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NONPARAMETRIC ESTIMATION OF SCALAR DIFFUSIONS BASED ON LOW FREQUENCY DATA[1]

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We study the problem of estimating the coefficients of a diffusion $(X_t, t \geq 0)$; the estimation is based on discrete data $X_{n\Delta}, n = 0, 1, \ldots, N$. The sampling frequency Δ^{-1} is constant, and asymptotics are taken as the number N of observations tends to infinity. We prove that the problem of estimating both the diffusion coefficient (the volatility) and the drift in a nonparametric setting is ill-posed: the minimax rates of convergence for Sobolev constraints and squared-error loss coincide with that of a, respectively, first- and second-order linear inverse problem. To ensure ergodicity and limit technical difficulties we restrict ourselves to scalar diffusions living on a compact interval with reflecting boundary conditions.

Our approach is based on the spectral analysis of the associated Markov semigroup. A rate-optimal estimation of the coefficients is obtained via the nonparametric estimation of an eigenvalue–eigenfunction pair of the transition operator of the discrete time Markov chain $(X_{n\Delta}, n = 0, 1, \ldots, N)$ in a suitable Sobolev norm, together with an estimation of its invariant density.

1. Introduction.

1.1. *Overview.* Since Feller's celebrated classification, stationary scalar diffusions have served as a representative model for homogeneous Markov processes in continuous time. Historically, diffusion processes were probably first seen as approximation models for discrete Markov chains, up to an appropriate rescaling in time and space. More recently, the development of financial mathematics has argued in favor of genuinely continuous time models, with simple dynamics governed by a local mean (drift) $b(\cdot)$ and local variance (diffusion coefficient, or volatility) $\sigma(\cdot)$ on the state space $S = \mathbb{R}$ or $S \subset \mathbb{R}$ with appropriate boundary condition. The dynamics are usually described by an Itô-type stochastic differential equation in the interior of S, which in the time-homogeneous case reads like

$$dX_t = b(X_t)\,dt + \sigma(X_t)\,dW_t, \qquad t \geq 0,$$

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where the driving process $(W_t, t \geq 0)$ is standard Brownian motion. The growing importance of diffusion models progressively raised among the community of statisticians a vast research program, from both quantitative and theoretical angles. We outline the main achievements of this program in Section 1.2.

In the late 1970s a statistician was able to characterize qualitatively the properties of a parametric ergodic diffusion model based on the continuous observation of a sample path

$$X^T := (X_t, 0 \leq t \leq T)$$

of the trajectory, as $T \to \infty$, that is, as the time length of the experiment grows to infinity, a necessary assumption to assure the growing of information thanks to the recurrence of the sample path. The 1980s explored various discretization schemes of the continuous time model: the data X^T could progressively be replaced by the more realistic observation

$$X^{(N,\Delta_N)} := \big(X_{n\Delta_N}, n = 0, 1, \ldots, N\big),$$

with asymptotics taken as $N \to \infty$. The discretization techniques used at that time required the high frequency sampling assumption $\Delta_N \to 0$ whereas $N\Delta_N \to \infty$ in order to guarantee the closeness of $X^{(N,\Delta_N)}$ and X^T, with $T = N\Delta_N$. Soon, a similar nonparametric program was achieved for both continuous time and high frequency data.

By the early to mid-1990s, the frontier remained the "fixed Δ case," that is, the case of low frequency data. This is the topic of the present paper. First, one must understand the importance and flexibility gained by being able to relax the assumption that the sampling time Δ between two data points is "small": indeed, one can hardly deny that, in practice, it may well happen that sampling with arbitrarily small Δ is simply not feasible. Put differently, the asymptotic statistical theory is a mathematical construct to assess the quality of an estimator based on discrete observations and it must be decided which asymptotics are adequate for the data at hand. Second, the statistical nature of the problem drastically changes when passing from high to low frequency sampling: the approximation properties of the sample path $X^{N\Delta_N}$ by $X^{(N,\Delta_N)}$ are not valid anymore; the observation $(X_0, X_\Delta, \ldots, X_{N\Delta})$ becomes a genuine Markov chain, and inference about the underlying coefficients of the diffusion process must be sought via the identification of the law of the observation $X^{(N,\Delta_N)}$. In the time-homogeneous case the mathematical properties of the random vector $X^{(N,\Delta_N)}$ are embodied in the transition operator

$$P_\Delta f(x) := \mathbb{E}[f(X_\Delta)|X_0 = x],$$

defined on appropriate test functions f. Under suitable assumptions, the operator P_Δ is associated with a Feller semigroup $(P_t, t \geq 0)$ with a densely defined infinitesimal generator L on the space of continuous functions given by

$$Lf(x) = L_{\sigma,b} f(x) := \frac{\sigma^2(x)}{2} f''(x) + b(x) f'(x).$$

The second-order term $\sigma(\cdot)$ is the diffusion coefficient, and the first-order term $b(\cdot)$ is the drift coefficient. Postulating the existence of an invariant density $\mu(\cdot) = \mu_{\sigma,b}(\cdot)$, the operator L is unbounded, but self-adjoint negative on $L^2(\mu) := \{f \mid \int |f|^2\mu < \infty\}$, and the functional calculus gives the correspondence

$$P_\Delta = \exp(\Delta L) \tag{1.1}$$

in the operator sense. Therefore, a consistent statistical program can be presumed to start from the observed Markov chain $X^{(N,\Delta)}$, estimate its transition operator P_Δ and infer about the pair $(b(\cdot), \sigma(\cdot))$, via the correspondence (1.1), in other words via the spectral properties of the operator P_Δ. Expressed in a diagram, we obtain the following line:

$$\text{data} = X^{(N,\Delta)} \xrightarrow{(E)} P_\Delta \xrightarrow{(I)} L \longleftrightarrow \big(b(\cdot), \sigma(\cdot)\big) = \text{parameter}. \tag{1.2}$$

The efficiency of a given statistical estimation procedure will be measured by the proficiency in combining the estimation part (E) and the identification part (I) of the model.

The works of Hansen, Scheinkman and Touzi (1998) and Chen, Hansen and Scheinkman (1997) paved the way: they formulated a precise and thorough program, proposing and discussing several methods for identifying scalar diffusions via their spectral properties. Simultaneously, the Danish school, given on impulse by the works of Kessler and Sørensen (1999), systematically studied the parametric efficiency of spectral methods in the fixed Δ setting described above. By constructing estimating functions based on eigenfunctions of the operator L, they could construct $\sqrt{N}$-consistent estimators and obtained precise asymptotic properties.

However, a quantitative study of nonparametric estimation in the fixed Δ context remained out of reach for some time, for both technical and conceptual reasons. The purpose of the present paper is to fill in this gap, by trying to understand and explain why the nonparametric case significantly differs from its parametric analogue, as well as from the high frequency data framework in nonparametrics.

We are going to establish minimax rates of convergence over various smoothness classes, characterizing upper and lower bounds for estimating $b(\cdot)$ and $\sigma(\cdot)$ based on the obervation of $X_0, X_\Delta, \ldots, X_{N\Delta}$, with asymptotics taken as $N \to \infty$. The minimax rate of convergence is an index of both accuracy of estimation and complexity of the model. We will show that in the nonparametric case the complexity of the problems of estimating $b(\cdot)$ and $\sigma(\cdot)$ is related to ill-posed inverse problems. Although we mainly focus on the theoretical aspects of the statistical model, the estimators we propose are based on feasible nonparametric smoothing methods: they can be implemented in practice, allowing for adaptivity and finite sample optimization. Some simulation results were performed by Reiß (2003).

The estimation problem is exactly formulated in Section 2, where also the main theoretical results are stated. The spectral estimation method we adopt is

explained in Section 3, which includes a discussion of related problems and possible extensions. The proofs of the upper bound for our estimator and its optimality in a minimax sense are given in Sections 4 and 5, respectively. Results of rather technical nature are deferred to Section 6.

1.2. *Statistical estimation for diffusions*: *an outlook.* We give a brief and selective summary of the evolution of the area over the last two decades. The nonparametric identification of diffusion processes from continuous data was probably first addressed in the reference paper of Banon (1978). More precise estimation results can be listed as follows:

1.2.1. *Continuous or high frequency data*: *the parametric case.* Estimation of a finite-dimensional parameter θ from $X^T = (X_t, 0 \le t \le T)$ with asymptotics as $T \to \infty$ when X is a diffusion of the form

$$dX_t = b_\theta(X_t)\,dt + \sigma(X_t)\,dW_t \tag{1.3}$$

is classical [Brown and Hewitt (1975) and Kutoyants (1975)]. Here $(W_t, t \ge 0)$ is a standard Wiener process. The diffusion coefficient is perfectly identified from the data by means of the quadratic variation of X. By assuming the process X to be ergodic (positively recurrent), a sufficiently regular parametrization $\theta \mapsto b_\theta(\cdot)$ implies the local asymptotic normality (LAN) property for the underlying statistical model, therefore ensuring the $\sqrt{T}$-consistency and efficiency of the ML-estimator [see Liptser and Shiryaev (2001)].

In the case of discrete data $X_{n\Delta_N}, n = 0, 1, \ldots, N$, with high frequency sampling $\Delta_N^{-1} \to \infty$, but long range observation $N\Delta_N \to \infty$ as $N \to \infty$, various discretization schemes and estimating procedures had been proposed [Yoshida (1992) and Kessler (1997)] until Gobet (2002) eventually proved the LAN property for ergodic diffusions of the form

$$dX_t = b_{\theta_1}(X_t)\,dt + \sigma_{\theta_2}(X_t)\,dW_t \tag{1.4}$$

in a general setting, by means of the Malliavin calculus: under suitable regularity conditions, the finite-dimensional parameter θ_1 in the drift term can be estimated with optimal rate $\sqrt{N\Delta_N}$, whereas the finite-dimensional parameter θ_2 in the diffusion coefficient is estimated with the optimal rate $\sqrt{N}$.

1.2.2. *Continuous or high frequency data*: *the nonparametric case.* A similar program was progressively obtained in nonparametrics: If the drift function $b(\cdot)$ is globally unknown in the model given by (1.3), but belongs to a Sobolev ball $S(s, L)$ (of smoothness order $s > 0$ and radius L) over a given compact interval $\mathcal{I}$, a certain kernel estimator $\hat{b}_T(\cdot)$ achieves the following upper bound in $L^2(\mathcal{I})$ and in a root-mean-squared sense:

$$\sup_{b \in S(s,L)} \mathbb{E}\big[\|\hat{b}_T - b\|^2_{L^2(\mathcal{I})}\big]^{1/2} \lesssim T^{-s/(2s+1)}.$$

This already indicates a formal analogy with the model of nonparametric regression or "signal + white noise" where the same rate holds. (Here and in the sequel, the symbol $\lesssim$ means "up to constants," possibly depending on the parameters of the problem, but that are continuous in their arguments.) See Kutoyants (1984) for precise mathematical results.

Similar extensions to the discrete case with high frequency data sampling for the model driven by (1.4) were given in Hoffmann (1999), where the rates $(N\Delta_N)^{-s/(2s+1)}$ for the drift function $b(\cdot)$ and $N^{-s/(2s+1)}$ for the diffusion coefficient $\sigma(\cdot)$ have been obtained and proved to be optimal. See also the pioneering paper of Pham (1981). Methods of this kind have been successfully applied to financial data [Aït-Sahalia (1996), Stanton (1997), Chapman and Pearson (2000) and Fan and Zhang (2003)]. In particular, it is investigated whether the usual parametric model assumptions are compatible with the data, and the use of nonparametric methods is advocated.

1.2.3. *From high to low frequency data.* As soon as the sampling frequency $\Delta_N^{-1} = \Delta^{-1}$ is not large anymore, the problem of estimating a parameter in the drift or diffusion coefficient becomes significantly more difficult: the trajectory properties that can be recovered from the data when Δ_N is small are lost. In particular, there is no evident approximating scheme that can efficiently compute or mimic the continuous ML-estimator in parametric estimation.

