

STATISTICAL GUARANTEES FOR BAYESIAN UNCERTAINTY QUANTIFICATION IN NONLINEAR INVERSE PROBLEMS WITH GAUSSIAN PROCESS PRIORS

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Bayesian inference and uncertainty quantification in a general class of nonlinear inverse regression models is considered. Analytic conditions on the regression model $\{\mathcal{G}(\theta) : \theta \in \Theta\}$ and on Gaussian process priors for θ are provided such that semiparametrically efficient inference is possible for a large class of linear functionals of θ . A general Bernstein–von Mises theorem is proved that shows that the (non-Gaussian) posterior distributions are approximated by certain Gaussian measures centred at the posterior mean. As a consequence, posterior-based credible sets are valid and optimal from a frequentist point of view. The theory is illustrated with two applications with PDEs that arise in nonlinear tomography problems: an elliptic inverse problem for a Schrödinger equation, and inversion of non-Abelian X -ray transforms. New analytical techniques are deployed to show that the relevant Fisher information operators are invertible between suitable function spaces.

1. Introduction. We are concerned here with a general class of nonlinear inverse regression problems that arise with partial differential equations (PDEs). They involve a functional parameter θ one wishes to make inference on, a nonlinear ‘forward map’ $\theta \mapsto \mathcal{G}(\theta)$ describing a set of regression functions $\{\mathcal{G}(\theta) : \theta \in \Theta\}$ defined on some domain $\mathcal{X}$, and statistical measurements

$$(1) \quad Y_i = \mathcal{G}(\theta)(X_i) + \sigma \varepsilon_i, \quad i = 1, \dots, N.$$

Here, the $(X_i)_{i=1}^N$ represent a finite ‘uniform’ discretisation of $\mathcal{X}$ and the ε_i are independent standard Gaussian variables scaled by a fixed noise level $\sigma > 0$.

The aim is to construct a statistically and computationally efficient algorithm that recovers θ from such data $(Y_i, X_i)_{i=1}^N$. In applications, often more is required and one is further interested in *data-driven performance guarantees for the output of the algorithm*. This task forms part of the evolving scientific paradigm of ‘uncertainty quantification’ [18]. In statistical terminology, one is concerned with the *construction of a confidence set* for aspects of the possibly infinite-dimensional parameter θ . In common language, this just expresses the desire to find valid ‘error bars’ for the output of the algorithm one has used.

Various methods aiming to ‘quantify inferential uncertainty’ for inverse problems involving PDEs are now available, particularly based on Bayesian posterior distributions arising from Gaussian process (and other) priors for θ , as advocated in influential work by A. Stuart [15, 58]. While these measures of uncertainty can be computed by MCMC methods (see [5, 12, 13, 31, 32, 54] and below), few statistical guarantees are available for the validity of such posterior inferences in typical PDE settings where $\mathcal{G}$ is nonlinear and θ is modelled as a Gaussian process. The present paper attempts to shed some light on this issue.

Received July 2020; revised April 2021.

MSC2020 subject classifications. 62F15, 65N21.

Key words and phrases. X -ray transforms, Schrödinger equation, credible sets, Bernstein–von Mises theorems.

The general results we obtain will be shown to apply to two prototypical ‘model problems’, which are concerned with nonlinear maps $f \mapsto u_f$ arising with solutions $u = u_f$ of a differential equation of the form

$$(2) \qquad \mathcal{D}u - fu = 0 \quad \text{on } M,$$

where $\mathcal{D}$ is a *given* differential operator and f an unknown potential defined on some domain M in $\mathbb{R}^d$. The aim is to recover f from certain measurements of u_f .

In our first example, one takes for $\mathcal{D}$ an elliptic second order differential operator, in fact, to simplify the exposition we only consider $\mathcal{D} = \Delta$ equal to the standard Laplacian. One then parameterises f via a link function mapping a linear space Θ (to which Gaussian process priors can be assigned) into positive potentials $f = f_\theta > 0$, and collects noisy measurements (1) with $\mathcal{X} = M$ of the solution $\mathcal{G}(\theta) = u_{f_\theta}$ of the corresponding (time-independent) *Schrödinger equation* (2) with prescribed boundary values. Various nonlinear inverse problems are of this form or can be reduced to one involving a Schrödinger-type equation [33]. To reduce the mathematical complexity of this first example, we assume that measurements *throughout all of* M are available, as is relevant, for example, in *photo-acoustic tomography* [3, 4].

In our second example, we consider a more challenging problem where only boundary measurements (‘scattering data’) of the solution u of (2) are given. Here, the differential operator $\mathcal{D}$ arises from the *geodesic vector field* on the 2-dimensional unit disk M and one observes *non-Abelian X-ray transforms* corresponding to the ‘influx’ boundary values at $\mathcal{X} = \partial_+ SM$ of matrix-valued solutions u_θ of (2) with $f = \theta$ a skew-symmetric matrix field. This nonlinear geometric inverse problem appears in physical imaging problems such as *neutron spin tomography*; see [28, 55] and has been studied in [17, 40, 47, 49]. Mathematically, the setting is fundamentally different from the Schrödinger case as the underlying PDE methods are not elliptic but of transport type. An important contribution of this article is to solve the analytical problem of inverting the Fisher information operator arising in this setting (see below for more details).

We will give rigorous frequentist ($N \rightarrow \infty$) guarantees for Bayesian uncertainty quantification methodology arising from sufficiently smooth Gaussian process priors for θ in such inverse problems. Specifically, conditions will be provided under which optimal asymptotic semiparametric inference is possible for linear functionals $\langle \theta, \psi \rangle$ for smooth $\psi \in C^\infty$, from data in (1), and we verify these conditions for the preceding examples with the Schrödinger equation and non-Abelian X-ray transforms. As a consequence, Bayesian credible sets for such parameters are shown to be valid frequentist confidence sets, providing objective large sample guarantees for uncertainty quantification. We numerically validate these theoretical findings for reasonable sample sizes ($N = 600, 1000$) in Section 2.6.

The idea behind our results is based on obtaining asymptotically exact Bernstein–von Mises type Gaussian approximations for the local fluctuations of the *non-Gaussian* posterior measure near θ_0 . In traditional regular statistical models, such approximations have a long history going back to Laplace [36], von Mises [63], Le Cam [37] and van der Vaart [61]. In more complex settings with infinite-dimensional parameter spaces and inverse problems, such results are more recent and the present article contributes to the programme developed in [6–10, 22, 39, 41–43, 52].

Next to some standard regularity assumptions on $\mathcal{G}$, our results involve *two key hypotheses*, which are specific to a given inverse problem. The first condition we require is that posterior inference is *globally consistent*, that is, that the posterior measure concentrates on a shrinking $\|\cdot\|_\infty$ neighbourhood of the ground truth θ_0 generating the data. Proving such results typically requires ‘global’ stability estimates for the inverse problem and the techniques involved are thus quite different from the ‘local’ techniques of the present paper. Consistency results of

this kind were recently obtained in relevant PDE settings in [1, 23, 40] building on ideas from Bayesian nonparametric statistics [62]. As we are dealing with difficult nonlinear ill-posed inverse problems, the contraction rates obtained in our concrete model examples are comparably slow in ‘low regularity settings’. Thus, in order to control the discretisation error and semiparametric ‘bias’ terms in our proofs, we will have to assume that the prior Gaussian process model employed is sufficiently regular (in a Sobolev sense).

The second key condition concerns the inverse of the so-called (‘Fisher’-) information operator of the inverse problem. If we denote by $\mathbb{I}_{\theta_0}$ the linear operator obtained from linearising the nonlinear map $\mathcal{G}$ near the ground truth parameter θ_0 (one may think of it as a derivative $(\partial\mathcal{G}/\partial\theta)|_{\theta=\theta_0}$ in a suitable sense), then general statistical theory (reviewed in Section 3.3 below) suggests that a canonical asymptotic approximation to the posterior measure for θ should arise from a Gaussian measure with covariance operator $\mathbb{I}_{\theta_0}(\mathbb{I}_{\theta_0}^*\mathbb{I}_{\theta_0})^{-1}$ where $\mathbb{I}_{\theta_0}^*$ is an appropriate adjoint of $\mathbb{I}_{\theta_0}$. Moreover, this operator provides a benchmark for the optimum any uncertainty quantification algorithm can achieve. What precedes can be made rigorous, however, only if the *information (or normal) operator* $\mathbb{I}_{\theta_0}^*\mathbb{I}_{\theta_0}$ is surjective onto a large enough range, and if the mapping properties of its inverse allow for the composition of $\mathbb{I}_{\theta_0}$ with $(\mathbb{I}_{\theta_0}^*\mathbb{I}_{\theta_0})^{-1}$. In the settings above, this is not at all clear a priori and, in fact, generates new PDE questions in its own right. For the Schrödinger equation problem, it was shown in [41] using elliptic theory that $\mathbb{I}_{\theta_0}^*\mathbb{I}_{\theta_0}$ indeed is invertible (in fact, its inverse equals a certain type of iterated Schrödinger operator). We extend here the results in [41] to allow for Gaussian priors and a more general discrete measurement setting (under suitable hypotheses). For the non-Abelian X-ray case, inversion of $\mathbb{I}_{\theta_0}^*\mathbb{I}_{\theta_0}$ is a more delicate problem that we successfully solve in this paper using recent techniques from [38]. We refer to Remark 2.3 for some context and perspectives on this result. At this point, it suffices to point out that the statistical questions explored here and in [39, 40] are drivers of new developments in geometric inverse problems.

This paper is organised as follows: The main results for the PDE models arising from (2) are given in Section 2, whereas the general theory for Bayesian inference in nonlinear random design regression models is developed in Section 3. All proofs are given in subsequent sections, and the results on the information geometry of non-Abelian X-ray transforms are presented in Section 6.1. Throughout, for $\mathcal{X}$ a suitable open subset of Euclidean space, we use standard notation for Hölder spaces $C^\beta(\mathcal{X})$ of $[\beta]$ -times ($[\cdot]$ denotes integer part) continuously differentiable functions whose partial derivatives of order $[\beta]$ satisfy a $\beta - [\beta]$ -Hölder continuity condition on $\mathcal{X}$, where $C^0(\mathcal{X}) = C(\mathcal{X})$ denotes the bounded continuous functions. Define Sobolev spaces $H^\alpha(\mathcal{X})$ of functions with $L^2(dx)$ -derivatives up to order α , defined for $\alpha \notin \mathbb{N}$ by interpolation. Finally, for V a normed vector space, $C^\infty(\mathcal{X}, V)$ denotes all smooth V -valued functions defined on $\mathcal{X}$, and $C_c^\infty(\mathcal{X}, V)$ denotes the subspace of $C^\infty(\mathcal{X}, V)$ consisting of functions that are compactly supported in the interior of $\mathcal{X}$. In Section 6.1 these definitions will also be used when $\mathcal{X} = M$ is a Riemannian manifold M with boundary.

2. Main results for PDE models.

2.1. General observation setting, prior and posterior. Let $(\mathcal{X}, \mathcal{A})$ and $(\mathcal{Z}, \mathcal{B})$ be measurable spaces equipped with measures λ, ζ , respectively. We assume that λ is a probability measure and that ζ a finite measure. Let further V, W be finite-dimensional vector spaces of fixed finite dimensions $p_V, p_W \in \mathbb{N}$, with inner products $\langle \cdot, \cdot \rangle_W, \langle \cdot, \cdot \rangle_V$, respectively. Let

$$L^\infty(\mathcal{X}), L^2(\mathcal{X}) = L_\lambda^2(\mathcal{X}, V) \quad \text{and} \quad L^\infty(\mathcal{Z}), L^2(\mathcal{Z}) = L_\zeta^2(\mathcal{Z}, W)$$

denote the bounded measurable, and λ - or ζ -square integrable, V or W -valued functions defined on $\mathcal{X}, \mathcal{Z}$, respectively. Denote by $\|\cdot\|_{L_\zeta^2(\mathcal{Z})}, \|\cdot\|_{L_\lambda^2(\mathcal{X})}$ the usual L^2 -norms on these

spaces, and by $\langle \cdot, \cdot \rangle_{L^2(\mathcal{Z})}$, $\langle \cdot, \cdot \rangle_{L^2(\mathcal{X})}$ the corresponding Hilbert space inner products; and write $\| \cdot \|_\infty$ for the supremum norm.

We will consider parameter spaces Θ that are (Borel-measurable) *linear* subspaces of $L^\infty(\mathcal{Z}, W)$, on which measurable ‘forward maps’

$$(3) \qquad \theta \mapsto \mathcal{G}(\theta), \qquad \mathcal{G} : \Theta \rightarrow L^2_\lambda(\mathcal{X}, V),$$

are defined. Observations then arise in a general random design regression setup where one is given jointly i.i.d. random variables $(Y_i, X_i)_{i=1}^N$ of the form

$$(4) \qquad Y_i = \mathcal{G}(\theta)(X_i) + \varepsilon_i, \qquad \varepsilon_i \stackrel{\text{i.i.d.}}{\sim} N(0, \sigma^2 I_V), \quad \sigma > 0, i = 1, \dots, N,$$

where the X_i ’s are random i.i.d. covariates drawn from law λ on $\mathcal{X}$. We assume that the covariance I_V of each noise vector $\varepsilon_i \in V$ is diagonal for the inner product of V . Correlated Gaussian noise can be accommodated simply by adjusting the choice of inner product on V . Conditions on the ‘experiments’ underlying our regression model enter our results only through the probability measure λ generating the X_i ’s. In common cases where λ represents a uniform distribution on some bounded domain in Euclidean space, a deterministic design regression model with ‘equally spaced’ design $X_i = x_i$ can be seen to be statistically equivalent to (4), see [53], and our analysis thus also informs such measurement setups. We opt to present the theory here in a *random* design model as it allows for a unified probabilistic treatment of the numerical discretisation error in the proofs.

If the natural domain on which $\mathcal{G}$ is defined is not a linear space, one can employ ‘link functions’ that map Θ into the relevant domain. The new forward map then consists of the composition of that link function with the initial forward map. See Section 2.3 below for an example. We insist that Θ be a linear space so that Gaussian process priors can be assigned to it.

To fix notation: The joint law of the random variables $(Y_i, X_i)_{i=1}^N$ in (4) defines a product probability measure on $(V \times \mathcal{X})^N$, and it will be denoted by $P_\theta^N = \bigotimes_{i=1}^N P_\theta^i$, where we note $P_\theta^i = P_\theta^1$ for all i . The infinite product probability measure $\bigotimes_{i=1}^\infty P_\theta^i$ describing the law of all possible infinite sequences of observations (in $(V \times \mathcal{X})^\mathbb{N}$) will be denoted by $P_\theta^\mathbb{N}$. We also write shorthand

$$(5) \qquad D_N = \{Y_1, \dots, Y_N, X_1, \dots, X_N\}, \quad N \in \mathbb{N},$$

for the given data vector.

Now given a prior probability measure Π on Θ to be specified, and assuming $\theta \sim \Pi$, we make the Bayesian model assumption that

$$(Y_i, X_i)_{i=1}^N | \theta \sim P_\theta^N$$

which by Bayes’ rule generates a conditional posterior distribution of $\theta | (Y_i, X_i)_{i=1}^N$ on Θ – it will be denoted by $\Pi(\cdot | (Y_i, X_i)_{i=1}^N) \equiv \Pi(\cdot | D_N)$. The posterior distribution arises from a dominated family of probability measures (assuming joint measurability of the map $(\theta, x) \rightarrow \mathcal{G}(\theta)(x)$) and is hence given by

$$(6) \qquad \Pi(A | D_N) \equiv \Pi(A | Y_1, \dots, Y_N, X_1, \dots, X_N) = \frac{\int_A e^{\ell_N(\theta)} d\Pi(\theta)}{\int_\Theta e^{\ell_N(\theta)} d\Pi(\theta)},$$

for any Borel set A in Θ . Here, by independence

$$(7) \qquad \ell_N(\theta) = \sum_{i \leq N} \ell_i(\theta), \quad \text{where } \ell_i(\theta) = -\frac{1}{2\sigma^2} \|Y_i - \mathcal{G}(\theta)(X_i)\|_V^2,$$

is, up to additive constants, the log-likelihood function of the observations.

2.2. *Gaussian process priors for inverse problems.* Gaussian priors are widely used in Bayesian inverse problems since [31, 32], among others for uncertainty quantification purposes as discussed in the [Introduction](#). In the ‘nonparametric’ setting advocated by Stuart [58], when the parameter of interest is a function $\theta : \mathcal{Z} \rightarrow W$, the infinite-dimensional notion of a Gaussian prior is the one of a random map arising from a centred *Gaussian process* (see, e.g., [19, 21] for background).

For example, if $\mathcal{Z}$ is a bounded smooth domain in $\mathbb{R}^d$, a *Whittle–Matérn process* with index set $\mathcal{Z}$ and regularity parameter α (cf. Example 11.8 in [19]) arises as the stationary centred Gaussian process $G = \{G(z), z \in \mathcal{Z}\}$ with covariance kernel

$$K(x, y) = \int_{\mathbb{R}^d} e^{-i\langle x-y, \xi \rangle_{\mathbb{R}^d}} \bar{\mu}(d\xi), \quad \bar{\mu}(d\xi) = (1 + \|\xi\|_{\mathbb{R}^d}^2)^{-\alpha} d\xi, \quad x, y \in \mathcal{Z}.$$

From the results in Chapter 11 in [19], we see that the *reproducing kernel Hilbert space* (RKHS) of $(G(z) : z \in \mathcal{Z})$ equals the set of restrictions to $\mathcal{Z}$ of elements in the Sobolev space $H^\alpha(\mathbb{R}^d)$, which coincides, with equivalent norms, with the Sobolev space $H^\alpha(\mathcal{Z})$ over $\mathcal{Z}$. Moreover, one shows (as in the proof of Lemma I.4 in [19]) that G has a version with paths belonging almost surely to the Hölder spaces $C^{\beta'}(\mathcal{Z})$ for all $\beta' < \alpha - d/2$, and thus defines a Gaussian Borel probability measure on $\Theta = C(\mathcal{Z})$ whenever $\alpha > d/2$ (and, in fact, in $C^\beta(\mathcal{Z})$ for any $\beta < \beta'$).

A key challenge for implementation is of course the computation of the posterior distribution in such settings. When the forward map $\mathcal{G}$ is *linear* then one can show that the posterior distribution (6) will also be a Gaussian measure on Θ so that posterior sampling is fairly straightforward (see [31] and, for concrete implementation with Whittle–Matérn priors, e.g., [39]). In the case where $\mathcal{G}$ is nonlinear, so that the posterior is *not Gaussian* any more, MCMC methods can be readily used as long as the forward map (and possibly its gradient) can be numerically evaluated, providing feasible statistical methodology for nonlinear problems; see, for example, [5, 12, 13, 29, 31, 32, 40, 54] and also Section 2.6 below. Computational guarantees for convergence of such algorithms are also available in the high-dimensional and nonlog-concave setting relevant here; see [27, 45] and references therein.

Regarding statistical (frequentist) properties of posterior measures, the case of linear $\mathcal{G}$ is again fairly well understood due to the explicit Gaussian structure of the posterior distribution, we refer here only to [2, 22, 26, 34, 35, 39, 51] and references therein. The nonlinear case, however, remains a formidable challenge. While consistency and contraction rates for Bayesian methods have been established very recently in some settings [1, 23, 40], no guarantees are currently available for the task of uncertainty quantification investigated here (except for [41] to be discussed below).

To address this challenge, we will prove Bernstein–von Mises theorems, which entail that under suitable hypotheses the *non-Gaussian* posterior measure $\Pi(\cdot|D_N)$ is approximated, in the sense of weak convergence, by a Gaussian distribution with a canonical covariance structure. Our results will hold in $P_{\theta_0}^N$ -probability, where θ_0 is the ground truth parameter generating the data (4), and for all linear functionals $\langle \theta, \psi \rangle_{L^2}$, $\theta \sim \Pi(\cdot|D_N)$, with ψ a test function. To limit technicalities, we assume that both θ_0 and ψ are *smooth*—relaxing such conditions is possible (adapting arguments from [41]) but not the scope of the present paper.

Rigorous statements will involve an arbitrary metric d_{weak} for weak convergence of probability measures on $\mathbb{R}$ (see [16]). If $E^\Pi[\theta|D_N]$ is the posterior mean (a Bochner integral in $C(\mathcal{Z})$), if $\Pi^\psi(\cdot|D_N)$ denotes the (through D_N random) probability law of

$$\sqrt{N}(\theta - E^\Pi[\theta|D_N], \psi)_{L^2_\zeta(\mathcal{Z})}, \quad \theta \sim \Pi(\cdot|D_N),$$

and for a normal $N(0, \sigma_\psi^2)$ distribution with variance σ_ψ^2 to be specified, we will prove limit theorems of the form

$$(8) \quad d_{\text{weak}}(\Pi^\psi(\cdot|D_N), N(0, \sigma_\psi^2)) \xrightarrow{P_{\theta_0}^N, N \rightarrow \infty} 0.$$

When (8) holds, we shall often just say that

$$\sqrt{N} \langle \theta - E^\Pi[\theta | D_N], \psi \rangle_{L^2_\zeta(\mathcal{Z})} \rightarrow^d N(0, \sigma_\psi^2)$$

in $P_{\theta_0}^N$ -probability, where $\rightarrow^d$ denotes convergence in distribution. We obtain general results of this kind in Section 3 but first give their explicit consequences for the main examples (2) of the Schrödinger equation and non-Abelian X -ray transforms.

2.3. Normal approximation for the Schrödinger equation. We now consider an inverse problem for a steady state Schrödinger equation. Such problems have applications in photo-acoustic tomography [3, 4] and have been studied recently in the Bayesian inference setting in [41]. For a bounded smooth domain $\mathcal{X} = \mathcal{Z}$ in $\mathbb{R}^d$, $d \in \mathbb{N}$, with boundary $\partial\mathcal{X}$, let $\lambda = \zeta$ equal the Lebesgue measure on $\mathcal{X}$ normalised to one. Then consider solutions u_f of the elliptic boundary value problem

$$(9) \qquad \begin{cases} \frac{1}{2} \Delta u - fu = 0 & \text{on } \mathcal{X}, \\ u = g & \text{on } \partial\mathcal{X}, \end{cases}$$

where $f : \mathcal{X} \rightarrow (0, \infty)$, is a positive potential, where Δ is the Laplacian, and where $g : \partial\mathcal{X} \rightarrow [g_{\min}, \infty)$, $g_{\min} > 0$, are given smooth ‘boundary temperatures’. For $\theta \in C(\mathcal{X})$, we will parameterise $f = \phi \circ \theta$ where $\phi : \mathbb{R} \rightarrow (f_{\min}, \infty)$, $f_{\min} \geq 0$, is a smooth bijective ‘regular link’ function chosen as in [44], satisfying in particular $\phi(0) = 1$ and $\phi' > 0$. We shall write $\phi(\theta)$, $\phi'(\theta)$ for $\phi \circ \theta$ and $\phi' \circ \theta$, respectively, when no confusion can arise. In the notation from earlier in this section, we set

$$\mathcal{G}(\theta) \equiv u_{\phi \circ \theta} \in L^2_\lambda(\mathcal{X}), \qquad V = W = \mathbb{R},$$

where we note that for $f = \phi \circ \theta$, $\theta \in C^\beta(\mathcal{X})$, $\beta > 0$, a unique C^2 -solution u_f of (9) exists by standard results for elliptic PDEs [20]. Measurements in (4) are thus collected *throughout* the domain $\mathcal{X}$ —results for the case where only boundary measurements at $\partial\mathcal{X}$ are available (‘Calderón type problems’) will require a different approach as the inverse problem is then statistically ‘severely-ill-posed’ (see [1]).

Now draw θ' from an α -regular Whittle–Matérn Gaussian process (cf. Section 2.2) supported in $C^\beta(\mathcal{X})$ for $0 < \beta < \alpha - d/2$, and let the prior $\Pi = \Pi_N$ be the law on $\Theta \equiv C^\beta(\mathcal{X})$ of the random function

$$(10) \qquad \frac{\theta'(x)}{Nd/(4\alpha+2d)}, \qquad x \in \mathcal{X}.$$

The N -dependent rescaling provides additional regularisation of the posterior distribution which is crucial to deal with the global nonlinearity of the inverse problem in the proofs (cf. also Remark 3.5 in [40]).

