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GAUSSIAN RECIPROCAL DIFFUSIONS AND POSITIVE DEFINITE STURM-LIOUVILLE OPERATORS*

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This paper examines the connection between Gaussian reciprocal diffusions (GRDs) on a finite interval $[0, T]$ and positive definite Sturm–Liouville boundary values problems (BVPs) on the same interval. We show that there exists a bijection between the set of GRDs on $[0, T]$ and the set of positive definite Sturm–Liouville BVPs on $[0, T]$. The bijection occurs through the identification of GRD covariances with Sturm–Liouville Green's functions. Furthermore, every GRD $x(t)$ can be formulated as a weak solution of its corresponding Sturm–Liouville BVP, where the interior forcing terms and the boundary forcing terms form a stochastic object whose covariance structure is determined by that of $x(t)$. This formulation differs from the one presented in [20] in that it represents $x(t)$ as the solution of its matching positive definite Sturm–Liouville BVP, as opposed to a Dirichlet BVP. Finally, for GRDs with a negative stress tensor [11], it is shown that the Sturm–Liouville BVP they satisfy can be reformulated as a first-order BVP with twice the dimension of the original problem, whose solution can be expressed as a standard Wiener integral plus an independent boundary term.

KEY WORDS: Gaussian reciprocal diffusion, Sturm–Liouville operator, Green's function.

1 INTRODUCTION

Reciprocal processes were introduced in 1932 by Bernstein [5], who was motivated by an attempt of Schrödinger [30, 31] at developing a stochastic interpretation of quantum mechanics in terms of a class of Markov processes for which boundary conditions are imposed at *both ends* of the interval of definition. A stochastic process $x(t)$ on $[0, T]$ taking values in $\mathbb{R}^n$ is called reciprocal if for any two times $t_0 < t_1$, the process interior to $[t_0, t_1]$ is independent of the process exterior to $[t_0, t_1]$, given $x(t_0)$ and $x(t_1)$. Reciprocal processes contain Markov processes as a subclass. Also, Markov random fields in the sense of Paul Lévy [23, 29] reduce in the single parameter case to reciprocal, rather than Markov processes. The properties of reciprocal processes have been examined in detail by a number of authors, and in particular Jamison [14, 15], who showed that they can be obtained by first conditioning the trajectories of a Markov process to arbitrary fixed values at both ends of the interval $[0, T]$, and then assigning an arbitrary joint probability

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distribution to the values $x(0)$ and $x(T)$ of the process at the end points. Other studies of reciprocal processes include [8, 6, 7, 25, 1, 27], among others.

In this paper, we shall be concerned with the class of Gaussian reciprocal diffusions (GRDs). Arbitrary, i.e. not necessarily Gaussian, reciprocal diffusions, were introduced by Krener [19] (see also [9, 22, 33]), who showed they admit second-order stochastic dynamics and satisfy a set of conservation laws which generalize to the reciprocal case the Fokker–Planck equation of Markov diffusions. However, a number of aspects of the theory of reciprocal diffusions, such as the development of a general theory of second-order stochastic differential equations, need to be fully worked out. For the Gaussian case, this theory was developed in [20], where it was shown that the covariance of a GRD satisfies a second order self-adjoint differential equation, which was then used to construct GRDs as weak solutions of linear second-order stochastic differential equations with Dirichlet conditions. In this paper, building on a characterization of discrete–time Gaussian reciprocal processes given in [21], we explore further the connection existing between positive Sturm–Liouville operators and GRDs.

Following [20], a continuous-time process $x(t)$ is called a Gaussian reciprocal diffusion if it satisfies the following four axioms:

A1. $x(t)$ is a zero mean Gaussian reciprocal process on $[0, T]$ and assumes values in $\mathbb{R}^n$. The sample paths of the process are continuous almost surely.

A2. Let $R(t,s) = E\{x(t)x^*(s)\}$, where "$*$" denotes the transpose operation. R is C^2 on the triangle $0 \leq s \leq t \leq T$ in the sense that continous limits of R and it first and second partials exist on the boundary of this triangle.

A3. For $0 < t_0 < t_1 < T$ the two time covariance matrix

$$\begin{bmatrix} R(t_0,t_0) & R(t_0,t_1) \\ R(t_1,t_0) & R(t_1,t_1) \end{bmatrix} \tag{1.1}$$

is invertible.

A4. The matrix

$$Q(t) = \frac{\partial R}{\partial t}(t^-,t) - \frac{\partial R}{\partial t}(t^+,t) \tag{1.2}$$

is positive definite for all t.

A4 is referred to as the full rank noise assumption. The terminology arises from the fact that when the stochastic 2nd order differential equation satisfied by $x(t)$ is discretized, the leading term of the covariance of the driving noise is proportional to $Q(t)$. It turns out that A3 is actually a consequence of A1, A2 and A4. However, this is not obvious, and it is most convenient to develop the theory of GRDs using the above (slightly redundant) set of axioms.