Likewise, the usual nonparametric kernel estimators, based on differencing, do not provide consistent estimation of the drift $b(\cdot)$ or the diffusion coefficient $\sigma(\cdot)$. As a concrete example, consider the standard Nadaraya–Watson estimator $\hat{b}(x)$ of the drift $b(x)$ in the point $x \in \mathbb{R}$:

$$\hat{b}(x) := \frac{(N\Delta)^{-1}\sum_{n=0}^{N-1} K_h(x - X_{n\Delta})(X_{(n+1)\Delta} - X_{n\Delta})}{N^{-1}\sum_{n=0}^{N-1} K_h(x - X_{n\Delta})}$$

with a kernel function $K(\cdot)$ and $K_h(x) := h^{-1}K(h^{-1}x)$ for $h > 0$. If we let $N \to \infty$ and $h \to 0$, then by the ratio ergodic theorem and by kernel properties we obtain almost surely the limit

$$\mathbb{E}[\Delta^{-1}(X_\Delta - X_0)|X_0 = x] = \Delta^{-1}\int_0^\Delta P_t b(x)\,dt.$$

Hence, this estimator is not consistent. It merely yields a highly blurred version of $b(x)$, which of course tends to $b(x)$ in the high frequency limit $\Delta \to 0$. Note that the transition operators P_t involved depend on the unknown functions $b(\cdot)$ and $\sigma(\cdot)$ as a whole. The situation for estimators of $\sigma(\cdot)$ based on the approximation of the quadratic variation is even worse, because the drift $b(\cdot)$ enters directly into the limit expression.

1.2.4. *Spectral methods for parametric estimation.* Kessler and Sørensen (1999) suggested the use of eigenvalues κ_θ and eigenvectors $\varphi_\theta(\cdot)$ of the parametrized infinitesimal generator

$$L_\theta f(x) = \frac{\sigma_\theta^2(x)}{2} f''(x) + b_\theta(x) f'(x),$$

that is, such that $L_\theta \varphi_\theta(x) = \kappa_\theta \varphi_\theta(x)$. Indeed, since the pair $(\kappa_\theta, \varphi_\theta)$ also satisfies

$$P_\Delta \varphi_\theta(X_{n\Delta}) = \mathbb{E}\big[\varphi_\theta\big(X_{(n+1)\Delta}\big)\big|X_{n\Delta}\big] = \exp(\kappa_\theta \Delta)\varphi_\theta(X_{n\Delta}),$$

whenever it is easy to compute, the knowledge of a pair $(\kappa_\theta, \varphi_\theta)$ can be translated into a set of conditional moment conditions to be used in estimating functions. With their method, Kessler and Sørensen can construct $\sqrt{N}$-consistent estimators that are nearly efficient. See also the paper of Hansen, Scheinkman and Touzi (1998) that we already mentioned.

In a sense, in this idea also lies the essence of our method. However, the strategy of Kessler and Sørensen is not easily extendable to nonparametrics: there is no straightforward way to pass from a finite-dimensional parametrization of the generator L_θ with explicit eigenpairs $(\kappa_\theta, \varphi_\theta)$ to a full nonparametric space with satisfactory approximation properties. Besides, there would be no evident route to treat the variance of such speculative nonparametric estimators either, because the behavior of the parametric Fisher information matrix for a growing number of parameters is too complex to be easily controlled. We will see in Section 3 how to pass over these objections by estimating directly an eigenpair nonparametrically.

1.2.5. *Prospectives.* A quick summary yields Table 1 for optimal rates of convergence.

Table 1 can be interpreted as follows: the difficulty of the estimation problem is increasing from top to bottom and from left to right. A blank line separates the continuous–high-frequency (HF) data domain from the low-frequency (LF) data domain. The breach for LF data opened by Kessler and Sørensen as well as by Hansen, Scheinkman and Touzi shows that $\sqrt{N}$-consistent estimators usually exist in the parametric case. The remaining case are the rates of convergence for LF data in the nonparametric case u_N for the drift $b(\cdot)$ and v_N for the diffusion coefficient $\sigma(\cdot)$, for which we are aiming.

TABLE 1

	Parametric		**Nonparametric**	
	b	σ	b	σ
Continuous	$T^{-1/2}$	known	$T^{-s/(2s+1)}$	known
HF data	$(N\Delta_N)^{-1/2}$	$N^{-1/2}$	$(N\Delta_N)^{-s/(2s+1)}$	$N^{-s/(2s+1)}$
LF data	$N^{-1/2}$	$N^{-1/2}$	u_N	v_N

2. Main results.

2.1. *A diffusion model with boundary reflections.* We shall restrict ourselves to reflecting diffusions on a one-dimensional interval to avoid highly nontrivial technical issues; see the discussion in Section 3.3.

Choosing for convenience the interval $[0, 1]$, we suppose the following.

ASSUMPTION 2.1. The function $b : [0, 1] \to \mathbb{R}$ is measurable and bounded, the function $\sigma : [0, 1] \to (0, \infty)$ is continuous and positive and the function $\nu : [0, 1] \to \mathbb{R}$ satisfies $\nu(0) = 1$, $\nu(1) = -1$.

We consider the stochastic differential equation

$$\begin{aligned} dX_t &= b(X_t)\,dt + \sigma(X_t)\,dW_t + \nu(X_t)\,dL_t(X), \\ X_0 &= x_0 \quad \text{and} \quad X_t \in [0, 1] \qquad \forall\, t \geq 0. \end{aligned} \tag{2.1}$$

The process $(W_t,\ t \geq 0)$ is a standard Brownian motion and $(L_t(X), t \geq 0)$ is a nonanticipative continuous nondecreasing process that increases only when $X_t \in \{0, 1\}$. The boundedness of $b(\cdot)$ and the ellipticity of $\sigma(\cdot)$ ensure the existence of a weak solution; see for instance Stroock and Varadhan (1971). Note that the process $L(X)$ is part of the solution and is given by a difference of local times of X at the boundary points of $[0, 1]$.

Due to the compactness of $[0, 1]$ and the reflecting boundary conditions, the Markov process X has a spectral gap, which implies geometric ergodicity; compare with Lemmas 6.1 and 6.2. In particular, a unique invariant measure μ exists and the one-dimensional distributions of X_t converge exponentially fast to μ as $t \to \infty$ so that the assumption of stationarity can be made without loss of generality for asymptotic results.

We denote by $\mathbb{P}_{\sigma,b}$ the law of the associated stationary diffusion on the canonical space $\Omega = \mathcal{C}(\mathbb{R}_+, [0, 1])$ of continuous functions over the positive axis with values in $[0, 1]$, equipped with the topology of uniform convergence and endowed with its Borel σ-field $\mathcal{F}$. We denote by $\mathbb{E}_{\sigma,b}$ the corresponding expectation operator. Given $N \geq 1$ and $\Delta > 0$, we observe the canonical process $(X_t, t \geq 0)$ at equidistant times $n\Delta$ for $n = 0, 1, \ldots, N$. Let $\mathcal{F}_N$ denote the σ-field generated by $\{X_{n\Delta} | n = 0, \ldots, N\}$.

DEFINITION 2.2. An estimator of the pair $(\sigma(\cdot), b(\cdot))$ is an $\mathcal{F}_N$-measurable function on Ω with values in $L^2([0, 1]) \times L^2([0, 1])$.

To assess the L^2-risk in a minimax framework, we introduce the nonparametric set Θ_s, which consists of pairs of functions of regularity s and $s - 1$, respectively.

DEFINITION 2.3. For $s > 1$ and given constants $C \geq c > 0$, we consider the class $\Theta_s := \Theta(s, C, c)$ defined by

$$\left\{(\sigma, b) \in H^s([0,1]) \times H^{s-1}([0,1]) \big| \|\sigma\|_{H^s} \leq C,\ \|b\|_{H^{s-1}} \leq C,\ \inf_x \sigma(x) \geq c\right\},$$

where H^s denotes the L^2-Sobolev space of order s.

Note that all $(\sigma(\cdot), b(\cdot)) \in \Theta_s$ satisfy Assumption 2.1.

2.2. *Minimax rates of convergence.* We are now in position to state the main theorems. By (3.12) and (3.13) in the next section we define estimators $\hat{\sigma}^2$ and $\hat{b}$ using a spectral estimation method based on the observation $(X_0, X_\Delta, \ldots, X_{N\Delta})$. These estimators, which of course depend on the number N of observations, satisfy the following uniform asymptotic upper bounds.

THEOREM 2.4. *For all $s > 1$, $C \geq c > 0$ and $0 < a < b < 1$ we have*

$$\sup_{(\sigma,b)\in\Theta_s} \mathbb{E}_{\sigma,b}\big[\|\hat{\sigma}^2 - \sigma^2\|^2_{L^2([a,b])}\big]^{1/2} \lesssim N^{-s/(2s+3)},$$

$$\sup_{(\sigma,b)\in\Theta_s} \mathbb{E}_{\sigma,b}\big[\|\hat{b} - b\|^2_{L^2([a,b])}\big]^{1/2} \lesssim N^{-(s-1)/(2s+3)}.$$

Recall that $A \lesssim B$ means that A can be bounded by a constant multiple of B, where the constant depends continuously on other parameters involved. Similarly, $A \gtrsim B$ is equivalent to $B \lesssim A$ and $A \sim B$ holds if both relations $A \lesssim B$ and $A \gtrsim B$ are true.

As the following lower bounds prove, the rates of convergence of our estimators are optimal in a minimax sense over Θ_s.

THEOREM 2.5. *Let E_N denote the set of all estimators according to Definition* 2.2. *Then for all $0 \leq a < b \leq 1$ and $s > 1$ the following hold*:

$$\inf_{\hat{\sigma}^2 \in E_N} \sup_{(\sigma,b)\in\Theta_s} \mathbb{E}_{\sigma,b}\big[\|\hat{\sigma}^2 - \sigma^2\|^2_{L^2([a,b])}\big]^{1/2} \gtrsim N^{-s/(2s+3)}, \tag{2.2}$$

$$\inf_{\hat{b} \in E_N} \sup_{(\sigma,b)\in\Theta_s} \mathbb{E}_{\sigma,b}\big[\|\hat{b} - b\|^2_{L^2([a,b])}\big]^{1/2} \gtrsim N^{-(s-1)/(2s+3)}. \tag{2.3}$$

If we set $s_1 = s - 1$ and $s_2 = s$, then the drift $b(\cdot) \in \Theta_s$ with regularity s_1 can be estimated with the minimax rate of convergence $u_N = N^{-s_1/(2s_1+5)}$, whereas the diffusion coefficient $\sigma(\cdot) \in \Theta_s$ has regularity s_2 and the corresponding minimax rate of convergence is $v_N = N^{-s_2/(2s_2+3)}$. Hence, Table 1 in Section 1.2.5 can be filled with two rather unexpected rates of convergence u_N and v_N. In Section 3.3 the rates are explained in the terminology of ill-posed problems and reasons are given why the tight connection between the regularity assumptions on $b(\cdot)$ and $\sigma(\cdot)$ is needed.

3. Spectral estimation method.

3.1. *The basic idea.* We shall base our estimator of the diffusion coefficient $\sigma(\cdot)$ and of the drift coefficient $b(\cdot)$ on spectral methods for passing from the transition operator P_Δ, which is approximately known to us, to the infinitesimal generator L, which more explicitly encodes the functions $\sigma(\cdot)$ and $b(\cdot)$. In the sequel, we shall rely on classical results for scalar diffusions; for example, consult Bass [(1998), Chapter 4]. We use the specific form of the invariant density

$$\mu(x) = 2C_0\sigma^{-2}(x)\exp\left(\int_0^x 2b(y)\,\sigma^{-2}(y)\,dy\right) \tag{3.1}$$

and the function $S(\cdot) = 1/s'(\cdot)$, derived from the scale function $s(\cdot)$,

$$S(x) = \tfrac{1}{2}\sigma^2(x)\mu^{-1}(x) = C_0\exp\left(-\int_0^x 2b(y)\sigma^{-2}(y)\,dy\right), \tag{3.2}$$

with the normalizing constant $C_0 > 0$ depending on $\sigma(\cdot)$ and $b(\cdot)$. The action of the generator in divergence form is given by

$$Lf(x) = L_{\sigma,b}f(x) = \frac{1}{2}\sigma^2(x)f''(x) + b(x)f'(x) = \frac{1}{\mu(x)}\big(S(x)f'(x)\big)', \tag{3.3}$$

where the domain of this unbounded operator on $L^2(\mu)$ is given by the subspace of the L^2-Sobolev space H^2 with Neumann boundary conditions

$$\operatorname{dom}(L) = \{f \in H^2([0,1]) \mid f'(0) = f'(1) = 0\}.$$

The generator L is a self-adjoint elliptic operator on $L^2(\mu)$ with compact resolvent so that it has nonpositive point spectrum only. If ν_1 denotes the largest negative eigenvalue of L with eigenfunction u_1, then due to the reflecting boundary of $[0,1]$ the Neumann boundary conditions $u_1'(0) = u_1'(1) = 0$ hold and thus

$$Lu_1 = \mu^{-1}(Su_1')' = \nu_1 u_1 \quad\Longrightarrow\quad S(x)u_1'(x) = \nu_1\int_0^x u_1(y)\mu(y)\,dy. \tag{3.4}$$

From (3.2) we can derive an explicit expression for the diffusion coefficient:

$$\sigma^2(x) = \frac{2\nu_1\int_0^x u_1(y)\mu(y)\,dy}{u_1'(x)\mu(x)}. \tag{3.5}$$

The corresponding expression for the drift coefficient is

$$b(x) = \nu_1\frac{u_1(x)u_1'(x)\mu(x) - u_1''(x)\int_0^x u_1(y)\mu(y)\,dy}{u_1'(x)^2\mu(x)}. \tag{3.6}$$

Hence, if we knew the invariant measure μ, the eigenvalue ν_1 and the eigenfunction u_1 (including its first two derivatives), we could exactly determine the drift and diffusion coefficient. Of course, these identities are valid for any eigenfunction u_k with eigenvalue ν_k, but for better numerical stability we shall use only the largest

nondegenerate eigenvalue ν_1. Moreover, it is known that only the eigenfunction u_1 does not have a vanishing derivative in the interior of the interval (cf. Proposition 6.5) so that by this choice indeterminacy at interior points is avoided.