To state the following theorem, define the space $C^{\infty,2}(\mathcal{X})$ consisting of real-valued functions $f \in C^\infty(\mathcal{X})$ such that the partial derivatives $(D^j f)|_{\partial\mathcal{X}} = 0$ vanish for all multiindices j of order $0 \leq |j| \leq 2$. Evidently, $C_c^\infty(\mathcal{X}) \subset C^{\infty,2}(\mathcal{X})$. We also introduce the Schrödinger operator

$$\mathbb{S}_f[w] = \frac{1}{2} \Delta w - fw, \qquad w \in C^2(\mathcal{X}),$$

appearing in the expression for the asymptotic variance. The following theorem extends related results in [41] to Gaussian process priors, and to the more realistic measurement setting (1), if the true parameter θ_0 and test function ψ define appropriate elements of $C^\infty(\mathcal{X})$.

THEOREM 2.1. Consider the prior Π_N from (10) with integer regularity α satisfying

$$(11) \quad \frac{\alpha}{2\alpha + d} \frac{\alpha - d}{\alpha + 2 - d/2} > \frac{1}{3}.$$

Let $\theta \sim \Pi(\cdot | D_N)$ where $\Pi(\cdot | D_N)$ is the posterior measure (6) on Θ arising from observations D_N in model (4) with $\mathcal{G}(\theta)$ the solution of the Schrödinger equation (9), $f = \phi \circ \theta$, and where $\phi : \mathbb{R} \rightarrow (f_{\min}, \infty)$, $f_{\min} \geq 0$, is a regular link function. Denote the posterior mean by $\bar{\theta}_N = E^\Pi[\theta | D_N]$, and let $\psi \in C^{\infty,2}(\mathcal{X})$. Assume $f_0 = \phi \circ \theta_0$ for some $\theta_0 \in C^\infty(\mathcal{X})$ such that $\inf_{x \in \mathcal{X}} f_0(x) > f_{\min}$. Then we have, as $N \rightarrow \infty$,

$$\sqrt{N} \langle \theta - \bar{\theta}_N, \psi \rangle_{L^2_\lambda(\mathcal{X})} | D_N \rightarrow^d N(0, \sigma^2(f_0, \psi)) \quad \text{in } P_{\theta_0}^N\text{-probability,}$$

and moreover, that

$$\sqrt{N} \langle \bar{\theta}_N - \theta_0, \psi \rangle_{L^2_\lambda(\mathcal{X})} \rightarrow^d N(0, \sigma^2(f_0, \psi))$$

where the asymptotic variance is given by

$$(12) \quad \sigma^2(f_0, \psi) = \left\| \mathbb{S}_{f_0} \left[\frac{\psi}{u_{f_0} \phi'(\theta_0)} \right] \right\|_{L^2_\lambda(\mathcal{X})}^2.$$

The boundary conditions $u = g > 0$ on $\partial \mathcal{X}$ and regularity assumption $\theta_0 \in C^\infty(\mathcal{X})$ ensure that the inverse of the underlying information operator (which is an elliptic order-4 type operator; see (44) below) exists and maps $C^{\infty,2}(\mathcal{X})$ into $C^\infty(\mathcal{X})$. This fact is used crucially in the proofs and also implies finiteness of $\sigma^2(f_0, \psi)$ in (12).

In the proofs, we establish a nonparametric contraction rate $\bar{\delta}_N \rightarrow 0$ of the posterior measure about θ_0 in $\|\cdot\|_\infty$ -distance. The rate $\bar{\delta}_N$ improves if the Gaussian process prior model is more regular. To control nonlinear semiparametric bias terms in the Bernstein–von Mises approximation, we require $N\bar{\delta}_N^3 = o(1)$ in our proofs, giving rise to the condition (11). For instance when $d = 2$, this requires $\alpha > 10$. This can be weakened by obtaining a faster rate than $\bar{\delta}_N$ (the optimal rate is obtained in [41] for more restrictive measurements and non-Gaussian priors), but we do not pursue this issue here as we require $\theta_0 \in C^\infty(\mathcal{X})$ at any rate (for the mapping properties of the information operator).

2.4. Normal approximation for non-Abelian X -ray transforms. We now present results comparable to those from the previous subsection for the non-Abelian X -ray transform as considered in [40, 49]. Applications to neutron spin tomography can be found in [28, 55]; see also Section 1.2 in [40].

We let $M \subset \mathbb{R}^2$ be the closed unit disk with boundary ∂M . We consider lines in the plane (i.e., geodesics) parametrised by $\gamma(t) = x + tv$, where $x \in \mathbb{R}^2$ and v is a direction on the unit circle S^1 . We only want those lines intersecting our region M of interest and further introduce the influx and outflux boundaries as

$$\partial_+ SM = \{(x, v) \in \partial M \times S^1 : x \cdot v \leq 0\},$$

$$\partial_- SM = \{(x, v) \in \partial M \times S^1 : x \cdot v \geq 0\},$$

where $\cdot$ is the standard dot product in the plane. If we take $(x, v) \in \partial_+ SM$, then the line $\gamma(t) = x + tv$ will exit the disk in time

$$\tau(x, v) := -2x \cdot v.$$

Let $\Phi : M \rightarrow \mathbb{C}^{n \times n}$ be a continuous matrix field. Given a line segment (geodesic) $\gamma : [0, \tau] \rightarrow M$ with endpoints $\gamma(0), \gamma(\tau) \in \partial M$, we consider $\mathbb{C}^{n \times n}$ -valued functions $U = U(t)$, $0 \leq t \leq \tau$, solving the matrix ODE

$$\frac{d}{dt}U(t) + \Phi(\gamma(t))U(t) = 0, \quad U(\tau) = \text{Id}.$$

We define the scattering data of Φ on γ to be $C_\Phi(\gamma) := U(0)$. This problem, backward in time for convention here, is well posed and leads to a unique definition of $U(0)$, containing information about Φ along the geodesic γ . Note that when Φ is scalar, we obtain $\log U(0) = \int_0^\tau \Phi(\gamma(t)) dt$, which is the classical X -ray/Radon transform of Φ along the ray γ . Considering the collection of all such data makes up the *non-Abelian X -ray transform* of Φ , viewed here as a map

(13)
$$C_\Phi : \partial_+ SM \rightarrow \mathbb{C}^{n \times n},$$

and the goal is to recover Φ from C_Φ . Inverting Abelian and non-Abelian X -ray transforms are examples of inverse problems in integral geometry, an active field permeating several tomographic imaging methods; see also the recent topical review [30]. We are most interested here in the case where Φ takes values in the Lie algebra $\mathfrak{so}(n)$ of skew-symmetric matrices associated to the special orthogonal group $\text{SO}(n)$. In this case, the scattering data C_Φ maps into $\text{SO}(n)$ and the map $\Phi \mapsto C_\Phi$ is known to be injective [17, 47, 49]. Also, for $n = 3$ this is the relevant problem for neutron spin tomography [28, 55].

Since M is the unit disk, we can parametrise its boundary (the unit circle) ∂M with an angular variable ϕ ; similarly, the vectors v pointing inside M can be parametrised with an angular variable $\varphi \in [-\pi/2, \pi/2]$ (fan-beam coordinates). The influx boundary $\partial_+ SM$ can hence be equipped with a normalized area form λ , $d\lambda := d\phi d\varphi/2\pi^2$. The other common measure in use is $\cos \varphi d\lambda$ (the symplectic measure) and as we comment below in Remark 2.3 the ramifications of choosing one over the other in terms of the Fisher information operator go quite deeply. In this paper, we work exclusively with λ as in [40].

The non-Abelian X -ray transform can be cast into the general statistical model setting from (4) as follows: We set $\mathcal{Z} = M$ endowed with its volume element $\zeta = dx$, and $\mathcal{X} = \partial_+ SM$ with λ defined above. The vector spaces $V = W$ can be taken to equal the space of $n \times n$ real matrices with Frobenius inner product $\langle \cdot, \cdot \rangle_F$. The standard elementwise basis $e_{jk} = \delta_{jk}$, $1 \leq j, k \leq n$, of V then allows to realise the random vector $\varepsilon \sim N(0, I_V)$ as the i.i.d. sequence $\varepsilon_{j,k} \sim N(0, 1)$, $1 \leq j, k \leq n$, considered in the noise model in [40]. Next, we let $\Theta = \bigtimes_{j=1}^{\dim(\mathfrak{so}(n))} C(M)$ denote the space of all continuous maps defined on M taking values in $\mathfrak{so}(n)$. Identifying $\theta = \Phi$, the nonlinear forward map is then $\mathcal{G}(\theta) = C_\theta = C_\Phi$ from (13).

The linearisation $\mathbb{I}_{\theta_0}$ of $\mathcal{G}$ at θ_0 provides a bounded linear map from $L^2_\zeta(M)$ to $L^2_\lambda(\partial_+ SM)$ with adjoint $\mathbb{I}^*_{\theta_0} : L^2_\lambda(\partial_+ SM) \rightarrow L^2_\zeta(M)$; see Section 6.1. There it is further shown that for $\theta_0 \in C^\infty_c(M, \mathfrak{so}(n))$ the information operator $\mathbb{I}^*_{\theta_0} \mathbb{I}_{\theta_0}$ is invertible on $C^\infty(M) = C^\infty(M, V)$, in particular,

(14)
$$\psi \in C^\infty(M, \mathfrak{so}(n)) \implies \tilde{\psi} = (\mathbb{I}^*_{\theta_0} \mathbb{I}_{\theta_0})^{-1} \psi \in C^\infty(M, \mathfrak{so}(n)).$$

To construct a prior Π on Θ , we follow [40] and construct a $\mathfrak{so}(n)$ valued matrix Gaussian random field on M by taking i.i.d. copies of Gaussian process priors $B_j : j = 1, \dots, \dim(\mathfrak{so}(n))$. For each component B_j , we first draw an α -regular ($\alpha \in \mathbb{N}$) planar Whittle–Matérn Gaussian process θ' on M (cf. Section 2.2), with law on $C(M)$ denoted by Π' . Then we choose as prior for B_j the law of

$$\theta_j = \frac{\theta'_j}{N^{1/(2\alpha+2)}}, \quad \theta'_j \sim \Pi',$$

the rescaling playing a comparable role to (10). The product prior probability measure on $\Theta = \times_{j=1}^{\dim(\mathfrak{so}(n))} C(M)$ arising from these coordinate distributions will be denoted by Π_N . The following theorem holds for arbitrary smooth test functions $\psi : M \rightarrow \mathfrak{so}(n)$. As the prior and posterior are measures concentrated in $\mathfrak{so}(n)$ valued matrix fields, it is natural to require the same range constraint on the test function ψ appearing in the dual pairing $\langle \theta, \psi \rangle_{L^2}$. Further remarks paralleling those following Theorem 2.1 about the conditions on θ_0, α apply to the next theorem as well.

THEOREM 2.2. *Consider the preceding Gaussian prior Π_N with integer $\alpha > 8$. Let θ be drawn from the posterior distribution $\Pi(\cdot|D_N)$ from (6) on Θ arising from observations D_N in model (4), where $\mathcal{G}(\theta)$ is the non-Abelian X-ray transform. Denote the posterior mean by $\bar{\theta}_N = E^\Pi[\theta|D_N]$, and let $\psi \in C^\infty(M, \mathfrak{so}(n))$. Assume $\theta_0 \in C_c^\infty(M, \mathfrak{so}(n))$. Then we have as $N \rightarrow \infty$ and in $P_{\theta_0}^N$ -probability, the weak convergence*

$$\sqrt{N} \langle \theta - \bar{\theta}_N, \psi \rangle_{L_\xi^2(M)|D_N} \rightarrow^d N(0, \|\mathbb{I}_{\theta_0}(\mathbb{I}_{\theta_0}^* \mathbb{I}_{\theta_0})^{-1} \psi\|_{L_\lambda^2(\partial_+ SM)}^2),$$

and moreover, that

$$\sqrt{N} \langle \bar{\theta}_N - \theta_0, \psi \rangle_{L_\xi^2(M)} \rightarrow^d N(0, \|\mathbb{I}_{\theta_0}(\mathbb{I}_{\theta_0}^* \mathbb{I}_{\theta_0})^{-1} \psi\|_{L_\lambda^2(\partial_+ SM)}^2).$$

REMARK 2.3. The inversion of $\mathbb{I}_{\theta_0}^* \mathbb{I}_{\theta_0}$ as stated in (14) has its own independent interest and it is one of the innovations of the present paper. In general, for geodesic X-ray transforms, the inversion of the Fisher information operator is a delicate problem and its solution depends on the measure chosen on the influx boundary $\partial_+ SM$ as this choice determines the adjoint $\mathbb{I}_{\theta_0}^*$. There are two commonly used measures and in both cases the Fisher information operator becomes an elliptic pseudo-differential operator of order -1 in the interior of M . However, its boundary behaviour is sensitive to the choice of measure, and given the non-local nature of $\mathbb{I}_{\theta_0}^* \mathbb{I}_{\theta_0}$, one must understand finer mapping properties that include boundary effects. In [39], we considered (in the Abelian case) the Fisher information operator for the symplectic measure, that is, the natural measure on the space of geodesics (also the measure naturally produced by Santaló's formula). In this case, it turns out that $\mathbb{I}_{\theta_0}^* \mathbb{I}_{\theta_0}$ extends as a pseudo-differential operator to a slightly larger manifold containing M and one can make use of transmission properties as developed by Hörmander and Grubb [25]. The upshot of this analysis is the need to incorporate a blow up at the boundary of type $\rho^{-1/2}$ (where ρ is distance to the boundary) when proving Bernstein–von Mises theorems. In contrast, the second choice of measure, which is given by the canonical volume form λ on the influx boundary—and the one chosen in this paper—exhibits different behaviour and $\mathbb{I}_{\theta_0}^* \mathbb{I}_{\theta_0}$ does not extend as a pseudo-differential operator to any neighbourhood of M . To study the behaviour near the boundary in the case of the disk, we take advantage of the recent developments in [38] which deliver nonstandard Sobolev scales with suitable degenerations at the boundary. The inversion in (14) is the first result of its kind and hints at a more general picture valid on any nontrapping manifold with strictly convex boundary and no conjugate points.

2.5. Application to uncertainty quantification. Bayesian uncertainty quantification for functionals $\langle \theta, \psi \rangle_{L_\xi^2(\mathcal{Z})}$, is based on level $1 - \xi$ Bayesian credible sets

$$(15) \quad C_N = \{v \in \mathbb{R} : |v - \langle \bar{\theta}, \psi \rangle_{L_\xi^2(\mathcal{Z})}| \leq R_N\}, \quad \Pi(C_N|D_N) = 1 - \xi, \quad 0 < \xi < 1,$$

where $\bar{\theta} = E^\Pi[\theta|D_N]$ is the posterior mean. Construction of the interval C_N requires only computation of that mean and of the quantiles R_N of the posterior distribution, both of which

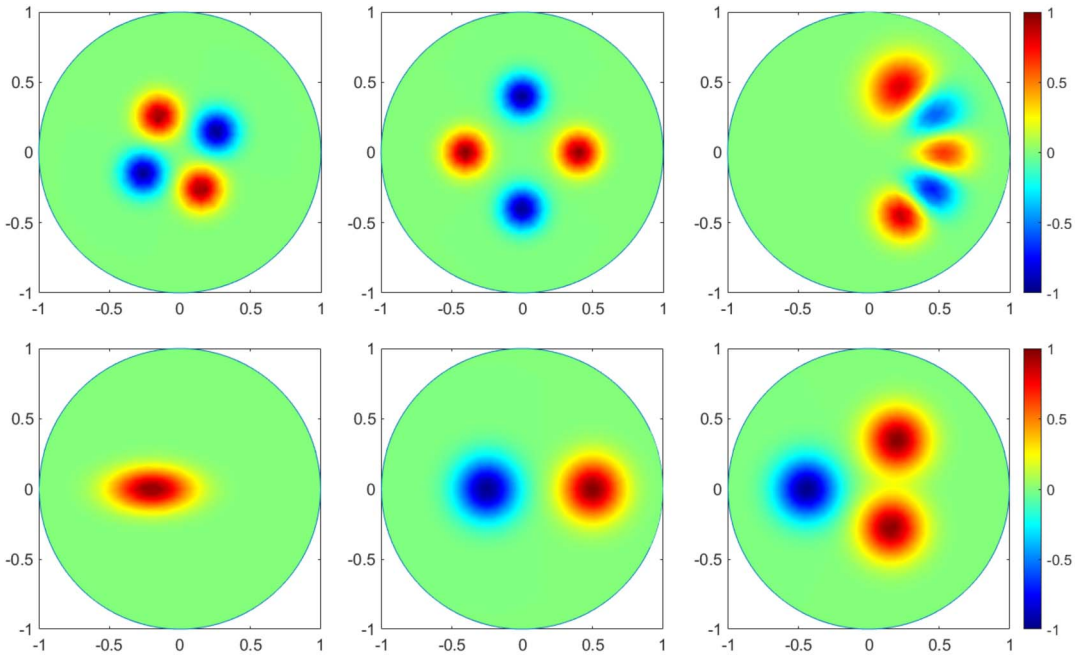


FIG. 1. The six functions used (top row: a, b, c ; bottom row: d, e, f), all drawn on the same color scale.

can be calculated approximately along a chain of MCMC samples (see also Section 2.6). In particular, the asymptotic variances appearing in Theorems 2.1 and 2.2 need not be estimated.

Now using Theorems 2.1 and 2.2 with $0 \neq \psi \in C^\infty$, and arguing as in Remark 2.9 in [39] one shows that the credible interval C_N has valid frequentist coverage of the true parameter θ_0 in the sense that, as $N \rightarrow \infty$,

$$P_{\theta_0}^N(\langle \theta_0, \psi \rangle_{L^2_\zeta(\mathcal{Z})} \in C_N) \rightarrow 1 - \xi, \quad \sqrt{N}R_N \xrightarrow{P_{\theta_0}^N} Q^{-1}(1 - \xi),$$

with $Q(t) = \Pr(|Z| \leq t)$, $t \in \mathbb{R}$, where Z is the (for $\psi \neq 0$ nondegenerate) limiting normal distribution occurring in Theorems 2.1 or 2.2. In particular, the diameter of this confidence interval is optimal in an asymptotic minimax sense; see Section 3.3 for details.

2.6. Numerical illustration. We illustrate our theory by numerical experiments for non-Abelian X -ray transforms, following the implementation detailed in Section 4 of [40] with $\mathfrak{so}(3)$ replaced by the (isomorphic) $\mathfrak{su}(2)$. We fix the Euclidean metric on the unit disk, and represent the disk as an unstructured mesh with 886 vertices. We choose an $\mathfrak{su}(2)$ -valued matrix field $\Phi = a\sigma_1 + b\sigma_2 + c\sigma_3$ as in [40] with $\sigma_1, \sigma_2, \sigma_3$ the Pauli basis matrices, and a, b, c smooth scalar components characterised by their values at the 886 vertices; see Figure 1.

For $N = 600$, then $N = 1000$, we compute C_Φ over N geodesics drawn at random, whose entries are then corrupted by additive noise with $\sigma = 0.1$. The prior is set to be of Matérn type with parameters $\alpha = 3$ (and length-scale parameter $\ell = 0.2$; see [40] for full details).

The preconditioned Crank–Nicolson (pCN) algorithm is then used to compute $N_s = 10^5$ iterations of a Markov chain $\{\Phi_n\}_{n \leq N_s}$ targeting the posterior distribution of $\Phi|D_N$; cf. Section 4, [40]. As the purpose here is to explore and display the main features of the posterior, the initial condition is chosen as the ground truth Φ , which shortens the burn-in phase. The sequence $\{\Phi_n\}_{n=1000}^{N_s}$ represents a family of posterior draws.

We fix three $\mathfrak{su}(2)$ -valued test functions

$$\Psi_1 = d\sigma_1 + e\sigma_2 + f\sigma_3, \quad \Psi_2 = e\sigma_1 + f\sigma_2 + d\sigma_3, \quad \Psi_3 = f\sigma_1 + d\sigma_2 + e\sigma_3,$$

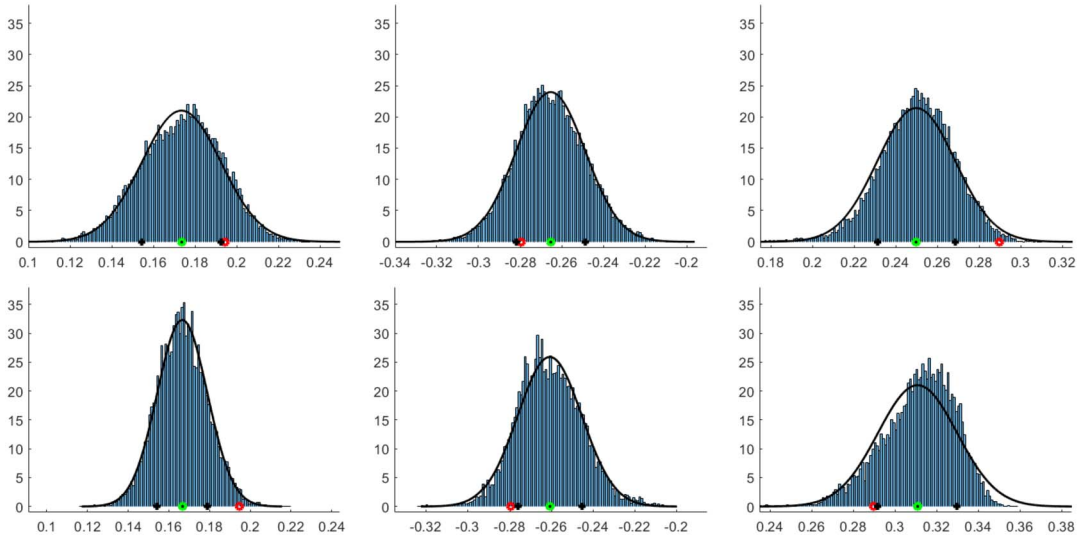


FIG. 2. Histograms of the MCMC chains for (left to right): $\langle \Phi_n, \Psi_1 \rangle$, $\langle \Phi_n, \Psi_2 \rangle$, $\langle \Phi_n, \Psi_3 \rangle$, rescaled as probability densities, and Gaussians with empirical mean $\hat{m}$ and variance $\hat{\sigma}^2$ superimposed. Axes scales are uniform across all plots. Red dot: true value; green dot: mean; black dots: $\hat{m} \pm 1\hat{\sigma}$. Top to bottom: $N = 600$, $N = 1000$. The spreads decrease from the top row to the bottom row, most noticeably by 25% on the left plot.

where the functions d , e , f appear on Figure 1, and we are interested in the statistics of the smooth aspects $\langle \Phi, \Psi_1 \rangle_{L^2}$, $\langle \Phi, \Psi_2 \rangle_{L^2}$, $\langle \Phi, \Psi_3 \rangle_{L^2}$ of the posterior measure. Figure 2 displays histograms of the tracked quantities $\{\langle \Phi_n, \Psi_j \rangle_{L^2}, 0 \leq n \leq N_s, j \in \{1, 2, 3\}\}$ along each chain, illustrating both approximate posterior normality and concentration as N increases as predicted by Theorem 2.2. Note that although all three test functions used have the same $L^2(M)$ norm, the predicted asymptotic variances $\|\mathbb{I}_{\theta_0}(\mathbb{I}_{\theta_0}^* \mathbb{I}_{\theta_0})^{-1} \Psi_j\|_{L^2_{\lambda}(\partial_+ SM)}^2$ should differ for $1 \leq j \leq 3$, as observed on Figure 2. The empirical posterior standard deviations further corroborate the frequentist validity of the uncertainty quantification provided by these credible sets established in Section 2.5.

3. BvM in regression models with Gaussian process priors. In this section, we provide general conditions under which Bernstein–von Mises type approximations can be proved for posterior distributions arising from Gaussian process priors in the general nonlinear regression model (4). Theorems 2.1 and 2.2 will be deduced by verifying these conditions.

3.1. Analytical hypotheses. We start with the key hypotheses on the forward map $\mathcal{G}$ from (3). Recall that Θ is a parameter set arising as a linear subspace of $L^\infty(\mathcal{Z}, W)$. The first condition concerns the uniform boundedness as well as the global Lipschitz continuity of $\mathcal{G}$ on Θ both for L^2 and $\|\cdot\|_\infty$ norms. While restrictive, such assumptions are often satisfied due to ‘compactification’ or ‘energy preservation’ properties of the PDEs describing the forward map $\mathcal{G}$. The second condition requires that $\mathcal{G}$ is differentiable at the ‘true value’ $\theta_0 \in \Theta$ in a suitable sense.

