, variable, and that partial derivative cannot vanish on \( \mathcal{O}_0 \). In view of (90), (91) this implies that the corresponding eigenfunction \( e_{1,f,m} \) on \( \mathcal{O} \) has a partial derivative for the first variable that is strictly positive while the other partial derivatives are bounded (in fact can be made arbitrarily close to zero). One can then easily adapt the steps V and VI in the proof of Theorem 10 in [58] (with \( \varepsilon^{-2} \) there equal to our \( N \)) to establish, for all \( N \) large enough, the required bound

\[
\|\nabla \cdot [(f_m - f_{m'})\nabla e_{1,f,m'}]\|_{L^2} \gtrsim N^{-(s-1)/(2s+2+d)}.
\]
3.6. Bayesian contraction results.

3.6.1. Results for general priors. In this subsection we follow general ideas from Bayesian nonparametrics [24] and specifically in our diffusion context adapt the results from [56] to our multi-dimensional setting to obtain a contraction theorem for posteriors arising from general possibly $N$-dependent priors $\Pi$. Recall the information distance $KL$ from (44) on parameter spaces $\mathcal{F} \subset C^2(\mathcal{O}) \cap \{f \geq f_{\text{min}}\}, f_{\text{min}} > 0$.

**Lemma 3.** For $\delta > 0$ define

$$B_\delta = \{f \in \mathcal{F} : KL(f, f_0) \leq \delta^2, \ Var_{f_0}\left(\log \frac{p_{D,f}(X_0, X_D)}{p_{D,f_0}(X_0, X_D)}\right) \leq 2\delta^2\}.$$

Then for any probability measure $\nu$ on $B_\delta$, any $c > 0$ and $\rho_D \in [0, r_D]$ from (71),

$$\mathbb{P}_{f_0}\left(\int_{B_\delta} \prod_{i=1}^N \frac{p_{D,f}(X_{(i-1)D}^i, X_{iD}^i)}{p_{D,f_0}(X_{(i-1)D}^i, X_{iD}^i)} d\nu(f) \leq \exp\{-(1+c)N\delta^2\}\right) \leq \frac{6(1+\rho_D)}{c^2(1-\rho_D)N\delta^2}.$$

**Proof.** The proof is the same as the one Lemma 25 in [56], ignoring the term involving invariant measures $\mu_{a,b}$ there as in our case $\mu_f = \mu_{f_0} = \text{const}$ for all $f$. The key variance estimate in that lemma can then be replaced by our (72) with $h = \log \frac{p_{D,f}(X_0, X_D)}{p_{D,f_0}(X_0, X_D)}$.

**Theorem 12.** Let $\Pi = \Pi_N$ be a sequence of priors on $\mathcal{F}$ and suppose for $f_0 \in \mathcal{F}$, some sequence $\delta_N \to 0$ such that $\sqrt{N}\delta_N \to \infty$ and constant $A > 0$ we have

$$\Pi_N(B_{\delta_N}) \geq e^{-AN\delta_N^2}.$$ 

Suppose further for a sequence of subsets $\mathcal{F}_N \subset \mathcal{F}$ and constant $B > A + 2$ we have

$$\Pi_N(\mathcal{F} \setminus \mathcal{F}_N) \leq e^{-BN\delta_N^2},$$

and that there exists tests $\Psi_N = \Psi(X_0, \ldots, X_{ND})$ and a sequence $\bar{\delta}_N \to 0$ such that

$$\mathbb{E}_{f_0} \Psi_N \to_{N \to \infty} 0, \quad \sup_{f \in \mathcal{F}_N, d(f, f_0) > \bar{\delta}_N} \mathbb{E}_f[1 - \Psi_N] \leq e^{-BN\delta_N^2},$$

where $d$ is some distance function on $\mathcal{F}$. Then we have for $0 < b < B - A - 2$ that

$$\Pi(\mathcal{F}_N \cap \{f : d(f, f_0) \leq \bar{\delta}_N\} | X_0, \ldots, X_{ND}) = 1 - O_{f_0}(e^{-bN\delta_N^2}).$$

**Proof.** The proof is the same as the one as of Theorem 13 in [56]. We can track the constants in this proof (similar as in Theorem 1.3.2 in [54]) to further include the set $\mathcal{F}_N$ in, and to obtain the explicit convergence rate bound on the r.h.s. of (78).

3.6.2. Proof of Theorems 9 and 10. With these preparations we can now prove Theorem 9 and a version of it with distance functions $d(f, f_0) = \|P_{D,f} - P_{D,f_0}\|_{L^2 \to L^2}$ replaced by $d(f, f_0) = \|P_{D,f} - P_{D,f_0}\|_{H^s \to H^s}$, relevant to prove Theorem 10. We will choose

$$\delta_N = MN^{-(s+1)/(2s+2+d)}$$

throughout, for $M$ a large enough constant. We consider the prior $\Pi_N$ from (17) and use standard theory for Gaussian processes (e.g., Ch.2 in [26]). In particular, recalling the cut-off function $\zeta$, we note that the reproducing kernel Hilbert space (RKHS) $\mathbb{H}_N$ of the Gaussian process $\theta$ generating $\Pi_N$ is given by $\mathbb{H}_N = \{\zeta h : h \in E_K\} \subset C_c^\infty$, with RKHS norm

$$\|g\|_{\mathbb{H}_N} \simeq \sqrt{N}\delta_N \left(\|\zeta^{-1}g, (1)L^2\|^2 + \|\zeta^{-1}(g - \langle g, 1 \rangle_{L^2})\|^2_{H^1}\right), \quad g \in \mathbb{H}_N.$$
i) Verification of (75). Proposition 3 with \( k > d/2 \) and Proposition 4 imply the two sided estimate \( 0 < c_{\theta} \leq p_{D,f}(x,y) \leq c_{\theta} \) with constants that are uniform in \( \|f\|_{H^s} \leq U \). This applies as well to \( f_0 \in H^s \) and so, by standard inequalities (e.g., Appendix B in [24]),

\[
E_{f_0} \left| \log \frac{p_{D,f}(X_0,X_D)}{p_{D,f_0}(X_0,X_D)} \right|^2 \lesssim \|p_{D,f} - p_{D,f_0}\|_{L^2(O \times O)}^2 = \|P_{D,f} - P_{D,f_0}\|_{HS}^2
\]

for such \( f \), with constants depending on \( U, s, d, O \).