Using semigroup theory [Engel and Nagel (2000), Theorem IV.3.7] we know that u_1 is also an eigenfunction of P_Δ with eigenvalue $\kappa_1 = e^{\Delta\nu_1}$. Our procedure consists of determining estimators $\hat{\mu}$ of μ and $\hat{P}_\Delta$ of P_Δ, to calculate the corresponding eigenpair $(\hat{\kappa}_1, \hat{u}_1)$ and to use (3.5) and (3.6) to build a plug-in estimator of $\sigma(\cdot)$ and $b(\cdot)$.

3.2. *Construction of the estimators.* We use projection methods, taking advantage of approximating properties of abstract operators by finite-dimensional matrices, for which the spectrum is easy to calculate numerically. A similar approach was already suggested by Chen, Hansen and Scheinkman (1997). More specifically, we make use of wavelets on the interval $[0, 1]$. For the construction of wavelet bases and their properties we refer to Cohen (2000).

DEFINITION 3.1. Let (ψ_λ) with multiindices $\lambda = (j, k)$ be a compactly supported L^2-orthonormal wavelet basis of $L^2([0, 1])$. The approximation spaces (V_J) are defined as L^2-closed linear spans of the wavelets up to the frequency level J,

$$V_J := \overline{\operatorname{span}}\{\psi_\lambda \,|\, |\lambda| \le J\} \qquad \text{where } |(j,k)| := j.$$

The L^2-orthogonal projection onto V_J is called π_J; the $L^2(\mu)$-orthogonal projection onto V_J is called π_J^μ.

In the sequel we shall regularly use the Jackson and Bernstein inequalities with respect to the L^2-Sobolev spaces $H^s([0, 1])$ of regularity s:

$$\|(\mathrm{Id} - \pi_J) f\|_{H^t} \lesssim 2^{-J(s-t)} \|f\|_{H^s}, \qquad 0 \le t \le s,$$
$$\forall\, v_J \in V_J, \qquad \|v_J\|_{H^s} \lesssim 2^{J(s-t)} \|v_J\|_{H^t}, \qquad 0 \le t \le s.$$

The canonical projection estimate of μ based on $(X_{n\Delta})_{0 \le n \le N}$ is given by

$$\hat{\mu} := \sum_{|\lambda| \le J} \hat{\mu}_\lambda \psi_\lambda \qquad \text{with } \hat{\mu}_\lambda := \frac{1}{N+1} \sum_{n=0}^{N} \psi_\lambda(X_{n\Delta}). \tag{3.7}$$

By the ergodicity of X it follows that $\hat{\mu}_\lambda$ is a consistent estimate of $\langle \mu, \psi_\lambda \rangle$ for $N \to \infty$. To estimate the action of the transition operator on the wavelet basis $(\mathbf{P}_\Delta^J)_{\lambda,\lambda'} := \langle P_\Delta \psi_\lambda, \psi_{\lambda'} \rangle_\mu$, we introduce the symmetrized matrix estimator $\hat{\mathbf{P}}_\Delta$ with entries

$$(\hat{\mathbf{P}}_\Delta)_{\lambda,\lambda'} := \frac{1}{2N} \sum_{n=1}^{N} \big(\psi_\lambda(X_{(n-1)\Delta}) \psi_{\lambda'}(X_{n\Delta}) + \psi_{\lambda'}(X_{(n-1)\Delta}) \psi_\lambda(X_{n\Delta}) \big). \tag{3.8}$$

This yields an approximation of $\langle P_\Delta \psi_{\lambda'}, \psi_\lambda \rangle_\mu$, that is, of the action of the transition operator on V_J with respect to the unknown scalar product $\langle \cdot, \cdot \rangle_\mu$

in $L^2(\mu)$. We therefore introduce a third statistic $\hat{\mathbf{G}}$, which approximates the $\dim(V_J) \times \dim(V_J)$-dimensional Gram matrix $\mathbf{G}$ with entries $\mathbf{G}_{\lambda,\lambda'} = \langle \psi_\lambda, \psi_{\lambda'} \rangle_\mu$, and which is given by

$$\hat{\mathbf{G}}_{\lambda,\lambda'} := \frac{1}{N}\left(\frac{1}{2}\psi_\lambda(X_0)\psi_{\lambda'}(X_0) + \frac{1}{2}\psi_\lambda(X_{N\Delta})\psi_{\lambda'}(X_{N\Delta}) + \sum_{n=1}^{N-1} \psi_\lambda(X_{n\Delta})\psi_{\lambda'}(X_{n\Delta})\right). \tag{3.9}$$

The particular treatment of the boundary terms will be explained later. If we put $\mathbf{\Sigma} = (w_n \psi_\lambda(X_n))_{|\lambda| \le J,\, n \le N}$ with $w_0 = w_N = \frac{1}{2}$ and $w_n = 1$ otherwise, we have $\hat{\mathbf{G}} = N^{-1}\mathbf{\Sigma}\mathbf{\Sigma}^T$, $\mathbf{\Sigma}^T$ being the transpose of $\mathbf{\Sigma}$. Our construction can thus be regarded as a least squares type estimator, as in a usual regression setting; see the argument developed in Section 3.3.1.

We combine the last two estimators in order to determine estimates for the eigenvalue κ_1 and the eigenfunction u_1 of P_Δ. As will be made precise in Proposition 4.5, the operators P_Δ and $\pi_J^\mu P_\Delta$ are close for large values of J. Note that all eigenvectors of $\pi_J^\mu P_\Delta$ lie in V_J, the range of $\pi_J^\mu P_\Delta$. The eigenfunction u_1^J corresponding to the second largest eigenvalue κ_1^J of $\pi_J^\mu P_\Delta$ is characterized by

$$\langle P_\Delta u_1^J, \psi_\lambda \rangle_\mu = \kappa_1^J \langle u_1^J, \psi_\lambda \rangle_\mu \qquad \forall\, |\lambda| \le J. \tag{3.10}$$

We pass to vector-matrix notation and use from now on bold letters to define for a function $v \in V_J$ the corresponding coefficient column vector $\mathbf{v} = (\langle v, \psi_\lambda \rangle)_{|\lambda| \le J}$. Observe carefully the different L^2-scalar products used; here they are with respect to the Lebesgue measure. Thus, we can rewrite (3.10) as

$$\mathbf{P}_\Delta^J \mathbf{u}_1^J = \kappa_1^J \mathbf{G}\mathbf{u}_1^J. \tag{3.11}$$

As $\mathbf{v}^T\mathbf{G}\mathbf{v} = \langle v, v \rangle_\mu > 0$ holds for $v \in V_J \setminus \{0\}$, the matrix $\mathbf{G}$ is invertible and $(\kappa_1^J, \mathbf{u}_1^J)$ is an eigenpair of $\mathbf{G}^{-1}\mathbf{P}_\Delta^J$. This matrix is self-adjoint with respect to the scalar product induced by $\mathbf{G}$:

$$\begin{aligned}\langle \mathbf{G}^{-1}\mathbf{P}_\Delta^J \mathbf{v}, \mathbf{w} \rangle_{\mathbf{G}} &:= (\mathbf{G}^{-1}\mathbf{P}_\Delta^J \mathbf{v})^T \mathbf{G}\mathbf{w} \\ &= \mathbf{v}^T \mathbf{P}_\Delta^J \mathbf{w} = \langle \mathbf{v}, \mathbf{G}^{-1}\mathbf{P}_\Delta^J \mathbf{w} \rangle_{\mathbf{G}}.\end{aligned}$$

Similarly, $\mathbf{v}^T\hat{\mathbf{G}}\mathbf{v} = N^{-1}(\mathbf{\Sigma}^T\mathbf{v})^T\mathbf{\Sigma}^T\mathbf{v} \ge 0$ holds and the matrix $\hat{\mathbf{G}}$ can be shown to be even strictly positive definite with high probability (see Lemma 4.12). In this case, we similarly infer that $\hat{\mathbf{G}}^{-1}\hat{\mathbf{P}}$ is self-adjoint with respect to the $\hat{\mathbf{G}}$-scalar product. The Cauchy–Schwarz inequality and the inequality between geometric

and arithmetic mean yield the estimate

$$\begin{aligned}\langle \hat{\mathbf{G}}^{-1}\hat{\mathbf{P}}_\Delta \mathbf{v}, \mathbf{v}\rangle_{\hat{\mathbf{G}}} &= \frac{1}{N}\sum_{n=1}^{N} v(X_{(n-1)\Delta})v(X_{n\Delta}) \\ &\le \frac{1}{N}\left(\sum_{n=0}^{N-1} v(X_{n\Delta})^2\right)^{1/2}\left(\sum_{n=1}^{N} v(X_{n\Delta})^2\right)^{1/2} \\ &\le \frac{1}{N}\left(\frac{1}{2}v(X_0)^2 + \frac{1}{2}v(X_{N\Delta})^2 + \sum_{n=1}^{N-1} v(X_{n\Delta})^2\right) \\ &= \langle \mathbf{v}, \mathbf{v}\rangle_{\hat{\mathbf{G}}}.\end{aligned}$$

We infer that all eigenvalues of $\hat{\mathbf{G}}^{-1}\hat{\mathbf{P}}_\Delta$ are real and not larger than 1. Hence, the second largest eigenvalue $\hat{\kappa}_1$ of $\hat{\mathbf{G}}^{-1}\hat{\mathbf{P}}_\Delta$ is well defined, which is why we downweighted the boundary terms of $\hat{\mathbf{G}}$. The eigenvalue $\hat{\kappa}_1$ of $\hat{\mathbf{G}}^{-1}\hat{\mathbf{P}}_\Delta$ and its corresponding eigenvector $\hat{\mathbf{u}}_1$ yield estimators of κ_1^J and u_1^J.

Plugging the estimator $\hat{\mu}$ as well as $\hat{\kappa}_1$ and $\hat{u}_1$ into (3.5) and (3.6), we obtain our estimators of $\sigma^2(\cdot)$ and $b(\cdot)$:

$$\hat{\sigma}^2(x) := \frac{2\Delta^{-1}\log(\hat{\kappa}_1)\int_0^x \hat{u}_1(y)\hat{\mu}(y)\,dy}{\hat{u}_1'(x)\hat{\mu}(x)}, \tag{3.12}$$

$$\hat{b}(x) := \Delta^{-1}\log(\hat{\kappa}_1)\frac{\hat{u}_1(x)\hat{u}_1'(x)\hat{\mu}(x) - \hat{u}_1''(x)\int_0^x \hat{u}_1(y)\hat{\mu}(y)\,dy}{\hat{u}_1'(x)^2\hat{\mu}(x)}. \tag{3.13}$$

To avoid indeterminacy, the denominators of the estimators are forced to remain above a certain minimal level, which depends on the subinterval $[a, b] \subset [0, 1]$ for which the loss function is taken. See (4.5) for the exact formulation in the case of $\hat{\sigma}^2(\cdot)$ and proceed analogously for $\hat{b}(\cdot)$.