CONDITION 3.1. There exists a fixed constant $C > 0$ such that we have

$$\|\mathcal{G}(\theta)\|_\infty \leq C, \quad \text{and} \quad \|\mathcal{G}(\theta) - \mathcal{G}(\theta')\|' \leq C\|\theta - \theta'\|, \quad \text{for all } \theta, \theta' \in \Theta,$$

where either $\|\cdot\|' = \|\cdot\| = \|\cdot\|_\infty$ or $\|\cdot\|' = \|\cdot\|_{L^2_\lambda(\mathcal{X})}$ and $\|\cdot\| = \|\cdot\|_{L^2_\lambda(\mathcal{Z})}$.

CONDITION 3.2. For $\theta_0 \in \Theta$ and any $h \in \Theta$ suppose that as $\|h\|_\infty \rightarrow 0$,

$$\|\mathcal{G}(\theta_0 + h) - \mathcal{G}(\theta_0) - D\mathcal{G}_{\theta_0}[h]\|_{L^2_\lambda(\mathcal{X}, V)} \equiv \rho_{\theta_0}[h] = o(\|h\|_\infty)$$

for some operator

$$\mathbb{I}_{\theta_0} \equiv D\mathcal{G}_{\theta_0} : (\Theta, \langle \cdot, \cdot \rangle_{L^2_\zeta(\mathcal{Z}, W)}) \rightarrow L^2_\lambda(\mathcal{X}, V)$$

that is a continuous linear map. Moreover, we assume that $\mathbb{I}_{\theta_0}$ is also continuous as a map from $(\Theta, \|\cdot\|_\infty) \rightarrow L^\infty(\mathcal{X})$.

When considering inference on linear functionals $\langle \psi, \theta \rangle_{L^2(\mathcal{Z})}$ of θ , the invertibility of the ‘information’ (or normal) operator $\mathbb{I}^*_{\theta_0} \mathbb{I}_{\theta_0}$ induced by $\mathbb{I}_{\theta_0}$ in directions ψ will be required. Here,

$$\mathbb{I}^*_{\theta_0} : L^2_\lambda(\mathcal{X}, V) \rightarrow \overline{(\Theta, \langle \cdot, \cdot \rangle_{L^2_\zeta(\mathcal{Z}, W)})}$$

denotes the adjoint map of $\mathbb{I}_{\theta_0}$, and we will employ the following condition on ψ .

CONDITION 3.3. Given $\psi \in \Theta$ and $\mathbb{I}_{\theta_0}$ from Condition 3.2, suppose there exists $\tilde{\psi} = \tilde{\psi}_{\theta_0} \in \Theta$ such that $\langle \mathbb{I}^*_{\theta_0} \mathbb{I}_{\theta_0} \tilde{\psi} - \psi, h \rangle_{L^2_\zeta(\mathcal{Z}, W)} = 0$ for all $h \in \Theta$.

We now turn to the choice of Gaussian process priors and their reproducing kernel Hilbert spaces (RKHS). As is common in Bayesian nonparametric statistics [19, 62], we will require assumptions on the small deviation asymptotics of the prior measure Π . While the displayed probability in the following condition still involves the map $\mathcal{G}$, one can readily use (3.1) to simplify the condition to one involving only the prior small probabilities of $\|\theta - \theta_0\|_{L^2_\zeta(\mathcal{Z})}$.

CONDITION 3.4. The priors $\Pi = \Pi_N$ consist of Gaussian–Borel probability measures on the measurable linear subspace Θ of $L^\infty(\mathcal{Z})$. The RKHS of Π_N is given by the linear subspace $\mathcal{H}_N$ of Θ , with RKHS inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}_N}$. Suppose further that $\sup_N E^{\Pi_N} \|\theta\|_{L^2(\mathcal{Z})}^4 < \infty$ and that for some sequence $\delta_N \rightarrow 0$ satisfying $e^{-N\delta_N^2} N^2 \rightarrow_{N \rightarrow \infty} 0$, some $\bar{d} > 0$ and all N large enough,

$$\pi(\delta_N) := \Pi_N(\|\mathcal{G}(\theta) - \mathcal{G}(\theta_0)\|_{L^2_\lambda(\mathcal{X})} \leq \delta_N) \geq \exp\{-\bar{d}N\delta_N^2\}.$$

Note that norms of tight Gaussian probability measures always have all higher moments finite, but we require this bound to be uniform in N , hence the condition.

The next condition concerns an initial result about global contraction properties of the posterior measure near the true value $\theta_0 \in \Theta$. For nonlinear inverse problems with Gaussian process priors such results have recently been obtained in [1, 23, 40].

CONDITION 3.5. For a prior Π_N as in Condition 3.4, consider the posterior distribution $\Pi(\cdot | D_N)$ in (6) arising from data D_N in the model (4). Let the ‘ground truth’ $\theta_0 \in \Theta$ generate data $D_N \sim P^N_{\theta_0}$, and let $(\mathcal{R}, \|\cdot\|_{\mathcal{R}})$ be a normed linear measurable subspace of $L^\infty(\mathcal{Z})$. Assume that as $N \rightarrow \infty$ and for real sequences $\bar{\delta}_N \rightarrow 0$, $M_N \geq 1$, such that $\sqrt{N}\bar{\delta}_N \rightarrow \infty$,

(16) $\Pi(\theta : \|\theta\|_{\mathcal{R}} \leq M_N, \|\theta - \theta_0\|_\infty \leq \bar{\delta}_N | D_N) = 1 - o_{P^N_{\theta_0}}(\eta_N).$

Here, $\eta_N = e^{-(L+1)N\delta_N^2}$ with $L = 2(2C^2 + 1) + \bar{d}$ where C is as in Condition 3.1 and $\bar{d}$, δ_N as in Condition 3.4.

Following ideas in [40], verification of Condition 3.5 can be based on i) a global *stability (or inverse continuity) estimate* for the map $\theta \mapsto \mathcal{G}(\theta)$, ii) a ‘forward’ contraction rate result for the posterior law of $\mathcal{G}(\theta)$ about $\mathcal{G}(\theta_0)$ and iii) the fact that for *rescaled* Gaussian priors, posteriors automatically concentrate (with high probability) on suitable bounded sets in regularisation spaces $\mathcal{R} = C^\beta$ for some β related to the path regularity of the Gaussian process. A general result providing bounds for (ii) and (iii) can be found in Theorem 14 in the Appendix of [23]. Stability estimates (i) are more problem specific—for the applications from Sections 2.3 and 2.4 we rely on Lemma 28 in [44] and Corollary 2.3 in [40], respectively.

The preceding ‘regularised parameter spaces’

$$(17) \quad \Theta_N = \{\theta \in \Theta : \|\theta\|_{\mathcal{R}} \leq M_N, \|\theta - \theta_0\|_{\infty} \leq \bar{\delta}_N\}$$

play a key role in our proofs via the following quantitative condition that allows to control the nonlinearity of the likelihood function of the model (4), the discretisation errors arising from statistical sampling, and the sensitivity of Π_N with respect to small perturbations in $\tilde{\psi}$ -directions. Let $\mathcal{J}_N$ be an upper bound for the following (‘Dudley’-type) integral of the Kolmogorov metric entropy of Θ_N :

$$(18) \quad \mathcal{J}_N(s, t) \geq \int_0^s \sqrt{\log 2N(\Theta_N, \|\cdot\|_{\infty}, t\epsilon)} d\epsilon, \quad s, t > 0,$$

where $N(\Theta_N, \|\cdot\|_{\infty}, \epsilon)$ are the usual ϵ -covering numbers of the set Θ_N for the $\|\cdot\|_{\infty}$ -distance (i.e., the minimal number of ϵ -balls for $\|\cdot\|_{\infty}$ required to cover Θ_N).

CONDITION 3.6. Suppose that $\tilde{\psi} = \tilde{\psi}_{\theta_0}$ from Condition 3.3 belongs to $\mathcal{H}_N \cap \mathcal{R}$ and that it satisfies, for δ_N from Condition 3.4 and $\|\cdot\|_{\mathcal{H}_N}$ the norm induced by $\langle \cdot, \cdot \rangle_{\mathcal{H}_N}$,

$$(19) \quad \lim_{N \rightarrow \infty} \delta_N \|\tilde{\psi}\|_{\mathcal{H}_N} = 0.$$

Moreover, for $\bar{\delta}_N$ as in Condition 3.5, suppose that as $N \rightarrow \infty$,

$$(20) \quad \sqrt{N} \bar{\delta}_N^2 \mathcal{J}_N(1, \bar{\delta}_N^2) \rightarrow 0.$$

Further for σ_N a sequence such that for all N large enough and all $t \in \mathbb{R}$ fixed,

$$\sigma_N \geq \sup_{\theta \in \Theta_N} \rho_{\theta_0}[\theta - \theta_0 - (t/\sqrt{N})\tilde{\psi}],$$

assume that as $N \rightarrow \infty$,

$$(21) \quad \max(N(\sigma_N^2 + \sigma_N \bar{\delta}_N), \sqrt{N} \mathcal{J}_N(\sigma_N, 1), \bar{\delta}_N \sqrt{\log N} \mathcal{J}_N^2(\sigma_N, 1)/\sigma_N^2) \rightarrow 0.$$

In prototypical situations where $\mathcal{R}$ equals a fixed ball in a Hölder space $C^\beta(\mathcal{Z})$ for a d -dimensional domain $\mathcal{Z}$, and when the approximation in Condition 3.2 is quadratic ($\rho_{\theta_0}(h) = O(\|h\|_{\infty}^2)$), it can be shown (see Section 5.3) that Conditions (20) and (21) reduce to the much simpler conditions

$$(22) \quad N \bar{\delta}_N^3 \rightarrow 0, \quad \text{and} \quad \beta > 2d.$$

The requirements on α in Theorems 2.1 and 2.2 ultimately arise from (22) via the initial uniform contraction rate $\bar{\delta}_N$ obtained for the posterior distribution.

3.2. *Bernstein–von Mises theorems.* Our first main theorem shows that the posterior distribution in our nonlinear inverse problem is asymptotically Gaussian when integrated against fixed test functions $\psi \in \Theta$, and when centred at

$$(23) \qquad \hat{\Psi}_N = \langle \theta_0, \psi \rangle_{L^2_\zeta(\mathcal{Z}, W)} + \frac{1}{N} \sum_{i=1}^N \langle \mathbb{I}_{\theta_0} \tilde{\psi}_{\theta_0}(X_i), \varepsilon_i \rangle_V.$$

We recall that the next limit is to be understood in the sense of (8).

THEOREM 3.7. *Let $\theta \sim \Pi(\cdot|D_N)$ be a posterior draw and assume Conditions 3.1–3.6 are satisfied. Then we have as $N \rightarrow \infty$ and in $P_{\theta_0}^N$ -probability,*

$$\sqrt{N}(\langle \theta, \psi \rangle_{L^2_\zeta(\mathcal{Z})} - \hat{\Psi}_N) | D_N \rightarrow^d N(0, \|\mathbb{I}_{\theta_0} \tilde{\psi}_{\theta_0}\|_{L^2_\lambda(\mathcal{X}, V)}^2).$$

To use an approximation as the last one for uncertainty quantification (as in Section 2.5), we need to choose a *feasibly computable centring statistic* instead of the (infeasible) $\hat{\Psi}_N$. A desirable choice, both for inference and computation purposes via MCMC, is the mean

$$\langle \bar{\theta}_N, \psi \rangle_{L^2_\zeta(\mathcal{Z}, W)}, \quad \text{where } \bar{\theta}_N = E^\Pi[\theta | D_N],$$

of the posterior distribution. [By uniform boundedness of $\mathcal{G}$, (6) and Condition 3.4, the Bochner integral $E^\Pi[\theta | D_N]$ can be shown to exists for any given data vector D_N .]

THEOREM 3.8. *In the setting of Theorem 3.7, if $\bar{\theta}_N = E^\Pi[\theta | D_N]$ denotes the posterior mean, then we have as $N \rightarrow \infty$,*

$$\sqrt{N} \langle \theta - \bar{\theta}_N, \psi \rangle_{L^2_\zeta(\mathcal{Z})} | D_N \rightarrow^d N(0, \|\mathbb{I}_{\theta_0} \tilde{\psi}_{\theta_0}\|_{L^2_\lambda(\mathcal{X}, V)}^2) \quad \text{in } P_{\theta_0}^N - \text{probability}.$$

Moreover, as $N \rightarrow \infty$, we also have

$$\sqrt{N} \langle \bar{\theta}_N - \theta_0, \psi \rangle_{L^2_\zeta(\mathcal{Z}, W)} \rightarrow^d N(0, \|\mathbb{I}_{\theta_0} \tilde{\psi}_{\theta_0}\|_{L^2_\lambda(\mathcal{X}, V)}^2).$$

3.3. *LAN expansion and asymptotic optimality.* We finally establish the local asymptotically normal (LAN) expansion of our model and deduce from it the semiparametric information bound (cf. [60, 61]) for inference on $\langle \theta, \psi \rangle_{L^2(\mathcal{Z})}$. This implies the optimality of Theorem 3.8 as long as $\mathbb{I}_{\theta_0}$ is injective on Θ , as is the case in our model examples. [In the Schrödinger case, injectivity of $\mathbb{I}_{\theta_0}$ from (43) follows from the uniqueness of solutions of (38) and positivity of $u_{f_0}, \phi'(\theta_0)$, while the injectivity of $\mathbb{I}_{\theta_0}$ in the setting of Theorem 2.2 is proved in [49].]

PROPOSITION 3.9. *Suppose Conditions 3.1 and 3.2 hold true. Then the log-likelihood ratio process in the model (4) satisfies, for every fixed $h \in L^\infty(\mathcal{Z})$ and as $N \rightarrow \infty$, the asymptotic expansion*

$$(24) \qquad \log \frac{dP_{\theta_0+h/\sqrt{N}}^N}{dP_{\theta_0}^N}(D_N) = W_N(h) - \frac{1}{2} \|\mathbb{I}_{\theta_0}[h]\|_{L^2_\lambda(\mathcal{X}, V)}^2 + o_{P_{\theta_0}^N}(1)$$

for random variables

$$(25) \qquad W_N \equiv \frac{1}{\sqrt{N}} \sum_{i=1}^N \langle \mathbb{I}_{\theta_0} h(X_i), \varepsilon_i \rangle_V \rightarrow_{N \rightarrow \infty}^d N(0, \|\mathbb{I}_{\theta_0}[h]\|_{L^2_\lambda(\mathcal{X}, V)}^2).$$

Assuming also Condition 3.3 and that $\mathbb{I}_{\theta_0} : \Theta \rightarrow L^2_{\lambda}(\mathcal{X})$ is injective, the semiparametric information bound for optimal inference on the functional $\kappa(\theta) = \langle \theta, \psi \rangle_{L^2(\mathcal{Z})}$ based on observations D_N is given by

$$(26) \quad \|\mathbb{I}_{\theta_0} \tilde{\psi}_{\theta_0}\|_{L^2_{\lambda}(\mathcal{X}, V)}^2.$$

PROOF. An expansion for $\ell_N(\theta_0 + h/\sqrt{N}) - \ell_N(\theta_0)$ under $P_{\theta_0}^N$ can be obtained as in the proof of Proposition 4.2 (replacing $\theta, t\tilde{\psi}_{\theta_0}$ by θ_0 and h , resp.), from which the LAN expansion (24) can be derived without difficulty, and (25) follows directly from the central limit theorem. To find the information lower bound for estimating the functional $\kappa(\theta)$, we need to find the Riesz representer $\tilde{\kappa}$ of

$$\kappa : (\Theta, \langle \cdot, \cdot \rangle_{\text{LAN}}) \rightarrow \mathbb{R}, \quad \text{where } \langle \cdot, \cdot \rangle_{\text{LAN}} = \langle \mathbb{I}_{\theta_0}[\cdot], \mathbb{I}_{\theta_0}[\cdot] \rangle_{L^2_{\lambda}(\mathcal{X})}$$

is a Hilbert space inner product since $\mathbb{I}_{\theta_0}$ is linear and injective. But Condition 3.3 implies

$$(27) \quad \langle h, \tilde{\psi}_{\theta_0} \rangle_{\text{LAN}} = \langle h, \mathbb{I}_{\theta_0}^* \mathbb{I}_{\theta_0}[\tilde{\psi}_{\theta_0}] \rangle_{L^2_{\lambda}(\mathcal{Z})} = \langle h, \psi \rangle_{L^2_{\lambda}(\mathcal{Z})} = \kappa(h), \quad h \in \Theta,$$

hence $\tilde{\kappa} = \tilde{\psi}_{\theta_0} \in \Theta$, and arguing as in, for example, Section 7.5 in [41], the information lower bound is given by $\langle \tilde{\kappa}, \tilde{\kappa} \rangle_{\text{LAN}}$, as desired. $\square$

REMARK 3.10. By convergence of moments established in the proof of Theorem 3.8,

$$NE_{\theta_0}^N \langle \bar{\theta}_N - \theta_0, \psi \rangle_{L^2_{\lambda}(\mathcal{Z})}^2 \rightarrow \|\mathbb{I}_{\theta_0} \tilde{\psi}\|_{L^2_{\lambda}(\mathcal{X})}^2$$

as $N \rightarrow \infty$, and this is optimal in the minimax sense by the preceding proposition, as then, by the semiparametric asymptotic minimax theorem [61],

$$\lim_N \inf_{\tilde{\psi}_N : (V \times \mathcal{X})^N \rightarrow \mathbb{R} : \|\theta - \theta_0\|_{L^2(\mathcal{Z})} \leq 1/\sqrt{N}} \sup NE_{\theta}^N (\tilde{\psi}_N - \langle \theta, \psi \rangle_{L^2(\mathcal{Z})})^2 = \|\mathbb{I}_{\theta_0} \tilde{\psi}\|_{L^2_{\lambda}(\mathcal{X})}^2.$$

In particular, no confidence region can have a smaller uniform asymptotic diameter as the one constructed in Section 2.5.

4. Proofs of Theorems 3.7 and 3.8. We set $\sigma^2 = 1$ to simplify notation. We follow ideas from [7, 9, 41, 43] and prove a Bernstein–von Mises theorem by proving convergence of the moment generating functions (Laplace transforms) of $\sqrt{N}(\langle \theta, \psi \rangle_{L^2(\mathcal{Z})} | D_N - \hat{\Psi}_N)$ with centring as in (23), which implies weak convergence (in probability), and thus Theorem 3.7. This follows by obtaining LAN-type approximations of suitable likelihood-ratios within the support of a suitably ‘localised’ posterior distribution. The stochastic linearisation as well as the discretisation error are controlled by tools from empirical process theory in Section 4.3. That one can centre at the posterior mean instead of $\hat{\Psi}_N$ (i.e., Theorem 3.8) will be proved in Section 4.5.

4.1. Localisation of the posterior measure. We first record a standard stochastic lower bound on the posterior denominator commonly used in Bayesian nonparametric statistics.

LEMMA 4.1. Assume Condition 3.4 holds for some $\delta_N, \bar{d}$ and let C be the constant from Condition 3.1. Then $P_{\theta_0}^N(C_N) \rightarrow 1$ as $N \rightarrow \infty$ where

$$C_N = \left\{ \int_{\Theta} e^{\ell_N(\theta) - \ell_N(\theta_0)} d\Pi(\theta) \geq e^{-LN\delta_N^2} \right\}, \quad L = 2(2C^2 + 1) + \bar{d}.$$

Moreover, if T_N is a measurable subset of Θ such that

$$\Pi(T_N) \leq e^{-D_0 N \delta_N^2} \quad \text{for some } D_0 > L,$$

then as $N \rightarrow \infty$,

$$\Pi(T_N|D_N) = O_{P_{\theta_0}^N}(e^{-(D_0-L)N\delta_N^2}) = o_{P_{\theta_0}^N}(1).$$

PROOF. We apply Lemma 7.3.2 in [21] with $\mathcal{P}$ there equal to our Θ and with $p = dP_{\theta}^1$, $p_0 = dP_{\theta_0}^1$ the model densities for variables $X = (Y_1, X_1)$ on $(V \times \mathcal{X})$ generating the i.i.d. data (4) for respective choices of θ , and with probability measure $\nu = \Pi(\cdot \cap B)/\Pi(B)$ on the set $B = B_{\epsilon} \subset \Theta$ defined in that lemma. If we define sets

$$B_{(N)} = \{\theta \in \Theta : \|\mathcal{G}(\theta) - \mathcal{G}(\theta_0)\|_{L^2_{\lambda}(\mathcal{X})} \leq \delta_N\}$$

then $B_{(N)} \subset B_{\epsilon}$ for $\epsilon = \sqrt{2C^2 + 1}\delta_N$ since, noting that $-\log(p/p_0) = \ell_1(\theta_0) - \ell_1(\theta)$ in the notation (7), standard computations with likelihood ratios (e.g., Lemma 23 in [23], or page 224 in [19]) and Condition 3.1 imply

$$\begin{aligned} E_{\theta_0}^1[\ell_1(\theta_0) - \ell_1(\theta)] &= \frac{1}{2}\|\mathcal{G}(\theta) - \mathcal{G}(\theta_0)\|_{L^2_{\lambda}(\mathcal{X})}^2, \\ E_{\theta_0}^1[\ell_1(\theta_0) - \ell_1(\theta)]^2 &\leq (2C^2 + 1)\|\mathcal{G}(\theta) - \mathcal{G}(\theta_0)\|_{L^2_{\lambda}(\mathcal{X})}^2. \end{aligned}$$

We hence obtain from that lemma (with $c = 1$), as $N \rightarrow \infty$,

$$P_{\theta_0}^N\left(\int_{B_{\epsilon}} e^{\ell_N(\theta) - \ell_N(\theta_0)} d\Pi(\theta) \geq e^{-2(2C^2+1)N\delta_N^2} \Pi(B_{\epsilon})\right) \leq \frac{1}{(2C^2 + 1)N\delta_N^2} \rightarrow 0.$$

Now the first limit follows since $\Theta \supset B_{\epsilon}$ and since $\Pi(B_{\epsilon}) \geq \Pi(B_{(N)}) \geq \pi(\delta_N) \geq e^{-\bar{d}N\delta_N^2}$ by Condition 3.4. Finally, we see on the event $\mathcal{C}_N$ that

$$\Pi(T_N|D_N) = \frac{\int_{T_N} e^{\ell_N(\theta) - \ell_N(\theta_0)} d\Pi(\theta)}{\int_{\Theta} e^{\ell_N(\theta) - \ell_N(\theta_0)} d\Pi(\theta)} \leq e^{LN\delta_N^2} Z_N$$

where $Z_N := \int_{T_N} e^{\ell_N(\theta) - \ell_N(\theta_0)} d\Pi(\theta) = O_{P_{\theta_0}^N}(e^{-D_0 N \delta_N^2})$ by Markov's inequality since Fubini's theorem and $E_{\theta_0}^N e^{\ell_N(\theta) - \ell_N(\theta_0)} = 1$ imply $E_{\theta_0}^N Z_N \leq \Pi(T_N) \leq e^{-D_0 N \delta_N^2}$. $\square$

Now since $\tilde{\psi}$ from Condition 3.3 defines an element of the RKHS $\mathcal{H}_N$ of Π_N by Condition 3.6, if $\theta \sim \Pi_N$ then by properties of RKHS the variable $\langle \theta, \tilde{\psi} \rangle_{\mathcal{H}_N}$ has distribution $N(0, \|\tilde{\psi}\|_{\mathcal{H}_N}^2)$. Hence if we define

$$T_N = \left\{ \theta : \frac{|\langle \theta, \tilde{\psi} \rangle_{\mathcal{H}_N}|}{\|\tilde{\psi}\|_{\mathcal{H}_N}} > \sqrt{2L + 1} \sqrt{N} \delta_N \right\},$$

then the tail inequality for standard normal random variables implies that $\Pi(T_N) \leq e^{-(2L+1)N\delta_N^2}$, and hence the previous lemma applies, so that for Θ_N from (17) and

$$(28) \quad \bar{\Theta}_N := \Theta_N \cap T_N^c \quad \text{we have } \Pi(\bar{\Theta}_N^c|D_N) = O_{P_{\theta_0}^N}(e^{-(L+1)N\delta_N^2}) = o_{P_{\theta_0}^N}(1)$$

as $N \rightarrow \infty$, using also Condition 3.5. In the proofs that follow we consider $\theta \sim \Pi^{\bar{\Theta}_N}(\cdot|D_N)$ where the posterior (6) is taken to arise from prior probability measure

$$\Pi^{\bar{\Theta}_N} \equiv \frac{\Pi(\cdot \cap \bar{\Theta}_N)}{\Pi(\bar{\Theta}_N)}$$

equal to Π restricted to $\bar{\Theta}_N$ from (17) and renormalised. Indeed, Condition 3.5 and standard arguments (e.g., page 142 in [61]) then imply, for $\|\cdot\|_{\text{TV}}$ the total variation distance on probability measures on Θ , that as $N \rightarrow \infty$,

$$(29) \quad \|\Pi(\cdot|D_N) - \Pi^{\bar{\Theta}_N}(\cdot|D_N)\|_{\text{TV}} \leq 2\Pi(\bar{\Theta}_N^c|D_N) \xrightarrow{P_{\theta_0}^N} 0,$$

and then also $d_{\text{weak}}(\Pi(\cdot|D_N), \Pi^{\bar{\Theta}_N}(\cdot|D_N)) \xrightarrow{P_{\theta_0}^N} 0$ for any metric d_{weak} for weak convergence. It hence suffices to prove Theorem 3.7 for $\Pi^{\bar{\Theta}_N}(\cdot|D_N)$ instead of $\Pi(\cdot|D_N)$.