Let us define \( \theta_0 = \log(4f_0 - 1) \) which is zero outside of \( O_{00} \) and lies in \( H^s \) by the hypotheses on \( f_0 \). This implies that \( \theta_0 - \langle \theta_0, 1 \rangle_{L^2} \in H^s / R \cap L^2_0 \subset H^s \) by Proposition 2. If \( \theta_{0,K} \) is the \( L^2 \)-projection of \( \theta_0 \) onto \( E_K \), then \( \theta_{0,K} \in L^2 \) and

\[
\|\theta_{0,K}\|_{H^s} \lesssim \|\langle \theta_0, 1 \rangle_{L^2}\| + \|\theta_{0,K} - \langle \theta_0, 1 \rangle_{L^2}\|_{H^s} \lesssim \|\theta_0\|_{H^s} \lesssim U.
\]

Since \( H^s / R \cap L^2 \subset H^s \) (Proposition 2) implies that \( H^s \) embeds continuously into \( H^s / R \cap L^2 \), we can use (26) and choose \( M \) large enough s.t.

\[
\|\theta_0 - \theta_{0,K}\|_{H^s} \lesssim \|\langle \theta_0, 1 \rangle_{L^2}\| + \|\theta_{0,K} - \langle \theta_0, 1 \rangle_{L^2}\|_{H^s} \lesssim \|\theta_0\|_{H^s} \lesssim U.
\]

for any given \( c, U > 0 \). Now using Theorem 11, (80) and for \( C_1 > 0 \), with \( M, B \) large enough,

\[
\Pi_N(B_{\delta_N}) \geq \Pi_N(\|f - \theta_0\|_{H^s} \leq C_1 \delta_N) \cap \{ \theta : \|\theta\|_{H^s} \leq 2B \}
\]

\[
\geq \Pi_N(\{ \theta : \|\theta - \theta_{0,K}\|_{H^s} \leq C_2 \delta_N, \|\theta - \theta_{0,K}\|_{H^s} \leq B \})
\]

\[
\geq \Pi_N(\{ \theta : \|\theta - \theta_{0,K}\|_{H^s} \leq C_3 \delta_N, \|\theta - \theta_{0,K}\|_{H^s} \leq B \})
\]

where we have used that the map \( \theta \mapsto e^\theta \) is Lipschitz on bounded sets of \( H^s \) for the \( (H^s) \) norm (cf. the argument on p.27 in [54]). We apply Corollary 2.6.18 in [26] with `shift` vector \( \theta_{0,K} \in L^2 \) and the Gaussian correlation inequality (in the form of Theorem B.1.2 in [54]) to further lower bound the r.h.s. in the last display by

\[
ge^{-\|\theta_{0,K}\|_{B_{\delta_N}}^2/2} \Pi_N(\{ \theta : \|\theta\|_{H^s} \leq C_3 \delta_N, \|\theta\|_{H^s} \leq B \})
\]

\[
ge^{-\tilde{c}N^2\delta_N^2} \Pi_N(\|\theta\|_{(H^s)} \leq C_3 \delta_N) \Pi_N(\|\theta\|_{H^s} \leq B),
\]

using also (79), (80) and for some \( \tilde{c} = c(U) > 0 \). Next, since the RKHS of the base prior \( \theta' = \sqrt{N} \delta_N \theta \) embeds continuously into \( H^s \subset H^2_0 \) (cf. (79)), we obtain

\[
\Pi_N(\|\theta\|_{H^s} \leq C_3 \delta_N) \leq \Pi_N(\|\theta'\|_{H^s} \leq C_3 \sqrt{N} \delta_N) \geq e^{-aN\delta_N^2}
\]

as in eq. (2.4) in [54] with \( \kappa = 1 \) there. In concluding this step we now also construct the regularisation sets \( \mathcal{F}_N \) for (76). If we define

\[
\Theta_N = \{ \theta : \theta_{\vartheta}, \vartheta \in E_K, \vartheta = \vartheta_1 + \vartheta_2, |\vartheta_1, 1\rangle_{L^2} | + \vartheta_2 - |\vartheta_2, 1\rangle_{L^2} | \leq \delta \}
\]

then for every \( B \) we can choose \( m \) large enough so that \( \Pi_N(\Theta_N) \geq 1 - e^{-BN\delta_N^2} \), by an application of the Gaussian isoperimetric theorem in [26] as in step iii) in the proof of Theorem 2.2.2 in [54] with \( \kappa = 1 \). Now we have

\[
|\vartheta - |\vartheta_1, 1\rangle_{L^2} | \leq |\vartheta_1 - |\vartheta_1, 1\rangle_{L^2} | + |\vartheta_2 - |\vartheta_2, 1\rangle_{L^2} | \leq c + m.
\]
where we have used (26) in the estimate
\[ \|\vartheta_1 - \langle \vartheta_1, 1 \rangle L^2\|_{H_t}^2 = \sum_{1 \leq j \leq K} \frac{\lambda_j^{s+1}}{\lambda_j} \langle \vartheta_1, e_j, 1 \rangle_{L^2}^2 \lesssim K^{2(s+1)} \|\vartheta_1 - \langle \vartheta_1, 1 \rangle L^2\|_{H_t}^2 \lesssim N^{2s+2} \delta_N^2, \]
and the last term is bounded by a fixed constant \(c^2\). In conclusion this proves \(\Pi_N(\|\theta\|_{H^s} \leq B) \geq 1/2\) for all \(B', N\) large enough so that (75) follows for our choice of \(\delta_N, A > a + \tilde{c}\), and all \(M\) large enough. Since \(\theta \mapsto f_0\) is Lipschitz on bounded subsets of \(H^s\), we have in fact proved the stronger result – to be used in the next step – that for some \(U > 0\) we have \( (82) \)
\[ \mathcal{F}_N := \{\theta : \theta \in \Theta_N\} \subseteq \{f : \|f\|_{H^s} \leq U\}, \quad \Pi_N(\mathcal{F} \setminus \mathcal{F}_N) \leq e^{-BN\delta_N^2}. \]

