On low frequency inference for
diffusions without the hot spots conjecture

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Abstract. We remove the dependence on the 'hot-spots' conjecture in two of the main theorems of the recent paper of Nickl (2024). Specifically, we characterise the minimax convergence rates for estimation of the transition operator P_f arising from the Neumann Laplacian with diffusion coefficient f on arbitrary convex domains with smooth boundary, and further show that a general Lipschitz stability estimate holds for the inverse map $P_f \mapsto f$ from $H^2 \to H^2$ to L^1.

1. Introduction

We revisit here two results of the recent paper of Nickl [12] and begin by recalling its setting. The density of a diffusing substance in an insulated medium, say a bounded convex domain $\mathcal{O}$ of $\mathbb{R}^d$ ($d \geq 1$) with smooth boundary $\partial\mathcal{O}$, is described by the solutions u to the parabolic partial differential equation (PDE) known as the heat equation, $\partial u/\partial t = \mathcal{L}_f u$. The divergence form elliptic second order differential operator

$$\mathcal{L}_f = \nabla \cdot (f\nabla)$$

is equipped with Neumann conditions $\frac{\partial u}{\partial \nu} = 0$ at $\partial\mathcal{O}$, where $\nu(x)$ is the (inward pointing) normal vector at $x \in \partial\mathcal{O}$. Here, ∇ and $\nabla\cdot$ are the usual gradient and divergence operators, and $f : \mathcal{O} \to [f_{\min}, \infty)$, $f_{\min} > 0$, is a positive, scalar 'diffusivity' function.

As is well known, solutions to this heat equation describe the probability densities of diffusing particles (X_t) solving the stochastic differential equation (SDE)

$$dX_t = \nabla f(X_t)\, dt + \sqrt{2f(X_t)}\, dW_t + \nu(X_t)\, dL_t, \quad t \geq 0, \tag{1}$$

started at $X_0 = x \in \mathcal{O}$, where W_t denotes d-dimensional Brownian motion. The process is *reflected* when hitting the boundary $\partial\mathcal{O}$ of its state space: L_t is a 'local time'

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process acting only when $X_t \in \partial \mathcal{O}$. In the statistical setting considered in [12], we are given equally spaced observations from (1): $X_0, X_D, \dots, X_{ND}$, where $D > 0$ is a fixed observation 'time' distance – one sometimes [8] speaks of low frequency measurements since we do not let $D \to 0$ in the asymptotic framework. By allowing a 'burn in' phase (i.e., waiting a fixed amount of time), one can assume that $X_0 \sim \text{Unif}(\mathcal{O})$, the uniform distribution (invariant measure).

The non-linear map $f \mapsto P_{D,f}$, where

$$P_{t,f} = e^{t\mathscr{L}_f}, \quad t \geq 0, \tag{2}$$

is the transition operator of the Markov process (X_t) (see Section 3), is injective for any D under mild assumptions on f ([12, Theorem 1]). Given the data $X_0, X_D, \dots,$ X_{ND}, we seek to recover the diffusivity f. This is possible by first recovering $P_{D,f}$ via an explicit estimator, and then by using inverse continuity estimates for the map $f \mapsto P_{D,f}$, following the general paradigm of Bayesian non-linear inverse problems [10, 11] and earlier ideas from [8] in the one-dimensional case. See [12] for the general setting as well as theoretical results and [7] where concrete MCMC algorithms for such low frequency diffusion data are studied.

Some of the results proved in [12] rely on arguments that are closely related to a conjecture in spectral geometry that is known as the *hot-spots conjecture*. Loosely speaking the conjecture is that the first non-constant eigenfunction of the Laplacian $\Delta = \mathscr{L}_1$ with Neumann conditions on a domain $\mathcal{O}$ attains its critical points on the boundary ∂O, see [3] for a review of some main ideas. The conjecture is still actively studied and believed to be true for convex planar domains, while it is known to be potentially false [4] in non-convex domains. A more complete list of recent references can be found in [12], where the validity of the hot spots conjecture is employed in various places in the proofs (including the construction of basic cylindrical domains where it indeed holds). While this conceivably gives the 'right' proofs of these theorems, at the time of this writing, the hot spots conjecture is still unproved in general and we wish to show here how it can be circumvented in the derivation of the results in [12].

2. Main results

Throughout, the $L^p(\mathcal{O})$ spaces with $p \in [1, \infty)$ refer to the space of p-th power integrable functions on $\mathcal{O}$ with respect to the Lebesgue measure, while $C^k(\mathcal{O})$ and $H^k(\mathcal{O})$ refer to the space of k-times differentiable (resp. weakly differentiable) functions on $\mathcal{O}$ whose derivatives define uniformly continuous functions (resp. $L^2(\mathcal{O})$ functions). The definition of $H^k(\mathcal{O})$ extends to real valued k, see [5]. When the domain is

clear, we omit it from the notation. Given any Hilbert space H, we denote the operator norm of linear maps from H to H by $\|\cdot\|_{H\to H}$.

To construct a lower bound (in the minimax sense) for the optimal convergence rate of estimation of $P_{D,f}$, a specific domain is constructed in [12] in which the hot spots conjecture can be verified (see [12, Proposition 1 and Theorem 8]). Moreover, the first eigenvalue of the Laplacian on this domain is simple. A first contribution of the present paper is to remove these restrictions and to obtain a matching lower bound to [12, Theorem 3] for arbitrary bounded convex domains with smooth boundary.

Theorem 2.1. *Let $s > \max(2d - 1, 2 + d/2)$ and $U > 0$. Consider data $X_0, X_D, \ldots,$ X_{ND} at a fixed observation distance $D > 0$, from the reflected diffusion model* (1) *on a bounded convex domain $\mathcal{O} \subset \mathbb{R}^d$ with smooth boundary, started at $X_0 \sim \mathrm{Unif}(\mathcal{O})$. Then, there exists a constant $c = c(s, D, U, \mathcal{O}, f_{\min}) > 0$ such that*

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

where the infimum extends over all estimators $\widetilde{P}_N$ 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 H^2), and where $\mathbb{P}_f$ denotes the probability law induced by the solution (X_t) to (1) *with diffusivity f and observation distance $D > 0$.*

Inspection of the proof shows that the supremum in the last display can be further restricted to f constant near $\partial\mathcal{O}$. The main obstruction in the proof compared to that of [12, Theorem 4] arises when the first non-zero eigenvalue of the Laplacian is not simple, as is generically the case in 'nice' domains, such as on the sphere. Since multiplicity of eigenvalues represents symmetries in the domain, one may expect that the convergence rate of estimators of $P_{D,f}$ could be improved by exploiting these symmetries in some way. Theorem 2.1 tells us that the effect of such symmetries is not sufficient to accelerate the minimax rates of convergence. However, the constant c is inversely proportional to the multiplicity of the first eigenvalue, so one could expect the constant factor to decrease in the convergence rate given symmetries (but note that the multiplicities of the eigenvalues of Δ in any fixed domain are necessarily finite).