4.2. Uniform LAN approximation of the posterior Laplace transform.

PROPOSITION 4.2. For $\theta, \psi \in \Theta$ and $\tilde{\psi} = \tilde{\psi}_{\theta_0}$ from Condition 3.3, define

$$\theta_{(t)} = \theta - \frac{t}{\sqrt{N}} \tilde{\psi}_{\theta_0}, \quad t \in \mathbb{R}.$$

Let $\hat{\Psi}_N$ be as in (23) and $\bar{\Theta}_N$ as in (28). Then we have for every fixed $t \in \mathbb{R}$ and a sequence $R_N = o_{P_{\theta_0}^N}(1)$ that as $N \rightarrow \infty$,

$$E^{\Pi^{\bar{\Theta}_N}}[\exp\{t\sqrt{N}(\langle \theta, \psi \rangle_{L^2(\mathcal{Z})} - \hat{\Psi}_N)\}|D_N] = e^{\frac{t^2}{2}\|\tilde{\psi}\|_{L^2(\mathcal{X})}^2} \times \frac{\int_{\bar{\Theta}_N} e^{\ell_N(\theta_{(t)})} d\Pi(\theta)}{\int_{\bar{\Theta}_N} e^{\ell_N(\theta)} d\Pi(\theta)} \times e^{R_N}.$$

PROOF. For W_N as in (25) with $h = \tilde{\psi}$, the posterior Laplace transform equals

$$\begin{aligned} E^{\Pi^{\bar{\Theta}_N}}[e^{t\sqrt{N}(\langle \theta, \psi \rangle_{L^2(\mathcal{Z})} - \hat{\Psi}_N)}|D_N] \\ = \frac{\int_{\bar{\Theta}_N} e^{t\sqrt{N}(\langle \theta - \theta_0, \psi \rangle_{L^2(\mathcal{Z})} - tW_N + \ell_N(\theta) - \ell_N(\theta_{(t)}) + \ell_N(\theta_{(t)})} d\Pi(\theta)}{\int_{\bar{\Theta}_N} e^{\ell_N(\theta)} d\Pi(\theta)} \end{aligned}$$

The main step in the proof is a uniform in $\theta \in \bar{\Theta}_N$ perturbation expansion of the log-likelihood ratios under $P_{\theta_0}^N$, recalling (7) and $\sigma = 1$,

$$\begin{aligned} \ell_N(\theta) - \ell_N(\theta_{(t)}) \\ &= -\frac{1}{2} \sum_{i=1}^N (\|Y_i - \mathcal{G}(\theta)(X_i)\|_V^2 - \|Y_i - \mathcal{G}(\theta_{(t)})(X_i)\|_V^2) \\ &= -\frac{1}{2} \sum_{i=1}^N (\|\mathcal{G}(\theta_0)(X_i) - \mathcal{G}(\theta)(X_i) + \varepsilon_i\|_V^2 - \|\mathcal{G}(\theta_0)(X_i) - \mathcal{G}(\theta_{(t)})(X_i) + \varepsilon_i\|_V^2) \\ &= -\sum_{i=1}^N (\langle \varepsilon_i, \mathcal{G}(\theta_0)(X_i) - \mathcal{G}(\theta)(X_i) \rangle_V - \langle \varepsilon_i, \mathcal{G}(\theta_0)(X_i) - \mathcal{G}(\theta_{(t)})(X_i) \rangle_V) \\ &\quad - \frac{1}{2} \sum_{i=1}^N (\|\mathcal{G}(\theta_0)(X_i) - \mathcal{G}(\theta)(X_i)\|_V^2 - \|\mathcal{G}(\theta_0)(X_i) - \mathcal{G}(\theta_{(t)})(X_i)\|_V^2) \equiv I + II. \end{aligned}$$

About term I, we ‘linearise’ the map $\mathcal{G}$ at θ_0 in each inner product to obtain

$$\begin{aligned} I &= \sum_{i=1}^N \langle \varepsilon_i, D\mathcal{G}_{\theta_0}(X_i)[\theta - \theta_{(t)}] \rangle_V \\ &\quad + \sum_{i=1}^N \langle \varepsilon_i, \mathcal{G}(\theta)(X_i) - \mathcal{G}(\theta_0)(X_i) - D\mathcal{G}_{\theta_0}(X_i)[\theta - \theta_0] \rangle_V \end{aligned}$$

$$\begin{aligned}
& - \sum_{i=1}^N \langle \varepsilon_i, \mathcal{G}(\theta_{(t)})(X_i) - \mathcal{G}(\theta_0)(X_i) - D\mathcal{G}_{\theta_0}(X_i)[\theta_{(t)} - \theta_0] \rangle_V \\
& = \frac{t}{\sqrt{N}} \sum_{i=1}^N \langle \varepsilon_i, D\mathcal{G}_{\theta_0}(X_i)[\tilde{\psi}] \rangle_V + R_{(0)}(\theta) - R_{(t)}(\theta) \\
& = tW_N + R_{(0)}(\theta) - R_{(t)}(\theta),
\end{aligned}$$

noting that $\theta_{(0)} = \theta$ and where the ‘remainder empirical processes’ are given by

$$R_{(t)} \equiv \sum_{i=1}^N \langle \varepsilon_i, \mathcal{G}(\theta_{(t)})(X_i) - \mathcal{G}(\theta_0)(X_i) - D\mathcal{G}_{\theta_0}(X_i)[\theta_{(t)} - \theta_0] \rangle_V.$$

We show in Lemma 4.3 below that for all $t \in \mathbb{R}$ fixed,

$$(30) \quad \sup_{\theta \in \Theta_N} |R_{(t)}(\theta)| = o_{P_{\theta_0}^N}(1)$$

so that these terms form a part of the sequence R_N .

For term II, we write E^X for the expectation under the X_i ’s only so that

$$\begin{aligned}
& - \frac{1}{2} \sum_{i=1}^N (\|\mathcal{G}(\theta_0)(X_i) - \mathcal{G}(\theta)(X_i)\|_V^2 - E^X \|\mathcal{G}(\theta_0)(X_i) - \mathcal{G}(\theta)(X_i)\|_V^2 \\
& - \|\mathcal{G}(\theta_0)(X_i) - \mathcal{G}(\theta_{(t)})(X_i)\|_V^2 + E^X \|\mathcal{G}(\theta_0)(X_i) - \mathcal{G}(\theta_{(t)})(X_i)\|_V^2) \\
& - \frac{N}{2} \|\mathcal{G}(\theta_0) - \mathcal{G}(\theta)\|_{L^2(\mathcal{X})}^2 + \frac{N}{2} \|\mathcal{G}(\theta_0) - \mathcal{G}(\theta_{(t)})\|_{L^2(\mathcal{X})}^2.
\end{aligned}$$

The sums in the first two lines are empirical processes and are shown in Lemma 4.4 below to be $o_{P_{\theta_0}^N}(1)$ uniformly in $\theta \in \Theta_N$ for every fixed t , and can thus also be absorbed into R_N .

For the terms in the last line of the last display, we can further decompose

$$\begin{aligned}
& \|\mathcal{G}(\theta_0) - \mathcal{G}(\theta_{(t)})\|_{L^2(\mathcal{X})}^2 \\
& = \|\mathcal{G}(\theta_{(t)}) - \mathcal{G}(\theta_0) - D\mathcal{G}_{\theta_0}[\theta_{(t)} - \theta_0] + D\mathcal{G}_{\theta_0}[\theta_{(t)} - \theta_0]\|_{L^2(\mathcal{X})}^2 \\
& = \|D\mathcal{G}_{\theta_0}[\theta_{(t)} - \theta_0]\|_{L^2(\mathcal{X})}^2 \\
& \quad + 2\langle D\mathcal{G}_{\theta_0}[\theta_{(t)} - \theta_0], \mathcal{G}(\theta_{(t)}) - \mathcal{G}(\theta_0) - D\mathcal{G}_{\theta_0}[\theta_{(t)} - \theta_0] \rangle_{L^2(\mathcal{X})} \\
& \quad + \|\mathcal{G}(\theta_{(t)}) - \mathcal{G}(\theta_0) - D\mathcal{G}_{\theta_0}[\theta_{(t)} - \theta_0]\|_{L^2(\mathcal{X})}^2
\end{aligned}$$

including also the case $\theta = \theta_{(0)}$ by convention for $t = 0$. Now using Conditions 3.2, 3.6 and the Cauchy–Schwarz inequality the last two remainder terms are bounded by a constant multiple of

$$\sup_{\theta \in \Theta_N} [\rho_{\theta_0}^2(\theta_{(t)} - \theta_0) + \|\theta_{(t)} - \theta_0\|_{L^2} \rho_{\theta_0}(\theta_{(t)} - \theta_0)] \lesssim \sigma_N^2 + \sigma_N \bar{\delta}_N = o(1/N).$$

The remaining terms in the expansion are

$$\begin{aligned}
& \frac{N}{2} \left(\left\| D\mathcal{G}_{\theta_0} \left[\theta - \theta_0 - \frac{t}{\sqrt{N}} \tilde{\psi} \right] \right\|_{L^2(\mathcal{X}, V)}^2 - \|D\mathcal{G}_{\theta_0}[\theta - \theta_0]\|_{L^2(\mathcal{X}, V)}^2 \right) \\
& = -t\sqrt{N} \langle D\mathcal{G}_{\theta_0}[\theta - \theta_0], D\mathcal{G}_{\theta_0}[\tilde{\psi}] \rangle_{L^2(\mathcal{X}, V)} + \frac{t^2}{2} \|D\mathcal{G}_{\theta_0}[\tilde{\psi}]\|_{L^2(\mathcal{X}, V)}^2 \\
& = -t\sqrt{N} \langle \theta - \theta_0, \mathbb{I}_{\theta_0}^* \mathbb{I}_{\theta_0} \tilde{\psi} \rangle_{L^2(\mathcal{Z}, W)} + \frac{t^2}{2} \|\mathbb{I}_{\theta_0}[\tilde{\psi}]\|_{L^2(\mathcal{X}, V)}^2
\end{aligned}$$

which, combined with Condition 3.3, the bounds from term I and the identity in the first display in this proof, implies the result. $\square$

4.3. Stochastic bounds on remainder terms and discretisation error. The following two key lemmas use tools from infinite-dimensional probability to bound the collections of empirical processes appearing as remainder terms in the proof of Proposition 4.2. While that proposition considers localisation to the sets $\bar{\Theta}_N$, the following bounds actually hold uniformly in the larger classes Θ_N from (17).

LEMMA 4.3. *We have (30).*

PROOF. For t fixed, define new functions $g_\theta : \mathcal{X} \rightarrow V$ as

$$g_\theta = \mathcal{G}(\theta_{(t)})(\cdot) - \mathcal{G}(\theta_0)(\cdot) - D\mathcal{G}_{\theta_0}(\cdot)[\theta_{(t)} - \theta_0].$$

Then the remainder term from (30), viewed as a stochastic process indexed by $\theta \in \Theta_N$, equals a centred (since $E\varepsilon_i = 0$) empirical process for the jointly i.i.d. variables (X_i, ε_i) of the form

$$|R_{(t)}(\theta)| = \left| \sum_{i=1}^N \langle \varepsilon_i, g_\theta(X_i) \rangle_V \right| = \left| \sum_{j=1}^{p_V} \sum_{i=1}^N \varepsilon_{i,j} g_{\theta,j}(X_i) \right| \leq \sum_{j=1}^{p_V} \left| \sum_{i=1}^N \varepsilon_{i,j} g_{\theta,j}(X_i) \right|.$$

Here, $g_{\theta,j}$ are the entries of the vector field $g_\theta \in V$, and the $\varepsilon_{i,j}$ are all i.i.d. $N(0, 1)$ variables. We will now bound the supremum over Θ_N of the each of the last p_V summands by using a moment inequality for the empirical process $\{\sum_{i=1}^N f_\theta(Z_i) : f \in \mathcal{F}\}$ where, for every $1 \leq j \leq p$ fixed (and with e denoting a real variable in this proof in slight abuse of notation),

$$f_\theta \in \mathcal{F} \equiv \mathcal{F}_j = \{f_\theta(z) = e g_{\theta,j}(x) : \theta \in \Theta_N\}, \quad z = (e, x) \in \mathbb{R} \times \mathcal{X},$$

and $Z_1, \dots, Z_N$ are i.i.d. copies of the variables $Z = (\varepsilon, X) \sim N(0, 1) \times \lambda = P$.

We will apply Theorem 3.5.4 in [21] but to do so need to calculate some preliminary bounds: First, by independence of X, ε , the ‘weak’ variances of $\mathcal{F}$ are of order

$$\sup_{\theta \in \Theta_N} E f_\theta^2(Z) = \sup_{\theta \in \Theta_N} E g_\theta^2(X) \leq \sup_{\theta \in \Theta_N} \rho_{\theta_0}^2(\theta_{(t)} - \theta_0) \leq \sigma_N^2$$

by Conditions 3.2 and 3.6. Next, by Condition 3.1, the L^∞ -norm mapping properties of $D\mathcal{G}_{\theta_0}$ (Condition 3.2) and the definition of Θ_N we have

$$\sup_{\theta \in \Theta_N} \|g_{\theta,j}\|_\infty \lesssim \|\theta_{(t)} - \theta_0\|_\infty \lesssim \bar{\delta}_N(1 + \|\tilde{\psi}\|_\infty) \lesssim \bar{\delta}_N.$$

As a consequence, the preceding empirical process has pointwise envelopes

$$\sup_{\theta \in \Theta_N} |f_\theta(e, x)| \lesssim |e| \bar{\delta}_N \equiv F_N(e, x) \quad \forall (e, x) \in \mathbb{R} \times \mathcal{X},$$

in particular $F_N > 0$ P -a.s. and

$$\|F\|_{L^2(P)}^2 := \int_{\mathbb{R} \times \mathcal{X}} F_N^2(z) dP(z) \lesssim \bar{\delta}_N^2, \quad \|F\|_{L^2(Q)}^2 := \int_{\mathbb{R} \times \mathcal{X}} F_N^2(z) dQ(z) = \bar{\delta}_N^2 s_Q^2,$$

where, for any (discrete, finitely supported) probability measure Q on $\mathbb{R} \times \mathcal{X}$, we have set $s_Q^2 := \int_{\mathbb{R} \times \mathcal{X}} e^2 dQ(e, x)$. Finally, we have again from Conditions 3.1 and 3.2, and for any $\theta, \theta' \in \Theta$ and some fixed constant c_0 that

$$\begin{aligned} \|f_\theta - f_{\theta'}\|_{L^2(Q)} &:= \sqrt{\int_{\mathbb{R}} \int_{\mathcal{X}} e^2 (g_{\theta,j}(x) - g_{\theta',j}(x))^2 dQ(e, x)} \\ &\leq s_Q \|g_\theta - g_{\theta'}\|_\infty \\ &\leq s_Q (\|\mathcal{G}(\theta_{(t)}) - \mathcal{G}(\theta'_{(t)})\|_\infty + \|\mathbb{I}_{\theta_0}[\theta_{(t)} - \theta'_{(t)}]\|_\infty) \\ &\leq c_0 \|F_N\|_{L^2(Q)} \|\theta - \theta'\|_\infty / \bar{\delta}_N. \end{aligned}$$

We conclude that any $\bar{\delta}_N \epsilon / c_0$ -covering of Θ_N for the norm $\|\cdot\|_\infty$ induces a $\|F_N\|_{L^2(Q)} \epsilon$ -covering of $\mathcal{F}$ for the $L^2(Q)$ norm, and so $J(\mathcal{F}, F, s)$ in (3.169) in [21] is bounded by a constant multiple of our $\mathcal{J}_N(s, \bar{\delta}_N)$ (using also Lemma 3.5.3a in [21]). With these preparations, we can now apply Theorem 3.5.4 in [21] where for our choice of envelope F_N we can take $\|U\|_{L^2(P)}$ in that theorem bounded by a constant multiple of $\sqrt{\log N} \bar{\delta}_N$ (using independence of X , ϵ and also Lemma 2.3.3 in [21]). The upper bound (3.171) in [21] then implies that

$$E \sup_{\theta \in \Theta_N} \left| \sum_{i=1}^N f_\theta(Z_i) \right| \lesssim \sqrt{N} \max \left[\bar{\delta}_N \mathcal{J}_N(\sigma_N / \bar{\delta}_N, \bar{\delta}_N), \frac{\sqrt{\log N} \bar{\delta}_N^3 \mathcal{J}_N^2(\sigma_N / \bar{\delta}_N, \bar{\delta}_N)}{\sqrt{N} \sigma_N^2} \right]$$

which in turn, using the substitution $\bar{\delta}_N \epsilon = \rho$ in (18), is bounded by a constant multiple of the maximum of the second and third terms appearing in (21). Hence the remainder terms from (30) converge to zero in expectation, and then also in probability (by Markov’s inequality). (Let us finally note that, strictly speaking, the application of Theorem 3.5.4 in [21] requires $0 \in \mathcal{F}$ and $\mathcal{F}$ countable: If $\|\theta_0\|_{\mathcal{R}} < M_N$, then $g_\theta = 0$ for $\theta = \theta_0 - (t/\sqrt{N})\tilde{\psi} \in \Theta_N$ and N large enough, so $0 \in \mathcal{F}$. Otherwise we can recenter f_θ at f_{θ_*} for some arbitrary θ_* and use a standard (one-dimensional) moment bound for $E|\sum_{i=1}^N f_{\theta_*}(Z_i)| \leq \sqrt{N} \sigma_N \rightarrow 0$. One then applies the previous argument to the class $\mathcal{F} - f_{\theta_*}$, so that the same overall bound holds true also in this case. Finally, by continuity of $\theta \mapsto g_{\theta,j}$ on the totally bounded set Θ_N , the supremum of the empirical process can be realised over a countable dense subset of Θ_N , so the assumption that $\mathcal{F}$ be countable can be met, too.) $\square$

LEMMA 4.4. *We have for any $t \in \mathbb{R}$ that*

$$\sup_{\theta \in \Theta_N} \left| \sum_{i=1}^N (\|\mathcal{G}(\theta_0)(X_i) - \mathcal{G}(\theta_{(t)})(X_i)\|_V^2 - E^X \|\mathcal{G}(\theta_0)(X_i) - \mathcal{G}(\theta)(X_i)\|_V^2) \right| = o_{P_{\theta_0}^N}(1)$$

PROOF. We will obtain a bound for the supremum of the empirical process $\{\sum_{i=1}^N (f(X_i) - Ef(X_i)) : f \in \mathcal{F}\}$, this time with indexing class

$$\mathcal{F} = \{f_\theta = \|\mathcal{G}(\theta_0)(\cdot) - \mathcal{G}(\theta_{(t)})(\cdot)\|_V^2 : \theta \in \Theta_N\}.$$

Using Condition 3.1, the envelopes of $\mathcal{F}$ can be taken to be

$$\sup_{\theta \in \Theta_N} \|\mathcal{G}(\theta_0) - \mathcal{G}(\theta_{(t)})\|_\infty^2 \lesssim \sup_{\theta \in \Theta_N} \|\theta_0 - \theta_{(t)}\|_\infty^2 \lesssim \bar{\delta}_N^2 \equiv F,$$

and we also have, since $\|\mathcal{G}(\theta)\|_\infty \leq C$ by Condition 3.1, that

$$\|f_\theta - f_{\theta'}\|_\infty \lesssim \|\theta - \theta'\|_\infty \quad \forall \theta, \theta' \in \Theta_N.$$

This implies, similar to the proof in the previous lemma, that a $c_0 \bar{\delta}_N^2 \epsilon$ -covering of Θ_N for the $\|\cdot\|_\infty$ -norm (and c_0 a small but fixed constant) induces a $\|F\|_{L^2(Q)} \epsilon$ -covering of $\mathcal{F}$ for the $L^2(Q)$ -norm (Q any probability measure), and that the functional $J(\mathcal{F}, F, s)$ in (3.169) in [21] is bounded by a constant multiple of our $\mathcal{J}(s, \bar{\delta}_N^2)$. The convergence to zero required in the lemma now follows from Theorem 3.5.4 in [21], in fact, Remark 3.5.5 after it, the requirement (20) from Condition 3.6, and Markov’s inequality. $\square$

4.4. *Gaussian change of variables.* We now control the ratio of Gaussian integrals appearing in Proposition 4.2.

PROPOSITION 4.5. *As $N \rightarrow \infty$, we have for any fixed $t \in \mathbb{R}$ that*

$$\frac{\int_{\bar{\Theta}_N} e^{\ell_N(\theta_{(t)})} d\Pi(\theta)}{\int_{\bar{\Theta}_N} e^{\ell_N(\theta)} d\Pi(\theta)} \rightarrow_{P_{\theta_0}^N} 1.$$

PROOF. If we denote by Π_t the Gaussian law of $\theta_{(t)} = \theta - (t/\sqrt{N})\tilde{\psi}$, then the Cameron–Martin theorem (e.g., Theorem 2.6.13 in [21]) provides the formula for the Radon–Nikodym density of

$$\frac{d\Pi_t}{d\Pi}(\theta) = \exp\left\{\frac{t}{\sqrt{N}}\langle\theta, \tilde{\psi}\rangle_{\mathcal{H}_N} - \frac{t^2}{2N}\|\tilde{\psi}\|_{\mathcal{H}_N}^2\right\}, \quad \theta \sim \Pi, \tilde{\psi} \in \mathcal{H}_N.$$

The ratio in the proposition thus equals

$$\frac{e^{-\frac{t^2}{2N}\|\tilde{\psi}\|_{\mathcal{H}_N}^2} \int_{\bar{\Theta}_{N,t}} e^{\ell_N(\vartheta)} e^{\frac{t}{\sqrt{N}}\langle\vartheta, \tilde{\psi}\rangle_{\mathcal{H}_N}} d\Pi(\vartheta)}{\int_{\bar{\Theta}_N} e^{\ell_N(\theta)} d\Pi(\theta)}, \quad \text{where } \bar{\Theta}_{N,t} = \{\theta_{(t)} : \theta \in \bar{\Theta}_N\}.$$

Uniformly in $\theta \in T_N^c \subset \bar{\Theta}_N$ from (28), we have as $N \rightarrow \infty$ that $|(t/\sqrt{N})\langle\theta, \tilde{\psi}\rangle_{\mathcal{H}_N}| \lesssim \delta_N \|\tilde{\psi}\|_{\mathcal{H}_N} \rightarrow 0$ by the requirement (19) in Condition 3.6, which also implies that $(t^2/N)\|\tilde{\psi}\|_{\mathcal{H}_N}^2 = o(1)$ since $1/\sqrt{N} = o(\delta_N)$. Now since

$$\frac{|t|}{\sqrt{N}} \sup_{\vartheta \in \bar{\Theta}_{N,t}} |\langle\vartheta, \tilde{\psi}\rangle_{\mathcal{H}_N}| \leq \frac{|t|}{\sqrt{N}} \sup_{\theta \in T_N^c} |\langle\theta, \tilde{\psi}\rangle_{\mathcal{H}_N}| + \frac{t^2}{N} \|\tilde{\psi}\|_{\mathcal{H}_N}^2$$

we deduce from what precedes that the last ratio of integrals equals

$$e^{o(1)} \times \frac{\int_{\bar{\Theta}_{N,t}} e^{\ell_N(\vartheta)} d\Pi(\vartheta)}{\int_{\bar{\Theta}_N} e^{\ell_N(\theta)} d\Pi(\theta)} = e^{o(1)} \times \frac{\Pi(\bar{\Theta}_{N,t}|D_N)}{\Pi(\bar{\Theta}_N|D_N)}.$$

The denominator converges to 1 in $P_{\theta_0}^N$ -probability by (28), and so does then the numerator, using again (28) and that $t\|\tilde{\psi}\|_{\infty}/\sqrt{N} = o(\delta_N)$ and $t\|\tilde{\psi}\|_{\mathcal{R}}/\sqrt{N} = o(M_N)$ under the maintained assumptions. $\square$

Combining Propositions 4.2 and 4.5, we have shown that for all $t \in \mathbb{R}$, as $N \rightarrow \infty$,

$$(31) \quad E^{\Pi^{\bar{\Theta}_N}}[\exp\{t\sqrt{N}(\langle\theta, \psi\rangle_{L_\zeta^2(\mathcal{Z})} - \hat{\Psi}_N)\}|D_N] \rightarrow \exp\left\{\frac{t^2}{2}\|\mathbb{I}_{\theta_0}\tilde{\psi}\|_{L_\lambda^2(\mathcal{X})}^2\right\}$$

in $P_{\theta_0}^N$ -probability and, therefore, using also (29), for $\theta \sim \Pi(\cdot|D_N)$,

$$(32) \quad \sqrt{N}(\langle\theta|D_N, \psi\rangle_{L_\zeta^2(\mathcal{Z})} - \hat{\Psi}_N) \rightarrow^d N(0, \|\mathbb{I}_{\theta_0}\tilde{\psi}\|_{L_\lambda^2(\mathcal{X})}^2)$$

by the in $P_{\theta_0}^N$ -probability version of the usual implication that convergence of Laplace transforms implies convergence in distribution (see the Appendices of [41] or [9]). This completes the proof of Theorem 3.7.