ii) Construction of tests. We cannot rely on Hellinger testing theory as in \([24, 50, 54]\) because our data does not arise from an i.i.d. model. Instead (following ideas from \([25, 56]\)) we use concentration inequalities, specifically Proposition 5, to construct these tests. For the hypothesis \(H_0 : f = f_0\) consider the plug in test \(\Psi_N = 1\{\|\hat{P}_D - P_{D,f_0}\|_{L^2 \rightarrow L^2} \geq M\delta_N\}\), where \(\hat{P}_D\) is from (63) with choice \(J = BN\delta_N^2\). We verify (77) with \(\mathcal{F}_N\) from (82). By Proposition 5, the type-one error is then controlled, for \(M\) large enough, as
\[ \mathbb{E}_{f_0}\Psi_N = \mathbb{P}_{f_0}(\|\hat{P}_D - P_{D,f_0}\|_{L^2 \rightarrow L^2} \geq M\delta_N) \leq e^{-cN\delta_N^2} \]
and likewise, by the triangle inequality,
\[ \mathbb{E}_{f}(1 - \Psi_N) = \mathbb{P}_f(\|\hat{P}_D - P_{D,f_0}\|_{L^2 \rightarrow L^2} < M\delta_N) \]
\[ = \mathbb{P}_f(\|\hat{P}_D - P_{D,f}\|_{L^2 \rightarrow L^2} > \|P_{D,f_0} - P_{D,f}\|_{L^2 \rightarrow L^2} - M\delta_N) \leq e^{-cN\delta_N^2} \]
whenever \(\|P_{D,f_0} - P_{D,f}\|_{L^2 \rightarrow L^2} \geq \delta_N \geq 2M\delta_N\). Now we can apply Theorem 12 and deduce that for all \(b\) we can choose \(M\) and \(U\) large enough such that
\[ \Pi\{f : \|f\|_{H^s} \leq U, \|P_{D,f} - P_{D,f_0}\|_{L^2 \rightarrow L^2} \geq 2M\delta_N|X_0, \ldots, X_N\} = 1 - O_{\mathbb{P}_{f_0}}(e^{-BN\delta_N^2}). \]
This proves Theorem 9. To proceed, note that the same arguments work for \(\|\cdot\|_{H^s \rightarrow H^2}\) operator norms by appealing to Corollary 2 with the same choice of \(J\), resulting in the slower convergence rate \(\delta_N = N^{-(s-1)/(2s+2+d)}\) replacing \(\delta_N\). Now to prove Theorem 10 under hypothesis (10), we can invoke the stability estimate Theorem 6 and the set inclusion
\[ \left\{f : \|f - f_0\|_{L^2} \leq M\delta_N\right\} \supset \left\{f : \|f\|_{H^s} \leq U, \|P_{D,f} - P_{D,f_0}\|_{H^2 \rightarrow H^2} \leq 2M\delta_N\right\} \]
for \(M\) large enough such that \(M \geq \tilde{C}\). If (10) does not hold we can still use the stability estimate (8) from Theorem 5 and obtain the slower rate for the posterior distribution. This completes the proof of the contraction rate bounds for \(f_0\) in Theorem 10. The rate for the HS-norms follow in a similar way from (14), (13) instead of the previous stability estimates.

3.6.3. Posterior mean convergence and proof of Theorem 2. The above contraction results holds as well for the ‘linear’ parameter \(\theta - \theta_0\), as log is \(L^2\)-Lipschitz on \(\|\cdot\|_{H^s}\)-bounded sets of \(f\)’s bounded away from zero (and using that \(\|f - f_0\|_{\infty} \rightarrow 0\) for \(f \rightarrow f_0\) in \(L^2\) bounded in \(H^s\)). In turn we further deduce a convergence rate for the posterior mean vectors
\[ \|E^{\Pi}[\theta|X_0, \ldots, X_N] - \theta_0\|_{L^2} = O_{\mathbb{P}_{f_0}}(\delta_N) \]
using that we have exponential convergence to zero in (78) for any \(b > 0\) if we just increase the constant \(M\), and by a uniform integrability argument as in Theorem 2.3.2 of [54] (or see also the proof of Theorem 3.2 in [50], to whom this argument is due). This then implies the same \(L^2(O)\)-rates for \(\hat{f}_N = f^{\Pi}[\theta|X_0, \ldots, X_N]\) towards \(f_0\) and in particular implies the second limit in Theorem 2. An argument parallel to the one leading to (83) further implies that \(\|E^{\Pi}[\theta|X_0, \ldots, X_N]\|_{H^s} = O_{P_{f_0}}(1)\) and we can then use (45) and the imbedding \(L^2 \subset (H^s_1)^*\) to obtain convergence to zero of the Hilbert-Schmidt norms \(\|P_{D,f_N} - P_{D,f_0}\|_{HS}\) (which bound \(\|\cdot\|_{L^2 \rightarrow L^2}\) norms) also at rate \(\tilde{\delta}_N\).
3.7. Neumann eigenfunctions on cylindrical domains.

3.7.1. Proof of Proposition 1. Let us decompose a point $x \in \mathcal{O}_1 \times (0, w)$ as $y = (x_1, \ldots, x_{d-1}), z = x_d$. The restricted Neumann Laplacians $\Delta_{\mathcal{O}_1}, \Delta_{(0,w)}$ have discrete non-positive spectrum on $L^2(\mathcal{O}_1)$ and $L^2((0, w))$, respectively, with eigenfunctions $e_{1,k}, e_{2,k}, k \in \mathbb{N}$, all orthogonal on constants on their respective domains. If we set $e_{1,0} = 1/(\text{vol}(\mathcal{O}_1))^{1/2}$, $e_{2,0} = 1/\sqrt{w}$ for eigenvalues $\lambda_{i,0} = 0 \leq \lambda_{i,k}$ then the eigenfunctions $(e_j : j \geq 0)$ of $\Delta$ on $L^2(\mathcal{O})$ tensorise by a standard separation of variables argument (that is left to the reader).