3.3. *Discussion.*

3.3.1. *Least squares approach.* The estimator matrix $\hat{\mathbf{G}}^{-1}\hat{\mathbf{P}}_\Delta$ is built as in the least squares approach for projection methods in classical regression. To estimate $P_\Delta\psi_{\lambda_0}(x) = \mathbb{E}_{\sigma,b}[\psi_{\lambda_0}(X_\Delta)|X_0 = x]$, the least squares method consists of minimizing

$$\sum_{n=1}^{N}\left|\psi_{\lambda_0}(X_{n\Delta}) - \sum_{|\lambda|\le J}\alpha_\lambda^0\psi_\lambda(X_{(n-1)\Delta})\right|^2 \longrightarrow \min! \tag{3.14}$$

over all real coefficients (α_λ^0), leading to the normal equations

$$\sum_{n=1}^{N}\left(\sum_{|\lambda|\le J}\alpha_\lambda^0\psi_\lambda(X_{(n-1)\Delta})\right)\psi_{\lambda'}(X_{(n-1)\Delta}) = \sum_{n=1}^{N}\psi_{\lambda'}(X_{(n-1)\Delta})\psi_{\lambda_0}(X_{n\Delta})$$

for all $|\lambda'| \leq J$. Up to the special treatment of the boundary terms, we thus obtain the vector (α_λ^0) as the column with index λ_0 in $\hat{\mathbf{G}}^{-1}\hat{\mathbf{P}}_\Delta$.

3.3.2. *Other than wavelet methods.* For our projection estimates to work, we merely need approximation spaces satisfying the Jackson and Bernstein inequalities. Hence, other finite element bases could serve as well.

The invariant density and the transition density could also be estimated using kernel methods, but the numerical calculation of the eigenpair $(\hat{\kappa}_1, \hat{u}_1)$ would then involve an additional discretization step.

3.3.3. *Diffusions over the real line.* Using a wavelet basis of $L^2(\mathbb{R})$, it is still possible to estimate μ and P_Δ over the real line; in particular the eigenvalue characterization (3.10) extends to this case. Hansen, Scheinkman and Touzi (1998) derive the same formulae as (3.5) and (3.6) under ergodicity and boundary conditions so that a plug-in approach is feasible. However, a theoretical study seems to require much more demanding theoretical tools. If the uniform separation of the spectral value ν_1 and a polynomial growth bound for the eigenfunction $u_1(\cdot)$ are ensured, we expect that the same minimax results hold with respect to an $L^2(\mu)$-loss function, where the invariant density $\mu(\cdot)$ is of course parameter-dependent. However, all spectral approximation results have to be reconsidered with extra care, in particular because the $L^2(\mu)$-norms are in general not equivalent for different parameters.

3.3.4. *Adaptation to unknown smoothness.* The knowledge of the smoothness s that is needed for the construction of our estimators is not realistic in practice. An adaptive estimation of the eigenpair $(u_1(\cdot), \kappa_1)$ and $\mu(\cdot)$ that yields adaptive estimators for $(\sigma(\cdot), b(\cdot))$ could be obtained by the following modifications: First, the adaptive estimation of $\mu(\cdot)$ in a classical mixing framework is fairly well known [e.g., Tribouley and Viennet (1998)]. Second, taking advantage of the multiresolution structure provided by wavelets, the adaptive estimation of P_Δ could be obtained by introducing an appropriate thresholding in the estimated matrices on a large approximation space.

3.3.5. *Interpretation as an ill-posed problem.* One can make the link with ill-posed inverse problems by saying that estimation of $\mu(\cdot)$ is well-posed (i.e., with achievable rate $N^{-s/(2s+1)}$), but for $S(\cdot)$ we need an estimate of the derivative $u_1'(\cdot)$ yielding an ill-posedness degree of 1 ($N^{-s/(2s+3)}$). Observe that the regularity conditions $\sigma \in H^s$ and $b \in H^{s-1}$ are translated into $\mu \in H^s$, $S \in H^s$. The transformation of (μ, S) to $\sigma^2(\cdot) = 2S(\cdot)/\mu(\cdot)$ is stable [L^2-continuous for $S(\cdot) \geq s_0 > 0$], whereas in $b(\cdot) = S'(\cdot)/\mu(\cdot)$ another ill-posed operation (differentiation) occurs with degree 1.

A brief stepwise explanation reads as follows. Step 1, the natural parametrization (μ, P_Δ) is well-posed (for P_Δ in the strong operator norm sense). Step 2, the

calculation of the spectral pair (κ_1, u_1) is well-posed. Step 3, the differentiation of u_1 that determines S has an ill-posedness of degree 1. Step 4, the calculation of σ^2 from (μ, S) is well-posed. Step 5, the calculation of b from (μ, S) is ill-posed of degree 1.

3.3.6. *Regularity restrictions on $b(\cdot)$ and $\sigma(\cdot)$.* It is noteworthy that in the continuous time or high frequency observation case, the parameter $b(\cdot)$ does not influence the asymptotic behavior of the estimator of $\sigma(\cdot)$ and vice versa. The estimation problems are separated. In our low frequency regime we had to suppose tight regularity connections between $\sigma(\cdot)$ and $b(\cdot)$. This stems from the fact that for the underlying Markov chain $X^{(N,\Delta)}$ the parameters $\mu(\cdot)$ and $S(\cdot)$ are more natural and the regularity of these functions depends on the regularity both of $b(\cdot)$ and of $\sigma(\cdot)$.

At a different level, in nonparametric regression, different smoothness constraints are needed between the mean and the variance function. Recommended references are Müller and Stadtmüller (1987) and Fan and Yao (1998).

Finally, although we ask for the tight connection $s_1 = s_2 - 1$ for the regularity s_1 of the drift $b(\cdot)$ and s_2 of the diffusion coefficient $\sigma(\cdot)$, our results readily carry over to the milder constraint $s_1 \geq s_2 - 1$.

3.3.7. *Estimation when one parameter is known.* If $\sigma(\cdot)$ is known, an estimate $\hat{\mu}$ of the invariant density yields an estimate of $b(\cdot)$, since

$$b(x) = \frac{(\sigma^2(x)\mu(x))'}{2\mu(x)}, \qquad x \in [0,1].$$

Estimation of $\mu \in H^s$, $s > 1$, in H^1-norm can be achieved with rate $N^{-(s-1)/(2s+1)}$ and this rate is thus also valid for estimating $b(\cdot)$ in L^2-norm. Given the drift coefficient $b(\cdot)$, we find

$$\sigma^2(x) = 2\frac{\int_0^x b(y)\mu(y)\,dy + C}{\mu(x)}, \qquad x \in [0,1],$$

where C is a suitable constant. If we knew $\sigma^2(0)$, we would obtain the rate $N^{-s/(2s+1)}$ for $\mu \in H^s$.

Using a preliminary nonparametric estimate $\hat{\sigma}_C^2$ depending on the parameter C and then fitting a parametric model for C, we are likely to find the same rate. In any case, the assumption of knowing one parameter seems rather artificial and no further investigations have been performed.

3.3.8. *Estimation at the boundary.* Our plug-in estimators can only be defined on the open subinterval $(0,1)$. Estimation at the boundary points leads to a risk increase due to $S^{-1}(0) = \nu_1 u_1(0)\mu(0)/u_1''(0)$ by de l'Hôspital's rule applied to (3.4). Thus, estimating $\sigma(0)$ and $b(0)$ involves taking the second and third

derivative, respectively, when using plug-in estimators. A pointwise lower bound result—along the lines of the L^2-lower bound proof—shows that this deterioration cannot be avoided.

4. Proof of the upper bound.

4.1. *Convergence of* $\hat{\mu}$. First, we recall the proof for the risk bound in estimating the invariant measure:

PROPOSITION 4.1. *With the choice* $2^J \sim N^{1/(2s+1)}$ *the following uniform risk estimate holds for* $\hat{\mu}$ *based on* N *observations*:

$$\sup_{(\sigma,b)\in\Theta_s} \mathbb{E}_{\sigma,b}\big[\|\hat{\mu}-\mu\|_{L^2}^2\big]^{1/2} \lesssim N^{-s/(2s+1)}.$$

PROOF. The explicit formula (3.1) for μ shows that $\|\mu\|_{H^s}$ is uniformly bounded over Θ_s. This implies that the bias term satisfies

$$\|\mu-\pi_J\mu\|_{L^2} \lesssim 2^{-Js}\|\mu\|_{H^s} \sim N^{-s/(2s+1)},$$

uniformly over Θ_s. Since $\hat{\mu}_\lambda$ is an unbiased estimator of $\langle\mu,\psi_\lambda\rangle$, we can apply the variance estimates of Lemma 6.2 to obtain

$$\mathbb{E}_{\sigma,b}\big[\|\hat{\mu}-\pi_J\mu\|_{L^2}^2\big] = \sum_{|\lambda|\le J} \mathrm{Var}_{\sigma,b}[\hat{\mu}_\lambda] \lesssim 2^J N^{-1},$$

which—in combination with the uniformity of the constants involved—gives the announced upper bound. □

4.2. *Spectral approximation.* We shall rely on the spectral approximation results given in Chatelin (1983); compare also Kato (1995). Since for $\hat{\sigma}(\cdot)$ we have to estimate not only the eigenvalue u_1, but also its derivative u_1', we will be working in the L^2-Sobolev space H^1. The general idea is that the error in the eigenvalue and in the eigenfunction can be controlled by the error of the operator on the eigenspace, once the overall error measured in the operator norm is small. Let $R(T,z)=(T-z\,\mathrm{Id})^{-1}$ denote the resolvent map of the operator T, $\sigma(T)$ its spectrum and $B(x,r)$ the closed ball of radius r around x.

PROPOSITION 4.2. *Suppose a bounded linear operator* T *on a Hilbert space has a simple eigenvalue* κ *such that* $\sigma(T)\cap B(\kappa,\rho)=\{\kappa\}$ *holds for some* $\rho>0$. *Let* T_ε *be a second linear operator with* $\|T_\varepsilon - T\| < \frac{R}{2}$, *where* $R := (\sup_{z\in B(\kappa,\rho)}\|R(T,z)\|)^{-1}$. *Then the operator* T_ε *has a simple eigenvalue* κ_ε *in* $B(\kappa,\rho)$ *and there are eigenvectors* u *and* u_ε *with* $Tu=\kappa u$, $T_\varepsilon u_\varepsilon=\kappa_\varepsilon u_\varepsilon$ *satisfying*

$$\|u_\varepsilon - u\| \le \sqrt{8}R^{-1}\|(T_\varepsilon - T)u\|. \tag{4.1}$$

PROOF. We use the resolvent identity and the Cauchy integral representation of the spectral projection P_ε on the eigenspace of T_ε contained in $B(\kappa,\rho)$ [see Chatelin (1983), Lemma 6.4]. By the usual Neumann series argument we find formally for an eigenvector u corresponding to κ,

$$\begin{aligned}\|u - P_\varepsilon u\| &= \frac{1}{2\pi}\left\| \oint_{B(\kappa,\rho)} \frac{R(T_\varepsilon, z)}{\kappa - z}\, dz\, (T_\varepsilon - T)u \right\| \\ &\le \frac{1}{2\pi} 2\pi\rho \sup_{z\in B(\kappa,\rho)} \|R(T_\varepsilon, z)\|\rho^{-1}\|(T_\varepsilon - T)u\| \\ &\le \sup_{z\in B(\kappa,\rho)} \frac{\|R(T,z)\|}{1 - \|R(T,z)\|\|T_\varepsilon - T\|}\|(T_\varepsilon - T)u\| \\ &= (R - \|T_\varepsilon - T\|)^{-1}\|(T_\varepsilon - T)u\|.\end{aligned}$$

Hence, for $\|T_\varepsilon - T\| < \frac{R}{2}$ this calculation is a posteriori justified and yields $\|u - P_\varepsilon u\| < 2R^{-1}\|(T_\varepsilon - T)u\|$. Applying $\|(T_\varepsilon - T)u\| < \frac{R}{2}\|u\|$ once again, we see that the projection P_ε cannot be zero. Consequently there must be a part of the spectrum of T_ε in $B(\kappa,\rho)$. By the argument in the proof of Theorem 5.22 in Chatelin (1983) this part consists of a simple eigenvalue κ_ε.

It remains to find eigenvectors that are close, too. Observe that, for arbitrary Hilbert space elements g, h with $\|g\| = \|h\| = 1$ and $\langle g, h\rangle \ge 0$,

$$\|g - h\|^2 = 2 - 2\langle g, h\rangle \le 2(1 + \langle g, h\rangle)(1 - \langle g, h\rangle) = 2\|g - \langle g, h\rangle h\|^2$$

holds. We substitute for g and h the normalized eigenvectors u and u_ε with $\langle u, u_\varepsilon\rangle \ge 0$; note that oblique projections only enlarge the right-hand side and thus infer (4.1). □

COROLLARY 4.3. *Under the conditions of Proposition* 4.2 *there is a constant* $C = C(R, \|T\|)$ *such that* $|\kappa_\varepsilon - \kappa| \le C\|(T_\varepsilon - T)u\|$.