4.5. *Convergence of the posterior mean.* The proof combines ideas from [6, 39–41]. The key lemma is the following stochastic bound on the posterior second moments.

LEMMA 4.6. *Under the hypotheses of Theorem 3.8, we have*

$$NE^{\Pi}[(\langle\theta, \psi\rangle_{L_\zeta^2(\mathcal{Z})} - \hat{\Psi}_N)^2|D_N] = O_{P_{\theta_0}^N}(1)$$

PROOF. The left-hand side in the last display is bounded by

$$2NE^\Pi[\langle\theta - \theta_0, \psi\rangle_{L^2_\zeta(\mathcal{Z})}^2 | D_N] + 2N(\hat{\Psi}_N - \langle\theta_0, \psi\rangle_{L^2_\zeta(\mathcal{Z})})^2$$

and in view of (23), the second term in the last decomposition is bounded in $P_{\theta_0}^N$ -probability by the central limit theorem applied to W_N from (25) with $h = \tilde{\psi}_{\theta_0}$ (one also applies the continuous mapping theorem for $x \mapsto x^2$ and Prohorov's theorem to deduce from convergence in distribution of NW_N^2 that it is uniformly tight.)

It hence remains to bound the first term in the last decomposition. Define $A_N = \{\|\theta - \theta_0\|_\infty \leq \bar{\delta}_N\} \subset \Theta$ and write the first quantity in the last display as (two times)

$$(33) \quad NE^\Pi[\langle\theta - \theta_0, \psi\rangle_{L^2_\zeta(\mathcal{Z})}^2 1_{A_N} | D_N] + NE^\Pi[\langle\theta - \theta_0, \psi\rangle_{L^2_\zeta(\mathcal{Z})}^2 1_{A_N^c} | D_N] = I + II.$$

To deal with term II, we apply the Cauchy–Schwarz inequality to obtain the bound

$$N\sqrt{E^\Pi[\langle\theta - \theta_0, \psi\rangle_{L^2(\mathcal{Z})}^4 | D_N]}\sqrt{\Pi(\|\theta - \theta_0\|_\infty > \bar{\delta}_N | D_N)}$$

and we now show that this term is bounded in $P_{\theta_0}^N$ -probability: Using Condition 3.5, Lemma 4.1, Markov's inequality and $E_{\theta_0}^N e^{\ell_N(\theta) - \ell_N(\theta_0)} = 1$, we indeed have

$$\begin{aligned} & P_{\theta_0}^N(E^\Pi[\langle\theta - \theta_0, \psi\rangle_{L^2(\mathcal{Z})}^4 | D_N]\Pi(\|\theta - \theta_0\|_\infty > \bar{\delta}_N | D_N) > N^{-2}) \\ & \leq P_{\theta_0}^N(E^\Pi[\langle\theta - \theta_0, \psi\rangle_{L^2(\mathcal{Z})}^4 | D_N]e^{-(L+1)N\delta_N^2} > N^{-2}) + o(1) \\ & = P_{\theta_0}^N\left(\frac{\int_\Theta \langle\theta - \theta_0, \psi\rangle_{L^2(\mathcal{Z})}^4 e^{\ell_N(\theta) - \ell_N(\theta_0)} d\Pi(\theta)}{\int_\Theta e^{\ell_N(\theta) - \ell_N(\theta_0)} d\Pi(\theta)} > e^{(L+1)N\delta_N^2} N^{-2}, \mathcal{C}_N\right) + o(1) \\ & \leq \|\psi\|_{L^2(\mathcal{Z})}^4 e^{-N\delta_N^2} N^2 \int_\Theta \|\theta - \theta_0\|_{L^2(\mathcal{Z})}^4 E_{\theta_0}^N e^{\ell_N(\theta) - \ell_N(\theta_0)} d\Pi(\theta) + o(1) \\ & \lesssim N^2 e^{-N\delta_N^2} + o(1) \rightarrow 0 \end{aligned}$$

as $N \rightarrow \infty$, by hypothesis on δ_N , Π_N . Collecting what precedes implies that the term II in (33) is indeed $O_{P_{\theta_0}^N}^N(1)$.

The next step is to bound the term I in (33). Recalling that $\Pi^{\bar{\Theta}_N}[\cdot | D_N]$ denotes the posterior distribution arising from prior restricted and renormalised to $\bar{\Theta}_N$, we decompose

$$\begin{aligned} & NE^\Pi[\langle\theta - \theta_0, \psi\rangle_{L^2(\mathcal{Z})}^2 1_{A_N} | D_N] \\ & = NE^{\Pi^{\bar{\Theta}_N}}[\langle\theta - \theta_0, \psi\rangle_{L^2(\mathcal{Z})}^2 1_{A_N} | D_N] \\ & \quad + NE^\Pi[\langle\theta - \theta_0, \psi\rangle_{L^2(\mathcal{Z})}^2 1_{A_N} | D_N] - NE^{\Pi^{\bar{\Theta}_N}}[\langle\theta - \theta_0, \psi\rangle_{L^2(\mathcal{Z})}^2 1_{A_N} | D_N] \\ & = A + B. \end{aligned}$$

For term A, using $x^2 \leq 2e^x$, $x \geq 0$, the definition of $\hat{\Psi}_N$ from (23) and $W_N = O_{P_{\theta_0}^N}(1)$ with $h = \tilde{\psi}_{\theta_0}$ from (25), the limit (31) at $t = 1$ implies that for all N large enough and some $r_N = o_{P_{\theta_0}^N}(1)$,

$$A \leq 2e^{W_N + r_N} e^{\frac{1}{2}\|\mathbb{I}_{\theta_0}\tilde{\psi}\|_{L^2(\mathcal{X}, V)}^2},$$

and hence this term is stochastically bounded.

Finally, by definition of the events A_N , the term $|B|$ can be written as

$$\begin{aligned} N \left| \int_{A_N} \langle \theta - \theta_0, \psi \rangle_{L^2(\mathcal{Z})}^2 [d\Pi(\theta|D_N) - d\Pi^{\tilde{\Theta}_N}(\theta|D_N)] \right| \\ \leq N \bar{\delta}_N^2 \|\psi\|_{L^1(\mathcal{Z})}^2 \|\Pi(\cdot|D_N) - \Pi^{\tilde{\Theta}_N}(\cdot|D_N)\|_{\text{TV}} \\ \lesssim N \bar{\delta}_N^2 \Pi(\tilde{\Theta}_N^c|D_N) \lesssim N \bar{\delta}_N^2 O_{P_{\theta_0}^N}(e^{-(L+1)N\bar{\delta}_N^2}) = o_{P_{\theta_0}^N}(1), \end{aligned}$$

where we have used (29) and (28), completing the proof of the lemma. $\square$

Now to prove the theorem note that by (32) and (8) we have for

$$Z_n|D_N \equiv \sqrt{N}(\langle \theta, \psi \rangle_{L_\xi^2(\mathcal{Z})} - \hat{\Psi}_N)|D_N, \quad Z \sim N(0, \|\mathbb{I}_{\theta_0} \tilde{\psi}\|_{L_\lambda^2(\mathcal{X})}^2)$$

and d_{weak} any metric for weak convergence of laws $\mathcal{L}(\cdot)$ on $\mathbb{R}$,

$$(34) \quad d_{\text{weak}}(\mathcal{L}(Z_n|D_N), \mathcal{L}(Z)) \xrightarrow{P_{\theta_0}^N} 0.$$

The idea of the proof of follow is that the previous lemma implies (by uniform integrability) convergence of moments in the last limit (34), and thus that, since $EZ = 0$, the posterior mean equals $\hat{\Psi}_N$ up to a stochastic term of order $o(1/\sqrt{N})$. However, as the probability measures $\mathcal{L}(Z_n|D_N)$ to which this argument is applied are *random* via the data D_N , the proof requires some care. We will employ a contradiction argument: To prove Theorem 3.8, it suffices by Theorem 3.7, Slutsky's lemma and (25) with $h = \tilde{\psi}_{\theta_0}$ to prove that as $N \rightarrow \infty$,

$$(35) \quad \sqrt{N}(\langle E^\Pi[\theta|D_N], \psi \rangle_{L_\xi^2(\mathcal{Z})} - \hat{\Psi}_N) \rightarrow^{\text{Pr}} 0,$$

where we write Pr for the probability measure $P_{\theta_0}^{\mathbb{N}}$ on the underlying measurable space $(\Omega, \mathcal{S}) := ((V \times \mathcal{X})^{\mathbb{N}}, \mathcal{S})$ supporting all data variables $(D_N, N \in \mathbb{N})$. Suppose the last limit does not hold true. Then there exists $\Omega' \in \mathcal{S}$ of positive probability $\text{Pr}(\Omega') > \tau$ and $\zeta' > 0$ such that along a subsequence of N (still denoted by N) we have

$$(36) \quad |\sqrt{N}(\langle E^\Pi[\theta|D_N(\omega)], \psi \rangle_{L_\xi^2(\mathcal{Z})} - \hat{\Psi}_N(\omega))| \geq \zeta' > 0 \quad \text{for } \omega \in \Omega'.$$

Now since convergence in Pr -probability implies Pr -almost sure convergence along a subsequence, we can extract a further subsequence of N such that (34) holds almost surely, that is, on an event $\Omega_0 \subset \Omega$ such that $\text{Pr}(\Omega_0) = 1$. For each fixed $\omega \in \Omega_0$, we can use the Skorohod imbedding (Theorem 11.7.2 in [16]) to construct (if necessary on a new probability space) new real random variables $\tilde{Z}_N, \tilde{Z}$ such that their laws satisfy

$$\mathcal{L}(\tilde{Z}_N) = \mathcal{L}(Z_n|D_N(\omega)), \quad \mathcal{L}(\tilde{Z}) = \mathcal{L}(Z), \quad \tilde{Z}_N \xrightarrow{a.s.} \tilde{Z},$$

and we also know by Lemma 4.6 that $E\tilde{Z}_N^2 = E[Z_N^2|D_N(\omega)] = O(1)$ for all $\omega \in \Omega'_0 \subset \Omega_0$ of probability $\text{Pr}(\Omega'_0) > 1 - \tau$ as close to one as desired. But this implies that the $(\tilde{Z}_N : N \in \mathbb{N})$ are uniformly integrable real random variables so that almost sure convergence implies convergence of first moments ([16], Theorem 10.3.6), that is,

$$E|Z_n|D_N(\omega) - Z| = E|\tilde{Z}_N - \tilde{Z}| \rightarrow_{N \rightarrow \infty} 0$$

for all $\omega \in \Omega'_0$. In particular then, using also Fubini's theorem,

$$\begin{aligned} (37) \quad \sqrt{N}(\langle E^\Pi[\theta|D_N(\omega)], \psi \rangle_{L_\xi^2(\mathcal{Z})} - \hat{\Psi}_N(\omega)) &= E^\Pi[\sqrt{N}(\langle \theta, \psi \rangle - \hat{\Psi}_N)|D_N(\omega)] \\ &\rightarrow EZ = 0 \end{aligned}$$

for $\omega \in \Omega'_0$. But if the last limit holds for all $\omega \in \Omega'_0$ with probability $\text{Pr}(\Omega'_0) > 1 - \tau$ we have a contradiction to (36) (as then $\text{Pr}(\Omega) \geq \text{Pr}(\Omega') + \text{Pr}(\Omega'_0) > 1 - \tau + \tau = 1$), completing the proof of (35), and thus of the theorem.

5. Proofs for non-Abelian X -ray and Schrödinger equation. The proofs proceed by verifying the hypotheses of Theorems 3.7 and 3.8.

5.1. Proof of Theorem 2.1. We follow ideas laid out in [41] for a more restrictive class of priors and a simpler noise model. In particular in our setting Θ is unbounded and we therefore need to explicitly track the growth of various constants in the PDE estimates used in [41]. These have been obtained in the recent article [44] in the study of a related problem, and we will refer repeatedly to [44] in the proofs that follow.

A key role is played by the linear $L^2(\mathcal{X})$ -self-adjoint ‘inverse Schrödinger’ integral operator $\mathbb{V}_f$, $f > 0$ smooth, furnishing unique solutions $u_{f,\psi} = \mathbb{V}_f[\psi]$ of the PDE,

$$(38) \quad \mathbb{S}_f(u_{f,\psi}) = \psi \quad \text{on } \mathcal{X}, \quad \text{s.t.} \quad u_{f,\psi} = 0 \quad \text{on } \partial\mathcal{X}, \quad \text{for all } \psi \in C(\mathcal{X}),$$

where we recall the Schrödinger operator $\mathbb{S}_f(h) = \frac{\Delta}{2}h - fh$. We also have for $\psi \in C_0^2(\mathcal{X}) := C^2(\mathcal{X}) \cap \{\psi|_{\partial\mathcal{X}} = 0\}$ that

$$(39) \quad \mathbb{V}_f[\mathbb{S}_f[\psi]] = \psi \quad \text{on } \mathcal{X}.$$

See Chapter 3 in [11] (or also Proposition 22 in [41]) for these facts. We will also repeatedly use below that the linear operator $\mathbb{V}_f$ is Lipschitz-continuous on $L_\lambda^p(\mathcal{X})$ for $p = 2, \infty$, with Lipschitz constant independent of f ; see, for example, Lemma 25 in [44] for a proof.

Condition 3.1: Let us write $\theta = \phi^{-1} \circ f$, $\theta' = \phi^{-1} \circ h$ for $\theta, \theta' \in \Theta$ so that

$$\mathcal{G}(\theta) - \mathcal{G}(\theta') = u_f - u_h = \mathbb{V}_f[(f - h)u_h].$$

Using L^p -continuity of $\mathbb{V}_f$ and that composition with regular link functions is Lipschitz for L^p -norms (Lemma 29 in [44]),

$$(40) \quad \|\mathbb{V}_f[(f - h)u_h]\| \lesssim \|u_h\|_\infty \|f - h\| \lesssim \|\theta - \theta'\|$$

both for $\|\cdot\|$ equal to the $L^2(\mathcal{X})$ and the $L^\infty(\mathcal{X})$ -norm, and with constants independent of f . Here, we have used also that

$$(41) \quad \|u_h\|_\infty \leq c \|g\|_\infty, \quad 0 \leq h \in C^\beta,$$

for a fixed constant $c > 0$, as follows, for example, from the Feynman–Kac representation of u_h (see (5.35) in [44]). Then (41) also implies the first inequality in Condition 3.1.

Conditions 3.2 and 3.3: If $f_0 = \phi(\theta_0)$, $f_h = \phi(\theta_0 + h)$, then Proposition 4 in [41] and again regularity of the link function ϕ imply, for $\mathbb{V}_f$ the inverse Schrödinger operator,

$$\|u_{f_h} - u_{f_0} - \mathbb{V}_{f_0}[u_{f_0}(f_h - f_0)]\|_{L^2(\mathcal{X})} = O(\|f_h - f_0\|_\infty^2) = O(\|h\|_\infty^2).$$

Then by the chain rule for $\phi \circ \theta$ and continuity of the operator $\mathbb{V}_{f_0}$ on $C(\mathcal{X})$,

$$(42) \quad \|u_{f_h} - u_{f_0} - \mathbb{V}_{f_0}[u_{f_0}\phi'(\theta_0)h]\|_{L^2(\mathcal{X})} = O(\|h\|_\infty^2)$$

which shows that the linearised ‘score’ operator $\mathbb{I}_{\theta_0} : L^2(\mathcal{X}) \rightarrow L^2(\mathcal{X})$ equals

$$(43) \quad \mathbb{I}_{\theta_0} = \mathbb{V}_{f_0}[u_{f_0}\phi'(\theta_0)\cdot] \quad \text{with adjoint } \mathbb{I}_{\theta_0}^* = u_{f_0}\phi'(\theta_0)\mathbb{V}_{f_0}[\cdot].$$

We see that $\mathbb{I}_{\theta_0}$ is a continuous operator on both $L^2(\mathcal{X})$ and $L^\infty(\mathcal{X})$ since $\mathbb{V}_{f_0}$ is and since both u_{f_0} and $\phi'(\theta_0)$ are bounded functions. Now as in Section 4.2 in [41] we can define

$$(44) \quad \tilde{\psi} \equiv (\mathbb{I}_{\theta_0}^* \mathbb{I}_{\theta_0})^{-1}(\psi) \equiv \frac{\mathbb{S}_{f_0} \mathbb{S}_{f_0}[\frac{\psi}{u_{f_0}\phi'(\theta_0)}]}{u_{f_0}\phi'(\theta_0)}, \quad \psi \in C^\infty(\mathcal{X}),$$

where we note that $\min(u_{f_0}, \phi'(\theta_0)) > 0$ throughout $\mathcal{X}$ by $g \geq g_{\min}$ and the Feynman–Kac formula (cf. (5.36) in [44]) and since $\theta_0 \in C^\infty(\mathcal{X})$ is bounded. Moreover, since f_0 is

smooth by assumption we also have $u_{f_0} \in C^\infty(\mathcal{X})$ (as in Lemma 27 in [44], for instance). Then, for all $\psi \in C^{\infty,2}(\mathcal{X})$ one checks directly from the definitions and the product rule that $\mathbb{S}_{f_0}[\psi/(u_{f_0}\phi'(\theta_0))] \in C_0^2(\mathcal{X})$. We can thus apply (39) to obtain

$$\mathbb{I}_{\theta_0}\tilde{\psi} = \mathbb{V}_{f_0}\left[\mathbb{S}_{f_0}\mathbb{S}_{f_0}\left[\frac{\psi}{u_{f_0}\phi'(\theta_0)}\right]\right] = \mathbb{S}_{f_0}\left[\frac{\psi}{u_{f_0}\phi'(\theta_0)}\right]$$

and another application of (39) implies $\mathbb{I}_{\theta_0}^*\mathbb{I}_{\theta_0}\tilde{\psi} = \psi$, and hence Condition 3.3, in particular, $(\mathbb{I}_{\theta_0}^*\mathbb{I}_{\theta_0})^{-1}$ is a proper inverse mapping $C^{\infty,2}(\mathcal{X})$ into $C^\infty(\mathcal{X})$. What precedes also explains the form of the asymptotic variance in Theorem 2.1.

Conditions 3.4 and 3.5: We will use results in [23] for general nonlinear inverse problems. Using the bounds (40) and (41), the conditions formulated at the beginning of Section A in [23] can be verified for the PDE arising from the Schrödinger equation with $\kappa = \gamma = 0$. Lemma 16 in [23] (which for $\kappa = 0$ permits to replace H_c^α by H^α in its Condition 3) then verifies the lower bound for $\pi(\delta_N)$ in Condition 3.4 for the rescaled prior Π_N with RKHS,

$$\mathcal{H}_N = (H^\alpha(\mathcal{X}), \sqrt{N}\delta_N \|\cdot\|_{H^\alpha(\mathcal{X})}) \quad \text{where } \delta_N = N^{-\alpha/(2\alpha+d)}.$$

Moreover, since $E\|\theta'\|_{L^2}^4 < \infty$ the moment condition is also verified. To verify Condition 3.5, we will choose as regularisation space $\mathcal{R} = C^\beta(\mathcal{X})$ equipped with the C^β -norm for any $\max(2, d/2) < \beta < \alpha - d/2$. We apply Theorem 14 in [23] to the effect that we can find $L_0, M > 0$ large enough depending on L such that the set

$$\tilde{\Theta}_N = \{\theta \in \mathcal{R} : \|u_{\phi(\theta)} - u_{\phi(\theta_0)}\|_{L^2} \leq L_0\delta_N; \|\theta\|_{C^\beta} \leq M\}$$

satisfies

$$\Pi(\tilde{\Theta}_N^c | D_N) = o_{P_{\theta_0}^N}(\eta_N), \quad \eta_N = e^{-(L+1)N\delta_N^2}.$$

We next show that for all N large enough

$$\tilde{\Theta}_N \subset \Theta_N = \{\theta \in \mathcal{R} : \|\theta - \theta_0\|_\infty \leq \bar{\delta}_N; \|\theta\|_{C^\beta} \leq M\},$$

and hence Condition 3.5, for convergence rate

$$\bar{\delta}_N \equiv N^{-r(\alpha)} \quad \text{for any } r(\alpha) < \frac{\alpha}{2\alpha+d} \cdot \frac{\beta - \frac{d}{2}}{\beta + 2}, \alpha > \beta - d/2 > 0.$$

Indeed, just as in Lemma 28 in [44], using the Sobolev imbedding theorem, standard interpolation inequalities for Sobolev spaces (e.g., (5.9) in [44]) and regularity estimates for the Schrödinger equation (e.g., Lemma 27 in [44]), we have

$$\begin{aligned} \|f - f_0\|_\infty &\lesssim \|u_f - u_{f_0}\|_{C^2} \\ &\lesssim \|u_f - u_{f_0}\|_{H^{2+d/2+\epsilon}} \\ &\lesssim \|u_f - u_{f_0}\|_{L^2}^\theta \|u_f - u_{f_0}\|_{H^{\beta+2}}^{1-\theta} \\ &\lesssim \delta_N^\theta (\|f\|_{C^\beta} + \|f_0\|_{C^\beta}) = o(\bar{\delta}_N) \end{aligned}$$

where $\theta = (\beta - d/2 - \epsilon)/(\beta + 2)$. By our hypotheses on β , the sequence $\bar{\delta}_N$ converges to zero and since $f_0 > f_{\min}$ we then also have $\inf_{x \in \mathcal{X}} f(x) > f_{\min}$ for all N large enough. Then composition with ϕ^{-1} is Lipschitz on $(f_{\min}, \infty)$ so that $\|\theta - \theta_0\|_\infty \lesssim \|f - f_0\|_\infty$ and we finally deduce the inclusion $\tilde{\Theta}_N \subset \Theta_N$ follows for all large enough N .

Conditions 3.4 and 3.6: The conditions (20) and (21) are checked, in Section 5.3. The RKHS-norm of the rescaled Whittle–Matérn prior from (10) equals

$$(45) \quad \delta_N \|\tilde{\psi}\|_{\mathcal{H}_N} = \sqrt{N}\delta_N^2 \|\tilde{\psi}\|_{H^\alpha(\mathcal{X})} \rightarrow 0$$

as $N \rightarrow \infty$ since $\tilde{\psi} \in C^\infty(\mathcal{X}) \subset \mathcal{R} \cap H^\alpha(\mathcal{X})$ (cf. after (44)) and $\alpha > d/2$, verifying (19).

5.2. *Proof of Theorem 2.2.* We again verify the general Conditions 3.1–3.6.