While the solution theory for equation (1) is more complex for general non-convex domains, in the cases when solutions exist, Theorem 2.1 still holds. However, the assumption of a smooth boundary remains crucial, as it is necessary in [12, Proposition 2], which is used extensively here and recalled in Appendix A for the reader.

Another result obtained in [12] that depends on the hot-spots conjecture was a Lipschitz stability estimate for the inverse map $P_{D,f} \mapsto f$ with respect to the $H^2(\mathcal{O}) \to H^2(\mathcal{O})$ and the $L^2(\mathcal{O})$ norms. We remove this dependence and obtain a Lipschitz estimate as long as one is satisfied to replace the $L^2(\mathcal{O})$ norm by the $L^1(\mathcal{O})$

norm (which for statistical convergence rates in this infinite-dimensional model is only a mild concession).

Theorem 2.2. *Let $\mathcal{O}$ be a bounded and smooth (not necessarily convex) domain in $\mathbb{R}^d$. Let $f, f_0 \in H^s(\mathcal{O}), s > \max(d, 2 + d/2)$, suppose that $f = f_0$ on $\mathcal{O} \setminus \mathcal{O}_0$ for some compact subset $\mathcal{O}_0 \subset \mathcal{O}$ and that $f, f_0 \geq f_{\min} > 0$ on $\mathcal{O}$. For $D > 0$ arbitrary but fixed, let $P_{D,f}$ denote the operator defined in (2). We then have the stability estimate*

$$\|f - f_0\|_{L^1(\mathcal{O})} \leq \overline{c} \, \|P_{D,f} - P_{D,f_0}\|_{H^2 \to H^2},$$

where the constant $\overline{c}$ depends on s, U, $\mathcal{O}_0$, $\mathcal{O}$, $f_{\min}$, and where $U \geq \|f\|_{H^s} + \|f_0\|_{H^s}$.

We emphasise that this stability estimate holds also if $\mathcal{O}$ is not convex, but for the interpretation of $P_{D,f}$ in (2) as the transition operator of a continuous time Markov process (X_t), the requirement of convexity is natural [15]. We further remark that the hypothesis that f needs to be known near the boundary is related to the fact that reflection – which is not informative about f – dominates the local dynamics near $\partial\mathcal{O}$.

Our proof of Theorem 2.2 relies on the use of the L^1 norm to deal with the sign of a certain transport operator, as well as on an idea of [2]. Note that a weaker logarithmic estimate for the L^2 norm holds without assuming the hot-spots conjecture, as was already shown in [12], but the stronger Lipschitz estimate is crucial for statistical applications. Indeed, by combining this stability estimate with the proof of [12, Theorem 10], we obtain the following contraction rate for the Bayesian posterior distribution arising from a natural K-dimensional Gaussian process model for f described in detail in [12, (17)].

Corollary 2.3. *Consider the data $X_0, X_D, \dots, X_{ND}$ from the reflected diffusion model on a bounded convex domain $\mathcal{O} \subset \mathbb{R}^d$ with smooth boundary started at $X_0 \sim \mathrm{Unif}(\mathcal{O})$. Assume that $f_0 \in H^s$, $s > \max(2 + d/2, 2d - 1)$, satisfies $\inf_{x \in \mathcal{O}} f_0(x) > 1/4$ and $f_0 \equiv 1/2$ on $\mathcal{O} \setminus \mathcal{O}_0$, where $\mathcal{O}_0 \subset \mathcal{O}$ is compact. Let $\Pi(\cdot | X_0, X_D, \dots, X_{ND})$ be the posterior distribution resulting from data $X_0, X_D, \dots, X_{ND}$ in model (1) and from the prior Π for f from [12, (17)] with $K \simeq N^{d/(2s+2+d)}$ and the given s. Then, as $N \to \infty$, we have*

$$\Pi\big(f : \|f - f_0\|_{L^1(\mathcal{O})} \geq \eta_N | X_0, X_D \dots X_{ND}\big) \to^{\mathbb{P}_{f_0}} 0,$$

where we can take $\eta_N = O(N^{-(s-1)/(2s+2+d)})$.

To deduce this corollary, one uses Theorem 2.2 (instead of [12, Theorem 6]) in the set-inclusion in [12, Section 3.6.2.ii]. The contraction rate η_N carries over to appropriate posterior mean 'point' estimates of f_0, as in [12, Section 3.6.3]. It shows that 'fast' algebraic convergence rates can be obtained under the standard 'non-parametric' assumption that f belongs to a Sobolev space only, which was previously an open problem except for the case $d = 1$ considered in [8, 12, 13].