The results of [20] concerning the connection between GRDs and positive definite Sturm–Liouville operators are extended here as follows. In [21] it was shown that a discrete time Gaussian reciprocal process $x(k)$ on an integer interval $[0, N]$ can be represented as the solution of two different types of stochastic BVPs, both involving a symmetric 2nd order difference operator, but with different BCs.

The first class of BVP admits Dirichlet BCs

$$\begin{bmatrix} x(0) \\ x(N) \end{bmatrix} = \begin{bmatrix} b_i \\ b_f \end{bmatrix} \sim \mathcal{N}(0, \mathbf{P}), \tag{1.3}$$

where the covariance matrix $\mathbf{P}$ is specified, and the random boundary vectors b_i and b_f are independent of the driving noise $e(k)$ for the difference equation satisfied by $x(k)$ in the interior of $[0, N]$. A second type of BVP examined in [21] corresponds to the BCs

$$M_0(0)x(0) - M_+(0)x(1) - M_-(0)x(N) = e(0) \tag{1.4a}$$

$$M_0(N)x(N) - M_-(N)x(N-1) - M_+(N)x(0) = e(N), \tag{1.4b}$$

which are called "cyclic" because they have exactly the same form as the 2nd order difference equation for $x(k)$ in the interior of $[0, N]$, provided we view $x(\cdot)$ as defined over a discretized circle. In (1.4a)–(1.4b), the coefficient matrices M are given, and the noises $e(0)$ and $e(N)$ on the boundary are defined in the same way as in the interior of $[0, N]$, by requiring that the covariance matrix of the full $e(\cdot)$ process should be the inverse of the covariance matrix of the $x(\cdot)$ of process, so that $e(\cdot)$ and $x(\cdot)$ are *conjugate processes* in the sense that

$$E\{e(k)x^*(l)\} = I_n \delta(k - l). \tag{1.5}$$

The case of Dirichlet BCs for a continuous time GRD $x(t)$ has been analyzed in [20]. The case of cyclic BCs in continuous time is a more delicate matter because continuous time GRDs do not have classical derivatives for which pointwise evaluations can be made at the boundary of $[0, T]$. Nonetheless, it is possible to make precise what is meant by "cyclic" BCs in the continuous case, and this paper does so. We should point out that the term "cyclic"does not imply that the BCs are periodic. Indeed, unlike the discrete–time case, where the $x(\cdot)$ process can be viewed as defined over a discretized circle, because of the continuity requirement for the trajectories of $x(\cdot)$, GRDs over $[0, T]$ cannot usually be considered as defined over a circle obtained by identifying the ends 0 and T of the interval $[0, T]$. However, an alternative interpretation of the discrete–time cyclic BCs (1.4a)–(1.4b) which can be extended to the continuous-time case consists in noting that the property (1.5) implies discrete time Gaussian reciprocal processes have a covariance matrix with a cyclic block tridiagonal inverse. In [21], this observation was used to show that the set of positive definite symmetric cyclic block tridiagonal matrices is bijective to the set of discrete–time Gaussian reciprocal processes on $[0, N]$. The bijection identifies covariance matrices with inverses of cyclic tridiagonal matrices. It is proved in Section 2 that there exists a similar bijection in the continuous case, between GRDs on $[0, T]$ and positive definite self-adjoint Sturm–Liouville operators on the same interval. Except for the requirement that the Sturm–Liouvile operator should be positive self-adjoint, the BCs are arbitrary, and are called "cyclic" only because they couple the functions in the domain of the operator, and their derivatives, at both ends of $[0, T]$.

In Section 3 it is shown that every GRD can be regarded as a weak solution of its corresponding Sturm–Liouville BVP. This makes precise the notion of cyclic BCs in the continuous time case. Here the "corresponding" Sturm–Liouville BVP we have in mind is the BVP for which the process covariance $R(t, s)$ is the Green's function. Finally, the section 4 explores the conditions under which the Sturm–Liouville stochastic BVP satisfied by a GRD can be formulated as a first-order two-point BVP of the type examined in [17, 2, 26]. It turns out that the class of GRDs that can be constructed in this manner are those with a negative definite stress tensor over the interval $[0, T]$, where the stress tensor is one of the quantities, together with the density and mean velocity, which are propagated by the conservation laws of GRDs. The first-order BVP implementing this subclass of GRDs has twice the dimension of the original Sturm–Liouville BVP, and its solution can be expressed as the sum of a Wiener integral plus a stochastically independent boundary term.