PROOF. The inverse triangle inequality yields

$$\begin{aligned}|\kappa_\varepsilon - \kappa| &= |\|T_\varepsilon u_\varepsilon\| - \|Tu\|| \le \|T_\varepsilon(u_\varepsilon - u) + (T_\varepsilon - T)u\| \\ &\le (\|T\| + \|T_\varepsilon - T\|)\|u_\varepsilon - u\| + \|(T_\varepsilon - T)u\| \\ &\le \left(\left(\|T\| + \frac{R}{2}\right)\sqrt{8}R^{-1} + 1\right)\|(T_\varepsilon - T)u\|,\end{aligned}$$

where the last line follows from Proposition 4.2. □

4.3. *Bias estimates.* In a first estimation step, we bound the deterministic error due to the finite-dimensional projection $\pi_J^\mu P_\Delta$ of P_Δ. We start with a lemma stating that π_J^μ and π_J have similar approximation properties.

LEMMA 4.4. *Let $m:[0,1]\to[m_0,m_1]$ be a measurable function with $m_1\geq m_0>0$. Denote by π_J^m the $L^2(m)$-orthogonal projection onto the multiresolution space V_J. Then there is a constant $C=C(m_0,m_1)$ such that*

$$\|(\mathrm{Id}-\pi_J^m)f\|_{H^1}\leq C\|(\mathrm{Id}-\pi_J)f\|_{H^1}\qquad\forall f\in H^1([0,1]).$$

PROOF. The norm equivalence $m_0\|g\|_{L^2}\leq\|g\|_m\leq m_1\|g\|_{L^2}$ implies

$$\|\pi_J^m\|_{L^2\to L^2}\leq m_1m_0^{-1}\|\pi_J^m\|_{L^2(m)\to L^2(m)}=m_1m_0^{-1}.$$

On the other hand, the Bernstein inequality in V_J and the Jackson inequality for $\mathrm{Id}-\pi_J$ in H^1 and L^2 yield, for $f\in H^1$,

$$\begin{aligned}\|(\mathrm{Id}-\pi_J^\mu)f\|_{H^1}&=\|(\mathrm{Id}-\pi_J^\mu)(\mathrm{Id}-\pi_J)f\|_{H^1}\\&\leq\|(\mathrm{Id}-\pi_J)f\|_{H^1}+\|\pi_J^\mu(\mathrm{Id}-\pi_J)f\|_{H^1}\\&\lesssim\|(\mathrm{Id}-\pi_J)f\|_{H^1}+2^J\|\pi_J^\mu(\mathrm{Id}-\pi_J)f\|_{L^2}\\&\lesssim\|(\mathrm{Id}-\pi_J)f\|_{H^1}+\|\pi_J^\mu\|_{L^2\to L^2}\|(\mathrm{Id}-\pi_J)f\|_{H^1},\end{aligned}$$

where the constants depend only on the approximation spaces. □

PROPOSITION 4.5. *Uniformly over Θ_s we have $\|\pi_J^\mu P_\Delta-P_\Delta\|_{H^1\to H^1}\lesssim 2^{-Js}$.*

PROOF. The transition density p_Δ is the kernel of the operator P_Δ. Hence, from Lemma 6.7 it follows that $P_\Delta:H^1\to H^{s+1}$ is continuous with a uniform norm bound over Θ_s. Lemma 4.4 yields

$$\|(P_\Delta-\pi_J^\mu P_\Delta)f\|_{H^1}\lesssim\|\mathrm{Id}-\pi_J\|_{H^{s+1}\to H^1}\|f\|_{H^1}.$$

The Jackson inequality in H^1 gives the result. □

COROLLARY 4.6. *Let κ_1^J be the largest eigenvalue smaller than 1 of π_J^μ with eigenfunction u_1^J. Then uniformly over Θ_s the following estimate holds*:

$$|\kappa_1^J-\kappa_1|+\|u_1^J-u_1\|_{H^1}\lesssim 2^{-Js}.$$

PROOF. We are going to apply Proposition 4.2 on the space H^1 and its Corollary 4.3. In view of Proposition 4.5, it remains to establish the existence of uniformly strictly positive values for ρ and R over Θ_s. The uniform separation of κ_1 from the rest of the spectrum is the content of Proposition 6.5.

For the choice of ρ in Proposition 6.5 we search a uniform bound R. If we regard P_Δ on $L^2(\mu)$, then P_Δ is self-adjoint and satisfies $\|R(P_\Delta,z)\|=\mathrm{dist}(z,\sigma(P_\Delta))^{-1}$ [see Chatelin (1983), Proposition 2.32].

By Lemma 6.3 and the commutativity between P_Δ and L we conclude

$$\begin{aligned}\|R(P_\Delta,z)f\|_{H^1} &\sim \|(\mathrm{Id}-L)^{1/2}R(P_\Delta,z)f\|_\mu \\ &\le \|R(P_\Delta,z)\|\|(\mathrm{Id}-L)^{1/2}f\|_\mu \\ &\sim \operatorname{dist}\bigl(z,\sigma(P_\Delta)\bigr)^{-1}\|f\|_{H^1}.\end{aligned}$$

Hence, $\|R(P_\Delta,z)\|_{H^1\to H^1} \lesssim \rho^{-1}$ holds uniformly over $z \in B(\kappa,\rho)$ and $(\sigma,b)\in\Theta_s$. $\square$

REMARK 4.7. The Kato–Temple inequality [Chatelin (1983), Theorem 6.21] on $L^2(\mu)$ even establishes the so-called superconvergence $|\kappa_1^J - \kappa_1| \lesssim 2^{-2Js}$.

4.4. *Variance estimates.* To bound the stochastic error on the finite-dimensional space V_J, we return to vector-matrix notation and look for a bound on the error involved in the estimators $\hat{\mathbf{G}}$ and $\hat{\mathbf{P}}_\Delta$. The Euclidean norm is denoted by $\|\cdot\|_{l^2}$.

LEMMA 4.8. *For any vector $\mathbf{v}\in\mathbb{R}^{|V_J|}$ we have, uniformly over Θ_s,*

$$\mathbb{E}_{\sigma,b}\bigl[\|(\hat{\mathbf{G}}-\mathbf{G})\mathbf{v}\|_{l^2}^2\bigr] \lesssim \|\mathbf{v}\|_{l^2}^2 N^{-1}2^J.$$

PROOF. We obtain, by (6.1) in Lemma 6.2,

$$\begin{aligned}&\mathbb{E}_{\sigma,b}\bigl[\|(\mathbf{G}-\hat{\mathbf{G}})\mathbf{v}\|_{l^2}^2\bigr] \\ &\quad= \sum_{|\lambda|\le J}\mathbb{E}_{\sigma,b}\Biggl[\frac{1}{N^2}\Biggl(\mathbb{E}_{\sigma,b}[\psi_\lambda(X_0)v(X_0)] - \frac{1}{2}\psi_\lambda(X_0)v(X_0) \\ &\qquad\qquad - \frac{1}{2}\psi_\lambda(X_{N\Delta})v(X_{N\Delta}) - \sum_{n=1}^{N-1}\psi_\lambda(X_{n\Delta})v(X_{n\Delta})\Biggr)^2\Biggr] \\ &\quad\lesssim \sum_{|\lambda|\le J} N^{-1}\mathbb{E}_{\sigma,b}\bigl[\bigl(\psi_\lambda(X_0)v(X_0)\bigr)^2\bigr] \\ &\quad\lesssim N^{-1}\Biggl\|\sum_{|\lambda|\le J}\psi_\lambda^2\Biggr\|_\infty \|v\|_{L^2}^2\|\mu\|_\infty \lesssim N^{-1}2^J\|\mathbf{v}\|_{l^2}^2,\end{aligned}$$

as asserted. $\square$

LEMMA 4.9. *For any vector $\mathbf{v}$ we have, uniformly over Θ_s,*

$$\mathbb{E}_{\sigma,b}\bigl[\|(\hat{\mathbf{P}}_\Delta-\mathbf{P}_\Delta)\mathbf{v}\|_{l^2}^2\bigr] \lesssim \|\mathbf{v}\|_{l^2}^2 N^{-1}2^J.$$

PROOF. We obtain, by (6.2) in Lemma 6.2,

$$\begin{aligned}
&\mathbb{E}_{\sigma,b}\big[\|(\hat{\mathbf{P}}_\Delta - \mathbf{P}_\Delta)v\|_{l^2}^2\big] \\
&\quad= \sum_{|\lambda|\le J} \mathbb{E}_{\sigma,b}\left[\left(\frac{1}{N}\sum_{n=1}^{N} \psi_\lambda\big(X_{(n-1)\Delta}\big)v(X_{n\Delta}) - \mathbb{E}_{\sigma,b}[\psi_\lambda(X_0)v(X_\Delta)]\right)^2\right] \\
&\quad\lesssim \sum_{|\lambda|\le J} N^{-1}\mathbb{E}_{\sigma,b}\big[\big(\psi_\lambda(X_0)v(X_1)\big)^2\big] \\
&\quad\le N^{-1}\sum_{|\lambda|\le J} \|\psi_\lambda\|_{L^2}^2\|v\|_{L^2}^2\|\mu p_\Delta\|_\infty \lesssim N^{-1}2^J\|\mathbf{v}\|_{l^2}^2,
\end{aligned}$$

as asserted. □

DEFINITION 4.10. We introduce the random set

$$\mathcal{R} = \mathcal{R}_{J,N} := \big\{\|\hat{\mathbf{G}} - \mathbf{G}\| \le \tfrac{1}{2}\|\mathbf{G}^{-1}\|^{-1}\big\}.$$

REMARK 4.11. Since $\mathbf{G}$ is invertible, so is $\hat{\mathbf{G}}$ on $\mathcal{R}$ with $\|\hat{\mathbf{G}}^{-1}\| \le 2\|\mathbf{G}^{-1}\|$ by the usual Neumann series argument.

LEMMA 4.12. *Uniformly over Θ_s we have $\mathbb{P}_{\sigma,b}(\Omega \setminus \mathcal{R}) \lesssim N^{-1}2^{2J}$.*

PROOF. By the classical Hilbert–Schmidt norm inequality,

$$\|\hat{\mathbf{G}} - \mathbf{G}\|_{l^2\to l^2}^2 \le \sum_{|\lambda|\le J} \|(\hat{\mathbf{G}} - \mathbf{G})\mathbf{e}_\lambda\|_{l^2\to l^2}^2$$

holds with unit vectors $(\mathbf{e}_\lambda)$. Then Lemma 4.8 gives uniformly

$$\mathbb{E}_{\sigma,b}\big[\|\hat{\mathbf{G}} - \mathbf{G}\|_{l^2\to l^2}^2\big] \lesssim N^{-1}2^{2J}.$$

Since the spaces $L^2([0,1])$ and $L^2(\mu)$ are isomorphic with uniform isomorphism constants, $\|\mathbf{G}^{-1}\| \sim 1$ holds uniformly over Θ_s and the assertion follows from Chebyshev's inequality. □

PROPOSITION 4.13. *For any $\varepsilon > 0$ we have, uniformly over Θ_s,*

$$\mathbb{P}_{\sigma,b}(\mathcal{R} \cap \{\|\hat{\mathbf{G}}^{-1}\hat{\mathbf{P}}_\Delta - \mathbf{G}^{-1}\mathbf{P}_\Delta\| \ge \varepsilon\}) \lesssim N^{-1}2^{2J}\varepsilon^{-2}.$$

PROOF. First, we separate the different error terms:

$$\begin{aligned}
\hat{\mathbf{G}}^{-1}\hat{\mathbf{P}}_\Delta - \mathbf{G}^{-1}\mathbf{P}_\Delta &= \hat{\mathbf{G}}^{-1}(\hat{\mathbf{P}}_\Delta - \mathbf{P}_\Delta) + (\hat{\mathbf{G}}^{-1} - \mathbf{G}^{-1})\mathbf{P}_\Delta \\
&= \hat{\mathbf{G}}^{-1}\big((\hat{\mathbf{P}}_\Delta - \mathbf{P}_\Delta) + (\mathbf{G} - \hat{\mathbf{G}})\mathbf{G}^{-1}\mathbf{P}_\Delta\big).
\end{aligned}$$

On the set $\mathcal{R}$ we obtain, by Remark 4.11,

$$\begin{aligned}\|\hat{\mathbf{G}}^{-1}\hat{\mathbf{P}}_\Delta - \mathbf{G}^{-1}\mathbf{P}_\Delta\| &\le \|\hat{\mathbf{G}^{-1}}\|(\|\hat{\mathbf{P}}_\Delta - \mathbf{P}_\Delta\| + \|\mathbf{G} - \hat{\mathbf{G}}\|\|\mathbf{G}^{-1}\|\|\mathbf{P}_\Delta\|)\\ &\le 2\|\mathbf{G}^{-1}\|(\|\hat{\mathbf{P}}_\Delta - \mathbf{P}_\Delta\| + \|\mathbf{G} - \hat{\mathbf{G}}\|\|\mathbf{G}^{-1}\|\|\mathbf{P}_\Delta\|)\\ &\lesssim \|\hat{\mathbf{P}}_\Delta - \mathbf{P}_\Delta\| + \|\mathbf{G} - \hat{\mathbf{G}}\|.\end{aligned}$$

By Lemmas 4.8 and 4.9 and the Hilbert–Schmidt norm estimate (cf. the proof of Lemma 4.12) we obtain the uniform norm bound over Θ_s,

$$\mathbb{E}_{\sigma,b}[\|\hat{\mathbf{G}}^{-1}\hat{\mathbf{P}}_\Delta - \mathbf{G}^{-1}\mathbf{P}_\Delta\|^2\mathbf{1}_{\mathcal{R}}] \lesssim N^{-1}2^{2J}.$$

It remains to apply Chebyshev's inequality. □

Having established the weak consistency of the estimators in matrix norm, we now bound the error on the eigenspace.