3. Proofs

To proceed without assuming the hot spots conjecture, the proofs of the theorems rely on the information gained by looking at multiple eigenfunctions simultaneously (see Lemma 3.1). We recall some notation from [12]: The transition operator of the Markov process (X_t) solving (1) is given by

$$P_{t,f} = e^{t\mathcal{L}_f}, \qquad\qquad t \geq 0,$$
$$P_{t,f}(\phi) = \sum_{k\in\mathbb{N}} e^{-t\lambda_{k,f}} e_{k,f} \langle e_{k,f}, \phi \rangle_{L^2}, \quad \phi \in L^2,$$

where $(e_{k,f}, -\lambda_{k,f})_{k\in\mathbb{N}}$ are the eigenpairs of $\mathcal{L}_f \equiv \nabla \cdot (f\nabla)$, that is,

$$\mathcal{L}_f e_{k,f} = -\lambda_{k,f} e_{k,f}$$

and the $e_{k,f}$ are orthonormal in $L^2(\mathcal{O})$ and satisfy Neumann boundary conditions. The eigenfunctions are ordered by increasing eigenvalues $0 = \lambda_{0,f} < \lambda_{1,f} \leq \cdots$ with $e_{0,f}$ constant on $\mathcal{O}$ for all f. We omit the subscript f when there is no danger of confusion. The usual Weyl asymptotics hold:

$$\lambda_k \sim k^{2/d}, \tag{3}$$

e.g., [17, p. 111], and as after [12, (26)], the inequalities in (3) can be taken to be uniform in $0 < f_{\min} \leq f \leq \|f\|_\infty \leq U$ (for a fixed domain $\mathcal{O}$). For $\mathcal{O} \subset \mathbb{R}^d$ a bounded domain, define

$$L_0^2(\mathcal{O}) = \Big\{ g \in L^2(\mathcal{O}) : \int_{\mathcal{O}} g(x)\, dx = 0 \Big\},$$

the $L^2(\mathcal{O})$-functions orthogonal to $e_{0,f}$. For $s \geq 0$, the Hilbert spaces $\bar{H}_f^s$ are defined by

$$\bar{H}_f^s(\mathcal{O}) = \{ g \in L_0^2(\mathcal{O}) : \|g\|_{\bar{H}_f^s} < \infty \},$$

where

$$\|g\|_{\bar{H}_f^s}^2 = \sum_{j\geq 1} \lambda_{j,f}^s \langle g, e_{j,f} \rangle_{L^2}^2.$$

Again, we omit the subscript f when there is no danger of confusion. The relation between these $\bar{H}_f^s$ spaces and the usual Sobolev spaces H^s is recalled in Appendix A.

3.1. Lower bounds for $\|P_{D,f} - P_{D,f_0}\|_{H^2 \to H^2}$ via eigenfunctions

Let $\mathcal{O} \subset \mathbb{R}^d$ be a bounded convex domain with smooth boundary and let $f, f_0 \in H^s(\mathcal{O}) \subset C^2(\mathcal{O})$, $s > \max(d, 2 + d/2)$, be bounded below by $f_{\min} > 0$ on $\mathcal{O}$. We also assume that $\|f\|_{H^s} + \|f_0\|_{H^s} \leq U$. From a perturbation analysis of the coefficients

of the underlying heat equation one can derive the following 'pseudo-linearisation identity': Specifically, using [12, (42)] with 'eigenblock' $E_{k,f_0,\iota}$ there selecting (via choice of ι) a fixed eigenfunction e_{k,f_0} of $\mathscr{L}_{f_0}$, we have

$$P_{t,f}(e_{k,f_0}) - P_{t,f_0}(e_{k,f_0}) = \sum_{l=1}^{\infty} b_{l,k} \langle e_{l,f}, G_k \rangle_{L^2} e_{l,f},$$

where

$$G_k = \nabla \cdot \left[(f - f_0) \nabla e_{k,f_0} \right],$$

$$b_{l,k} = \int_0^t e^{-s\lambda_{k,f_0}} e^{-(t-s)\lambda_{l,f}} \, ds.$$

We can then repeat the arguments leading to [12, (55)] for this selected eigenfunction, assuming the frequency $1 \le k \le \kappa$ does not exceed a fixed integer κ (which will be chosen later): From [12, Corollary 1] and monotonicity of eigenvalues, we know

$$\|e_{k,f_0}\|_{H^2} \lesssim \lambda_{\kappa,f_0} \lesssim \kappa^{2/d}$$

with constants depending on $\mathcal{O}, U$, and $f_{\min}$. Setting $t = D$, by definition of the operator norm, the preceding pseudo-linearisation identity, and Appendix A, we see

$$\|P_{D,f} - P_{D,f_0}\|_{H^2 \to H^2}^2 \gtrsim \|P_{D,f}(e_{k,f_0}) - P_{D,f_0}(e_{k,f_0})\|_{\bar{H}_f^2}^2$$

$$= \sum_{l=1}^{\infty} \lambda_{l,f}^2 |b_{l,k}|^2 |\langle G_k, e_{l,f} \rangle_{L^2}|^2 \tag{4}$$

with a constant depending only on κ and not k. We can write

$$b_{l,k} = e^{-D\lambda_{l,f}} \frac{e^{-D(\lambda_{k,f_0} - \lambda_{l,f})} - 1}{\lambda_{l,f} - \lambda_{k,f_0}} = D \frac{e^{-D\lambda_{k,f_0}} - e^{-D\lambda_{l,f}}}{D(\lambda_{l,f} - \lambda_{k,f_0})} = D e^{\xi(\lambda_{k,f_0}, \lambda_{l,f})}$$

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

By the Weyl asymptotics (3), we see that for $k \le \kappa$, $l \le K$ and any K fixed, the last displayed exponential is bounded below by a fixed constant depending on $f_{\min}$, U, K, and κ. The second to last term in the previous display is of order $\lambda_{l,f}^{-1}$ for fixed $D, k \le \kappa$, as $l \to \infty$. Hence, for all l and some $C = C(D, \mathcal{O}, f_{\min}, U, \kappa)$, we have

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

Combining this estimate with equation (4) and Parseval's identity gives a preliminary stability estimate.

Lemma 3.1. *Suppose* $\|f\|_{H^s} + \|f_0\|_{H^s} \leq U$ *for some* $U > 0$, $s > \max(d, 2 + d/2)$ *and that* $f, f_0 \geq f_{\min} > 0$ *in* $\mathcal{O}$. *We then have for any* $\kappa \in \mathbb{N}$ *the inequality*

$$\|P_{D,f} - P_{D,f_0}\|_{H^2 \to H^2} \geq \tilde{c} \max_{1 \leq k \leq \kappa} \|\nabla \cdot [(f - f_0)\nabla e_{k,f_0}]\|_{L^2},$$

where $\tilde{c} = \tilde{c}(D, \mathcal{O}, f_{\min}, s, U, \kappa)$ *is a positive constant.*

Note that as κ grows, $\tilde{c} \sim e^{-c\kappa^{2/d}}$, so it is important to keep κ fixed. A result similar to Lemma 3.1 is obtained in [12] considering only the first eigenfunction, which combined with the hot-spots conjecture was shown to give a lower bound proportional to $\|f - f_0\|_{L^2}$. The fact that our bound extends to any finite set of eigenfunctions will be essential in the proofs of Theorems 2.1 and 2.2 to be given.