2 POSITIVE STURM–LIOUVILLE OPERATORS AND GAUSSIAN RECIPROCAL DIFFUSIONS OVER $[0, T]$

Let $L_n^2[0, T]$ denote the real Hilbert space of functions taking values in $\mathbb{R}^n$, with inner product $\langle u, v\rangle = \int_0^T u^*(t)v(t)dt$. Consider the formal 2nd order differential operator

$$L = A_2(t)\frac{d^2}{dt^2} + A_1(t)\frac{d^1}{dt^1} + A_0(t)\frac{d^0}{dt^0}, \tag{2.1}$$

where we assume that the matrix coefficients $A_i(t)$ belong respectively to $C^i_{n\times n}[0, T]$ for $i = 0, 1, 2.$[1] Given the boundary condition

$$Bu \overset{\triangle}{=} \alpha_1 u(0) + \alpha_2 u(T) + \alpha_3 \dot{u}(0) + \alpha_4 \dot{u}(T) = 0 \tag{2.2a}$$

where the $2n \times n$ matrices α_k are such that the $2n \times 4n$ matrix

$$\alpha = [\alpha_1\ \alpha_2\ \alpha_3\ \alpha_4] \tag{2.2b}$$

has the full rank, we define the subspace $E \subset L_n^2[0, T]$ as

$$E = \{u \in L_n^2[0, T] : \dot{u} \text{ is absolutely continuous}, \ddot{u} \in L_n^2[0, T], \text{ and } Bu = 0\}. \tag{2.3}$$

Then the linear operator $L_E : E \to L_n^2[0, T]$ is defined by the rule $u \in E \to Lu \in L_n^2[0, T]$. Note that our notation distinguishes the formal differential "operator" L from the actual differential operator L_E. L_E is said to be a Sturm–Liouville

[1] This requirement can be weakened somewhat if we adopt the parametrization of L given in equation (2.59) below.

operator if it is self-adjoint, i.e. for all $u, v \in E$, $\langle Lu, v\rangle = \langle u, Lv\rangle$. Furthermore, it is positive definite if for all nonzero $u \in E$, $\langle Lu, u\rangle > 0$. We will repeatedly make use of the following two results from the theory of Sturm–Liouville BVPs [12, 28].

SL1. If L_E is positive definite self-adjoint, so is L_D, where D is the subspace of $L_n^2[0, T]$ specified by the homogeneous Dirichlet conditions, which correspond to the choice

$$\alpha_1 = \begin{bmatrix} I_n \\ 0 \end{bmatrix} \quad \alpha_2 = \begin{bmatrix} 0 \\ I_n \end{bmatrix} \quad \alpha_3 = \alpha_4 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{2.4}$$

SL2. Let $D[0, T]$ be the subspace defined in SL1, and let $D[t_0, t_1]$ be the subspace of $L_n^2[t_0, t_1]$ obtained by applying homogeneous Dirichlet conditions to the subinterval $[t_0, t_1]$ of $[0, T]$. Then, if $L_{D[0,T]}$ is positive definite self-adjoint, so is $L_{D[t_0,t_1]}$.

The results of this paper are based in large part on the following theorem, which establishes a bijection between the set of positive definite Sturm–Liouville operators on $[0, T]$ and the set of GRDs on the same interval. This bijection identifies the operator Green's function with the covariance of the corresponding process.

THEOREM 2.1 *Let $x(t)$ be a* GRD *on $[0, T]$ with covariance $R(t, s) = E\{x(t)x^*(s)\}$. Then there exists a unique positive definite self-adjoint operator L_E such that $R(t, s)$ is the Green's function of L_E. Conversely, if L_E is a positive definite self-adjoint operator with Green's function $G(t, s)$, there exists a unique GRD $x(t)$ on $[0, T]$ with covariance $E\{x(t)x^*(s)\} = G(t, s)$.*

Before proving Theorem 2.1, we introduce some notation and establish a basic lemma regarding the kinds of boundary conditions that can arise in positive definite Sturm–Liouville BVPs. We will formulate both the domain E and the formal operator L in terms that allow for streamlined proofs of not only Therorem 2.1, but also of results to be presented in subsequent sections of the paper.

We write the formal operator L in the form

$$L = Q^{-1}(t)\left(-\frac{d^2}{dt^2} + G(t)\frac{d^1}{dt^1} + F(t)\frac{d^0}{dt^0}\right), \tag{2.5}$$

where $Q(t)$ is symmetric positive definite on $[0, T]$, and where the following self-adjointness conditions [20] are satisfied

$$\frac{1}{2}(Q^{-1}G + G^*Q^{-1}) = -\frac{d}{dt}(Q^{-1}) \tag{2.6a}$$

$$Q^{-1}F - F^*Q^{-1} = \frac{1}{2}\frac{d}{dt}(Q^{-1}G - G^*Q^{-1}). \tag{2.6b}$$

Since we restrict our attention herein to positive definite self-adjoint operators, the reader may verify that there is no loss of generality in replacing the form (2.1) for L by (2.5).