**Proposition 7.** The eigenfunctions of $-\Delta$ on $\mathcal{O}$ for eigenvalues $\lambda_j = \lambda_{1,k} + \lambda_{2,l}$ are

$$e_j(y, z) = e_{1,k}(y) \times e_{2,l}(z), \quad j = (k, l) \in \mathbb{N}^2 \cup \{0, 0\}, \quad y \in \mathcal{O}_1, z \in (0, w).$$

To proceed, recall that for a convex domain $\mathcal{O}_1$, the Poincaré constant satisfies $p(\mathcal{O}_1) \leq (\text{diam}(\mathcal{O}_1)/\pi)^2$ by a classical result of [61]. For simple eigenvalues we then have:

**Proposition 8.** Suppose that the Poincaré constant $p(\mathcal{O}_1)$ of $\mathcal{O}_1$ satisfies $p(\mathcal{O}_1) \leq w^2/2\pi^2$. Then the first non-zero eigenvalue $\lambda_1$ of $\Delta$ on $\mathcal{O} = \mathcal{O}_1 \times (0, w)$ is simple, equals $\pi^2/w^2$ and the rest of the spectrum is separated from $\lambda_1$ by at least $\pi^2/w^2$. The corresponding eigenfunction is smooth in the strict interior of $\mathcal{O}$ and satisfies for all $\eta > 0$ small enough

$$\inf_{x : |x - \partial \mathcal{O}|_{\mathbb{R}^d} \geq \eta} |\nabla e_1(x)|_{\mathbb{R}^d} \geq \frac{\pi^2 \eta}{2w^2 \sqrt{\text{vol}(\mathcal{O}_1)}} > 0.$$

**Proof.** By the assumption and (25) we have $\lambda_{1,1} \geq 1/p(\mathcal{O}_1)$. The first eigenvalue $\lambda_{2,1}$ of $\Delta$ on $(0, w)$ is $\pi^2/w^2$, hence $\lambda_{2,1} < \lambda_{1,1}$ and the first non-constant eigenfunction of $\Delta$ on $\mathcal{O}$ corresponds to $\lambda_1 = 0 + \lambda_{2,1}$ and equals

$$e_1(y, z) = e_{1,0}(y)e_{2,1}(z) = \frac{\cos(\pi z/w)}{\sqrt{w} \sqrt{\text{vol}(\mathcal{O}_1)}}, \quad y \in \mathcal{O}_1, 0 < z < w.$$

By the hypotheses the next eigenvalue satisfies $\lambda_2 \geq \min\left(1/p(\mathcal{O}_1), \frac{4\pi^2}{w^2}\right)$ and so we have a ‘two-sided’ spectral gap around $\lambda_1$ in the spectrum $\sigma(\Delta) \cap \mathcal{O}$ in the sense that

$$\sigma(\Delta) \cap (\lambda_1 - \epsilon, \lambda_1 + \epsilon) = \{\lambda_1\} \quad \text{for } \epsilon = \min\left(\frac{\pi^2}{w^2}, \frac{1}{p(\mathcal{O}_1)} - \frac{\pi^2}{w^2}\right).$$

By the assumption on $p(\mathcal{O}_1)$ the first claim follows. Next for $x = (y, z)$ away from the boundary we have $\min(z, 1-z) \geq \eta > 0$ and so we have

$$|\nabla e_1(x)|^2_{\mathbb{R}^d} = \sum_{j=1}^{d} \left(\frac{\partial e_1(x)}{\partial x_j}\right)^2 = \frac{1}{w \text{vol}(\mathcal{O}_1)} \left(\frac{d}{dz} \cos\left(\frac{\pi z}{w}\right)\right)^2 \geq \frac{\pi^2 \eta^2}{4w^5 \text{vol}(\mathcal{O}_1)} > 0,$$

for $\eta$ small w.l.o.g. (so that we can use $\sin u \geq u/2$ for $u$ near zero). 

If in the previous proof we only assume $p(\mathcal{O}_1) \leq \frac{w^2}{\pi}$ then the first eigenvalue of $\Delta_{\mathcal{O}_1}$ may coincide with the one of $(0, w)$ and there may then be multiple eigenfunctions for $\lambda_1$. But the eigenfunction (86) is still one permissible choice, and we can choose the weight $i$ in (9) to choose that eigenfunction, so that Proposition 1 remains valid also in this case.
3.7.2. Proof of Theorem 8, Step I: perturbation. The remainder of this section is devoted to the proof of Theorem 8. It consists of combining Proposition 1 with perturbation theory for linear operators. The following result will be used repeatedly. For a proof see Sec.s IV.3.4-5 in Kato [39] (or cf. also Proposition 4.2 in [29]). The clusters of the eigenvalues converge also without simplicity of \( \lambda_{1,f_o} \), see the discussion in [39] or also in Sec 2.3 in [43].

**Proposition 9.** Let \( K \) be a bounded linear self-adjoint operator on a separable Hilbert space \( H \) with discrete spectrum \( \sigma(K) \) and simple eigenvalue \( \kappa \) such that \( \sigma(K) \cap [\kappa - \epsilon, \kappa + \epsilon] = \{ \kappa \} \) for some \( \epsilon > 0 \). Let \( K_\delta \) be another self-adjoint linear operator such that \( \| K - K_\delta \|_{H \to H} < \epsilon/4 \). Then \( K_\delta \) has a simple eigenvalue \( \kappa_\delta \in (\kappa - \epsilon/2, \kappa + \epsilon/2) \) and there are eigenvectors \( k, k_\delta \) of \( K, K_\delta \) for \( \kappa, \kappa_\delta \) such that \( \| k - k_\delta \|_H \to 0 \) as \( \epsilon \to 0 \).

3.7.3. Step II: rounding the corners. Let us fix \( w \geq 2 \) and agree to write \( \mathcal{O}_m \equiv \mathcal{O}_{m,w}, m \in \mathbb{N}, \) for the sequence of domains from (15), as well as \( \mathcal{O} = \mathcal{O}_\infty \) for the limit set, in this subsection. Note that \( \mathcal{O}_1 \) is the largest domain containing all the others and the perturbation argument below will be given on the Hilbert space \( L^2(\mathcal{O}_1) \supset L^2(\mathcal{O}_m) \supset L^2(\mathcal{O}) \), where the inclusions are to be understood by restriction to, and zero extension from, the domains \( \mathcal{O}, \mathcal{O}_m \). [Note a slight abuse of notation that \( \mathcal{O}_1 \) is not the cylinder base from earlier.]

Consider the linear operators on \( L^2(\mathcal{O}_m) \) given by \( T_{1,1} = (id + \Delta_{\mathcal{O}_m})^{-1} \) from after (24) in Section 3.1.2 with \( f = 1, \mathcal{O} = \mathcal{O}_m \). We extend them to operators denoted by \( T_{\mathcal{O}_m} \) on \( L^2(\mathcal{O}_1) \) by restriction of \( h \in L^2(\mathcal{O}_1) \) to \( \mathcal{O}_m \) and zero-extension of the resulting functions \( T_{1,1}(h) \) outside of \( \mathcal{O}_m \). Likewise we define \( T_{\mathcal{O}} \) on \( L^2(\mathcal{O}_1) \).