PROPOSITION 4.14. *Let $\mathbf{u}_1^J$ be the vector associated with the normalized eigenfunction u_1^J of $\pi_J^\mu P_\Delta$ with eigenvalue κ_1^J. Then uniformly over Θ_s the following risk bound holds*:

$$\mathbb{E}_{\sigma,b}\big[\|(\hat{\mathbf{G}}^{-1}\hat{\mathbf{P}}_\Delta - \mathbf{G}^{-1}\mathbf{P}_\Delta^J)\mathbf{u}_1^J\|_{l^2}^2\mathbf{1}_{\mathcal{R}}\big] \lesssim N^{-1}2^J.$$

PROOF. By the same separation of the error terms on $\mathcal{R}$ as in the preceding proof and by Lemmas 4.8 and 4.9 we find

$$\begin{aligned}&\mathbb{E}_{\sigma,b}\big[\|(\hat{\mathbf{G}}^{-1}\hat{\mathbf{P}}_\Delta - \mathbf{G}^{-1}\mathbf{P}_\Delta^J)\mathbf{u}_1^J\|_{l^2}^2\mathbf{1}_{\mathcal{R}}\big]\\ &\quad\le 8\|\mathbf{G}^{-1}\|^2\big(\mathbb{E}\big[\|(\hat{\mathbf{P}}_\Delta - \mathbf{P}_\Delta^J)\mathbf{u}_1^J\|_{l^2}^2\big] + \mathbb{E}\big[\|(\mathbf{G} - \hat{\mathbf{G}})\kappa_1^J\mathbf{u}_1^J\|_{l^2}^2\big]\big) \lesssim N^{-1}2^J.\end{aligned}$$

The uniformity over Θ_s follows from the respective statements in the lemmas. □

COROLLARY 4.15. *Let $\hat{\kappa}_1$ be the second largest eigenvalue of the matrix $\hat{\mathbf{G}}^{-1}\hat{\mathbf{P}}_\Delta$ with eigenvector $\hat{\mathbf{u}}_1$. If $\hat{\mathbf{G}}$ is not invertible or if $\|\hat{\mathbf{u}}_1\|_{l^2} \ge 2\sup_{\Theta_s}\|u_1\|_{L^2}$ holds, put $\hat{\mathbf{u}}_1 := \mathbf{0}$, $\hat{\kappa}_1 := 0$. If $N^{-1}2^{2J} \to 0$ holds, then uniformly over Θ_s the following bounds hold for $N, J \to \infty$*:

$$\mathbb{E}_{\sigma,b}\big[(|\hat{\kappa}_1 - \kappa_1^J|^2 + \|\hat{\mathbf{u}}_1 - \mathbf{u}_1^J\|_{l^2}^2)\mathbf{1}_{\mathcal{R}}\big] \lesssim N^{-1}2^J, \tag{4.2}$$

$$\mathbb{E}_{\sigma,b}\big[\|\hat{u}_1 - u_1^J\|_{H^1}^2\big] \lesssim N^{-1}2^{3J}. \tag{4.3}$$

PROOF. For the proof of (4.2) we apply Proposition 4.2 using the Euclidean Hilbert space $\mathbb{R}^{V_J}$ and Corollary 4.3. Then Proposition 4.14 in connection with Proposition 4.13 (using $\varepsilon < R/2$ and $N^{-1}2^{2J} \to 0$) yields the correct asymptotic rate on the event $\mathcal{R}$. For the uniform choice of ρ and R for $\mathbf{G}^{-1}\mathbf{P}_\Delta^J$ in

Proposition 4.2 just use the corresponding result for P_Δ and the convergence $\|\pi_J^\mu P_\Delta - P_\Delta\| \to 0$.

The precaution taken for undefined or too large $\hat{\mathbf{u}}_1$ is necessary for the event $\Omega \setminus \mathcal{R}$. Since the estimators $\hat{\kappa}_1$ and $\hat{\mathbf{u}}_1$ are now kept artificially bounded, the rate $\mathbb{P}_{\sigma,b}(\Omega \setminus \mathcal{R}) \lesssim N^{-1}2^{2J}$ established in Lemma 4.12 suffices to bound the risk on $\Omega \setminus \mathcal{R}$. Hence, the second estimate (4.3) is a consequence of (4.2) and the Bernstein inequality $\|\hat{u}_1 - u_1^J\|_{H^1} \lesssim 2^J \|\hat{u}_1 - u_1^J\|_{L^2}$. $\square$

REMARK 4.16. The main result of this section, namely (4.3), can be extended to pth moments for all $p \in (1, \infty)$:

$$\mathbb{E}_{\sigma,b}\big[\|\hat{u}_1 - u_1^J\|_{H^1}^p\big]^{1/p} \lesssim N^{-1/2}2^{3J/2}. \tag{4.4}$$

Indeed, tracing back the steps, it suffices to obtain bounds on the moments of order p in Lemmas 4.8 and 4.9, which on their part rely on the mixing statement in Lemma 6.2. By arguments based on the Riesz convexity theorem this last lemma generalizes to the corresponding bounds for pth moments, as derived in Section VII.4 of Rosenblatt (1971). For the sake of clarity we have restricted ourselves to the case $p = 2$ here.

4.5. *Upper bound for* $\sigma(\cdot)$. By Corollary 4.15 and our choice of J, $2^J \sim N^{1/(2s+3)}$,

$$\sup_{(\sigma,b)\in\Theta_s} \mathbb{E}_{\sigma,b}\big[|\hat{\kappa}_1 - \kappa_1^J|^2 + \|\hat{u}_1 - u_1^J\|_{H^1}^2\big] \lesssim N^{-1}2^{3J} \sim N^{-2s/(2s+3)}$$

holds. Using this estimate and the estimate for $\hat{\mu}$ in Proposition 4.1, the risk of the plug-in estimator $\hat{\sigma}^2(\cdot)$ in (3.12) is bounded as asserted in the theorem. We only have to ensure that the stochastic error does not increase from the plug-in and that the denominator is uniformly bounded away from zero. Using the Cauchy–Schwarz inequality and Remark 4.16 on the higher moments of our estimators, we encounter no problem in the first case. The second issue is dealt with by using the lower bound $c_{a,b} > 0$ in Proposition 6.5 so that an improvement of the estimate for the denominator by using

$$\widehat{\mu u}_1 := \max(\hat{\mu}\hat{u}_1, c_{a,b}) \tag{4.5}$$

instead of $\hat{\mu}\hat{u}_1$ guarantees the uniform lower bound away from zero.

4.6. *Upper bound for* $b(\cdot)$. Since $b(\cdot) = S'(\cdot)/\mu(\cdot)$ holds, it suffices to discuss how to estimate $S'(\cdot)$, which amounts to estimating the eigenfunction u_1 in H^2-norm; compare with (3.6). Substituting H^2 for H^1 in Proposition 4.5 and its proof, we obtain the bound

$$\|\pi_J^\mu P_\Delta - P_\Delta\|_{H^2 \to H^2} \lesssim 2^{-J(s-1)},$$

because $\|\mathrm{Id}-\pi_J\|_{H^{s+1}\to H^2}$ is of this order. As in Corollary 4.6 this is also the rate for the bias estimate. The only fine point is the uniform norm equivalence $\|f\|_{H^2}\sim\|(\mathrm{Id}-L)f\|_\mu$ for $f\in\mathrm{dom}(L)$, which follows by the methodology of perturbation and similarity arguments given in Section VI.4b of Engel and Nagel (2000). We omit further details.

The variance estimate is exactly the same. From (4.2) we infer, by Bernstein's inequality for H^2 and the estimate of $\mathbb{P}_{\sigma,b}(\Omega\setminus\mathcal{R})$,

$$\mathbb{E}_{\sigma,b}\big[\|\hat{u}_1-u_1^J\|_{H^2}^2\big]\lesssim N^{-1}2^{5J}.$$

Therefore balancing the bias and variance part of the risk by the choice $2^J\sim N^{1/(2s+3)}$—as before—yields the asserted rate of convergence $N^{-(s-1)/(2s+3)}$.

5. Proof of the lower bounds. First, the usual Bayes prior technique is applied for the reduction to a problem of bounding certain likelihood ratios. Then the problem is reduced to that of bounding the L^2-distance between the transition probabilities, which is finally accomplished using Hilbert–Schmidt norm estimates and the explicit form of the inverse of the generator.

5.1. *The least favorable prior.* The idea is to perturb the drift and diffusion coefficients of the reflected Brownian motion in such a way that the invariant measure remains unchanged. Let us assume that ψ is a compactly supported wavelet in H^s with one vanishing moment. Without loss of generality we suppose $C>1>c>0$ such that $(1,0)\in\Theta_s$ holds. We put $\psi_{jk}=2^{j/2}\psi(2^j\cdot-k)$ and denote by $K_j\subset\mathbb{Z}$ a maximal set of indices k such that $\mathrm{supp}(\psi_{jk})\subset[a,b]$ and $\mathrm{supp}(\psi_{jk})\cap\mathrm{supp}(\psi_{jk'})=\varnothing$ holds for all $k,k'\in K_j$, $k\neq k'$. Furthermore, we set $\gamma\sim 2^{-j(s+1/2)}$ such that, for all $\varepsilon=\varepsilon(j)\in\{-1,+1\}^{|K_j|}$,

$$\big(\sqrt{2S_\varepsilon},(S_\varepsilon)'\big)\in\Theta_s\qquad\text{with } S_\varepsilon(x):=S_\varepsilon(j,x):=\left(2+\gamma\sum_{k\in K_j}\varepsilon_k\psi_{jk}(x)\right)^{-1}.$$

We consider the corresponding diffusions with generator

$$L_{S_\varepsilon}f(x):=(S_\varepsilon f')'(x):=S_\varepsilon(x)f''(x)+S_\varepsilon'(x)f'(x),\qquad f\in\mathrm{dom}(L).$$

Hence, the invariant measure is the Lebesgue measure on $[0,1]$.