3.2. Proof of Theorem 2.1

For $d = 1$, all open bounded convex domains in $\mathbb{R}$ are intervals of the form (a, b) and the proof of [12, Theorem 4] is easily seen to apply. We assume $d \geq 2$ for the rest of the section. We start with the following auxiliary result.

Proposition 3.2. *Let* H *be a separable Hilbert space. Also, let* T *be a bounded linear self-adjoint operator on* H *with discrete spectrum* $\sigma(T)$, *and let* κ *be an eigenvalue with eigenspace* V, $\dim(V) = a$. *If*

$$\sigma(T) \cap [\kappa - \epsilon, \kappa + \epsilon] = \{\kappa\}$$

for some $\epsilon > 0$, *then there exists* $\delta > 0$ *such that for any self-adjoint operator* S *with* $\|T - S\|_{H \to H} < \delta$, *there is a unique subspace* W *such that* $\dim(W) = a$, *and* $S|_W$ *is diagonalizable with a (possibly repeated) eigenvalues* $\lambda_{1,S}, \ldots, \lambda_{a,S}$ *such that* $|\lambda_{i,S} - \kappa| < \epsilon$ *for all* i. *Moreover, any eigenspace of* S *with eigenvalue within* ϵ *of* κ *is contained in* W. *Finally, the choice of subspace is continuous in the sense that*

$$\|P_W - P_V\|_{H \to H} \to 0 \text{ as } \|T - S\|_{H \to H} \to 0,$$

where P_V *and* P_W *denote the orthogonal projection onto* V *and* W, *respectively.*

Proof. Proposition 3.2 is a special case of [9, Sections IV.3.4–5, Theorem 3.16], which simplifies substantially in our setting as we are dealing only with self-adjoint operators on a Hilbert space. In particular, they have real eigenvalues. The condition

$$\sigma(T) \cap [\kappa - \epsilon, \kappa + \epsilon] = \{\kappa\}$$

allows us to isolate the value κ from the rest of $\sigma(T)$ via a small ball with boundary Γ around κ in the complex plane. Noting that $\|T - S\|_{H \to H} \to 0$ is equivalent

to $\hat{\delta}(S, T) \to 0$ in the notation of [9], we can apply [9, Theorem 3.16] to the decomposition $H = V(T) \oplus M(T)$, where $V(T)$ is the eigenspace of κ, and where $M(T)$ is some complementary subspace. Thus for S sufficiently close to T, we get a corresponding decomposition

$$H = V(S) \oplus M(S)$$

such that the spectrum of $S|_{V(S)}$ is contained within Γ, and also

$$\dim(V(S)) = \dim(V(T)) = a.$$

Since S is self-adjoint, we get a (possibly repeated) real eigenvalues in $V(S)$.   ∎

Corollary 3.3. *In the setting of Proposition* 3.2, *given $e \in V$ a normalised eigenvector of T, there is a choice of $E \in W$ such that*

$$\|E\| = 1 \quad and \quad \|E - e\| \to 0 \ as \ \|S - T\|_{H \to H} \to 0.$$

Proof. Given $e \in V$, consider $P_W e$. Then, since $P_W \to P_V$ as $\|S - T\|_{H \to H} \to 0$, we see that

$$P_W e \to P_V e = e \text{ as } \|S - T\|_{H \to H} \to 0.$$

Since $\|e\| = 1$, this means in particular that for $\|P_W - P_V\|_{H \to H}$ small enough, $\|P_W e\| > 1/2$, say. Hence, we see that $E := P_W e / \|P_W e\|$ has the desired properties.   ∎

Now we return to the setting of Section 3.1 with f, f_0 satisfying the hypotheses introduced there. First we note that the perturbation result given in [12, Lemma 5] still holds for general domains, not just the 'rounded cylinder'.

Lemma 3.4. *Regarding $\mathcal{L}_f^{-1}, \mathcal{L}_1^{-1}$ as bounded linear operators on $L_0^2(\mathcal{O})$, we have*

$$\|\mathcal{L}_f^{-1} - \mathcal{L}_1^{-1}\|_{L_0^2 \to L_0^2} \lesssim \|f - 1\|_\infty,$$

where the constant depends only on $f_{\min}$, $\|f\|_\infty$, and $\mathcal{O}$.

In our setting, upon applying Corollary 3.3 to $\mathcal{L}_1^{-1}$, we obtain $E_f \in L_0^2$ such that

$$\|E_f - e_{1,1}\|_{L^2} \to 0 \text{ as } \|f - 1\|_\infty \to 0,$$

and such that E_f is a linear combination of a eigenfunctions (counted with multiplicity) of $\mathcal{L}_f$, where a is the degeneracy of the first eigenvalue of $\mathcal{L}_1$. Using the notation from Proposition 3.2, the eigenvalues of these eigenfunctions are within ϵ of $\lambda_{1,1}^{-1}$. Note that a and ϵ depend only on $\mathcal{O}$. Moreover, we observe that the largest eigenvalue of $\mathcal{L}_f^{-1}$ is $\lambda_{1,f}^{-1}$, and

$$|\lambda_{1,f}^{-1} - \lambda_{1,1}^{-1}| = \left|\|\mathcal{L}_f^{-1}\|_{L_0^2 \to L_0^2} - \|\mathcal{L}_1^{-1}\|_{L_0^2 \to L_0^2}\right| \leq \|\mathcal{L}_f^{-1} - \mathcal{L}_1^{-1}\| < \epsilon, \quad (5)$$

for $\|f - 1\|_\infty$ sufficiently small. Since the *first a* eigenvalues of $\mathcal{L}_f$ are the *largest a* eigenvalues of $\mathcal{L}_f^{-1}$, we deduce that E_f is a linear combination of the *first a* eigenfunctions of $\mathcal{L}_f$, say

$$E_f = \sum_{i=1}^{a} \alpha_{i,f} e_{i,f}, \quad \sum_{i=1}^{a} |\alpha_{i,f}|^2 = 1. \tag{6}$$

Note that in particular we have $|\alpha_{i,f}| \leq 1$ for every i.