**Lemma 4.** We have as \( m \to \infty \) that \( \| T_{\mathcal{O}_m} - T_{\mathcal{O}} \|_{L^2(\mathcal{O}_1) \to L^2(\mathcal{O}_1)} \to 0. \)

**Proof.** For any \( h \) such that \( \| h \|_{L^2(\mathcal{O}_m)} \leq \| h \|_{L^2(\mathcal{O}_1)} \leq 1 \) and writing \( u_m(h) = T_{\mathcal{O}_m}(h) \), we have from Theorem 3.1.3.3 in [31] (with \( \lambda = 1 \) there) that

\[
\| u_m(h) \|_{H^2(\mathcal{O}_m)} \leq C \| h \|_{L^2(\mathcal{O}_m)} \leq C,
\]

where \( C \) is a numerical constant independent of \( \mathcal{O}_m, h \). Following the argument given after (3.2.1.8) in [31] one shows that \( u_m(h) \rightharpoonup u(h) = T_{\mathcal{O}}(h) \) weakly in \( H^2(\mathcal{O}) \) and then by compactness also in the norm of \( L^2(\mathcal{O}) \) and in fact of \( L^2(\mathcal{O}_1) \) for the given \( h \). This convergence is uniform in \( h \); indeed, suppose \( u_m(h) \) does not converge to \( u(h) \) in \( L^2(\mathcal{O}_1) \) uniformly in \( \| h \|_{L^2(\mathcal{O}_1)} \leq 1 \). Then there exists \( \epsilon > 0 \) and a sequence \( h_m \in L^2(\mathcal{O}_1) \) such that

\[
\| h_m \|_{L^2(\mathcal{O}_1)} \leq 1 \quad \text{for which}
\]

\[
\| u_m(h_m) - u(h_m) \|_{L^2(\mathcal{O}_1)} \geq \epsilon_0 > 0 \quad \text{for all } m.
\]

The sequence \( h_m \) converges in the dual space \( (H^1(\mathcal{O}_1))^* \) to some \( h \) along a subsequence, by compactness of the inclusion \( L^2 \subset (H^1)^* \). As \( T_{\mathcal{O}_m} \) is self-adjoint on \( L^2(\mathcal{O}_m) \) we deduce

\[
\| u_m(h_m) - u_m(h) \|_{L^2} = \sup_{\| \psi \|_{L^2(\mathcal{O}_m)} \leq 1} \langle T_{\mathcal{O}_m} \psi, h_m - h \rangle_{L^2(\mathcal{O}_m)}
\]

\[
\leq \| h_m - h \|_{(H^1(\mathcal{O}_m))^*} \sup_{\| \psi \|_{L^2(\mathcal{O}_m)} \leq 1} \| T_{\mathcal{O}_m}(\psi) \|_{H^1(\mathcal{O}_m)}
\]

\[
\leq \| h_m - h \|_{(H^1(\mathcal{O}_1))^*} \to m \to \infty 0
\]

using also that the restriction operator from \( \mathcal{O}_1 \) to \( \mathcal{O}_m \) is continuous from \( (H^1(\mathcal{O}_1))^* \) to \( (H^1(\mathcal{O}_m))^* \), and where the last supremum was bounded using (24) (with \( f = 1 \)) and the Cauchy-Schwarz inequality, by \( \sup_{\| \psi \|_{L^2(\mathcal{O}_m)} \leq 1} \| T_{\mathcal{O}_m}(\psi) \|_{L^2(\mathcal{O}_m)}^{1/2} \leq 1 \), since \( T_{\mathcal{O}_m} \) has \( L^2 \to L^2 \) continuity.
where we use \( \|D\| \leq 1 \) on the lower bound in (85). Also we obtain convergence of \( (91) \).

The standard interpolation inequality for Sobolev norms in a strict interior subset (e.g., use [23], p.334, Thm 2) and so by a standard compactness argument for Sobolev norms and the Sobolev imbedding \( H^0 \subset C^2, \alpha > 2 + d/2 \), we obtain convergence of

\[
e_{1,1,m} \to e_{1,1} \text{ in } C^2(O_0).
\]

Thus the gradient condition (85) for \( e_{1,1} \) is inherited by \( e_{1,1,m} \) for all \( m \) large enough depending on the lower bound in (85). Also \( |\Delta e_{1,1,m}| \) remains bounded on \( O_0 \) by a fixed constant in view of (90), so we can verify (10) for \( \mu \) large enough and some \( c_0 > 0 \). This completes the proof of Theorem 8A).

3.7.4. Step III: neighbourhood of \( \Delta \). We now extend the previous result to a neighbourhood of \( f = 1 \). As the domain is fixed in what follows, we just write \( O \) for the bounded convex smooth domain \( O_m, u = O_m \) from the previous subsection.

**Lemma 5.** Regarding \( L_f^{-1}, L_1^{-1} \) as bounded linear operators on \( L_0^2(O) \) we have for some \( D' = D'(f_{\text{min}}, \|f\|_\infty, O) \) that \( \|L_f^{-1} - L_1^{-1}\|_{L_2^2 \to L_2^2} \leq D' \|f - 1\|_\infty \).

**Proof.** For \( \phi \in L_0^2 \) denote by \( u_f = L_f^{-1}(\phi) \) the solution to (58). By Proposition 2 we have \( H_1^1 \subset H^1 \) and so since \( L_1^{-1} \) is self-adjoint and using the divergence theorem,

\[
\|L_f^{-1} \phi - L_1^{-1} \phi\|_{L^2} \lesssim \|L_1^{-1} [\nabla \cdot (1 - f) \nabla u_f]\|_{L^2} = \sup_{\|\phi\|_{L^2} \leq 1, f \neq 0} \left| \int_O \nabla \cdot (1 - f) \nabla u_f L_1^{-1} \phi \right|
\]

\[
\lesssim \sup_{\|\psi\|_{H^1} \leq 1} \left| \int_O (f - 1) \nabla \psi \cdot \nabla u_f \right| \lesssim \|f - 1\|_\infty \sup_{\|\psi\|_{H^1} \leq 1} \|\nabla u_f\|_{L^2} \lesssim \|\phi\|_{L^2} \|f - 1\|_\infty
\]

where we use \( \|u_f\|_{H^1} \lesssim \|\phi\|_{L^2} \) as follows from the results in Section 3.1.2.