The usual Assouad cube techniques [e.g., see Korostelev and Tsybakov (1993)] give, for any estimator $\hat{\sigma}(\cdot)$ and for $N\in\mathbb{N}$, $\rho>0$, the lower bounds

$$\sup_{(\sigma,b)\in\Theta_s}\mathbb{E}_{\sigma,b}\big[\|\hat{\sigma}^2-\sigma^2\|_{L^2([a,b])}^2\big]\gtrsim 2^j\delta_{\sigma^2}^2e^{-\rho}p_0, \tag{5.1}$$

$$\sup_{(\sigma,b)\in\Theta_s}\mathbb{E}_{\sigma,b}\big[\|\hat{b}-b\|_{L^2([a,b])}^2\big]\gtrsim 2^j\delta_b^2e^{-\rho}p_0, \tag{5.2}$$

where, for all $\varepsilon, \varepsilon'$ with $\|\varepsilon - \varepsilon'\|_{l^1} = 2$ and with $\mathbb{P}_\varepsilon := \mathbb{P}_{\sqrt{2S_\varepsilon}, S'_\varepsilon}$,

$$\delta_{\sigma^2} \le \|2S_{\varepsilon'} - 2S_\varepsilon\|_{L^2}, \qquad \delta_b \le \|S'_{\varepsilon'} - S'_\varepsilon\|_{L^2}, \qquad p_0 \le \mathbb{P}_\varepsilon\left(\left.\frac{d\mathbb{P}_{\varepsilon'}}{d\mathbb{P}_\varepsilon}\right|_{\mathcal{F}_N} > e^{-\rho}\right).$$

We choose $\delta_{\sigma^2} \sim \gamma$ since, for $x \in \operatorname{supp}(\psi_{jk})$ with $\varepsilon_k = -\varepsilon'_k$,

$$S_{\varepsilon'}(x) - S_\varepsilon(x) = \pm 2\gamma\psi_{jk}(x)S_{\varepsilon'}(x)S_\varepsilon(x)$$

and $S_\varepsilon, S_{\varepsilon'} \to \frac{1}{2}$ holds uniformly so that the L^2-norm is indeed of order γ. Equivalently, we find $\delta_b \sim 2^j\gamma$. Due to $\gamma \sim 2^{-j(s+1/2)}$, the proof of the theorem is accomplished, once we have shown that a strictly positive p_0 can be chosen for fixed $\rho > 0$ and the asymptotics $2^j \sim N^{1/(2s+3)}$.

5.2. *Reduction to the convergence of transition densities.* If we denote the transition probability densities $\mathbb{P}_\varepsilon(X_\Delta \in dy | X_0 = x)$ by $p_\varepsilon(x, y)\,dy$ and the transition density of reflected Brownian motion by p_{BM}, then we infer, from Proposition 6.4,

$$\lim_{j\to\infty} \sup_{\varepsilon\in\{-1,+1\}^{K_j}} \|p_\varepsilon - p_{\mathrm{BM}}\|_\infty = 0$$

due to $\|S_\varepsilon - \frac{1}{2}\|_{C^1} \sim \gamma 2^{3j/2} \to 0$ for $s > 1$. We are now going to use the estimate $-\log(1+x) \le x^2 - x$, which is valid for all $x \ge -\frac{1}{2}$. For j so large that $\|1 - \frac{p_{\varepsilon'}}{p_\varepsilon}\|_\infty \le \frac{1}{2}$ holds, the Kullback–Leibler distance can be bounded from above (note that the invariant measure is Lebesgue measure):

$$\begin{aligned}
&\mathbb{E}_\varepsilon\left[-\log\left(\left.\frac{d\mathbb{P}_{\varepsilon'}}{d\mathbb{P}_\varepsilon}\right|_{\mathcal{F}_N}\right)\right] \\
&\quad= -\sum_{k=1}^N \mathbb{E}_\varepsilon\left[\log\left(\frac{p_{\varepsilon'}(X_{k-1}, X_k)}{p_\varepsilon(X_{k-1}, X_k)}\right)\right] \\
&\quad= -N\int_0^1\int_0^1 \log\left(\frac{p_{\varepsilon'}(x,y)}{p_\varepsilon(x,y)}\right)p_\varepsilon(x,y)\,dy\,dx \\
&\quad\le N\int_0^1\int_0^1 \frac{(p_{\varepsilon'}(x,y) - p_\varepsilon(x,y))^2}{p_\varepsilon(x,y)} - \big(p_{\varepsilon'}(x,y) - p_\varepsilon(x,y)\big)\,dy\,dx \\
&\quad= N\int_0^1\int_0^1 \frac{(p_{\varepsilon'}(x,y) - p_\varepsilon(x,y))^2}{p_\varepsilon(x,y)}\,dy\,dx \\
&\quad\le N\|p_\varepsilon^{-1}\|_\infty\|p_{\varepsilon'} - p_\varepsilon\|^2_{L^2([0,1]^2)}.
\end{aligned}$$

The square root of the Kullback–Leibler distance bounds the total variation distance in order, which by the Chebyshev inequality yields

$$\begin{aligned}\mathbb{P}_\varepsilon\left(\frac{d\mathbb{P}_{\varepsilon'}}{d\mathbb{P}_\varepsilon}\Big|_{\mathcal{F}_N} > e^{-\rho}\right) &= 1 - \mathbb{P}_\varepsilon\left(\frac{d\mathbb{P}_{\varepsilon'}}{d\mathbb{P}_\varepsilon}\Big|_{\mathcal{F}_N} - 1 \le e^{-\rho} - 1\right)\\ &\ge 1 - \mathbb{E}_\varepsilon\left[\left|\frac{d\mathbb{P}_{\varepsilon'}}{d\mathbb{P}_\varepsilon}\Big|_{\mathcal{F}_N} - 1\right|\right](1-e^{-\rho})^{-1}\\ &= 1 - (1-e^{-\rho})^{-1}\|(\mathbb{P}_{\varepsilon'} - \mathbb{P}_\varepsilon)|_{\mathcal{F}_N}\|_{\mathrm{TV}}\\ &\ge 1 - CN^{1/2}\|p_{\varepsilon'} - p_\varepsilon\|_{L^2([0,1]^2)},\end{aligned}$$

where $C > 0$ is some constant independent of γ, N, ε and j. Summarizing, we need the estimate

$$\limsup_{N,j\to\infty} N^{1/2}\|p_{\varepsilon'} - p_\varepsilon\|_{L^2([0,1]^2)} < C^{-1} \qquad \text{for } 2^j \sim N^{1/(2s+3)}. \tag{5.3}$$

5.3. *Convergence of the transition densities.* Observe first that $\|p_{\varepsilon'} - p_\varepsilon\|_{L^2([0,1]^2)}$ is exactly the Hilbert–Schmidt norm distance $\|P_\Delta^{\varepsilon'} - P_\Delta^\varepsilon\|_{\mathrm{HS}}$ between the transition operators derived from $L_{S_{\varepsilon'}}$ and L_{S_ε} acting on the Hilbert space $L^2([0,1])$. If we introduce

$$V := \left\{f \in L^2([0,1]) \Big| \int f = 0\right\} \quad \text{and} \quad V^\perp := \{f \in L^2([0,1]) | f \text{ constant}\},$$

then the transition operators coincide on $V^\perp$ and leave the space V invariant so that $\|P_\Delta^{\varepsilon'} - P_\Delta^\varepsilon\|_{\mathrm{HS}} = \|(P_\Delta^{\varepsilon'} - P_\Delta^\varepsilon)|_V\|_{\mathrm{HS}}$.

We take advantage of the key result that for Lipschitz functions f with Lipschitz constant Λ on the union of the spectra of two self-adjoint bounded operators T_1 and T_2 the continuous functional calculus satisfies

$$\|f(T_1) - f(T_2)\|_{\mathrm{HS}} \le \Lambda\|T_1 - T_2\|_{\mathrm{HS}}; \tag{5.4}$$

see Kittaneh (1985). We proceed by bounding the Hilbert–Schmidt norm of the difference of the inverses of the generators and by then transferring this bound to the transition operators via (5.4). By the functional calculus for operators on V, the function $f(z) = \exp(\Delta(z^{-1}))$ sends $(L_\varepsilon|_V)^{-1}$ to $P_\Delta^\varepsilon|_V$. Moreover, f is uniformly Lipschitz continuous on $(-\infty, 0)$ due to $\Lambda := \sup_{z<0}|f'(z)| = 4\Delta^{-1}e^{-2} < \infty$. Thus, we arrive at

$$\|p_{\varepsilon'} - p_\varepsilon\|_{L^2([0,1]^2)} = \big\|\big(P_\Delta^{\varepsilon'} - P_\Delta^\varepsilon\big)|_V\big\|_{\mathrm{HS}} \le \Lambda\|(L_{\varepsilon'}|_V)^{-1} - (L_\varepsilon|_V)^{-1}\|_{\mathrm{HS}}.$$

The inverse of the generator L_ε on V has for $g \in V$ the explicit form

$$(L_\varepsilon|_V)^{-1}g(x) = \int_0^1 \left(\int_y^1 S_\varepsilon^{-1}(v)\big(v - \mathbf{1}_{[x,1]}(v)\big)\,dv\right)g(y)\,dy. \tag{5.5}$$

Using $|S_{\varepsilon'}^{-1} - S_{\varepsilon}^{-1}| = 2\gamma\psi_{jk}$ for some $k \in K_j$ and denoting by Ψ the primitive of ψ with compact support, we obtain

$$\begin{aligned}
&\|(L_{\varepsilon'}|_V)^{-1} - (L_{\varepsilon}|_V)^{-1}\|_{\mathrm{HS}}^2 \\
&\quad = \int_0^1 \int_0^1 \left(\int_y^1 2\gamma\psi_{jk}(v)\big(v - \mathbf{1}_{[x,1]}(v)\big)\,dv \right)^2 dx\,dy \\
&\quad = 4\gamma^2 2^{-j} \int_0^1 \int_0^1 \Big(-\Psi(2^j y - k)\,y \\
&\qquad\qquad - \int_y^1 \Psi(2^j v - k)\,dv + \Psi\big(2^j(x \vee y) - k\big) \Big)^2 dx\,dy \\
&\quad \lesssim \gamma^2 2^{-j} \|\Psi(2^j \cdot)\|_{L^2}^2 \sim \gamma^2 2^{-2j}.
\end{aligned}$$

Consequently, $\|p_{\varepsilon'} - p_{\varepsilon}\|_{L^2}^2 \sim 2^{-j(2s+3)}$ holds with an arbitrarily small constant if $\gamma 2^{j(s+1/2)}$ is chosen sufficiently small. Hence, the estimate (5.3) is valid for this choice and the asymptotics $N 2^{-j(2s+3)} \to 1$, which remained to be proved.

6. Technical results. We shall need several technical results, mainly to describe the dependence of certain quantities on the underlying diffusion parameters. The following result is in close analogy with Section IV.5 in Bass (1998).

LEMMA 6.1. *The second largest eigenvalue ν_1 of the infinitesimal generator $L_{\sigma,b}$ can be bounded away from zero*:

$$\nu_1 \le -\inf_{x\in[0,1]} S(x) =: -s_0.$$

This eigenvalue is simple and the corresponding eigenfunction f_1 is monotone.

PROOF. The variational characterization of ν_1 [Davies (1995), Section 4.5] and partial integration yield

$$\nu_1 = \sup_{\substack{\|f\|_\mu = 1 \\ \langle f, \mathbf{1}\rangle_\mu = 0}} \langle Lf, f\rangle_\mu = -\inf_{\substack{\|f\|_\mu = 1 \\ \langle f, \mathbf{1}\rangle_\mu = 0}} \int_0^1 S(x) f'(x)^2\,dx.$$

Given the derivative f', the function $f \in \mathrm{dom}(L)$ with $\langle f, \mathbf{1}\rangle_\mu = 0$ is uniquely determined. Setting $M(x) := \mu([0,x])$, this function f satisfies

$$0 = \int_0^1 \left(f(0) + \int_0^x f'(y)\,dy \right) \mu(x)\,dx = f(0) + \int_0^1 f'(y)\big(1 - M(y)\big)\,dy.$$

For $f, g \in L^2(\mu)$ with $\langle f, \mathbf{1}\rangle_\mu = \langle g, \mathbf{1}\rangle_\mu = 0$ we find

$$\begin{aligned}
\langle f, g\rangle_\mu &= \int_0^1 \Big(f(0) + \int_0^x f'(y)\,dy\Big)\Big(g(0) + \int_0^x g'(z)\,dz\Big)\mu(x)\,dx \\
&= f(0)g(0) - f(0)\int_0^1 g'(z)\big(1 - M(z)\big)\,dz \\
&\quad - g(0)\int_0^1 f'(y)\big(1 - M(y)\big)\,dy \\
&\quad + \int_0^1\int_0^1 f'(y)g'(z)\big(1 - M(y \vee z)\big)\,dy\,dz \\
&= \int_0^1\int_0^1 \big(M(y \wedge z) - M(y)M(z)\big)f'(y)g'(z)\,dy\,dz \\
&=: \int_0^1\int_0^1 m(y, z)f'(y)g'(z)\,dy\,dz.
\end{aligned}$$

The kernel $m(y, z)$ is positive on $(0, 1)^2$ and bounded by 1, whence we obtain, by regarding $u = f'$,

$$-\nu_1 = \inf_u \frac{\int_0^1 S(x)u(x)^2\,dx}{\int_0^1\int_0^1 m(y, z)u(y)u(z)\,dy\,dz} \geq \frac{s_0\|u\|_{L^2}^2}{\|u\|_{L^1}^2} \geq s_0.$$