Condition 3.1: The Lipschitz estimate for L^2 and L^∞ norms follows from Theorem 2.2 (case $k = 0$) in [40]. The uniform boundedness of the forward map is clear since $\mathcal{G}(\theta)$ takes values in the compact group $\mathrm{SO}(n)$.

Conditions 3.2 and 3.3: The quadratic approximation for the linearisation is checked in Lemma 6.1 with $\rho_{\theta_0}(h) \lesssim \|h\|_\infty^2$. For the required mapping properties of $\mathbb{I}_{\theta_0}$ on L^2 and on L^∞ , see Remark 6.10. Theorem 6.5 allows us to define $\tilde{\psi}_{\theta_0} = (\mathbb{I}_{\theta_0}^* \mathbb{I}_{\theta_0})^{-1} \psi$, which determines another element of $C^\infty(M, \mathfrak{so}(n)) \subset H^\alpha(M)$.

Conditions 3.4 and 3.5: The verification of this condition is based on results in [40], with our prior satisfying Condition 3.1 there. The lower bound for $\pi(\delta_N)$ is given in Lemmas 5.15 and 5.16 in [40] with $\delta_N = N^{-\alpha/(2\alpha+2)}$, and the finiteness of fourth moments of the prior is also clear. Next, it is shown in Theorem 5.19 in [40], that we can take for $\mathcal{R}$ a C^β -Hölder-space, $M_N = M < \infty$, and for any integer β' s.t. $1 < \beta' < \beta < \alpha - 1$,

$$(46) \qquad \bar{\delta}_N = N^{-\frac{\alpha}{2\alpha+2} \frac{(\beta'-1)^2}{(\beta')^2}} = N^{-r(\alpha)},$$

since the $L^\infty(M)$ -rate can be bounded by the $H^{1+\epsilon}(M)$ -rate (Sobolev imbedding), which in turn can be bounded by the L^2 -rate to the power $(\beta - 1 - \epsilon)/\beta$ in view of the usual interpolation inequality for Sobolev norms. Also, we can choose η_N as desired (noting that the conclusion of Theorem 5.19 in [40], in fact, holds for any $C > 0$ large enough provided m', m'' are large enough).

Condition 3.6: The conditions (20) and (21) are checked in Section 5.3. For the prior-related conditions, we notice that the isomorphism theorem in Section 6.1 implies $\tilde{\psi}_{\theta_0} \in C^\infty(M) \subset \mathcal{R} \cap H^\alpha(M)$ and so as $N \rightarrow \infty$, since $\alpha > 1$,

$$(47) \qquad \delta_N \|\tilde{\psi}_{\theta_0}\|_{\mathcal{H}_N} = \sqrt{N} \delta_N^2 \|\tilde{\psi}_{\theta_0}\|_{H^\alpha(M)} \rightarrow 0.$$

5.3. *About conditions (20) and (21).* We finally check the quantitative conditions (20) and (21) for $\alpha - d/2 > \beta > 2d$ large enough—the proofs are the same for both inverse problems and, in fact, only depend on the fact that Θ_N is a subset of a C^β -ball and that its L^∞ -rate of contraction about θ_0 is $\bar{\delta}_N = N^{-r(\alpha)}$, $r(\alpha) > 0$, as well as on the quadratic approximation $\rho_{\theta_0}(h) = O(\|h\|_\infty^2)$ in Condition 3.2: The covering numbers of a β -Hölder ball in dimension d are of the order

$$\log N(\Theta_N, \|\cdot\|_\infty, \epsilon) \lesssim \left(\frac{1}{\epsilon}\right)^{d/\beta}, \quad \beta > 0,$$

see (4.184) in [21] for the case when the Hölder functions are defined over $[0, 1]^d$, and this bound applies to our setting by a standard extension arguments (and regarding $M, \mathcal{X}$ as subsets of $[0, 1]^d$, with $d = 2$ in the former case). Also, by the preceding proofs we can take

$$\rho_{\theta_0}(\theta - \theta_0 + (t/\sqrt{N})\tilde{\psi}) \lesssim \bar{\delta}_N^2 \equiv \sigma_N.$$

We first note that the quantity in (20) is bounded by

$$(48) \qquad \sqrt{N} \bar{\delta}_N^2 \int_0^1 (\bar{\delta}_N^2 \epsilon)^{-d/(2\beta)} d\epsilon \lesssim \sqrt{N} \bar{\delta}_N^{2-\frac{d}{\beta}}$$

since $\beta > d/2$. We will eventually show that the last bound converges to zero as $N \rightarrow \infty$, which also implies $N\sigma_N^2 \lesssim N\bar{\delta}_N^4 \rightarrow 0$. The middle term in the maximum in (21) can similarly be bounded by

$$\sqrt{N} \mathcal{J}_N(\sigma_N, 1) = \sqrt{N} \int_0^{\sigma_N} \epsilon^{-d/(2\beta)} d\epsilon \lesssim \sqrt{N} \bar{\delta}_N^{2-\frac{d}{\beta}},$$

and hence is of the same order as the one in (48). For the third member in the maximum (21) we have, by a similar calculation,

$$(49) \quad \frac{\bar{\delta}_N \sqrt{\log N}}{\sigma_N^2} \mathcal{J}_N^2(\sigma_N, 1) \lesssim \sqrt{\log N} \bar{\delta}_N^{1-\frac{2d}{\beta}}.$$

We can conclude from what precedes that it suffices to show that

$$(50) \quad \max(\sqrt{N} \bar{\delta}_N^{2-\frac{d}{\beta}}, N \bar{\delta}_N^3, \sqrt{\log N} \bar{\delta}_N^{1-\frac{2d}{\beta}}) \rightarrow 0$$

as $N \rightarrow \infty$. This requires $\beta > 2d$ and then simplifies to the basic requirement $N \bar{\delta}_N^3 \rightarrow 0$. In both the Schrödinger and the X -ray case, we have $\bar{\delta}_N = N^{-r(\alpha)}$ with precise exponent $r(\alpha) > 0$ given in the preceding subsections, which thus simplifies to $r(\alpha) > 1/3$. For the rate $\bar{\delta}_N$ obtained in the Schrödinger model, this necessitates (11) to hold, while in the X -ray case the corresponding rate translates into the condition

$$(51) \quad \frac{\alpha}{2\alpha + 2} \frac{(\alpha - 2)^2}{(\alpha - 1)^2} > 1/3,$$

satisfied for $\alpha \geq 9$. Both requirements on α imply in particular that we can choose β such that $2d < \beta < \alpha - d/2$ (with $d = 2$ in the X -ray case).

6. Analytical results for non-Abelian X -ray transforms.

6.1. Main results. This section contains the definitions and statements for the main analytical results needed on the non-Abelian X -ray transform, whose proofs can be found in Sections 6.2, 6.3 and 6.4. In particular, we compute the linearization of the map $\Phi \mapsto C_\Phi$ defined in (13) and its associated Fisher information operator. We then prove forward mapping properties of these operators in a fairly general setting (convex, nontrapping Riemannian manifolds). Finally, we show in the case of the Euclidean disk that the Fisher information operator is a bijection in suitable spaces.

6.1.1. Linearization and forward mapping properties on convex, nontrapping manifolds. Consider (M, g) a d -dimensional Riemannian manifold with boundary that is nontrapping (in the sense that every geodesic reaches ∂M in finite time) and has strictly convex boundary (in the sense of having a positive definite second fundamental form Π). For background on such manifolds and the definitions that follow, we refer to [48, 57]. Let SM denote the unit sphere bundle on M , that is,

$$SM := \{(x, v) \in TM : |v|_g = 1\}$$

with footpoint projection $\pi : SM \rightarrow M$. We define the volume form on SM by $d\Sigma^{2d-1}(x, v) = dV^d(x) \wedge dS_x(v)$, where dV^d is the volume form on M and dS_x is the volume form on the fibre S_x . The boundary of SM is

$$\partial SM := \{(x, v) \in SM : x \in \partial M\}.$$

On ∂SM , the natural volume form is $d\Sigma^{2d-2}(x, v) = dV^{d-1}(x) \wedge dS_x(v)$, where dV^{d-1} is the volume form on ∂M . We distinguish two subsets of ∂SM (influx and outflux boundaries)

$$\partial_\pm SM := \{(x, v) \in \partial SM : \pm \langle v, \nu(x) \rangle_g \geq 0\},$$

where $\nu(x)$ is the inward unit normal vector on ∂M at x . It is easy to see that

$$\partial_0 SM := \partial_+ SM \cap \partial_- SM = S(\partial M).$$

Given $(x, v) \in SM$, we let $\tau(x, v)$ denote the first time where the geodesic determined by (x, v) hits ∂M and we set $\mu(x, v) := \langle v(x), v \rangle$ for $(x, v) \in \partial SM$. We let X denote the geodesic vector field.

Fixing $n \in \mathbb{N}$, in order to give the linearization of the map

$$C^\infty(M, \mathbb{C}^{n \times n}) \ni \Phi \mapsto C_\Phi \in C^\infty(\partial_+ SM, \mathbb{C}^{n \times n})$$

defined in (13), we first recall some definitions. Given m an integer and $\Theta \in C^\infty(M, \mathbb{C}^{m \times m})$ a skew-hermitian matrix field, we define the *attenuated X-ray transform* with attenuation Θ ,

$$I_\Theta : C^\infty(M, \mathbb{C}^m) \rightarrow C^\infty(\partial_+ SM, \mathbb{C}^m)$$

through $I_\Theta f := u|_{\partial_+ SM}$, where $u : SM \rightarrow \mathbb{C}^m$ solves the transport equation

$$Xu + \Theta u = -f \text{ (SM)}, \quad u|_{\partial_- SM} = 0.$$

Such a transform extends as a bounded map

(52)
$$I_\Theta : L^2(M, \mathbb{C}^m) \rightarrow L^2(\partial_+ SM \rightarrow \mathbb{C}^m, (\mu/\tau) d\Sigma^{2d-2}),$$

and we denote I_Θ^* its adjoint in this functional setting (computed in (69) below). Note that this differs from the volume form $\mu d\Sigma^{2d-2}$ on $\partial_+ SM$ determined by Santaló’s formula (the symplectic volume form). For the unit disc in $\mathbb{R}^2$, $\mu/\tau = 1/2$, so the probability measure $(\mu/\tau) d\Sigma^2$ agrees with λ . In general, and thanks to Lemma 6.11 below, the measure $(\mu/\tau) d\Sigma^{2d-2}$ determines an *equivalent* L^2 -norm as $d\Sigma^{2d-2}$ since μ/τ is smooth and bounded away from zero.

These attenuated X-ray transforms are now well studied [17, 40, 46, 47, 49, 56], and their connection to the scattering map (13) is as follows: the linearization of the map (13) about a point Φ involves an attenuated X-ray transform whose integrands belong to $C^\infty(M, \mathbb{C}^{n \times n})$, with attenuation $\Theta(\Phi, \Phi)$, a matrix field described through the formula (pointwise on M)

$$\Theta(\Phi, \Phi) \cdot U := \Phi U - U \Phi, \quad U \in \mathbb{C}^{n \times n}.$$

The matrix field $\Theta(\Phi, \Phi)$ is skew-hermitian on $\mathbb{C}^{n \times n}$ equipped with the hermitian inner product $(A, B) \mapsto \text{tr}(AB^*)$.

More precisely, we prove in Section 6.2 the following lemma.

LEMMA 6.1. *Let (M, g) be a nontrapping manifold with strictly convex boundary. Given $\Phi \in C(M, \mathfrak{u}(n))$ and upon setting*

(53)
$$\mathbb{I}_\Phi(h) := I_{\Theta(\Phi, \Phi)}(h)C_\Phi$$

for $h \in C(M, \mathbb{C}^{n \times n})$ we have

$$\|C_{\Phi+h} - C_\Phi - \mathbb{I}_\Phi(h)\|_{L^2} \lesssim \|h\|_{L^\infty} \|h\|_{L^2},$$

where the norm on the left-hand side is the $L^2(\partial_+ SM \rightarrow \mathbb{C}^m, (\mu/\tau) d\Sigma^{2d-2})$ norm.

In addition to (53), since $C_\Phi(x, v) \in U(n)$ for all $(x, v) \in \partial_+ SM$, the Fisher information operator $\mathbb{N}_\Phi := \mathbb{I}_\Phi^* \mathbb{I}_\Phi$ of the problem is directly related to the associated normal operator $I_{\Theta(\Phi, \Phi)}^* I_{\Theta(\Phi, \Phi)}$, namely:

(54)
$$\mathbb{N}_\Phi := \mathbb{I}_\Phi^* \mathbb{I}_\Phi = I_{\Theta(\Phi, \Phi)}^* I_{\Theta(\Phi, \Phi)}.$$

In particular, the forward mapping properties of $\mathbb{N}_\Phi$ are a special case of a more general result on the mapping properties of ‘normal’ operators $I_\Theta^* I_\Theta$, which we prove in Section 6.3.

THEOREM 6.2. *Let (M, g) be a nontrapping manifold with strictly convex boundary, and let $\Theta \in C^\infty(M, \mathbb{C}^{m \times m})$. The operator $I_\Theta^* I_\Theta$ maps $C^\infty(M, \mathbb{C}^m)$ into itself.*

From this result, it becomes straightforward to deduce that the Fisher information operator (54) maps $C^\infty(M, \mathbb{C}^{n \times n})$ into itself. However, since Φ is often valued into a strict subalgebra of $\mathbb{C}^{n \times n}$, the last result below requires a Lie-algebra specific refinement. Let G be any compact Lie group. Without loss of generality, we may assume that $G \subset U(n)$, where $U(n)$ is the unitary group of $n \times n$ matrices and let $\mathfrak{g}$ be the Lie algebra of G . We are essentially interested in the case of $G = \text{SO}(n)$, where $\mathfrak{g} = \mathfrak{so}(n)$. Let us denote

$$(55) \quad \mathbb{C}^{n \times n} = \mathfrak{g} \oplus \mathfrak{g}^\perp$$

the orthogonal splitting of $\mathbb{C}^{n \times n}$ for the Frobenius inner product. (When $\mathfrak{g} = \mathfrak{u}(n)$, $\mathfrak{g}^\perp$ is the space of hermitian matrices.)

THEOREM 6.3. *Let (M, g) be a nontrapping manifold with strictly convex boundary, and let $\Phi \in C^\infty(M, \mathbb{C}^{n \times n})$. Then the following hold:*

- (1) *The Fisher information operator $\mathbb{N}_\Phi$ (54) maps $C^\infty(M, \mathbb{C}^{n \times n})$ into itself.*
- (2) *If $\Phi \in C^\infty(M, \mathfrak{g})$, then in the splitting (55), the operator $\mathbb{N}_\Phi$ maps $C^\infty(M, \mathfrak{g})$ into itself and $C^\infty(M, \mathfrak{g}^\perp)$ into itself.*

6.1.2. Isomorphism properties on the Euclidean disk. In light of Theorem 6.2, the next question is then whether an isomorphism property holds. With the current tools available, such a question cannot be answered within the level of generality of the previous section. However, if the manifold M is the Euclidean disk and the attenuation matrix Θ is compactly supported, then the normal operator $I_\Theta^* I_\Theta$ can be viewed as a relatively compact perturbation of the unattenuated case ($\Theta = 0$), whose sharp mapping properties have recently been described in [38]. This allows to prove in Section 6.4 an isomorphism property, using microlocal tools as well as Fredholm theory on a suitable scale of Hilbert spaces.

THEOREM 6.4. *Suppose M is the unit disk $\{(x, y) \in \mathbb{R}^2, x^2 + y^2 \leq 1\}$, equipped with the Euclidean metric, and let Θ be a smooth, skew-hermitian $m \times m$ matrix field on M , with compact support in M^{int} . Then the map*

$$I_\Theta^* I_\Theta : C^\infty(M, \mathbb{C}^m) \rightarrow C^\infty(M, \mathbb{C}^m)$$

is an isomorphism.

Theorem 6.4 is an abridged version of Theorem 6.18 below, where additional isomorphism properties on a special Sobolev scale (defined in equations (72) and (74)) are also given.

Finally, we explain how Theorem 6.4 yields the Fisher information result that is needed for the proof of the Bernstein–von Mises theorem for the non-Abelian X-ray transform. Let G be any compact Lie group and $\mathfrak{g}$ as in Section 6.1.1.

THEOREM 6.5. *Let M be the unit disk with the Euclidean metric and let $\Phi \in C_c^\infty(M, \mathfrak{g})$. Then*

$$\mathbb{N}_\Phi = I_{\Theta(\Phi, \Phi)}^* I_{\Theta(\Phi, \Phi)} : C^\infty(M, \mathfrak{g}) \rightarrow C^\infty(M, \mathfrak{g})$$

is a bijection.

PROOF. Theorem 6.4 implies right away that

$$\mathbb{N}_\Phi : C^\infty(M, \mathbb{C}^{n \times n}) \rightarrow C^\infty(M, \mathbb{C}^{n \times n})$$

is a bijection. The further isomorphism property on $C^\infty(M, \mathfrak{g})$ is a direct consequence of item (2) in Theorem 6.3 and the fact that $C^\infty(M, \mathbb{C}^{n \times n}) = C^\infty(M, \mathfrak{g}) \oplus C^\infty(M, \mathfrak{g}^\perp)$. $\square$

6.2. *Linearizing C_Φ . Proof of Lemma 6.1.* Fix (M, g) a compact, nontrapping manifold with strictly convex boundary. We let φ_t denote the geodesic flow of g ; the integrals that appear below in the variable t are all compositions of functions with φ_t ; we avoid writing this explicitly in order to prevent notation cluttering. An *integrating factor* for Φ is a function $R_\Phi \in C(SM, \text{GL}(n, \mathbb{C}))$, which is differentiable along the geodesic vector field X and $XR_\Phi + \Phi R_\Phi = 0$. If Φ is smooth, then it is not hard to see that smooth integrating factors always exist; cf. [48].

Let U_Φ denote the unique integrating factor with $U_\Phi|_{\partial_- SM} = \text{Id}$. Then $C_\Phi : \partial_+ SM \rightarrow \text{GL}(n, \mathbb{C})$ is defined as

$$C_\Phi := U_\Phi|_{\partial_+ SM}.$$

We can also consider the unique integrating factor u_Φ with $u_\Phi|_{\partial_+ SM} = \text{Id}$. It is immediate to check that $u_\Phi|_{\partial_- SM} = [C_\Phi]^{-1} \circ \alpha$, where $\alpha : \partial SM \rightarrow \partial SM$ denotes the scattering relation of the metric.

The next lemma will be useful for our purposes.

LEMMA 6.6. *Let R_Φ and R_Ψ be integrating factors for continuous matrix fields Φ and Ψ , respectively. Then*

$$\begin{aligned} C_\Phi - C_\Psi &= R_\Phi \left[\int_0^{\tau(x,v)} R_\Phi^{-1}(\Phi - \Psi) R_\Psi dt \right] (R_\Psi^{-1}) \circ \alpha \\ &= R_\Phi [I(R_\Phi^{-1}(\Phi - \Psi) R_\Psi)] (R_\Psi^{-1}) \circ \alpha \end{aligned}$$

where $I : C(SM) \rightarrow C(\partial_+ SM)$ is the standard X -ray transform.

PROOF. We first note that if R solves $XR + \Phi R = 0$, then any other integrating factor has the form $RF^\sharp$, where $F^\sharp$ is the first integral (i.e., $XF^\sharp = 0$) determined by $F \in C(\partial_+ SM, \text{GL}(n, \mathbb{C}))$. Thus, $R_\Phi = U_\Phi F^\sharp$ and from this we deduce

(56)
$$C_\Phi = R_\Phi (R_\Phi^{-1} \circ \alpha).$$

Next, we observe that a computation gives

$$X(R_\Phi^{-1} R_\Psi) = R_\Phi^{-1}(\Phi - \Psi) R_\Psi.$$

Integrating this along a geodesic between boundary points gives

$$\int_0^{\tau(x,v)} R_\Phi^{-1}(\Phi - \Psi) R_\Psi dt = -R_\Phi^{-1} R_\Psi(x, v) + R_\Phi^{-1} R_\Psi \circ \alpha(x, v),$$

for $(x, v) \in \partial_+ SM$. The lemma follows from this and (56). $\square$

DEFINITION 6.7. Given $\Phi, \Psi \in C(M, \mathbb{C}^{n \times n})$ and $h \in C(M, \mathbb{C}^{n \times n})$, consider the unique matrix solution to $Xu + \Phi u - u\Psi = -h$ with $u|_{\partial_- SM} = 0$. We define the attenuated X -ray transform of h with attenuation $\Theta(\Phi, \Psi)$ as

$$I_{\Theta(\Phi, \Psi)}(h) := u|_{\partial_+ SM}.$$

In terms of arbitrary integrating factors R_Φ and R_Ψ , we can give an integral expression for $I_{\Theta(\Phi, \Psi)}$ as

(57)
$$I_{\Theta(\Phi, \Psi)}(h) = R_\Phi \left[\int_0^{\tau(x,v)} R_\Phi^{-1} h R_\Psi dt \right] R_\Psi^{-1}.$$

Indeed, consider the unique matrix solution to $Xu + \Phi u - u\Psi = -h$ with $u|_{\partial_- SM} = 0$. By definition $u|_{\partial_+ SM} = I_{\Theta(\Phi, \Psi)}(h)$. We compute

$$\begin{aligned} X(R_\Phi^{-1}uR_\Psi) &= R_\Phi^{-1}\Phi uR_\Psi + R_\Phi^{-1}XuR_\Psi - R_\Phi^{-1}u\Psi R_\Psi \\ &= -R_\Phi^{-1}hR_\Psi. \end{aligned}$$

Integrating along a geodesic between boundary points, we get

$$R_\Phi^{-1}I_{\Theta(\Phi, \Psi)}(h)R_\Psi = \int_0^{\tau(x, v)} R_\Phi^{-1}hR_\Psi dt,$$

and hence (57) follows.

REMARK 6.8. Lemma 6.6 already contains the pseudo-linearization identity from [40], Lemma 5.5. Indeed, using u_Φ and u_Ψ as integrating factors, the lemma and (56) give

$$(58) \quad C_\Phi - C_\Psi = \left[\int_0^{\tau(x, v)} u_\Phi^{-1}(\Phi - \Psi)u_\Psi dt \right] C_\Psi.$$

$$(59) \quad = I_{\Theta(\Phi, \Psi)}(\Phi - \Psi)C_\Psi.$$

To find the linearization of C_Φ , let Φ_s be a curve of matrix-valued maps such that $\Phi_0 = \Phi$ and $h := \partial_{s=0}\Phi_s$. Differentiating the equation $XU_{\Phi_s} + \Phi_s U_{\Phi_s} = 0$ at $s = 0$, we obtain

$$XH + hU_\Phi + \Phi H = 0$$

where $H := \partial_{s=0}U_{\Phi_s}$. Note that $H|_{\partial_+ SM} = dC_\Phi(h)$. Then the matrix $W := HU_\Phi^{-1}$ satisfies

$$XW + \Phi W - W\Phi = -h.$$

Hence

$$W|_{\partial_+ SM} = I_{\Theta(\Phi, \Phi)}(h),$$

and thus

$$(60) \quad dC_\Phi(h) = I_{\Theta(\Phi, \Phi)}(h)C_\Phi.$$

We can now combine this with (59) to obtain

$$(61) \quad C_{\Phi+h} - C_\Phi - dC_\Phi(h) = (I_{\Theta(\Phi+h, \Phi)}(h) - I_{\Theta(\Phi, \Phi)}(h))C_\Phi.$$

We now use this identity to prove Lemma 6.1.