By the arguments after (90), (24), the operator \( -L_1^{-1} \) has a simple eigenvalue \( \lambda_{1,1} \) with eigenfunction \( e_{1,1} \) satisfying (10). We apply the preceding lemma and Proposition 9 in the Hilbert space \( L_0^2(O) \), which implies the convergence of the eigenpair \( (\lambda_{1,1}, e_{1,1}) \) of \( -L_f^{-1} \) to \( (\lambda_{1,1}, e_{1,1}) \) as \( \|f - 1\|_\infty \to 0 \), in \( \mathbb{R} \times L_0^2(O) \). Under the hypotheses on \( f \), Theorem 2 on p.334 in [23] implies that the \( \|e_{1,f}\|_{L^k(V)} \) norms in a strict interior subset \( V \supset O_0 \) of \( O \) are all uniformly bounded for \( k > 2 + d/2 \). The standard interpolation inequality for Sobolev norms (p.44 in [45]) implies for some \( 0 < c(k, \alpha) < 1 \), and \( 2 + d/2 < \alpha < k \) (if necessary considering fractional Sobolev norms)

\[
(91) \quad \|e_{1,f} - e_{1,1}\|_{H^\alpha} \leq \|e_{1,f} - e_{1,1}\|_{L^2}^{c(k,\alpha)} \|e_{1,f} - e_{1,1}\|_{H^k}^{1-c(k,\alpha)} \to 0
\]
as \( \| f - 1 \|_\infty \to 0 \), where all Sobolev norms are over \( V \). Since \( H^\alpha \) embeds continuous into \( C^2 \) this implies convergence to zero of \( \| e_{j,f} - e_{j,1} \|_{C^2(V)} \). We can then verify (10) just as after (90), for \( \kappa \) small enough, completing the proof of Theorem 8.

3.8. Proofs of auxiliary results.

3.8.1. Proof of Proposition 2. We require a few preparatory remarks that will be used: For any \( \eta > 0 \) the Sobolev imbedding gives \( \| f \|_\infty \leq \| f \|_{C^1} \leq \| f \|_{H^{1+d/2+\eta}} \leq U \). The multiplier inequality

\[
\| fh \|_{H^r} \leq \| f \|_{B^r} \| h \|_{H^r} \leq U \| h \|_{H^r}, \quad r \leq s,
\]

where \( B^r = H^r \) for \( r > d/2 \) and \( B^r = C^r \) for \( r \leq d/2 \), is also standard, and where we use that \( H^s \) imbeds continuously into \( C^{s-d/2-\eta} \subset C^r \) for \( r \leq d/2 \) in case B) of the proposition. We also recall the standard result from elliptic PDEs that \( (\Delta, \partial/\partial \nu) \) is a continuous isomorphism between \( H^k(\Omega) \cap L^2_0(\Omega) \) and \( H^{k-2}(\Omega) \cap L^2 \times H^{k-3/2}(\partial \Omega) \) (e.g, Theorem II.5.4 in [45] or Theorem 4.3.3 in [72]), specifically

\[
\| u \|_{H^k} \sim \| \Delta u \|_{H^{k-2}} + \| \partial u / \partial \nu \|_{H^{k-3/2}}, \quad u \in H^k, \quad k \geq 2,
\]

with constants depending only on \( d, \Omega, k \). [Here the \( H^\alpha \)-spaces on the boundary \( \partial \Omega \) are naturally defined as in [45], and we note that the result is also true when \( d = 1 \) if we replace the boundary spaces simply by the values of \( u \) at the endpoints of the interval \( \Omega \).]

Now any \( \phi \in H^1 \) is the limit in \( H^1 \) of and in \( L^2 \) of its partial sum \( \varphi_J = \sum_{j \leq J} e_{j,f} \langle \phi, e_{j,f} \rangle L^2 \). Moreover the \( \varphi_J \) lie in \( H^1 \cap H^1_\nu \) since the \( e_j \)'s do. We then have from (22) and for constants in \( \nu \) depending only on \( f_{\min}, U \geq \| f \|_{\infty} \), the two-sided inequality

\[
\| \varphi_J \|_{H^1} = \| \nabla \varphi_J \|_{L^2} \leq \| \sqrt{f} \nabla \varphi_J \|_{L^2} = (L_J \varphi, \varphi_J)_{L^2} = \| \varphi_J \|_{H^2_{\nu}}.
\]

Taking limits, these inequalities extend to all \( \phi \in H^1 \), in particular \( H^1_{\nu} \subset H^1 \). The inclusion \( H^1 \subset H^1_{\nu} \) is also valid (p.474 in [71], or see Exercise 38.1 in [7]) but will be left to the reader. This proves the required assertions when \( k = 1 \).

For \( k = 2 \), using (93), (94), \( \phi_J \in H^1_{\nu} \), we have with constants depending on \( U, f_{\min}, \)

\[
\| \varphi_J \|_{H^2} \leq \| \Delta \varphi_J \|_{L^2} = \| \Delta f \varphi_J - \nabla f \cdot \nabla \varphi_J \|_{L^2} \leq \| L_J f \varphi_J \|_{L^2} + \| f \|_{C^1} \| \varphi_J \|_{H^1} \leq \| \varphi_J \|_{H^2_{\nu}}
\]

and again taking limits the result extends to all \( \phi \in \tilde{H}^2_{\nu} \), in particular \( \tilde{H}^2_{\nu} \subset H^2 \). We see that any \( \phi \in \tilde{H}^2_{\nu}, k \geq 2 \), is the \( H^2 \)-limit of elements in \( H^2 \) satisfying Neumann boundary conditions. From this and Theorem I.9.4 in [45] we deduce that \( \tilde{H}^2_{\nu} \subset H^2 \). Then for \( h \in H^2 \cap H^1_{\nu} \cap L^2 \) and \( f \in C^1 \) we have \( \| L_f h \|_{L^2} \leq C(U) \| h \|_{H^2} \) and by the spectral representations of \( L_f, h \in L^2 \), we deduce \( L_f h \in L^2 \). The inclusion of the r.h.s. in (28) into \( \tilde{H}^2_{\nu} \) is also clear since for such \( \phi \) we have from the divergence and Parseval’s theorem

\[
\| \varphi \|_{H^2} = \sum_{j \geq 1} \lambda^2_{j,f} \| \varphi, e_{j,f} \|_{L^2} = \sum_{j \geq 1} \langle L_f \varphi, e_{j,f} \rangle_{L^2} = \| L_f \varphi \|_{L^2} < \infty,
\]

so that combining what precedes, (28) is proved. The desired norm equivalence for \( k = 2 \) then also follows from the last estimates.