Lemma 3.5. *We have* $\|E_f - e_{1,1}\|_{C^2(\mathcal{O})} \to 0$ *as* $\|f - 1\|_\infty \to 0$.

Proof. We know from Corollary 3.3 and Lemma 3.4 that

$$\|E_f - e_{1,1}\|_{L^2} \to 0 \text{ as } \|f - 1\|_\infty \to 0.$$

By standard interpolation inequalities (see [12, (91)]), we see that for any $s + 1 > \alpha > 2 + d/2$ there is some $0 < c(s, \alpha) < 1$ such that

$$\|E_f - e_{1,1}\|_{H^\alpha} \leq \|E_f - e_{1,1}\|_{L^2}^{c(s,\alpha)} \|E_f - e_{1,1}\|_{H^{s+1}}^{1-c(s,\alpha)}. \tag{7}$$

By [12, Corollary 1], we obtain a constant $C = C(\mathcal{O}, d, s, U, f_{\min})$ such that

$$\|e_{j,f}\|_{H^{s+1}} \leq Cj^{(s+1)/d}.$$

So, by equation (6), we observe

$$\|E_f\|_{H^{s+1}} \leq \sum_{j=1}^{a} |\alpha_{j,f}| \|e_{j,f}\|_{H^{s+1}}$$
$$\leq Ca \cdot a^{(s+1)/d}.$$

Since a depends only on $\mathcal{O}$, this means that the second factor in the right-hand side of (7) is uniformly bounded, and the conclusion of the lemma follows from the Sobolev embedding $H^\alpha \subset C^2$. ∎

Proof of Theorem 2.1. We follow the argument as in [14, Theorem 10], but instead of considering solutions for the standard elliptic Dirichlet problem, we consider eigenproblems for the Neumann Laplacian: Let e_{1,f_0} be the first eigenfunction of $\mathcal{L}_{f_0}$, where $f_0 \equiv 1$ on $\mathcal{O}$. Since $\lambda_{1,f_0} > 0$, e_{1,f_0} cannot be constant. Thus, $\nabla e_{1,f_0}$ is not zero on all of $\mathcal{O}$. Without loss of generality, we assume the first component of $\nabla e_{1,f_0}$ is positive at some x_0. Since $\nabla e_{1,f_0}$ is continuous, pick some $C, \varepsilon > 0$, and $\delta > 0$ such that $\partial_1 e_{1,f_0} > \varepsilon$ and $|\partial_i e_{1,f_0}| \leq C$ ($i \neq 1$) on a ball $B_\delta(x_0)$ in $\mathcal{O}$ of radius δ centred at x_0. Next, choose diffusivities ($f_m : m = 1, \ldots, M$) as

$$f_m := f_0 + \eta 2^{-j(s+d/2)} \sum_{r=1}^{n_j} \beta_{r,m} \Psi_{j,r}, \quad j \in \mathbb{N},$$

where n_j are integers such that $n_j \simeq 2^{jd}$ and the $\Psi_{j,r}$, $r = 1, \ldots, n_j$, are orthonormal tensor Daubechies wavelets supported in $B_\delta(x_0)$, chosen as in [14, (4.17)], so that in particular $f_m \equiv f_{m'} \equiv 1$ on $\mathcal{O} \setminus \overline{B_\delta(x_0)}$. Specifically, the ∂_1 derivative of $\Psi_{j,r}$ is scaled to be a constant factor c larger than the other partial derivatives. Both $\eta > 0$ and $1/c$ will be chosen small enough below. The coefficients $\beta_{r,m}, m = 1, \ldots, M$, of f_m will be sufficiently separated elements of the discrete hypercube, $\beta_m \in \{-1, 1\}^{n_j}$, for a suitable sequence $j = j_N \to \infty$ detailed below. By standard wavelet characterisations of Sobolev norms ([6, Chapter 4.3]), these f_m's lie in a H^s-ball centred at f_0 of radius $C\eta \leq U$ for some fixed $C = C(s) > 0$ and η small enough.

Choose j large enough so that $\|f_m - f_0\|_\infty$ is small enough as in (5) and so that

$$\|E_{f_m} - e_{1,f_0}\|_{C^2(\mathcal{O})} < \varepsilon/2, \quad m = 1, \ldots, M, \tag{8}$$

by Lemma 3.5. We see that in particular $\partial_1 E_{f_m} > \varepsilon/2$ and $|\partial_i E_{f_m}| \leq C + \varepsilon/2 = C'$ on $B_\delta(x_0)$. From the statement of Lemma 3.1, setting f to be f_m, f_0 to be $f_{m'}$ for any $m \neq m'$, and using (6) we see for $c_a > 0$ the constant $\tilde{c}$ with $\kappa = a$, that

$$\frac{c_a}{a} \|\nabla \cdot [(f_m - f_{m'})\nabla E_{f_{m'}}]\|_{L^2} \leq \frac{c_a}{a} \sum_{k=1}^a |\alpha_{k,f_{m'}}| \|\nabla \cdot [(f_m - f_{m'})\nabla e_{k,f_{m'}}]\|_{L^2}$$

$$\leq c_a \max_{1 \leq k \leq a} \|\nabla \cdot [(f_m - f_{m'})\nabla e_{k,f_{m'}}]\|_{L^2}$$

$$\leq \|P_{D,f_m} - P_{D,f_{m'}}\|_{H^2 \to H^2}.$$

Next, we lower bound out

$$\|\nabla \cdot [(f_m - f_{m'})\nabla E_{f_{m'}}]\|_{L^2}$$
$$\geq \underbrace{\|\nabla(f_m - f_{m'}) \cdot \nabla E_{f_{m'}}\|_{L^2}}_{\text{I}} - \underbrace{\|(f_m - f_{m'})\Delta E_{f_{m'}}\|_{L^2}}_{\text{II}}.$$