In the following we will make use of the $n \times n$ boundary-value transition matrices $\psi_1(t)$ and $\psi_2(t)$ for the operator L_D, which satisfy

$$L\psi_1(t) = L\psi_2(t) = 0 \tag{2.7}$$

with boundary conditions

$$\begin{bmatrix} \psi_1(0) & \psi_2(0) \\ \psi_1(T) & \psi_2(T) \end{bmatrix} = \begin{bmatrix} I_n & 0 \\ 0 & I_n \end{bmatrix} = \mathbf{I}. \tag{2.8}$$

If L_E is positive self-adjoint, the existence of ψ_1 and ψ_2 is ensured by SL1. As in (2.8), $2n \times 2n$ matrices will be denoted by boldface in the remainder of this paper.

Next we assert that the BCs of a positive definite Sturm–Liouville problem can always be cast in a certain form. This form will prove quite convenient for linking the study of positive definite Sturm–Liouville operators to the study of GRDs.

LEMMA 2.1 *Consider a formal operator L of the form* (2.5) *and a subspace $E \subset L_n^2[0, T]$ of the form* (2.3), *such that the resulting operator L_E is positive definite self-adjoint. Let $G(t, s)$ be the Green's function for L_E. Then, in the parametrization* (2.3) *of E, we can replace the boundary condition $Bu = 0$ by*

$$B'u \triangleq (\mathbf{I} + \mathbf{PQ}^{-1}\mathbf{\Psi})\begin{bmatrix} u(0) \\ u(T) \end{bmatrix} - \mathbf{PQ}^{-1}\begin{bmatrix} \dot{u}(0) \\ \dot{u}(T) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \tag{2.9}$$

where

$$\mathbf{P} = \begin{bmatrix} G(0,0) & G(0,T) \\ G(T,0) & G(T,T) \end{bmatrix} \tag{2.10a}$$

$$\mathbf{Q} = \begin{bmatrix} Q(0) & 0 \\ 0 & -Q(T) \end{bmatrix} \tag{2.10b}$$

$$\mathbf{\Psi} = \begin{bmatrix} \dot{\psi}_1(0) & \dot{\psi}_2(0) \\ \dot{\psi}_1(T) & \dot{\psi}_2(T) \end{bmatrix}. \tag{2.10c}$$

Remark Lemma 2.1 asserts, in effect, that the $2n \times 4n$ matrix α given by (2.2b) can always be premultiplied by an invertible $2n \times 2n$ matrix to yield the $2n \times 4n$ matrix

$$[\mathbf{I} + \mathbf{PQ}^{-1}\mathbf{\Psi} \quad -\mathbf{PQ}^{-1}]. \tag{2.11}$$

Proof of Lemma 2.1 It suffices to show that the Green's function $G(t, s)$ of L_E satisfies

$$(\mathbf{I} + \mathbf{PQ}^{-1}\mathbf{\Psi})\begin{bmatrix} G(0,s) \\ G(T,s) \end{bmatrix} - \mathbf{PQ}^{-1}\begin{bmatrix} \frac{\partial G}{\partial t}(0,s) \\ \frac{\partial G}{\partial t}(T,s) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \tag{2.12}$$

for $0 < s < T$. To do so, we obtain a representation of G that allows for a proof of (2.12) by direct calculation.

Let $\tilde{G}(t,s)$ denote the Green's function of L_D, where D is the subspace of $L_n^2[0,T]$ corresponding to homogeneous Dirichlet BCs (i.e. $\mathbf{P}=0$ in (2.9)). Then standard Green's function construction techniques yield the representation

$$\tilde{G}(t,s) = \begin{cases} \psi_2(t)K\psi_1^*(s), & 0 \le t \le s \le T \\ \psi_1(t)K^*\psi_2^*(s), & 0 \le s \le t \le T, \end{cases} \tag{2.13}$$

where K is a constant matrix. K admits several representations [10], two of which are

$$K = [\dot{\psi}_2(s) - \dot{\psi}_1(s)\psi_1^{-1}(s)\psi_2(s)]^{-1}Q(s)\psi_1^{-*}(s) \tag{2.14a}$$

$$= \psi_2^{-1}(s)Q(s)[\dot{\psi}_2(s)\psi_2^{-1}(s)\psi_1(s) - \dot{\psi}_1(s)]^{-*}, \tag{2.14b}$$

where "$-*$' denotes the inverse transpose. Since K is constant, the above representations do not really depend on s. Setting $s=0$ and $s=T$ in (2.14a) and (2.14b), respectively, gives the simplified expressions

$$K = (\dot{\psi}_2(0))^{-1}Q(0) = -Q(T)(\dot{\psi}_1(T))^{-*}, \tag{2.15}$$

which will prove useful below. Next, let

$$\hat{G}(t,s) = [\psi_1(t) \quad \psi_2(t)]\begin{bmatrix} G(0,0) & G(0,T) \\ G(T,0) & G(T,T) \end{bmatrix}\begin{bmatrix} \psi_1^*(s) \\ \psi_2^*(s) \end{bmatrix}. \tag{2.16}$$