The claims for integer \( k > 2 \) follow by induction. We assume the result has been proved for \( k - 1 \) and \( k - 2 \). Then we have \( \tilde{H}^k_{\nu} \subset H^k_{\nu} \cap H^{k-2} \). We then see from (93) that on \( \tilde{H}^k_{\nu} \), the norms \( \| \cdot \|_{H^k} \) are equivalent to the norms \( \| \Delta (\cdot) \|_{H^{k-2}} \). In particular for \( \varphi \in \tilde{H}^k_{\nu}, \)

\[
\| \varphi \|_{H^k} \leq \| \Delta \varphi \|_{H^{k-2}} = \| f^{-1} (L_f \varphi - \Delta f \cdot \nabla \varphi) \|_{H^{k-2}} \leq \| L_f \varphi \|_{H^k_{\nu}} + \| f \|_{H^{k-1}} \| \varphi \|_{H^{k-1}_{\nu}} \leq \| L_f \varphi \|_{\tilde{H}^k_{\nu}} + \| \varphi \|_{\tilde{H}^{k-1}_{\nu}} \leq \| \varphi \|_{\tilde{H}^k_{\nu}}
\]
using also the induction hypothesis, the multiplier inequality, and the definition of $\bar{H}^k$. The preceding bound for $\|\Delta \varphi\|_{H^{k-2}}$ in particular implies $\varphi \in H^k$. In the other direction, by similar arguments,

$$\|\varphi\|_{\bar{H}^1} = \|L_f \varphi\|_{H^2} \lesssim \|H_0\|_{H^{k-2}} + \|f\|_{H^{k-1}} \|\varphi\|_{H^{k-1}} \lesssim \|\Delta \varphi\|_{H^{k-2}} + \|\varphi\|_{H^{k-1}} \lesssim \|\varphi\|_{H^k}.$$ 

The last assertions follow for $k = 1$ from $\bar{H}^1 = \bar{H}^1_0 = \bar{H}^1_1$, and for $k = 2$ from (28). The general case follows again by induction: indeed suppose the result holds for some $k$. Just as when showing (28), the space $\bar{H}^{k+2}$ consists precisely of all $\varphi \in \bar{H}^k$ satisfying Neumann boundary conditions and such that $L_f \varphi \in \bar{H}^k$. This immediately implies $H^k_0/\mathbb{R} \cap L^2_0 \subset \bar{H}^k_1$ as elements of $H^k_0/\mathbb{R} \cap L^2_0$ are of the form $\bar{\varphi} = \varphi - \int \varphi$ for some $\varphi \in H^k_c$ so its normal derivatives of all orders vanish at $\partial \mathcal{O}$, and $H^k_0 \varphi \in H^{k-2}/\mathbb{R} \subset \bar{H}^{k-2}_1$ by the induction hypothesis. Finally, since $\bar{H}^k = \bar{H}^k_1$, by the induction hypothesis, we have $L_f \varphi \in \bar{H}^k_1$, and so $\varphi \in \bar{H}^k$. The equivalence of norms then follows from the first part of the proposition.

3.8.2. Proof of Proposition 4. We will apply Theorem 3.1 in [17] with semi-group $e^{-tE_f}$ acting on $L^2(\mathcal{O})$, where $E_f$ is the closure of $-L_f$ from before (23) on the domain $\bar{H}^1$. We note that any bounded convex domain satisfies the ‘chain condition’ employed in that reference. Further, the doubling condition (D) there is satisfied with scaling constant $\nu = d$. The upper bound heat kernel estimate for $p_t$ required in (3.1) in Theorem 3.1 in [17] is proved in Theorem 3.2.9 in [20] for the value $w = 2$ (noting that a bounded domain with smooth boundary satisfies the ‘extension property’ for Sobolev spaces required in [20]). Finally

$$\sup_{x,y \in \mathcal{O}} \frac{|\varphi(x) - \varphi(y)|}{|x-y|^{\alpha-d/2}} \lesssim L^\alpha_{f} \varphi \|_{L^2} \forall \varphi \in \bar{H}^\alpha_f, \alpha > d/2$$

where $L^\alpha_{f}$ is the $\alpha/2$-fold application of $L_f$. This verifies Condition (3.2) in [17] (for the choice of $\varphi = p_{t,f}$ relevant in the proof of Theorem 3.1 there). To prove (95), the Sobolev imbedding $H^\alpha \subset C^{\alpha-(d/2)}$ and Proposition 2 imply that it suffices to bound $\|\varphi\|_{\bar{H}^2}$, which for $\varphi \in \bar{H}^\alpha_f$ equals the graph norm $\|L^\alpha_{f} \varphi\|_{2}$ by the argument given in the last paragraph of the proof of Proposition 2. This completes the proof.

REFERENCES

[1] Abraham, K. and Nickl, R. (2019). On statistical Calderón problems. Math. Stat. Learn. 2 165–216.
[2] Ackerle-Willems, C. and Strauch, C. (2022). Sup-norm adaptive drift estimation for multivariate non-reversible diffusions. Ann. Statist. 50 3484–3509.
[3] Atar, R. and Burdzy, K. (2004). On Neumann eigenfunctions in lip domains. J. Amer. Math. Soc. 17 243–265. https://doi.org/10.1090/S0894-0347-04-00453-9 MR2051611
[4] Bañuelos, R. and Burdzy, K. (1999). On the hot spots conjecture of J. Rauch. J. Funct. Anal. 164 1–33.
[5] Bakry, D., Gentil, I. and Ledoux, M. (2014). Analysis and geometry of Markov diffusion operators 348. Springer, Cham. https://doi.org/10.1007/978-3-319-00022-7-9 MR3155209
[6] Bass, R. F. (1998). Diffusions and elliptic operators. Springer, New York. MR1483890
[7] Bass, R. F. (2011). Stochastic processes. Cambridge Univ. Press, Cambridge. MR2856623
[8] Beskos, A., Girolami, M., Lan, S., Farrell, P. E. and Stuart, A. M. (2017). Geometric MCMC for infinite-dimensional inverse problems. J. Comput. Phys. 335 327–351.
[9] Bohr, J. and Nickl, R. (2021). On log-concave approximations of high-dimensional posterior measures and stability properties in non-linear inverse problems. Ann. Inst. H. Poincaré (Prob. Stat.), to appear.
[10] Bonito, A., Cohen, A., DeVore, R., Petrova, G. and Welper, G. Diffusion coefficients estimation for elliptic partial differential equations. SIAM J. Math. Anal. 2 1570–1592. MR3639575
[11] Burdzy, K. (2006). Neumann eigenfunctions and Brownian couplings. In Potential theory in Matsue. Adv. Stud. Pure Math. 44 11–23. Math. Soc. Japan, Tokyo.
[12] Burdzy, K. and Werner, W. (1999). A counterexample to the “hot spots” conjecture. Ann. of Math. (2) 149 309–317.
[44] Law, K., Stuart, A. and Zygalakis, K. (2015). Data assimilation. Texts in Applied Mathematics 62. Springer, Cham A mathematical introduction.