PROOF OF LEMMA 6.1. From (58) and (59), we know that

$$I_{\Theta(\Phi, \Psi)}(h) = \int_0^\tau u_\Phi^{-1}hu_\Psi dt.$$

Thus,

$$I_{\Theta(\Phi+h, \Phi)}(h) - I_{\Theta(\Phi, \Phi)}(h) = \int_0^\tau (u_{\Phi+h}^{-1} - u_\Phi^{-1})hu_\Phi dt.$$

Since u_Φ takes values in the unitary group, we can estimate using the Frobenius norm

$$|(I_{\Theta(\Phi+h, \Phi)}(h) - I_{\Theta(\Phi, \Phi)}(h))C_\Phi|_F(x, v) \leq \int_0^\tau |(u_{\Phi+h}^* - u_\Phi^*)h|_F dt.$$

Using that $\tau \leq C_0\mu(x, v)$ (cf. Lemma 6.11 below) and Cauchy–Schwarz,

$$|(I_{\Theta(\Phi+h, \Phi)}(h) - I_{\Theta(\Phi, \Phi)}(h))C_\Phi|_F^2(x, v) \leq C_0 \int_0^\tau |(u_{\Phi+h}^* - u_\Phi^*)h|_F^2 dt \mu(x, v)$$

for $(x, v) \in \partial_+ SM$. Integrating now over $\partial_+ SM$ and using Santaló’s formula, we derive

$$\| (I_{\Theta(\Phi+h,\Phi)}(h) - I_{\Theta(\Phi,\Phi)}(h))C_\Phi \|_{L^2} \lesssim \| (u_{\Phi+h}^* - u_\Phi^*)h \|_{L^2}.$$

Using [40], equation (5.8), we have (strictly speaking the proof in [40] is for U_Φ but the same proof applies to u_Φ^*)

$$\| u_{\Phi+h}^* - u_\Phi^* \|_{L^2} \lesssim \| h \|_{L^2}$$

and putting everything together using (61)

$$\| C_{\Phi+h} - C_\Phi - dC_\Phi(h) \|_{L^2} \lesssim \| h \|_{L^\infty} \| h \|_{L^2}. \tag*{$\square$}$$

LEMMA 6.9. *We have*

$$\mathbb{N}_\Phi := \mathbb{I}_\Phi^* \mathbb{I}_\Phi = I_{\Theta(\Phi,\Phi)}^* I_{\Theta(\Phi,\Phi)}.$$

PROOF. Since the matrix C_Φ is unitary, we have

$$\langle \mathbb{I}_\Phi(\cdot), \mathbb{I}_\Phi(\cdot) \rangle_{L^2} = \langle I_{\Theta(\Phi,\Phi)}(\cdot), I_{\Theta(\Phi,\Phi)}(\cdot) \rangle_{L^2}$$

and the lemma follows. $\square$

REMARK 6.10. Since the attenuated X-ray transform $I_{\Theta(\Phi,\Phi)}$ extends as a bounded map from $L^2(M) \rightarrow L^2(\partial_+ SM)$, the same is true for $\mathbb{I}_\Phi$. Boundedness in L^∞ for $\mathbb{I}_\Phi$ is also obvious from the integral expression,

$$I_{\Theta(\Phi,\Phi)}(h) = \int_0^\tau u_\Phi^{-1} h u_\Phi \, dt.$$

6.3. *Forward mapping properties. Proof of Theorems 6.2 and 6.3.* Let (M, g) be a non-trapping manifold with strictly convex boundary. We need the following facts (cf. [48, 57]).

1. The function

$$\tilde{\tau}(x, v) = \begin{cases} \tau(x, v), & (x, v) \in \partial_+ SM, \\ -\tau(x, -v), & (x, v) \in \partial_- SM \end{cases}$$

belongs to $C^\infty(\partial SM)$. Actually, $\tau : SM \rightarrow \mathbb{R}$ solves transport problem $X\tau = -1$ with $\tau|_{\partial_- SM} = 0$ and the function $\tilde{\tau} = \tau(x, v) - \tau(x, -v)$ belongs to $C^\infty(SM)$.

2. The scattering relation $\alpha : \partial SM \rightarrow \partial SM$ is the diffeomorphism defined by

$$\alpha(x, v) = \varphi_{\tilde{\tau}(x,v)}(x, v).$$

3. The scattering relation satisfies $\alpha^2 = id$, based on the property $\tilde{\tau} \circ \alpha = -\tilde{\tau}$.

For what follows, it is convenient to consider (M, g) isometrically embedded in a closed manifold (N, g) , so that the geodesic flow can run for all times. Let $\rho \in C^\infty(N)$ be a boundary defining function for ∂M . That means that ρ coincides with $M \ni x \mapsto d(x, \partial M)$ in a neighbourhood of ∂M , $\rho \geq 0$ on M and $\partial M = \rho^{-1}(0)$. If we let v be the inward unit normal, then $\nabla \rho(x) = v(x)$ for all $x \in \partial M$. Consider the function $h : \partial SM \times \mathbb{R} \rightarrow \mathbb{R}$ given by

$$h(x, v, t) := \rho(\pi \circ \varphi_t(x, v)).$$

Note

$$h(x, v, 0) = 0, \quad \left. \frac{d}{dt} \right|_{t=0} h(x, v, t) = \langle v(x), v \rangle, \quad \left. \frac{d^2}{dt^2} \right|_{t=0} h(x, v, t) = \text{Hess}_x \rho(v, v).$$

Hence there is a smooth function $R : \partial SM \times \mathbb{R} \rightarrow \mathbb{R}$ such that we can write

$$(62) \quad h(x, v, t) = \langle v(x), v \rangle t + \frac{1}{2} \text{Hess}_x \rho(v, v) t^2 + R(x, v, t) t^3.$$

Since $h(x, v, \tilde{\tau}(x, v)) = 0$, it follows that

$$(63) \quad \langle v(x), v \rangle + \frac{1}{2} \text{Hess}_x \rho(v, v) \tilde{\tau} + R(x, v, \tilde{\tau}) \tilde{\tau}^2 = 0.$$

Note that $\tilde{\tau}(x, v) = 0$ iff $(x, v) \in \partial_0 SM$. Hence if we let

$$H(x, v, t) := \langle v(x), v \rangle + \frac{1}{2} \text{Hess}_x \rho(v, v) t + R(x, v, t) t^2$$

we see that H is smooth, $H(x, v, \tilde{\tau}(x, v)) = 0$ and

$$\left. \frac{d}{dt} \right|_{t=0} H(x, v, t) = \frac{1}{2} \text{Hess}_x \rho(v, v).$$

But for $(x, v) \in \partial_0 SM$, $\text{Hess}_x \rho(v, v) = -\Pi_x(v, v) < 0$, and thus by the implicit function theorem, $\tilde{\tau}$ is smooth in a neighbourhood of $\partial_0 SM$. Since $\tilde{\tau}$ is smooth in $\partial SM \setminus \partial_0 SM$, this gives smoothness of $\tilde{\tau}$ in ∂SM . A tweak of this argument gives the following lemma that is probably well known to experts. Recall that $\mu(x, v) = \langle v(x), v \rangle$ for $(x, v) \in \partial SM$.

LEMMA 6.11. *Let (M, g) be a nontrapping manifold with strictly convex boundary. The function $\mu/\tilde{\tau}$ extends to a smooth positive function on ∂SM with values on $\partial_0 SM$ given by*

$$\frac{\mu}{\tilde{\tau}}(x, v) = \frac{\Pi_x(v, v)}{2}, \quad (x, v) \in \partial_0 SM.$$

PROOF. Using (63), we can write

$$\mu(x, v) = -\frac{1}{2} \text{Hess}_x \rho(v, v) \tilde{\tau} - R(x, v, \tilde{\tau}) \tilde{\tau}^2$$

and hence for $(x, v) \in \partial SM \setminus \partial_0 SM$ near $\partial_0 SM$, we can write

$$(64) \quad \mu/\tilde{\tau} = -\frac{1}{2} \text{Hess}_x \rho(v, v) - R(x, v, \tilde{\tau}) \tilde{\tau}.$$

But the right-hand side of the last equation is a smooth function near $\partial_0 SM$ since R and $\tilde{\tau}$ are; its value at $(x, v) \in \partial_0 SM$ is $\Pi_x(v, v)/2$. Finally, observe that μ and $\tilde{\tau}$ are both positive for $(x, v) \in \partial_+ SM \setminus \partial_0 SM$ and both negative for $(x, v) \in \partial_- SM \setminus \partial_0 SM$. $\square$

6.3.1. The maps Υ and F . We now introduce two important maps for what follows.

Consider the map

$$(65) \quad \Upsilon : \partial_+ SM \times [0, 1] \rightarrow SM, \quad \Upsilon(x, v, u) := \varphi_{u\tilde{\tau}(x, v)}(x, v).$$

This map is smooth and it extends smoothly to

$$\Upsilon : \partial(SM) \times [0, 1] \rightarrow SM$$

by setting $\Upsilon(x, v, u) = \varphi_{u\tilde{\tau}(x, v)}(x, v)$. Note that $\Upsilon(x, v, 0) = \text{Id}$, $\Upsilon(x, v, 1) = \alpha(x, v)$ and $\Upsilon(\alpha(x, v), u) = \Upsilon(x, v, 1 - u)$. In other words, if we let $\Gamma : \partial(SM) \times [0, 1] \rightarrow \partial(SM) \times [0, 1]$ be $\Gamma(x, v, u) := (\alpha(x, v), 1 - u)$, then $\Upsilon \circ \Gamma = \Upsilon$. The map Υ is a 2-1 cover with deck transformation Γ away from $\partial_0 SM \times [0, 1]$.

For brevity, we shall denote $p := \mu/\tilde{\tau} \in C^\infty(\partial SM)$. We let $F : \partial SM \setminus \partial_0 SM \times (0, 1) \rightarrow \mathbb{R}$ be

$$(66) \quad F(x, v, u) := \frac{\rho(\pi \circ \varphi_{u\tilde{\tau}}(x, v))}{\tilde{\tau}^2 u(1 - u)} = \frac{h(x, v, u\tilde{\tau})}{\tilde{\tau}^2 u(1 - u)} > 0.$$

PROPOSITION 6.12. *The function F extends to a smooth positive function $F : \partial SM \times [0, 1] \rightarrow \mathbb{R}$ such that:*

- (a) $F(\alpha(x, v), u) = F(x, v, 1 - u)$;
- (b) $F(x, v, 0) = p(x, v)$ and $F(x, v, 1) = p \circ \alpha(x, v)$;
- (c) $F(x, v, u) = \Pi_x(v, v)$ for $(x, v, u) \in \partial_0 SM \times [0, 1]$.

PROOF. Using the definition of F and (62), we can write

$$F(x, v, u) = \frac{\mu(x, v) + \frac{1}{2} \operatorname{Hess}_x \rho(v, v) u \tilde{\tau} + R(x, v, u \tilde{\tau}) u^2 \tilde{\tau}^2}{\tilde{\tau}(1 - u)}.$$

Since R and $\tilde{\tau}$ are smooth, there is a smooth function $Q : \partial SM \times \mathbb{R} \rightarrow \mathbb{R}$ such that

$$R(x, v, u \tilde{\tau}(x, v)) - R(x, v, \tilde{\tau}(x, v)) = (1 - u)Q(x, v, u).$$

Combining this with (63), we can write F as

$$(67) \quad F(x, v, u) = -\frac{1}{2} \operatorname{Hess}_x \rho(v, v) - R(x, v, \tilde{\tau}) \tilde{\tau}(1 + u) + u^2 Q(x, v, u) \tilde{\tau}.$$

The right-hand side of this equation is a smooth function on $\partial SM \times \mathbb{R}$ thus showing that F extends to a smooth function on $\partial SM \times [0, 1]$ as claimed.

To check item (a), we check it first for $(x, v, u) \in \partial SM \setminus \partial_0 SM \times (0, 1)$. This is straight-forward from the definition of F and the fact that $\tilde{\tau} \circ \alpha = -\tilde{\tau}$. Since $\partial SM \setminus \partial_0 SM \times (0, 1)$ is dense in $\partial SM \times [0, 1]$, item (a) follows. To check item (b), we use (67) for $u = 0$; it yields

$$F(x, v, 0) = -\frac{1}{2} \operatorname{Hess}_x \rho(v, v) - R(x, v, \tilde{\tau}) \tilde{\tau}$$

and from (64) we see that it agrees with p . Combining this with item (b), we see that $F(x, v, 1) = F(\alpha(x, v), 0) = p \circ \alpha(x, v)$ as claimed. Item (c) follows from (67) and the facts that $\tilde{\tau}(x, v) = 0$ and $\operatorname{Hess}_x \rho(v, v) = -\Pi_x(v, v)$ for $(x, v) \in \partial_0 SM$. Finally, the positivity of F is a consequence of the positivity of p and the second fundamental form Π . $\square$

6.3.2. *General mapping properties and proof of Theorems 6.2 and 6.3.* Fix m, p two arbitrary integers. Given a weight $w \in C^\infty(SM, \mathbb{C}^{m \times p})$ and for $f \in C^\infty(SM, \mathbb{C}^m)$, we define the weighted transform $\mathcal{I}^w : L^2(SM, \mathbb{C}^p) \rightarrow L^2(\partial_+ SM \rightarrow \mathbb{C}^m, \frac{\mu}{\tau} d\Sigma^{2d-2})$ as

$$\mathcal{I}^w f(x, v) := \int_0^{\tau(x, v)} w(\varphi_t(x, v)) f(\varphi_t(x, v)) dt, \quad (x, v) \in \partial_+ SM.$$

An important space for what follows is given by

$$\begin{aligned} C^\infty_\alpha(\partial_+ SM) &:= \{u \in C^\infty(\partial_+ SM), u_\psi \in C^\infty(SM)\} \\ &= \{u \in C^\infty(\partial_+ SM), A_+ u \in C^\infty(\partial SM)\}, \end{aligned}$$

where for $u \in C^\infty(\partial_+ SM)$, we have defined $A_+ u \in C^\infty(\partial SM \setminus \partial_0 SM)$ as

$$A_+ u(x, v) = \begin{cases} u(x, v), & (x, v) \in \partial_+ SM, \\ u(\alpha(x, v)), & (x, v) \in \partial_- SM. \end{cases}$$

Such a space was first introduced in [50] as a ‘natural’ space of functions, which are mapped into $C^\infty(M)$ through the traditional adjoint of the X -ray transform, and the second equality is a characterization proved in [50]. We extend this definition to vector-valued functions, namely $C^\infty_\alpha(\partial_+ SM, \mathbb{C}^m) := (C^\infty_\alpha(\partial_+ SM))^m$. With ρ a boundary defining function for M as above, we now show the following result.

PROPOSITION 6.13. *Fix m , p and a smooth weight w as above. For every $s < 1$, the following mapping property holds:*

$$\mathcal{I}^w : \rho^{-s} C^\infty(SM, \mathbb{C}^p) \rightarrow \tau^{1-2s} C_\alpha^\infty(\partial_+ SM, \mathbb{C}^m).$$

PROOF. Given $f \in C^\infty(SM)$ and the function F defined in (66), we consider the change of variable $t = \tau(x, v)u$, so that we may rewrite

$$\begin{aligned} I^w(\rho^{-s} f)(x, v) &= \tau(x, v)^{1-2s} \int_0^1 w(\Upsilon(x, v, u)) f(\Upsilon(x, v, u)) F^{-s}(x, v, u) \frac{du}{(u(1-u))^s}, \\ &= \tau(x, v)^{1-2s} g(x, v), \end{aligned}$$

where

$$g(x, v) := \int_0^1 w(\Upsilon(x, v, u)) f(\Upsilon(x, v, u)) F^{-s}(x, v, u) \frac{du}{(u(1-u))^s}$$

and Υ is the map defined in (65).

All functions of (x, v, u) involved in the definition of g are defined and smooth for $(x, v) \in \partial SM$ (noninteger powers of F are well defined and smooth since F is positive everywhere), and thus we may think of g as $\tilde{g}|_{\partial_+ SM}$ for some $\tilde{g}$ whose definition is the same as above, but extended to ∂SM . Since all the functions participating in the definition of $\tilde{g}$ satisfy the property $q(\alpha(x, v), u) = q(x, v, 1-u)$, we have $\tilde{g} \circ \alpha = \tilde{g} = A_+ g$, and $\tilde{g}$ is smooth on ∂SM . In particular, the function g belongs to $C_\alpha^\infty(\partial_+ SM, \mathbb{C}^m)$, which completes the proof. $\square$

The case of interest to us is when $s = 0$, for which we obtain

$$\mathcal{I}^w : C^\infty(SM, \mathbb{C}^p) \rightarrow \tau C_\alpha^\infty(\partial_+ SM, \mathbb{C}^m),$$

and for $w \equiv 1$ and $m = p$, we will denote $\mathcal{I}^w = \mathcal{I}$.

On to the attenuated X -ray transform I_Θ with $p = m$ and $\Theta \in C^\infty(M, \mathfrak{u}(m))$: fixing a smooth integrating factor $R : SM \rightarrow U(m)$ solution of $XR + \Theta R = 0$, we can write $I_\Theta f$ as

$$(68) \quad I_\Theta f(x, v) = R(x, v) \mathcal{I}(R^{-1} f)(x, v), \quad (x, v) \in \partial_+ SM.$$

In the functional setting (52), we then compute the adjoint:

$$\begin{aligned} (I_\Theta f, h)_{\frac{\mu}{\tau}} &= \int_{\partial_+ SM} \langle R(x, v) \mathcal{I}(R^{-1} f(x, v)), h(x, v) \rangle_{\mathbb{C}^m} \frac{\mu}{\tau} d\Sigma^{2d-2} \\ &= \int_{\partial_+ SM} \left\langle \mathcal{I}(R^{-1} f)(x, v), \frac{1}{\tau} R^*(x, v) h(x, v) \right\rangle_{\mathbb{C}^m} \mu d\Sigma^{2d-2} \\ &\stackrel{(s)}{=} \int_{SM} \left\langle R^{-1} f, \left(\frac{1}{\tau} R^* h \right) \circ \psi \right\rangle_{\mathbb{C}^m} d\Sigma^{2d-1} \\ &= \int_M \left\langle f(x), \int_{S_x} \left((R^{-1})^*(x, v) \left(\frac{1}{\tau} R^* h \right) \circ \psi(x, v) \right) dS_x(v) \right\rangle_{\mathbb{C}^m} dV^d(x), \end{aligned}$$

where Santaló's formula was used at step (s). Note that we have used that the (component-wise) adjoint of $\mathcal{I} : L^2(SM) \rightarrow L^2(\partial_+ SM, \frac{\mu}{\tau} d\Sigma^{2d-2})$ is given by $\mathcal{I}^* h(x) = \frac{h}{\tau}(\psi(x, v))$, where $\psi : SM \rightarrow \partial_+ SM$ denotes the footpoint map, defined by $\psi(x, v) = \varphi_{-\tau(x, -v)}(x, v)$. This implies the following expression for the adjoint:

$$(69) \quad I_\Theta^* h(x) = \int_{S_x} \left((R^{-1})^*(x, v) \left(\frac{1}{\tau} R^* h \right) \circ \psi(x, v) \right) dS_x(v).$$

Notice that since Θ is skew-hermitian, we also have the pointwise relation $(R^{-1})^*(x, v) = R(x, v)$. We are now ready to compute associated normal operator $I_\Theta^* I_\Theta$:

(70)

$$\begin{aligned} I_\Theta^* I_\Theta f(x) &= \int_{S_x} R(x, v) \left(\frac{1}{\tau} R^* I_\Theta f \right) \circ \psi(x, v) \, dS_x(v) \\ &= \int_{S_x} R(x, v) \left(\frac{1}{\tau} R^* R \mathcal{I}(R^{-1} f) \right) \circ \psi(x, v) \, dS_x(v) \\ &= \int_{S_x} R(x, v) \left(\frac{1}{\tau} \mathcal{I}(R^{-1} f) \right) \circ \psi(x, v) \, dS_x(v), \end{aligned}$$

where we have used that $R^* R = id_{m \times m}$ pointwise. We can now prove Theorem 6.2.

PROOF OF THEOREM 6.2. Take f smooth on M , then $R^{-1} f$ is smooth on SM , then by Proposition 6.13, $\frac{1}{\tau} \mathcal{I}(R^{-1} f) \in C^\infty_\alpha(\partial_+ SM, \mathbb{C}^m)$. In particular, $(\frac{1}{\tau} \mathcal{I}(R^{-1} f)) \circ \psi(x, v)$ is smooth on SM , and so is its product with $R(x, v)$. Since $I_\Theta^* I_\Theta f$ is the fiberwise average of the latter product, it is smooth on M as well. Theorem 6.2 is proved. $\square$

We finally make the adjustments needed to incorporate restrictions to certain Lie-algebra valued elements, proving Theorem 6.3.

PROOF OF THEOREM 6.3. The proof of (1) follows directly from Theorem 6.2 and the fact that when $\Phi \in C^\infty(M, \mathbb{C}^{n \times n})$, then $\Theta(\Phi, \Phi)$ is a smooth matrix field on $\mathbb{C}^{n \times n}$.

On to the proof of (2), suppose that Φ is $\mathfrak{g}$ -valued. Equation (57) allows us to write

$$I_{\Theta(\Phi, \Phi)}(f) = \int_0^\tau u_\Phi^{-1} f u_\Phi \, dt = \int_0^\tau \text{Ad}_{u_\Phi^{-1}}(f) \, dt$$

where $\text{Ad}_g(f) = gfg^{-1}$ is the Adjoint representation. The map $I_{\Theta(\Phi, \Phi)}^*$ can be easily computed using (69) to obtain

$$I_{\Theta(\Phi, \Phi)}^*(h) = \int_{S_x} \text{Ad}_{u_\Phi}((h/\tau)^\sharp)(x, v) \, dS_x.$$

But the Adjoint representation preserves $\mathfrak{g}$ and thus $\mathbb{N}_\Phi$ maps $C^\infty(M, \mathfrak{g})$ into itself. In fact, since Ad_g for $g \in G \subset U(n)$ is unitary with respect to the Frobenius inner product we may F -orthogonally split $\mathbb{C}^{n \times n} = \mathfrak{g} \oplus \mathfrak{g}^\perp$ and from the expressions above we see that also

$$\mathbb{N}_\Phi : C^\infty(M, \mathfrak{g}^\perp) \rightarrow C^\infty(M, \mathfrak{g}^\perp).$$

$\square$

6.4. *Isomorphism property—proof of Theorem 6.4.* Let us denote $N_\Theta := I_\Theta^* I_\Theta$. As previously pointed out in Remark 2.3, unlike the case where L^2_μ (for μ the symplectic measure from Section 6.1.1) is chosen as co-domain for I_Θ , N_Θ is a pseudo-differential operator on M^{int} which does *not* extend to any simple neighbourhood of M . Understanding such an operator will require taking care of interior and boundary behaviour separately. The interior behaviour is well known and holds in a broad range of cases, while the boundary behaviour makes use of the recent results of [38]. The range of applicability of [38] is geodesic disks of constant curvature, and although what follows could apply to this class of surfaces, we will restrict to the Euclidean disk for simplicity.

6.4.1. *Interior behaviour.* In the interior, we now show that N_Θ is a classical elliptic Ψ DO of order -1 , and this actually holds for any simple manifold of dimension $d \geq 2$. Indeed, from the above calculation (70), we first write

$$N_\Theta f(x) = \int_{S_x} \int_0^{\tau(x,v)} \mathcal{N}_\Theta(x, \exp_x(tv)) f(\exp_x(tv)) j(x, v, t) dt dS_x(v),$$

where

$$(71) \quad \mathcal{N}_\Theta(x, \exp_x(tv)) := \frac{R(x, v)R^{-1}(\varphi_t(x, v)) + R(x, -v)R^{-1}(\varphi_{-t}(x, -v))}{\tau(\psi(x, v))j(x, v, t)},$$

and $j(x, v, t)$ denotes the Jacobian of the exponential map $S_x \times (0, \epsilon) \ni (v, t) \rightarrow \exp_x(tv) \in M$. The Schwartz kernel of N_Θ is then $\mathcal{N}_\Theta(x, y)$. Expansions for small t give

$$\frac{1}{j(x, v, t)} = t^{-d+1} + O(t^{-d+2}),$$

$$R(x, v)R^{-1}(\varphi_t(x, v)) = id_{N \times N} + t\Theta(x) + O(t^2),$$

and thus the part of the Schwartz kernel that contributes to the principal symbol is given by

$$\frac{2}{d_g(x, y)^{d-1}\ell(x, y)} id_{N \times N},$$

where ℓ denotes the length of the maximal geodesic passing through (x, y) .