If the derivative of an eigenfunction f_1 changed sign, we could write $f_1' = u^+ - u^-$ with two nonnegative functions u^+, u^- that are nontrivial. However, this would entail that the antiderivative f_0 of $f_0' := u^+ + u^-$ satisfies $\langle Lf_0, f_0\rangle_\mu = \langle Lf_1, f_1\rangle_\mu$, while $\|f_0\|_\mu$ would be strictly greater than $\|f_1\|_\mu$ due to the positivity of $m(u, v)$. This contradicts the variational characterization of ν_1 so that all eigenfunctions corresponding to ν_1 are monotone. Consequently, for any two eigenfunctions f_1 and g_1 the integrand in

$$\langle f_1, g_1\rangle_\mu = \int_0^1\int_0^1 m(y, z)f_1'(y)g_1'(z)\,dy\,dz$$

does not change sign and the whole integral does not vanish. We infer that the eigenspace of ν_1 cannot contain two orthogonal functions and is thus one-dimensional. □

LEMMA 6.2. *For H_1, $H_2 \in L^2([0, 1])$ we have the following two uniform variance estimates over Θ_s:*

$$\mathrm{Var}_{\sigma,b}\left[\frac{1}{N}\sum_{n=1}^N H_1(X_{n\Delta})\right] \lesssim N^{-1}\mathbb{E}_{\sigma,b}[H_1(X_0)^2], \tag{6.1}$$

$$\mathrm{Var}_{\sigma,b}\left[\frac{1}{N}\sum_{n=1}^N H_1\big(X_{(n-1)\Delta}\big)H_2(X_{n\Delta})\right] \lesssim N^{-1}\mathbb{E}_{\sigma,b}[H_1(X_0)^2 H_2(X_1)^2]. \tag{6.2}$$

PROOF. Due to the uniform spectral gap s_0 over Θ_s (Proposition 6.1), P_Δ satisfies $\|P_\Delta f\|_\mu \le \gamma \|f\|_\mu$ with $\gamma := e^{-|s_0|\Delta} < 1$ for all $f \in L^2(\mu)$ with $\langle f, \mathbf{1}\rangle_\mu = 0$.

We obtain the first estimate by considering the centered random variables $f_1(X_{k\Delta}) := H_1(X_{k\Delta}) - \mathbb{E}_{\sigma,b}[H_1(X_{k\Delta})]$, $k \in \mathbb{N}$:

$$\operatorname{Var}_{\sigma,b}\left[\sum_{n=1}^N H_1(X_{n\Delta})\right] = \sum_{m,n=1}^N \mathbb{E}_{\sigma,b}[f_1(X_{m\Delta}) f_1(X_{n\Delta})] = \sum_{m,n=1}^N \langle f_1, P_\Delta^{|m-n|} f_1\rangle_\mu$$
$$\le \sum_{m,n=1}^N \gamma^{|m-n|} \|f_1\|_\mu^2 \lesssim N \mathbb{E}_{\sigma,b}[H_1(X_0)^2].$$

The second estimate follows along the same lines. Merely observe that for $m > n$, by the projection property of conditional expectations

$$\mathbb{E}_{\sigma,b}\big[H_1\big(X_{(n-1)\Delta}\big) H_2(X_{n\Delta}) H_1\big(X_{(m-1)\Delta}\big) H_2(X_{m\Delta})\big]$$
$$= \big\langle H_1 \cdot (P_\Delta H_2),\, P_\Delta^{m-n-1}\big(H_1 \cdot (P_\Delta H_2)\big)\big\rangle_\mu$$

holds, where "$\cdot$" is the usual multiplication operator. □

LEMMA 6.3. *Uniformly over Θ_s the following norm equivalence holds*:

$$\|f\|_{H^1} \sim \|(\mathrm{Id} - L)^{1/2} f\|_\mu \qquad \textit{for all } f \in H^1.$$

PROOF. The invariant measure μ and the function S are uniformly bounded away from zero and infinity so that we obtain, with uniform constants for $f \in \operatorname{dom}(L)$,

$$\|f\|_{H^1}^2 = \langle f, f\rangle + \langle f', f'\rangle \sim \langle f, f\rangle_\mu + \langle Sf', f'\rangle$$
$$= \langle (\mathrm{Id} - L) f, f\rangle_\mu = \|(\mathrm{Id} - L)^{1/2} f\|_\mu^2.$$

By an approximation argument this extends to all $f \in H^1 = \operatorname{dom}(L^{1/2})$. □

PROPOSITION 6.4. *Suppose* $((\sigma_n(\cdot), b_n(\cdot)) \in \Theta_s$, $n \ge 0$, *and*

$$\lim_{n\to\infty} \|\sigma_n - \sigma_0\|_\infty = 0, \qquad \lim_{n\to\infty} \|b_n - b_0\|_\infty = 0.$$

Then the corresponding transition probabilities $(p_t^{(n)})$ *converge uniformly*:

$$\lim_{n\to\infty} \big\| p_t^{(n)}(\cdot,\cdot) - p_t^{(0)}(\cdot,\cdot)\big\|_\infty = 0.$$

PROOF. An application of the results by Stroock and Varadhan (1971) yields that the corresponding diffusion processes $X^{(n)}$ converge weakly to $X^{(0)}$ for any

fixed initial value $X^{(n)}(0) = x$. This implies in particular

$$\lim_{n\to\infty} \int_0^1 p_t^{(n)}(x, y)\varphi(y)\,dy = \int_0^1 p_t^{(0)}(x, y)\varphi(y)\,dy$$

for all test functions $\varphi \in L^\infty([0, 1])$ and all $x \in [0, 1]$.

On the other hand, the functions $(p_t^{(n)})_n$ form a relatively compact subset of $\mathcal{C}([0, 1]^2)$ by Proposition 6.7 and Sobolev embeddings. Any point of accumulation of $(p_t^{(n)})_n$ in $\mathcal{C}([0, 1]^2)$ must equal $p_t^{(0)}$, which follows from testing with suitable functions $\varphi \in L^\infty([0, 1])$. Consequently, $(p_t^{(n)})_n$ is a relatively compact sequence with only one point of accumulation and thus converges. □

PROPOSITION 6.5. *For the class Θ_s there is a constant $\rho > 0$ such that for all parameters $(\sigma(\cdot), b(\cdot))$ the eigenvalue $\kappa_1 = \kappa_1(\sigma, b)$ of P_Δ is uniformly separated*: $\sigma(P_\Delta) \cap B(\kappa_1, 2\rho) = \{\kappa_1\}$.

Furthermore, for all $0 < a < b < 1$ there is a uniform constant $c_{a,b} > 0$ such that the associated first eigenfunction $u_1 = u_1(\sigma, b)$ satisfies, for all $(\sigma, b) \in \Theta_s$,

$$\min_{x\in[a,b]} |u_1'(x)| \geq c_{a,b}.$$

PROOF. Proceeding indirectly, assume that there is a sequence $(\sigma_n, b_n) \in \Theta_s$ such that the corresponding eigenvalues satisfy $\kappa_1^{(n)} \to 1$ (or $\kappa_1^{(n)} - \kappa_2^{(n)} \to 0$, resp.). By the compactness of the Sobolev embedding of H^s into C^0 we can pass to a uniformly converging subsequence. Hence, Proposition 6.4 yields that the corresponding transition densities converge uniformly, which implies that the transition operators $P_\Delta^{(n)}$ converge in operator norm on $L^2([0, 1])$. By Proposition 5.6 and Theorem 5.20 in Chatelin (1983), this entails the convergence of their eigenvalues with preservation of the multiplicities. Since the limiting operator is again associated with an elliptic reflected diffusion, the fact that the eigenvalue $\kappa_1 = e^{\Delta\nu_1}$ is always simple (Lemma 6.1) gives the contradiction.

By the same indirect arguments, we construct transition operators $P_\Delta^{(n)}$ on the space $\mathcal{C}([0, 1])$ and infer that the eigenfunctions $u_1^{(n)}$ [Chatelin (1983), Theorem 5.10], the invariant measures $\mu^{(n)}$ [see (3.1)] and the inverses of the functions $S^{(n)}$ [see (3.2)] converge in supremum norm. Therefore $(u_1^{(n)})' = \nu_1^{(n)}(S^{(n)})^{-1} \int u_1^{(n)}\mu^{(n)}$ also converges in supremum norm. Due to $u_1'|_{[a,b]} \neq 0$ (Lemma 6.1) this implies that $(u_1^{(n)})'$ cannot converge to zero on $[a, b]$. □

LEMMA 6.6. *The $L^2(\mu)$-normalized eigenfunction u_k of the generator L corresponding to the $(k + 1)$st largest eigenvalue ν_k satisfies*

$$\|u_k\|_{H^{s+1}} \leq C(s, s_0, \|S^{-1}\|_s, \|\mu\|_{s-1})|\nu_k|^{\lceil s\rceil},$$

where C is a continuous function of its arguments.

PROOF. We know that $\mu^{-1}(Su_k')' = \nu_k u_k$ and $u_k'(0) = 0$ holds, which imply

$$u_k'(x) = \nu_k S^{-1}(x) \int_0^x u_k(u)\mu(u)\,du.$$

Suppose $u_k \in H^{r+1}$ with $r \in [0, s]$. Then the function $u_k\mu$ is in $H^{r\wedge(s-1)}$ due to $u_k \in C^r$ (Sobolev embeddings). Hence, the antiderivative is in $H^{(r+1)\wedge s}$. As $S^{-1} \in H^s$ holds, the right-hand side is an element of $H^{s\wedge(r+1)}$. We conclude that the regularity r of u_k is larger by 1, which implies that u_k is in H^{s+1}.

In quantitative terms we obtain for $r \in [1, s]$, where we use the seminorm $|f|_s := \|f^{(s)}\|_{L^2}$,

$$\begin{aligned}
|u_k'|_r &\le |\nu_k| C(r)\left(|S^{-1}|_r \left\| \int_0^{\cdot} u_k\mu \right\|_\infty + \|S^{-1}\|_\infty \left| \int_0^{\cdot} u_k\mu \right|_r \right) \\
&\le |\nu_k| C(r) \|S^{-1}\|_r \left(\|u_k\|_{L^1(\mu)} + |u_k\mu|_{r-1} \right) \\
&\le |\nu_k| C(r) \|S^{-1}\|_s (1 + |u_k|_{r-1}\|\mu\|_\infty + \|u_k\|_\infty \|\mu\|_{r-1}) \\
&\le |\nu_k| C(r) \|S^{-1}\|_s (1 + 2\|u_k\|_{r-1}\|\mu\|_{s-1}).
\end{aligned}$$

By applying this estimate $\|u_k\|_{r+1} \lesssim |\nu_k| \|S^{-1}\|_s (1 + \|u_k\|_{r-1}\|\mu\|_{s-1})$ successively for $r = 1, 2, \ldots, \lfloor s \rfloor$ and finally, for $r = s - 1$, the estimate follows. □

PROPOSITION 6.7. *For $(\sigma, b) \in \Theta_s$ the corresponding transition probability density $p_\Delta = p_{\Delta,\sigma,b}$ satisfies*

$$\sup_{(\sigma,b)\in\Theta_s} \|p_\Delta\|_{H^{s+1}\times H^s} < \infty.$$

PROOF. The spectral decomposition of $P_\Delta : L^2(\mu) \to L^2(\mu)$ yields

$$p_\Delta(x, y) = \mu(y) \sum_{k=0}^{\infty} e^{\nu_k \Delta} u_k(x) u_k(y), \qquad x, y \in [0, 1].$$

Due to the uniform ellipticity and uniform boundedness of the coefficients, we have $\nu_k \in [-C_1 k^2, -C_2 k^2]$ with uniform constants $C_1, C_2 > 0$ on Θ_s [see Davies (1995), adapting Example 4.6.1, page 93, to our situation]. From the preceding Lemma 6.6 and the Sobolev embedding $H^{s+1} \subset C^s$ we infer

$$\begin{aligned}
\|p_\Delta\|_{H^{s+1}\times H^s} &\le \sum_{k=0}^{\infty} e^{-C_2\Delta k^2} \|u_k\|_{s+1} \|\mu u_k\|_s \\
&\le \sum_{k=0}^{\infty} C(s, s_0, \|S^{-1}\|_s, \|\mu\|_{s-1})^2 e^{-C_2\Delta k^2} (C_1 k^2)^{s+1} \|\mu\|_s,
\end{aligned}$$

which gives the desired uniform estimate. □

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