[45] Lions, J. L. and Magenes, E. (1972). Non-homogeneous boundary value problems and applications. Vol. I. Springer-Verlag, New York-Heidelberg. MR0350177

[46] Loeffler, M. and Picard, A. (2021). Spectral thresholding for the estimation of Markov chain transition operators. Electron. J. Stat. 15 6281–6310. https://doi.org/10.1214/21-ejs1935 MR4355708

[47] Lunardi, A. (1995). Analytic semigroups and optimal regularity in parabolic problems. Modern Birkhäuser Classics. Birkhäuser/Springer Basel AG, Basel.

[48] Majda, A. J. and Harlim, J. (2012). Filtering complex turbulent systems. Cambridge University Press, Cambridge. https://doi.org/10.1017/CBO9781139061308 MR2934167

[49] Milo, R. and Phillips, R. (2015). Cell biology by the numbers. Garland, New York.

[50] Monard, F., Nickl, R. and Paternain, G. P. (2021). Consistent inversion of noisy non-Abelian X-ray transforms. Comm. Pure Appl. Math. 74 1045–1099.

[51] Monard, F., Nickl, R. and Paternain, G. P. (2021). Statistical guarantees for Bayesian uncertainty quantification in nonlinear inverse problems with Gaussian process priors. Ann. Statist. 49 3255–3298.

[52] Nachman, A. I. (1988). Reconstructions from boundary measurements. Ann. of Math. (2) 128 531–576.

[53] Nickl, R. (2020). Bernstein–von Mises theorems for statistical inverse problems I: Schrödinger equation. J. Eur. Math. Soc. (JEMS) 22 2697–2750. https://doi.org/10.4171/JEMS/975 MR4118619

[54] Nickl, R. (2023). Bayesian non-linear statistical inverse problems. Zurich Lectures in Advanced Mathematics. European Mathematical Society (EMS) press, Berlin.

[55] Nickl, R. and Ray, K. (2020). Nonparametric statistical inference for drift vector fields of multidimensional diffusions. Ann. Statist. 48 1383–1408.

[56] Nickl, R. and Sohler, J. (2017). Nonparametric Bayesian posterior contraction rates for discretely observed scalar diffusions. Ann. Statist. 45 1664–1693.

[57] Nickl, R. and Titi, E. S. (2023). On posterior consistency of data assimilation with Gaussian process priors: the 2D Navier-Stokes equations. arXiv 2023.

[58] Nickl, R., van de Geer, S. and Wang, S. (2020). Convergence rates for penalized least squares estimators in PDE constrained regression problems. SIAM/ASA J. Uncertain. Quantif. 8 374–413.

[59] Nickl, R. and Wang, S. (2022). On polynomial-time computation of high-dimensional posterior measures by Langevin-type algorithms. J. Eur. Math. Soc. (JEMS), to appear.

[60] Paulin, D. (2015). Concentration inequalities for Markov chains by Marton couplings and spectral methods. Electron. J. Probab. 20 no. 79, 32. https://doi.org/10.1214/EJP.v20-4039 MR3383563

[61] Payne, L. E. and Weinberger, H. F. (1960). An optimal Poincaré inequality for convex domains. Arch. Rational Mech. Anal. 5 286–292 (1960). https://doi.org/10.1007/BF00252910 MR117419

[62] Reich, S. and Cotter, C. (2015). Probabilistic forecasting and Bayesian data assimilation. Cambridge University Press, New York. https://doi.org/10.1017/CBO97811077076804 MR3242790

[63] Richter, G. R. (1981). An inverse problem for the steady state diffusion equation. SIAM J. Appl. Math. 41 210–221. https://doi.org/10.1137/0141016 MR628945

[64] Steinerberger, S. (2020). Hot spots in convex domains are in the tips (up to an inradius). Comm. Partial Differential Equations 45 641–654. https://doi.org/10.1080/03605302.2020.1750427 MR4107000

[65] Strauch, C. (2016). Exact adaptive pointwise drift estimation for multidimensional ergodic diffusions. Probab. Theory Related Fields 164 361–400.

[66] Strauch, C. (2018). Adaptive invariant density estimation for ergodic diffusions over anisotropic classes. Ann. Statist. 46 3451–3480. https://doi.org/10.1214/17-AOS1664 MR3852658

[67] Stuart, A. M. (2010). Inverse problems: a Bayesian perspective. Acta Numer. 19 451–559.

[68] Sylvester, J. and Uhlmann, G. (1987). A global uniqueness theorem for an inverse boundary value problem. Ann. of Math. (2) 125 153–169. https://doi.org/10.2307/1971291 MR873380

[69] Tanaka, H. (1979). Stochastic differential equations with reflecting boundary condition in convex regions. Hiroshima Math. J. 9 163–177. MR529332

[70] Taylor, M. E. (2011). Partial differential equations II. Springer, New York. MR2743652

[71] Taylor, M. E. (2011). Partial differential equations I. Springer, New York. MR2743652

[72] Triebel, H. (1983). Theory of function spaces 78. Birkhäuser Verlag, Basel.

[73] Uhlmann, G. (2009). Electrical impedance tomography and Calderón’s problem. Inverse Problems 25.

[74] van der Meulen, F. and Schauer, M. (2017). Bayesian estimation of discretely observed multidimensional diffusion processes using guided proposals. Electron. J. Stat. 11 2358–2396.

[75] van der Vaart, A. W. and van Zanten, J. H. (2008). Rates of contraction of posterior distributions based on Gaussian process priors. Ann. Statist. 36 1435–1463. MR2418663

[76] Wang, S. (2019). The nonparametric LAN expansion for discretely observed diffusions. Electron. J. Stat. 13 1329–1358. https://doi.org/10.1214/19-ejs1545 MR3935851