Following the arguments in [14],

$$\text{I} = \left\| \sum_{i=1}^d \partial_i (f_m - f_{m'})\partial_i E_{f_{m'}} \right\|_{L^2}$$

$$\geq \|\partial_1 (f_m - f_{m'})\partial_1 E_{f_{m'}}\|_{L^2} - \left\| \sum_{i=2}^d \partial_i (f_m - f_{m'})\partial_i E_{f_{m'}} \right\|_{L^2}$$

$$\geq \frac{\varepsilon}{2} \|\partial_1 (f_m - f_{m'})\|_{L^2} - C' \left\| \sum_{i=2}^d \partial_i (f_m - f_{m'}) \right\|_{L^2}.$$

Next, we note that by construction of the f_m, for $i \neq 1$,

$$\|\partial_i (f_m - f_{m'})\|_{L^2} = \frac{1}{c} \|\partial_1 (f_m - f_{m'})\|_{L^2}.$$

Hence, we observe

$$
\begin{aligned}
\mathrm{I} &\geq \frac{\varepsilon}{2} \left\| \partial_1 (f_m - f_{m'}) \right\|_{L^2} - \frac{C'(d-1)}{c} \left\| \partial_1 (f_m - f_{m'}) \right\|_{L^2} \\
&\geq \frac{\varepsilon}{4} \left\| \partial_1 (f_m - f_{m'}) \right\|_{L^2}
\end{aligned}
$$

for a sufficiently large choice of c. Finally, choosing the β_m vectors as in the display after [14, (4.22)], we have

$$
\mathrm{I} \gtrsim \left\| \partial_1 (f_m - f_{m'}) \right\|_{L^2} \gtrsim 2^{-j(s-1)}, \quad \text{and } M \simeq 2^{c_1 2^{jd}}, \, c_1 > 0. \tag{9}
$$

Next we show II is of smaller order than I. We have

$$
\begin{aligned}
\mathrm{II}^2 &\leq \| f_m - f_{m'} \|_{L^2}^2 \| E_{f_{m'}} \|_{C^2}^2 \\
&= \eta^2 2^{-2j(s+d/2)} \sum_{r=1}^{n_j} | \beta_{r,m} - \beta_{r,m'} |^2 \| E_{f_{m'}} \|_{C^2}^2 \\
&\lesssim \sup_{m'} \| E_{f_{m'}} \|_{C^2}^2 2^{-2js}.
\end{aligned}
$$

Therefore, we need only to show that $\sup_{m'} \| E_{f_{m'}} \|_{C^2}^2$ can be bounded by a constant independent of j, which follows from (8). In summary, we have shown

$$
\| P_{D,f_m} - P_{D,f_{m'}} \|_{H^2 \to H^2} \gtrsim 2^{-j(s-1)}, \quad m \neq m'. \tag{10}
$$

Next, let $KL(f, f')$ denote the Kullback–Leibler divergence (see Appendix B) between the distributions of $(X_0, X_D, \ldots, X_{ND})$ and $(X'_0, X'_D, \ldots, X'_{ND})$ corresponding to the solutions of (1) with diffusivities f and f', respectively. Note that $p_{D,f}$ from [12, (33)] can be regarded as the joint probability density of (X_0, X_D) given diffusivity f. For each $i = 0, \ldots, N$, we know $X_{iD} \sim \mathrm{Unif}(\mathcal{O})$, and $(X_t : t \geq 0)$ is a Markov process, so the joint distribution of $(X_0, \ldots, X_{ND})$ has density which splits into the product $p_{D,f}(X_0, X_D) \cdots p_{D,f}(X_{(N-1)D}, X_{ND})$. Hence,

$$
KL(f_m, f_0) = \sum_{i=0}^{N-1} \mathbb{E}_{f_0} \log \frac{p_{D,f_0}(X_{iD}, X_{(i+1)D})}{p_{D,f_m}(X_{iD}, X_{(i+1)D})}.
$$

Using standard arguments with the wavelet characterization of the $H^{-1}(\mathbb{R}^d)$-norm (see [6, p. 370], noting that $B_{2,2}^{-1} = H^{-1}$) and [12, Theorem 11], we have

$$
KL(f_m, f_0) \lesssim N \| f_m - f_0 \|_{H^{-1}}^2 \simeq \eta^2 N 2^{-2j(s+1)}.
$$

Now, we choose $2^j \simeq N^{1/(2s+2+d)}$, so that $N 2^{-2j(s+1)} \simeq 2^{jd} \lesssim \log M$, where we recall that M from (9) is the number of 'hypotheses' f_m lying in a ball of H^s for which the distances from (10) are lower bounded by $N^{(-s+1)/(2s+2+d)}$. Choosing η small enough we can apply Theorem B.1 from Appendix B with a sufficiently small α to complete the proof. ∎

3.3. Proof of Theorem 2.2

3.3.1. Stability for a transport operator. Consider the transport operator

$$h \to \nabla \cdot (h\nabla u)$$

acting on $H^1(\mathcal{O})$ functions, where $u \in C^2(\mathcal{O})$ is fixed. In view of Lemma 3.1, we have in mind $u = e_{k,f_0}$ for some k and $h = f - f_0$, so h changes sign over $\mathcal{O}$. To deal with this, let us first consider the operator $\nabla \cdot (|h|\nabla u)$.

Lemma 3.6. *For any vector field $v \in C^1(\mathcal{O}, \mathbb{R}^d)$ and $h \in H^1(\mathcal{O})$, we have*

$$\left| \nabla \cdot (|h|v) \right| \leq \left| \nabla \cdot (hv) \right|$$

almost everywhere on $\mathcal{O}$. In particular, for $u \in C^2(\mathcal{O})$,

$$\left\| \nabla \cdot (|h|\nabla u) \right\|_{L^2} \leq \left\| \nabla \cdot (h\nabla u) \right\|_{L^2}.$$

Proof. For $x \in \mathbb{R}$, define

$$\mathrm{sign}(x) = \begin{cases} 1 & x > 0, \\ 0 & x = 0, \\ -1 & x < 0. \end{cases}$$

By [5, Lemma 7.6], we have $|h| \in H^1(\mathcal{O})$ and the chain rule holds: $\nabla|h| = \mathrm{sign}(h)\nabla h$ almost everywhere. Thus, by the product rule (see, e.g., [5, (7.18)]), we have

$$\begin{aligned} \nabla \cdot (|h|v) &= \mathrm{sign}(h)\nabla h \cdot v + |h|\nabla \cdot v \\ &= \mathrm{sign}(h)(\nabla h \cdot v + h\nabla \cdot v) \\ &= \mathrm{sign}(h)\nabla \cdot (hv). \end{aligned}$$

Hence, since $|\mathrm{sign}(h)| \leq 1$, we have

$$\left| \nabla \cdot (|h|v) \right| \leq \left| \nabla \cdot (hv) \right|$$

almost everywhere. The last conclusion of the lemma follows by taking $v = \nabla u$ and integrating the square of both sides in the last inequality. ∎

We can now prove the following lemma.