We claim that G can be represented as

$$G(t,s) = \tilde{G}(t,s) + \hat{G}(t,s). \tag{2.17}$$

To see this, observe that $L_t[\tilde{G}(t,s) + \hat{G}(t,s)] = \delta(t-s)$, so that $L_t[G(t,s) - \tilde{G}(t,s) - \hat{G}(t,s)] = 0$, and that $G - \tilde{G} - \hat{G} = 0$ on the corners of $[0,T]\times[0,T]$. It then follows from SL1 that $G - \tilde{G} - \hat{G} = 0$ everywhere on $[0,T]\times[0,T]$. Using the representation (2.17) for $G(t,s)$, we can prove (2.12) by direct calculation as follows. For $0 < s < T$, we have

$$\begin{aligned} &(\mathbf{I} + \mathbf{PQ}^{-1}\mathbf{\Psi})\begin{bmatrix} G(0,s) \\ G(T,s) \end{bmatrix} - \mathbf{PQ}^{-1}\begin{bmatrix} \frac{\partial G}{\partial t}(0,s) \\ \frac{\partial G}{\partial t}(T,s) \end{bmatrix} \\ &= \begin{bmatrix} \hat{G}(0,s) \\ \hat{G}(T,s) \end{bmatrix} + \mathbf{PQ}^{-1}\left(\begin{bmatrix} \frac{\partial \hat{G}}{\partial t}(0,s) \\ \frac{\partial \hat{G}}{\partial t}(T,s) \end{bmatrix} - \begin{bmatrix} \frac{\partial G}{\partial t}(0,s) \\ \frac{\partial G}{\partial t}(T,s) \end{bmatrix}\right) \\ &= \begin{bmatrix} \hat{G}(0,s) \\ \hat{G}(T,s) \end{bmatrix} - \mathbf{PQ}^{-1}\begin{bmatrix} \frac{\partial \tilde{G}}{\partial t}(0,s) \\ \frac{\partial \tilde{G}}{\partial t}(T,s) \end{bmatrix}. \end{aligned} \tag{2.18}$$

But

$$Q^{-1}(0)\frac{\partial\tilde{G}}{\partial t}(0,s)=\psi_1^*(s) \tag{2.19a}$$

$$-Q^{-1}(T)\frac{\partial\tilde{G}}{\partial t}(T,s)=\psi_2^*(s), \tag{2.19b}$$

so that (2.18) is zero by the definitions of **P** and $\hat{G}$. □

We are now in position to establish Theorem 2.1.

Proof of Theorem 2.1 We must show that:

(1) If $x(t)$ is a GRD on $[0,T]$ with covariance $R(t,s)$, there exists a unique positive definite self-adjoint operator L_E such that $R(t,s)$ is the Green's function of L_E.
(2) If $G(t,s)$ is the Green's function for a positive definite self-adjoint operator L_E, there exists a unique GRD $x(t)$ on $[0,T]$ such that $G(t,s)=E\{x(t)x^*(s)\}$.

Proof of (1) Let $x(t)$ be a GRD on $[0,T]$ with covariance function $R(t,s)$. To $x(t)$, we can associate a formal self-adjoint operator L of the form (2.5) with

$$Q(t)=-\left(\frac{\partial R}{\partial t}(t^+,t)-\frac{\partial R}{\partial t}(t^-,t)\right) \tag{2.20a}$$

$$G(t)=-\left(\frac{\partial^2 R}{\partial t^2}(t^+,t)-\frac{\partial^2 R}{\partial t^2}(t^-,t)\right)Q^{-1}(t) \tag{2.20b}$$

$$F(t)=\left(\frac{\partial^2 R}{\partial t^2}(t^+,t)-G(t)\frac{\partial R}{\partial t}(t^+,t)\right)R^{-1}(t,t) \tag{2.20c}$$

It is shown in [20] that the corresponding L_D is positive definite self-adjoint, and $R(t,s)$ satisfies

$$L_tR(t,s)=\delta(t-s). \tag{2.21}$$

It is also proved in [20] and [10] that

$$R(t,s)=\tilde{R}(t,s)+\hat{R}(t,s), \tag{2.22}$$

where $\tilde{R}(t,s)$ has exactly the form given by the RHS of (2.13), and $\hat{R}(t,s)$ has the form given by the RHS of (2.16), with the symbol "G" replaced by "R". In both cases the ψ matrices are defined by the conditions (2.7–2.8), and their existence is ensured since L_D is positive. Now, applying the calculations in (2.18) to $R(t,s)$, we conclude that, for $0<s<T$,

$$(\mathbf{I}+\mathbf{P}\mathbf{Q}^{-1}\mathbf{\Psi})\begin{bmatrix}R(0,s)\\R(T,s)\end{bmatrix}-\mathbf{P}\mathbf{Q}^{-1}\begin{bmatrix}\frac{\partial R}{\partial t}(0,s)\\\frac{\partial R}{\partial t}(T,s)\end{bmatrix}=\begin{bmatrix}0\\0\end{bmatrix}, \tag{2.23}$$

where $\mathbf{P}$ is the matrix obtained by replacing "G" with "R" in (2.10a). From (2.21) and (2.23) we conclude that $R(t,s)$ is the Green's function of L_E, where we use the boundary condition (2.9) to parametrize E. The uniqueness of L_E is due to the fact that R can have only one inverse. This completes the proof of (1). Next we carry out the proof of (2) in five steps.