6.4.2. *Boundary behaviour.* We now focus on the case of the *Euclidean disk*, where $g = e$, $d = 2$ and the geodesic flow takes the form $\varphi_t(x, v) = (x + tv, v)$. We now recall the theory described in the case $\Theta = 0$, as outlined in [38]. Consider $x = (\rho \cos \omega, \rho \sin \omega)$ polar coordinates on the unit disk, and define¹ the unbounded operator

$$\mathcal{L} := (4\pi)^{-2} [-((1 - \rho^2)\partial_\rho^2 + (\rho^{-1} - 3\rho)\partial_\rho + \rho^{-2}\partial_\omega^2) + 1],$$

with domain $C^\infty(M)$. Then $\mathcal{L}$ is essentially self-adjoint on $L^2(M)$ with known (pure point) spectral decomposition

$$\{Z_{n,k}, n \in \mathbb{N}_0, 0 \leq k \leq n\}, \quad \lambda_n = (4\pi)^{-2}(n+1)^2.$$

The eigenfunctions are (Zernike) polynomials, hence smooth on M . We then define the Hilbert scale $\{\tilde{H}^s(M)\}_{s \geq 0}$ by

$$(72) \quad \tilde{H}^s = \tilde{H}^s(M) := \left\{ f = \sum_{n,k} f_{n,k} \widehat{Z_{n,k}}, (4\pi)^{-2s} \sum_{n=0}^{\infty} (n+1)^{2s} \sum_{k=0}^n |f_{n,k}|^2 < \infty \right\},$$

where the hat denotes L^2 -normalization. It is then proved in [38], Lemma 3, that $\bigcap_{s \geq 0} \tilde{H}^s = C^\infty(M)$. Moreover, following [38], Lemmas 13–14, there exists $\alpha > 3/2$ and $\ell > 2$ such that for any $u \in C^\infty(M)$ and $s \in \mathbb{N}_0$, we have

$$(73) \quad \|u\|_{\tilde{H}^{2s}} = \|\mathcal{L}^s u\|_{L^2(M)} \lesssim \|u\|_{C^{2s}} \lesssim \|u\|_{\tilde{H}^{\alpha+2s\ell}},$$

where for $k \in \mathbb{N}_0$, we define the C^k norm $\|u\|_{C^k} = \sup_{x \in M} \sum_{|\alpha| \leq k} |\partial^\alpha u(x)|$. Therefore, the topological dual of $C^\infty(M)$ equipped with the family of seminorms $\{\|\cdot\|_{\tilde{H}^s}\}_{s \in \mathbb{N}_0}$ coincides with that of $C^\infty(M)$ equipped with the family of $C^k(M)$ norms, the latter being the space of *supported distributions* $\dot{C}^{-\infty}(M)$.

¹The 4π factor is not directly incorporated in the definition of $\mathcal{L}$ in [38], though it helps avoid a proliferation of constants here, and only changes the results of [38] by powers of 4π .

As a result, $\mathcal{L}$ can be extended by duality to $\dot{C}^{-\infty}(M)$ through the pairing $\langle \mathcal{L}u, \phi \rangle := \langle u, \mathcal{L}\phi \rangle$ (if by $\langle \cdot, \cdot \rangle$ we denote the $(\dot{C}^{-\infty}(M), C^\infty(M))$ pairing). An element $u \in \dot{C}^{-\infty}(M)$ will be said to be in $L^2(M)$ if there exists a constant C such that for any $\phi \in C^\infty(M)$, $|\langle u, \phi \rangle| \leq C \|\phi\|_{L^2(M)}$. Definition (72) may then be extended to $s \in \mathbb{R}$, and each space can be identified as

$$(74) \quad \tilde{H}^s = \{u \in \dot{C}^{-\infty}(M), \mathcal{L}^{s/2}u \in L^2\}, \quad \|u\|_{\tilde{H}^s} := \|\mathcal{L}^{s/2}u\|_{L^2}.$$

As this Sobolev scale is not the classical one (it is modeled after an elliptic operator whose ellipticity degenerates at the boundary), we state a few facts which are reminiscent of the traditional scales:

LEMMA 6.14. *The scale $\{\tilde{H}^s\}_{s \in \mathbb{R}}$ satisfies the following:*

- (a) *Using L^2 as pivot space, for every $s \geq 0$, we have $(\tilde{H}^s)' = \tilde{H}^{-s}$.*
- (b) *For any $s, t \in \mathbb{R}$ such that $t < s$, the injection $\tilde{H}^s \subset \tilde{H}^t$ is compact.*
- (c) *For any $0 \leq s < t$ and $\theta \in [0, 1]$, we have $[\tilde{H}^t, \tilde{H}^s]_\theta = \tilde{H}^{\theta s + (1-\theta)t}$.*

PROOF. The definition (72) makes each $\tilde{H}^s$ isomorphic to a weighted ℓ^2 space. Then (a) follows directly from the fact that for any sequence of positive numbers $\{\lambda_n\}_n$,

$$\sum_{n \in \mathbb{N}} u_n \overline{v_n} \leq \left(\sum_{n \in \mathbb{N}} \lambda_n^2 u_n^2 \right)^{1/2} \left(\sum_{n \in \mathbb{N}} \lambda_n^{-2} v_n^2 \right)^{1/2}.$$

Then (b) is an immediate consequence of the fact that for any sequence $\{\lambda_n\}_n$ decreasing to zero, the operator $T_\lambda: \ell^2 \rightarrow \ell^2$ given by $\{u_j\}_{j \in \mathbb{N}} \mapsto \{\lambda_j u_j\}_{j \in \mathbb{N}}$ is compact.

Finally, (c) follows readily from the general complex interpolation result [59], Proposition 2.2, bearing in mind that $\tilde{H}^s$ is nothing but the domain space $\mathcal{D}(\mathcal{L}^{s/2})$. $\square$

Furthermore, we have that for any $s \in \mathbb{R}$ and any $u \in \tilde{H}^s$, $\|N_0 u\|_{\tilde{H}^{s+1}} = \|u\|_{\tilde{H}^s}$. Moreover, the following identity is given in [38], Theorem 11,

$$(75) \quad \mathcal{L}N_0^2 = id|_{C^\infty(M)},$$

and this equality extends to $\dot{C}^{-\infty}(M)$ by density. Therefore, N_0 is an isomorphism of $C^\infty(M)$ (in fact, a bijection of $\dot{C}^{-\infty}(M)$), and the work below will imply that this remains true for N_Φ , by showing that N_Φ is a relatively compact perturbation of N_0 on the $\tilde{H}^s$ scale.

Morally, the $\tilde{H}^s$ scale behaves like the usual Sobolev scale in the interior of M (while allowing for faster radial oscillations near the boundary). This is summarized in Lemma 6.15 below, in stark contrast with (73). Here and below, we write $U \Subset M^{\text{int}}$ for a set U which is relatively compact in M^{int} . If U is open, we have the natural operators of extension-by-zero $e_U: C_c^\infty(U) \rightarrow C^\infty(M)$ and restriction $r_U: C^\infty(M) \rightarrow C^\infty(U)$, which extend by duality to $e_U = r_U^t: \mathcal{E}'(U) \rightarrow \dot{C}^{-\infty}(M)$ and $r_U = e_U^t: \dot{C}^{-\infty}(M) \rightarrow \mathcal{D}'(U)$. We also have $r_U e_U = id|_{\mathcal{E}'(U)}$, and $\mathcal{L}e_U = e_U \mathcal{L}$ (where $\mathcal{L}$, being a differential operator, will be viewed either as continuous on $\mathcal{E}'(U) \rightarrow \mathcal{E}'(U)$ or $\dot{C}^{-\infty}(M) \rightarrow \dot{C}^{-\infty}(M)$).

LEMMA 6.15. *Fix an open set $U \Subset M^{\text{int}}$ and an integer $p \geq 0$. Then for any $u \in \mathcal{E}'(U)$, we have that $u \in H^{2p}(U)$ if and only if $e_U u \in \tilde{H}^{2p}$. Moreover, there exist constants $C_1(U, p)$ and $C_2(U, p)$ such that*

$$(76) \quad C_1 \|u\|_{H^{2p}(U)} \leq \|e_U u\|_{\tilde{H}^{2p}} \leq C_2 \|u\|_{H^{2p}(U)}, \quad \forall u \in H^{2p}(U) \cap \mathcal{E}'(U).$$

PROOF. We then have

$$\|e_U u\|_{\tilde{H}^{2p}} = \|\mathcal{L}^p e_U u\|_{L^2(M)} = \|\mathcal{L}^p u\|_{L^2(U)} \leq C \|u\|_{H^{2p}(U)},$$

where the last inequality comes from the fact that $\mathcal{L}^p$ is a differential operator of order $2p$. For the other inequality, notice that for any $u \in \mathcal{E}'(U)$ and any $p \in \mathbb{N}_0$, we have $e_U u = N_0^{2p} \mathcal{L}^p e_U u$, and upon applying r_U we obtain $u = r_U N_0^{2p} e_U \mathcal{L}^p u$. We now claim that there is a constant such that

$$(77) \quad \|r_U N_0^{2p} e_U v\|_{H^{2p}(U)} \leq \|v\|_{L^2(U)}, \quad \forall v \in L^2(U).$$

In that case, we write

$$\begin{aligned} \|u\|_{H^{2p}(U)} &= \|r_U N_0^{2p} e_U \mathcal{L}^p u\|_{H^{2p}(U)} \\ &\leq C \|\mathcal{L}^p u\|_{L^2(U)} = C \|\mathcal{L}^p e_U u\|_{L^2(M)} = C \|e_U u\|_{\tilde{H}^{2p}}, \end{aligned}$$

completing the proof of the lemma.

To prove (77): given U' an open set such that $U \Subset U' \Subset M^{\text{int}}$, define $e_{U,U'}: \mathcal{E}'(U) \rightarrow \mathcal{E}'(U')$ and $r_{U',U}: \mathcal{D}'(U') \rightarrow \mathcal{D}'(U)$ the operators of extension by zero and restriction. With $\chi \in C_c^\infty(U')$ equal to 1 in a neighbourhood of U , the operators $r_U N_0^{2p} e_U$ and $r_{U',U} \chi r_{U'} N_0^{2p} e_{U'} \chi e_{U,U'}$ agree. The operator $\chi r_{U'} N_0^{2p} e_{U'} \chi$ is a properly supported element of $\Psi^{-2p}(U')$, and thus by [24], Theorem 4.7,

$$\chi r_{U'} N_0^{2p} e_{U'} \chi: L_{\text{loc}}^2(U') \rightarrow H_{\text{loc}}^{2p}(U')$$

is continuous. In particular, there exists $U'' \Subset U'$ and a constant C such that

$$\|r_{U',U} \chi r_{U'} N_0^{2p} e_{U'} \chi w\|_{H^{2p}(U)} \leq C \|r_{U',U''} w\|_{L^2(U'')}, \quad \forall w \in \mathcal{E}'(U').$$

Applying this inequality to $w = e_{U,U'} v$ for some $v \in \mathcal{E}'(U)$ yields the result. $\square$

Everything we have done in this section so far generalizes straightforwardly to $\mathbb{C}^N$ -valued functions. We may define $\tilde{H}^s(M; \mathbb{C}^N)$ as in (72) by making the coefficients $f_{n,k}$ to be valued in $\mathbb{C}^N$ with $|f_{n,k}|^2$ the standard Euclidean norm. This scale corresponds to a Sobolev scale with respect to $\mathcal{L}$ acting on each scalar component. Now denoting $\tilde{H}^s = \tilde{H}^s(M; \mathbb{C}^N)$, Lemmas 6.14 and 6.15 still hold true with minor modifications. We now turn to the study of N_Θ , and write $N_\Theta = N_0 + K_\Theta$, where the ‘unattenuated’ normal operator N_0 is thought of as acting diagonally on each component of a $\mathbb{C}^N$ -valued function.

LEMMA 6.16. *For any open set $U \Subset M^{\text{int}}$, the following hold:*

- (i) *The operator $r_U N_\Theta e_U$ is an elliptic element of $\Psi^{-1}(U)$.*
- (ii) *The operator $r_U K_\Theta e_U$ belongs to $\Psi^{-2}(U)$.*

PROOF. Fix an open set $U \Subset M^{\text{int}}$. For $f \in C_0(U)$ extended by zero outside of U , we may write

$$r_U N_\Theta e_U f(x) = \int_{S_x} \int_0^\infty A(x, v, t) f(x + tv) dt dS_x(v), \quad x \in U,$$

where $A(x, v, t) := \frac{R(x, v) R^{-1}(x + tv, v) + R(x, -v) R^{-1}(x + tv, -v)}{\tau(\psi(x, v))} \chi(x + tv)$ for $(x, v, t) \in \mathcal{D}_U$ with

$$\mathcal{D}_U := \{(x, v, t), (x, v) \in SU, t \in \mathbb{R}\},$$

and where $\chi \in C_c^\infty(M^{\text{int}})$ is equal to 1 on U . Then $A \in C^\infty(\mathcal{D}_U)$ and by [14], Lemma B.1, $r_U N_\Theta e_U$ is a classical Ψ DO of order -1 on U with full symbol $\sigma(x, \xi) \sim \sum_{k=0}^\infty \sigma_k(x, \xi)$, where

$$\sigma_k(x, \xi) = \pi \frac{i^k}{k!} \int_{S_x U} \partial_t^k A(x, v, 0) \delta^{(k)}(\langle \xi, v \rangle) dS_x(v).$$

The principal symbol of N_Θ is thus given by

$$\begin{aligned} \sigma_0(x, \xi) &= 2\pi \int_{S_x} \frac{\delta(\langle \xi, v \rangle)}{\tau(x, v) + \tau(x, -v)} dS_x(v) id_{N \times N} \\ &= \frac{4\pi}{|\xi|} \frac{1}{\tau(x, \hat{\xi}_\perp) + \tau(x, -\hat{\xi}_\perp)} id_{N \times N}. \end{aligned}$$

We also notice that σ_0 actually does not depend on Θ , in other words, $r_U K_\Theta e_U = r_U(N_\Theta - N_0)e_U \in \Psi^{-2}(U)$. Hence the result. $\square$

The next lemma is in essence the reason why N_Θ is a relatively compact perturbation of N_0 on the $\tilde{H}^s$ scale.

LEMMA 6.17. *For any $s \geq 0$, the operators $\mathcal{L}K_\Theta$ and $K_\Theta \mathcal{L}$ are $\tilde{H}^s \rightarrow \tilde{H}^s$ bounded.*

PROOF. It is enough to prove boundedness for $s = 2p$ with $p \in \mathbb{N}_0$, and the general case follows from Lemma 6.14.(c) and the interpolation result [59], Proposition 2.1.

An important observation is that since Θ is compactly supported inside M^{int} , there exists $\delta > 0$ such that for any $x_0 \in \partial M$, if $x, y \in B_\delta(x_0) \cap M$, then $\mathcal{K}_\Theta(x, y) = 0$. Indeed, if δ is so small that $B_\delta(x_0)$ does not intersect the support of Θ , and by convexity of the set $B_\delta(x_0) \cap M$, the geodesic segment $[x, y]$ is completely included outside the support of Θ , thus in (71), writing $y = \text{Exp}_x(tv)$ for some t, v , we have that $R(x, v)R^{-1}(\varphi_t(x, v)) = id_{N \times N}$, and hence $\mathcal{N}_0(x, y) = \mathcal{N}_\Phi(x, y)$ there.

Let us then cover M by open balls $\{U_i\}_i$ of small enough diameter that if $U_i \cap U_j \neq \emptyset$ and if either intersects ∂M , then $U_i \cup U_j \subset B_\delta(x_0)$ for some $x_0 \in \partial M$. In this scenario, $\mathcal{K}_\Phi(x, y) = 0$ for any $x \in U_i$ and $y \in U_j$. Consider $\{\psi_i\}_i$ a locally finite partition of unity subordinated to $\{U_i\}_i$, and write $K_\Theta = \sum_{i,j} K_{ij}$ with $K_{ij}(x, y) = \psi_i(x)K(x, y)\psi_j(y)$. Denote by $S_i \Subset U_i$ the support of ψ_i . By the comment above, K_{ij} is trivial whenever $U_i \cap U_j \neq \emptyset$ and either set intersects ∂M and we may assume that the nontrivial terms arise either from (I) $U_i \cap U_j = \emptyset$, or (II) $U_i \cap U_j \neq \emptyset$ and $U_i \cup U_j \Subset M^{\text{int}}$.

In case (I), then $K_{ij}, \mathcal{K}_{ji} \in C^\infty(M \times M)$, since these are supported away from the diagonal and the corner of $M \times M$. In particular for any $p \in \mathbb{N}$, the Schwartz kernel of $\mathcal{L}^p K_{ij}$ and $\mathcal{L}^p K_{ji}$ belongs to $C^\infty(M \times M)$ as well as those of $K_{ji}\mathcal{L}^p$ and $K_{ij}\mathcal{L}^p$ by duality. Then for any p, q , the Schwartz kernel of $\mathcal{L}^q K_{ij}\mathcal{L}^p$ belongs to $C^\infty(M \times M)$, thus $\mathcal{L}^q K_{ij}\mathcal{L}^p$ is $L^2 \rightarrow L^2$ bounded. In particular, $\mathcal{L}^p K_{ij}\mathcal{L}$ and $\mathcal{L}^p \mathcal{L}K_{ij}$ are $L^2 \rightarrow L^2$ bounded, which is equivalent to $K_{ij}\mathcal{L}$ and $\mathcal{L}K_{ij}$ being $L^2 \rightarrow \tilde{H}^{2p}$ bounded, and in particular, $\tilde{H}^{2p} \rightarrow \tilde{H}^{2p}$ bounded.

In case (II), take open sets U, U' such that $S_i \cup S_j \subset U \Subset U' \Subset M^{\text{int}}$. Then from the composition calculus of Ψ DO's and Lemma 6.16.(ii), $K_{ij}\mathcal{L}$ and $\mathcal{L}K_{ij}$ are properly supported elements of $\Psi^0(U')$, and thus by [24], Theorem 4.7, we have $\mathcal{L}K_{ij}, K_{ij}\mathcal{L}: H_{\text{loc}}^s(U') \rightarrow H_{\text{loc}}^s(U')$ for all s . In particular, there exists $V \Subset U'$ and a constant C such that for every $v \in \mathcal{E}'(U)$, $\|\mathcal{L}K_{ij}v\|_{H^{2p}(U)} \leq C\|v\|_{H^{2p}(V)}$. Using Lemma 6.15, this gives

$$\|e_U \mathcal{L}K_{ij}v\|_{\tilde{H}^{2p}} \lesssim \|\mathcal{L}K_{ij}v\|_{H^{2p}(U)} \lesssim \|v\|_{H^{2p}(V)} \lesssim \|e_V v\|_{\tilde{H}^{2p}},$$

similarly for $K_{ij}\mathcal{L}$.

On to the proof, for $v \in \dot{C}^{-\infty}(M)$, we write $\mathcal{L}K_{\Theta}v = \sum_{i,j} \mathcal{L}K_{ij}v_j$, where $v_j = \chi_j v$ and where $\chi_j \in C_c^{\infty}(U_j)$ is equal to 1 on S_j . Then

$$\|\mathcal{L}K_{\Theta}v\|_{\tilde{H}^{2p}} \leq \sum_{(I)} \|\mathcal{L}K_{ij}v_j\|_{\tilde{H}^{2p}} + \sum_{(II)} \|\mathcal{L}K_{ij}v_j\|_{\tilde{H}^{2p}}.$$

From the work above, each term involving v_j is $\lesssim \|v_j\|_{\tilde{H}^{2p}}$, which by Leibniz's rule is bounded by $C\|v\|_{\tilde{H}^{2p}}$. The proof for $\mathcal{L}K_{\Theta}$ is identical. $\square$

Since K_{Θ} is $L^2 \rightarrow L^2$ self-adjoint and $\mathcal{L}$ is essentially $L^2 \rightarrow L^2$ self-adjoint, the transpose of $\mathcal{L}K_{\Theta}: \tilde{H}^s \rightarrow \tilde{H}^s$ is $K_{\Theta}\mathcal{L}: \tilde{H}^{-s} \rightarrow \tilde{H}^{-s}$, and the transpose of $K_{\Theta}\mathcal{L}: \tilde{H}^s \rightarrow \tilde{H}^s$ is $\mathcal{L}K_{\Theta}: \tilde{H}^{-s} \rightarrow \tilde{H}^{-s}$, both of which are then bounded by virtue of Lemma 6.17. A consequence of the previous lemma is also that $K_{\Theta} = \mathcal{L}^{-1} \circ \mathcal{L}K_{\Phi}: \tilde{H}^s \rightarrow \tilde{H}^{s+2}$ is bounded for every $p \in \mathbb{N}_0$, and thus that $N_{\Theta} = N_0 + K_{\Theta}$ is $\tilde{H}^s \rightarrow \tilde{H}^{s+1}$ bounded for all $s \geq 0$. Dualizing, the operator $N_{\Theta}: \tilde{H}^{-s-1} \rightarrow \tilde{H}^{-s}$ is bounded for all $s \geq 0$.

We now prove the main theorem of this section.

THEOREM 6.18. *For all $s \geq 0$, the operator $N_{\Theta}: \tilde{H}^s \rightarrow \tilde{H}^{s+1}$ is a Hilbert space isomorphism. As a consequence, the operator $N_{\Theta}: C^{\infty}(M, \mathbb{C}^N) \rightarrow C^{\infty}(M, \mathbb{C}^N)$ is a Fréchet space isomorphism.*

PROOF. We know that $N_{\Theta}: L^2(M, \mathbb{C}^N) \rightarrow L^2(M, \mathbb{C}^N)$ is self-adjoint by construction, and injective [49], and in particular, injective on $\tilde{H}^s$ for any $s \geq 0$. We now prove that this is also true for negative s . Indeed for $s < 0$, if $u \in \tilde{H}^s$ satisfies $0 = N_{\Theta}u = N_0u + K_{\Theta}u$, composing with $\mathcal{L}^{1/2}$, we obtain the equation $u = -\mathcal{L}^{1/2}K_{\Theta}u$. Now from Lemma 6.17, we have that $\mathcal{L}^{1/2}K_{\Theta} = \mathcal{L}^{-1/2} \circ \mathcal{L}K_{\Theta}: \tilde{H}^t \rightarrow \tilde{H}^{t+1}$ is continuous for all $t \in \mathbb{R}$, and thus by bootstrapping, $u \in C^{\infty}(M, \mathbb{C}^N)$. Finally, by injectivity of N_{Θ} on $C^{\infty}(M, \mathbb{C}^N)$, we obtain that N_{Θ} is injective on $\tilde{H}^s$ for any $s \in \mathbb{R}$.

On to the surjectivity, fix $s \geq 0$: given $f \in \tilde{H}^{s+1}$, $u \in \tilde{H}^s$ solves $N_{\Theta}u = f$ if and only if u solves $N_0u + K_{\Theta}u = f$. Upon composing by $\mathcal{L}^{1/2}$, this is equivalent to solving for $u \in \tilde{H}^s$

$$(78) \quad u + \mathcal{L}^{1/2}K_{\Phi}u = \mathcal{L}^{1/2}f \in \tilde{H}^s.$$

As mentioned above the operator $\mathcal{L}^{1/2}K_{\Theta}: \tilde{H}^s \rightarrow \tilde{H}^{s+1}$ is bounded, hence $\tilde{H}^s \rightarrow \tilde{H}^s$ compact. As a result, the bounded operator $Id + \mathcal{L}^{1/2}K_{\Theta} = \mathcal{L}^{1/2}N_{\Theta}: \tilde{H}^s \rightarrow \tilde{H}^s$ has closed range. Finally, the Hilbert-space adjoint of $\mathcal{L}^{1/2}N_{\Theta}: \tilde{H}^s \rightarrow \tilde{H}^s$ is $\mathcal{L}^{-s}N_{\Theta}\mathcal{L}^{1/2}\mathcal{L}^s$, and thus,

$$\text{ran}(\mathcal{L}^{1/2}N_{\Theta}|_{\tilde{H}^s}) = \overline{\text{ran}(\mathcal{L}^{1/2}N_{\Theta}|_{\tilde{H}^s})} = (\ker(\mathcal{L}^{-s}N_{\Theta}\mathcal{L}^{1/2}\mathcal{L}^s|_{\tilde{H}^s}))^{\perp}.$$

The latter kernel is directly related to $\ker N_{\Theta}|_{\tilde{H}^{-s-1}}$, which was proved above to be trivial. As a result, $\mathcal{L}^{1/2}N_{\Theta}: \tilde{H}^s \rightarrow \tilde{H}^s$ is an isomorphism, and so is $N_{\Theta}: \tilde{H}^s \rightarrow \tilde{H}^{s+1}$. $\square$

Acknowledgments. The authors would like to thank the anonymous referees for their constructive comments that improved the quality of this paper.

Funding. F. Monard was supported by NSF Grant DMS-1814104 and NSF CAREER Grant DMS-1943580. R. Nickl was supported by the European Research Council under ERC Grant 647812 (UQMSI). G.P. Paternain was supported by the Leverhulme trust and EPSRC Grant EP/R001898/1.

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