Lemma 3.7. *Suppose $u_1, \ldots, u_\kappa \in C^2(\mathcal{O})$ are such that $\|u_k\|_{L^2(\mathcal{O})} = 1$ for every $k = 1, \ldots, \kappa$ and that*

$$\sum_{k=1}^{\kappa} |\nabla u_k(x)|^2 \geq c > 0, \quad x \in \bar{\mathcal{O}}_0,$$

for some subset $\mathcal{O}_0$ of $\mathcal{O}$. Then for all $h \in H^1(\mathcal{O})$ with boundary trace $h_{|\partial\Omega} = 0$, we have

$$\|h\|_{L^1(\mathcal{O}_0)} \leq c^{-1} \sum_{k=1}^{\kappa} \|\nabla \cdot (h\nabla u_k)\|_{L^2(\mathcal{O})}.$$

Proof. By the Cauchy–Schwarz inequality, we have the upper bound

$$\left| \int_{\mathcal{O}} u_k \nabla \cdot (|h|\nabla u_k) \right| \leq \|u_k\|_{L^2(\mathcal{O})} \|\nabla \cdot (|h|\nabla u_k)\|_{L^2(\mathcal{O})}$$
$$= \|\nabla \cdot (|h|\nabla u_k)\|_{L^2(\mathcal{O})}.$$

By the divergence theorem ([16, pp. 140ff]), we have

$$\left| \int_{\mathcal{O}} u_k \nabla \cdot (|h|\nabla u_k) \right| = \left| \int_{\mathcal{O}} |h|\nabla u_k \cdot \nabla u_k \right| \geq \int_{\mathcal{O}_0} |h| \, |\nabla u_k|^2.$$

Combining these two inequalities, and summing over k, by Lemma 3.6 we obtain

$$c\|h\|_{L^1(\mathcal{O}_0)} \leq \sum_{k=1}^{\kappa} \|\nabla \cdot (|h|\nabla u_k)\|_{L^2(\mathcal{O})}$$
$$\leq \sum_{k=1}^{\kappa} \|\nabla \cdot (h\nabla u_k)\|_{L^2(\mathcal{O})},$$

as required. ∎

3.3.2. Critical points of eigenfunctions. We now combine the results of the preceding sections and adapt an idea from Alberti [2] (see also [1]) to obtain the global Lipschitz stability estimate in Theorem 2.2. We often suppress f_0 in the notation, in particular setting $e_k = e_{k,f_0}$ and $\lambda_k = \lambda_{k,f_0}$ for all k.

Lemma 3.8. *For every compact $\mathcal{O}_0$ subset of $\mathcal{O}$, there exist $\kappa \in \mathbb{N}$ and $c > 0$ depending only on $\mathcal{O}$, $\mathcal{O}_0$, s, U, and $f_{\min}$ such that*

$$\sum_{k=1}^{\kappa} |\nabla e_k(x)|^2 \geq c, \quad x \in \bar{\mathcal{O}}_0.$$

Proof. All the constants left implicit in the proof depend only on $\mathcal{O}$, $\mathcal{O}_0$, s, U and $f_{\min}$. Let $\mathcal{O}'$ be a smooth domain such that $\mathcal{O}_0 \Subset \mathcal{O}' \Subset \mathcal{O}$. Let $\chi \in C_c^\infty(\mathcal{O})$ be a cut-off such that $\chi|_{\mathcal{O}'} \equiv 1$. Define

$$\phi(x) = \chi(x)x_1 - \frac{1}{|\mathcal{O}|} \int_{\mathcal{O}} \chi(z)z_1 \, dz,$$

so that $\phi \in C_c^\infty(\mathcal{O}) \cap L_0^2(\mathcal{O})$. Then $\nabla\phi(x) = (1, 0, \ldots, 0)$ for every $x \in \bar{\mathcal{O}}_0$.

Set $l = \lfloor 2 + d/2 \rfloor > 1 + d/2$. For $\kappa \geq 1$, set $\phi_\kappa = \phi - \sum_{k=1}^{\kappa} \langle \phi, e_k \rangle_{L^2} e_k$. By the Sobolev embedding theorem and by Proposition A.1, we have

$$\|\phi_\kappa\|_{C^1(\bar{\mathcal{O}}_0)}^2 \lesssim \|\phi_\kappa\|_{H^l(\mathcal{O})}^2 \lesssim \|\phi_\kappa\|_{\bar{H}_{f_0}^l}^2 = \sum_{k>\kappa} \lambda_k^l \langle \phi, e_k \rangle_{L^2}^2.$$

Thus

$$\|\phi_\kappa\|_{C^1(\bar{\mathcal{O}}_0)}^2 \lesssim \lambda_\kappa^{-1} \sum_{k>\kappa} \lambda_k^{l+1} \langle \phi, e_k \rangle_{L^2}^2$$

$$\leq \lambda_\kappa^{-1} \sum_{k=1}^{+\infty} \lambda_k^{l+1} \langle \phi, e_k \rangle_{L^2}^2 = \frac{\|\phi\|_{\bar{H}_{f_0}^{l+1}}^2}{\lambda_\kappa}.$$

Now, using that

$$\|\phi\|_{\bar{H}_{f_0}^{l+1}} \lesssim \|\phi\|_{H^{l+1}} \lesssim 1$$

(again by Proposition A.1, since $l + 1 \leq s + 1$) and the Weyl asymptotics (3), we obtain

$$\|\phi_\kappa\|_{C^1(\bar{\mathcal{O}}_0)} \leq C \kappa^{-1/d}$$

for some $C > 0$ depending only on $\mathcal{O}$, $\mathcal{O}_0$, s, U, and $f_{\min}$. Choose $\kappa = \lceil (2C)^d \rceil$, so that

$$\|\phi_\kappa\|_{C^1(\bar{\mathcal{O}}_0)} \leq 1/2.$$

As a consequence, for every $x \in \bar{\mathcal{O}}_0$, we have

$$|\nabla(\phi - \phi_\kappa)(x)| \geq |\nabla\phi(x)| - |\nabla\phi_\kappa(x)| \geq 1 - 1/2 = 1/2.$$