2-i) Prove that there exists a zero-mean Gaussian process $x(t)$ on $[0,T]$ such that $G(t,s) = R(t,s) = E\{x(t)x^*(s)\}$.
2-ii) Prove that $x(t)$ has continuous sample paths a.s.
2-iii) Prove that for $0 < t_0 < t_1 < T$ the two time covariance matrix

$$\begin{bmatrix} R(t_0,t_0) & R(t_0,t_1) \\ R(t_1,t_0) & R(t_1,t_1) \end{bmatrix} \tag{2.24}$$

is invertible.
2-iv) Prove that $x(t)$ satisfies the full rank noise assumption.
2-v) Prove that $x(t)$ is reciprocal.

2-i) To prove that there exists a zero-mean Gaussian process $x(t)$ on $[0,T]$ with covariance $G(t,s)$, we note first that since L_E is positive-definite, so is L_E^{-1}, i.e.

$$\langle L_E^{-1}v, v\rangle = \int_0^T\int_0^T v^*(t)G(t,s)v(s)dtds > 0 \tag{2.25}$$

for every nonzero $v \in L_n^2[0,T]$. Given $t_1,\dots,t_p$ in $[0,T]$, let $C(t_1,\dots,t_p)$ denote the $np \times np$ matrix whose (i,j)th block is $G(t_i,t_j), 1 \le i,j \le p$. The self–adjointness of L_E^{-1} implies that C is symmetric. Also, C is nonnegative (though not necessarily positive) definite. To see this, let $a^* = (a_1^*,\dots,a_p^*)$ be a row vector in $\mathbb{R}^{np}$, and define the sequence $\{v_k(t)\}$ by

$$v_k(t) = k(a_1I_{1k}(t) + \cdots + a_pI_{pk}(t)), \tag{2.26}$$

where $I_{mk}(t)$ is the indicator function of the interval $[t_m - 1/2k, t_m + 1/2k]$ (with the obvious modification in definition if $t_1 = 0$ or $t_p = T$). Then $a^*Ca = \lim_{k\to\infty}\langle L_E^{-1}v_k, v_k\rangle \ge 0$. Here we have used the continuity of $G(t,s)$ on $[0,T]\times[0,T]$. This continuity follows from the fact that G is the Green's function for a Sturm–Liouville operator.

Now consider the zero-mean Gaussian distribution on $\mathbb{R}^{np}$ whose covariance matrix is $C(t_1,\dots,t_p)$. These finite-dimensional distribution satisfy the consistency hypotheses of Kolmogorov's existence theorem (see Theorem 3.1 of [13]), so there exists a stochastic process $x(t)$ on $[0,T]$ having these finite-dimensional distributions. Clearly $G(t,s)$ is the covariance of this process.

2-ii) To prove that $x(t)$ has continuous sample paths a.s., observe that if $z(t) = b^*x(t)$, where b is an arbitrary vector of R^n, we have

$$E\{(z(t+h) - z(t))^2\} = b^*[G(t+h,t+h) - G(t+h,t) - G(t,t+h) + G(t,t)]b. \tag{2.27}$$

Then, using the moment factoring identity

$$E\{(z(t+h)-z(t))^4\} = 3(E\{(z(t+h)-z(t))^2\})^2 \tag{2.28}$$

for zero-mean Gaussian random variables, we can conclude that

$$E\{(z(t+h)-z(t))^4\} \leq Mh^2, \tag{2.29}$$

where M is a constant independent of t and h. It follows fromt the Kolmogorov continuity theorem ([32], p. 51) that $z(t)$, and thus $x(t)$, have sample path continuous versions.

2-(iii) To show that the two time covariance matrix

$$\begin{bmatrix} G(t_0,t_0) & G(t_0,t_1) \\ G(t_1,t_0) & G(t_1,t_1) \end{bmatrix} \tag{2.30}$$

is invertible for $0 < t_0 < t_1 < T$, we note from Lemma 2.1 that since $G(t,s)$ is the Green's function of L_E, it admits the representation $G = \tilde{G} + \hat{G}$. Thus

$$\begin{bmatrix} G(t_0,t_0) & G(t_0,t_1) \\ G(t_1,t_0) & G(t_1,t_1) \end{bmatrix} = \begin{bmatrix} \tilde{G}(t_0,t_0) & \tilde{G}(t_0,t_1) \\ \tilde{G}(t_1,t_0) & \tilde{G}(t_1,t_1) \end{bmatrix} + \begin{bmatrix} \hat{G}(t_0,t_0) & \hat{G}(t_0,t_1) \\ \hat{G}(t_1,t_0) & \hat{G}(t_1,t_1) \end{bmatrix}. \tag{2.31}$$

From the definitions (2.15) of $\hat{G}$ and (2.12) of $\tilde{G}$, it is clear that both matrices on the RHS of (2.31) are nonnegative definite. It suffices therefore to show that the first matrix on the RHS is invertible when $0 < t_0 < t_1 < T$.

Now, the matrix K defined in (2.12) is invertible, so that unless $t_0 = 0$ or $t_1 = T$, the $2n \times 1$ column vector in R^{2n}. But then the column vector

$$\begin{bmatrix} K^*\psi_2^*(t_0)a \\ K\psi_1^*(t_1)b \end{bmatrix} \tag{2.32}$$

must be nonzero, where $[a^*, b^*]^*$ is any nonzero column vector in $\mathbb{R}^{2n}$. But then the column vector

$$\begin{bmatrix} \psi_1(t_0) & \psi_2(t_0) \\ \psi_1(t_1) & \psi_2(t_1) \end{bmatrix} \begin{bmatrix} K^*\psi_2^*(t_0)a \\ K\psi_1^*(t_1)b \end{bmatrix} \tag{2.33}$$

must be nonzero. But from (2.12) we see that (2.33) is exactly

$$\begin{bmatrix} \tilde{G}(t_0,t_0) & \tilde{G}(t_0,t_1) \\ \tilde{G}(t_1,t_0) & \tilde{G}(t_1,t_1) \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix}. \tag{2.34}$$

Hence the first matrix on the RHS of (2.31) is invertible. This completes the proof of 2-iii.

2-iv) Next, to prove that $x(t)$ satisfies the full rank noise assumption, we observe that since $G(t,s)$ is the Green's function for L_E, it satisfies

$$\frac{\partial G(t^+,t)}{\partial t} - \frac{\partial G(t^-,t)}{\partial t} = -Q(t). \tag{2.35}$$

But Q must be positive definite symmetric, since L_E is positive definite and self-adjoint. This completes the proof of 2-iv).

2-v) We now prove that $x(t)$ is reciprocal. Let $[t_0, t_1]$ be a subinterval of $[0, T]$, and assume t and s are inside and outside this subinterval, respectively. For $t \in [0, T]$ define

$$y(t) = E\{x(t) | x(t_0), x(t_1)\}. \tag{2.36}$$

Then

$$y(t) = [G(t,t_0)\ G(t,t_1)] \begin{bmatrix} G(t_0,t_1) & G(t_0,t_1) \\ G(t_1,t_0) & G(t_1,t_1) \end{bmatrix}^{\dagger} \begin{bmatrix} x(t_0) \\ x(t_1) \end{bmatrix}, \tag{2.37}$$

where $\dagger$ denotes the matrix pseudoinverse. Of course, from 2-iii we know that this pseudoinverse will coincide with the actual inverse except possibly when $t_0 = 0$ or $t_1 = T$. In any case, using elementary properties of the pseudoinverse, we see that

$$E\{y(t)y^*(s)\} = [G(t,t_0)\ G(t,t_1)] \begin{bmatrix} G(t_0,t_0) & G(t_0,t_1) \\ G(t_1,t_0) & G(t_1,t_1) \end{bmatrix}^{\dagger} \begin{bmatrix} G(t_0,s) \\ G(t_1,s) \end{bmatrix}. \tag{2.38}$$

On (t_0, t_1) we have $L_t(E\{y(t)y^*(s)\}) = 0$. This follows from applying L to the RHS of (2.38). Moreover, it is clear from the definition of y in (2.36) that at times t_0 and t_1 the equalities $E\{y(t_0)y^*(s)\} = G(t_0,s)$ and $E\{y(t_1)y^*(s)\} = G(t_1,s)$ must hold, since $x(\cdot) - y(\cdot)$ is uncorrelated with $x(t_0)$ and $x(t_1)$. Thus $G(t,s) - E\{y(t)y^*(s)\}$ vanishes at the endpoints of $[t_0,t_1]$, and is in the nullspace of L on (t_0,t_1). Now, from SL1 we know that L_D is positive, so then by SL2 L has no conjugate points on subintervals of $[0,T]$. Hence $G(t,s) - E\{y(t)y^*(s)\}$ vanishes identically for $t \in [t_0,t_1]$. We conclude that $E\{y(t)y^*(s)\} = G(t,s)$, and applying this fact to (2.38) gives

$$G(t,s) = [G(t,t_0)\ G(t,t_1)] \begin{bmatrix} G(t_0,t_0)\ G(t_0,t_1) \\ G(t_1,t_0)\ G(t_1,t_1) \end{bmatrix}^{\dagger} \begin{bmatrix} G(t_0,s) \\ G(t_1,s) \end{bmatrix}. \tag{2.39}$$