On the other hand, by the Cauchy–Schwarz inequality, we have

$$|\nabla(\phi - \phi_\kappa)(x)| = \left| \sum_{k=1}^{\kappa} \langle \phi, e_k \rangle_{L^2} \nabla e_k(x) \right|$$

$$\leq \left(\sum_{k=1}^{\kappa} \langle \phi, e_k \rangle_{L^2}^2 \right)^{1/2} \left(\sum_{k=1}^{\kappa} |\nabla e_k(x)|^2 \right)^{1/2}.$$

Observing that $\sum_{k=1}^{\kappa} \langle \phi, e_k \rangle_{L^2}^2 \leq \|\phi\|_{L^2}^2 \lesssim 1$ concludes the proof. ∎

Just as in the proof of Lemma 3.5, we can combine the Sobolev embedding with $\|e_k\|_{H^a} < \infty$ for all $a \leq s + 1$ (in view of [12, Corollary 1]) to give the following result.

Lemma 3.9. *We have $e_k \in C^2(\mathcal{O})$ for all k.*

3.3.3. Completion of the proof of Theorem 2.2. By Lemma 3.8, there exist $\kappa \in \mathbb{N}$ and $c > 0$ depending only on $\mathcal{O}$, $\mathcal{O}_0$, s, U, and $f_{\min}$ such that

$$\sum_{k=1}^{\kappa} |\nabla e_k(x)|^2 \geq c, \quad x \in \bar{\mathcal{O}}_0.$$

By Lemma 3.9, we have that e_k is C^2 for every k. Then, by Lemma 3.7 applied with $u_k = e_k$ and $h = f - f_0$, we obtain

$$\begin{aligned}
\|f - f_0\|_{L^1(\mathcal{O}_0)} &\leq \frac{1}{c} \sum_{k=1}^{\kappa} \|\nabla \cdot ((f - f_0)\nabla e_k)\|_{L^2} \\
&\leq \frac{\kappa}{c} \max_{1 \leq k \leq \kappa} \|\nabla \cdot ((f - f_0)\nabla e_k)\|_{L^2}.
\end{aligned}$$

Recalling that $f = f_0$ in $\mathcal{O} \setminus \mathcal{O}_0$, Lemma 3.1 yields the result.

A. Proposition 2 in Nickl (2024)

The following proposition gives a relationship between the usual Sobolev spaces H^k and the spectral Sobolev spaces $\bar{H}_f^k$ defined in Section 3. The space H_c^k from [12] is the subspace of H^k of functions which 'vanish near the boundary' in the sense defined in Section 3.3.1. Let us also for convenience denote by $H_\nu^1(\mathcal{O})$ the space of those functions in H^1 whose inward normal derivatives exist in the trace sense (e.g., belong to $H^{3/2}$) and vanish almost everywhere at the boundary.

Proposition A.1. *Let $\mathcal{O}$ be a bounded convex domain in $\mathbb{R}^d$ with smooth boundary and let $f \in C^1(\mathcal{O})$ be such that $\inf_{x \in \mathcal{O}} f(x) \geq f_{\min} > 0$. Then*

$$\bar{H}_f^1(\mathcal{O}) = H^1(\mathcal{O}) \cap L_0^2$$

and

$$\bar{H}_f^2 = H^2 \cap H_\nu^1 \cap L_0^2 = \{h \in L_0^2 : \mathscr{L}_f h \in L_0^2, (\partial h/\partial \nu) = 0 \text{ on } \partial\mathcal{O}\}.$$

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 $s > d$ such that $k \leq s + 1$, then we have

$$\bar{H}_f^k(\mathcal{O}) \subset H^k(\mathcal{O}) \quad \text{and} \quad \|\phi\|_{H^k} \simeq \|\phi\|_{\bar{H}_f^k} \text{ for } \phi \in \bar{H}_f^k.$$

We further have the embedding $H_c^k \cap L_0^2 \subset \bar{H}_1^k$ and also if H_c^k is replaced by $H_c^k/\mathbb{R}$ (modulo constants). Finally, we have $\bar{H}_f^k = \bar{H}_{f'}^k$, for any pair f, f' satisfying (A) or (B), with equivalent norms. All embedding/equivalence constants depend only on $f_{\min}$, U, d, k, and $\mathcal{O}$.

B. A general mini-max lower bound

Let P and Q be probability laws on the same space. Then, $KL(P, Q)$ denotes the Kullback–Leibler divergence from P to Q and is given by

$$KL(P, Q) = \mathbb{E}_P \left[\log \frac{dP}{dQ} \right],$$

where $\frac{dP}{dQ}$ is the Radon–Nikodym derivative of P with respect to Q.

Theorem B.1. *Suppose that a parameter space $\mathcal{F}$ has a metric d and associated probability laws $\{P_f : f \in \mathcal{F}\}$. Next, suppose $\mathcal{F}$ contains*

$$\{f_m : m = 0, 1, \ldots, M\}, \quad M \geq 3,$$

which are $2r$ separated, i.e., $d(f_i, f_j) \geq 2r$ for $i \neq j$, and such that the P_{f_m} are all absolutely continuous with respect to P_{f_0}. Assume, for some $\alpha > 0$, that

$$\frac{1}{M} \sum_{m=1}^{M} KL(P_{f_m}, P_{f_0}) \leq \alpha \log M.$$

Then,

$$\inf_{\widetilde{f}} \sup_{f \in \mathcal{F}} P_f \left(d(\widetilde{f}, f) > r \right) \geq \frac{\sqrt{M}}{1 + \sqrt{M}} \left(1 - 2\alpha - \sqrt{\frac{8\alpha}{\log M}} \right),$$

where the infimum ranges over all estimators (measurable maps into $\mathcal{F}$) $\widetilde{f}$.

A proof can be found in [6, Theorem 6.3.2], see also [18].

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