But the equation (4) of [1] implies that a zero-mean Gaussian process is reciprocal if and only if (2.39) holds, so that $x(t)$ is reciprocal on $[0,T]$. □

A potential application of the above result concerns the computation of the Karhunen–Loève expansion of GRDs. The normal procedure for constructing this expansion [34], section 3.4 consists in finding the eigenvalues and eigenfunctions of the integral operator R over $L_n^2[0,T]$ with kernel $R(t,s)$. However, since $R(t,s)$ is the

Green's function of L_E, if $\phi(t)$ is an eigenfunction of R corresponding to the eigenvalue λ, it is also an eigenfunction of L_E corresponding to the eigenvalue $1/\lambda$. Thus, the problem of finding the Karhunen–Loève expansion of a GRD corresponding to a given positive Sturm–Liouville operator L_E reduces to one of finding the eigenvalues and eigenfunctions of L_E, an easier problem than the corresponding eigenvalue problem for R.

Also, it was shown in [21] that within the class of discrete-time Gaussian reciprocal processes, the Gauss–Markov processes are characterized by the property that the inverse of their covariance matrix is tridiagonal, instead of cyclic tridiagonal. Completing some earlier results of Beghi [4], we now extend this characterization to the continuous time case. To do so, we restrict our attention to Gauss–Markov diffusions (GMDs) for which the joint covariance matrix $\mathbf{P}$ of $x(0)$ and $x(T)$ is positive definite.

In the following, the forward and backward first-order differences of a stochastic processes $x(\cdot)$ are denoted respectively as

$$d^+x(t,h) = x(t+h) - x(t) \tag{2.40a}$$

$$d^-x(t,h) = x(t) - x(t-h). \tag{2.40b}$$

Then, if $x(t)$ is a Gauss–Markov diffusion over $[0, T]$, it satisfies a first-order stochastic differential equation of the form

$$d^+x(t) = \int_t^{t+h} A(s)x(s)ds + \int_t^{t+h} B(s)dw(s), \tag{2.41}$$

where $w(t)$ is a standard Wiener process, and $B(t)B^*(t) = Q(t)$. Its covariance can be expressed as

$$R(t,s) = \begin{cases} \phi(t,s)\Pi(s) & t \geq s \\ \Pi(t)\phi^*(s,t) & s \geq t, \end{cases} \tag{2.42}$$

where $\phi(t,s)$ denotes the transition matrix of A, i.e.

$$\frac{\partial\phi}{\partial t}(t,s) = A(t)\phi(t,s) \quad \phi(s,s) = I_n, \tag{2.43a}$$

and the state covariance $\Pi(t) = E\{x(t)x^*(t)\}$ satisfies the Lyapunov equation

$$\dot{\Pi}(t) = A(t)\Pi(t) + \Pi(t)A^*(t) + Q(t). \tag{2.43b}$$

From the representation (2.42) for $R(t,s)$ we immediately deduce that

$$\frac{\partial R}{\partial t}(t,s) = \begin{cases} A(t)R(t,s) & t \geq s \\ A_b(t)R(t,s) & s \geq t, \end{cases} \tag{2.44}$$

where $A_b(t) \triangleq A(t) + Q(t)\Pi^{-1}(t)$ denotes the state dynamics matrix of the backward stochastic differential equation satisfied by $x(t)$. This implies that if $x(t)$ is a GMD, its covariance $R(t,s)$ satisfies *separable* boundary conditions

$$\frac{\partial R}{\partial t}(0,s) = A_b(0)R(0,s) \tag{2.45a}$$

$$\frac{\partial R}{\partial t}(T,s) = A(T)R(T,s) \tag{2.45b}$$

for $0 < s < T$, where the positive-definiteness of $\mathbf{P}$ ensures that the matrices $A(T)$ and $A_b(0)$ remain finite. This suggests that within the larger class of GRDs, the GMDs are characterized by the feature that their corresponding Sturm–Liouville BVP admits separable boundary conditions, as we now demonstrate.

THEOREM 2.2 *$x(t)$ is a GMD on $[0,T]$ with $\mathbf{P}$ invertible, and with covariance $R(t,s)$ if and only if there exists a positive definite Sturm–Liouville operator L_E with separable boundary conditions*

$$\dot{u}(0) - A_0u(0) = 0 \tag{2.46a}$$

$$\dot{u}(T) - A_Tu(T) = 0 \tag{2.46b}$$

such that $R(t,s)$ is the Green's function of L_E.

Proof We have already proved necessity. To establish sufficiency, suppose L_E is a Sturm–Liouville operator obeying the boundary conditions (2.46a)–(2.46b). Denoting

$$\mathbf{A} = \begin{bmatrix} A_0 & 0 \\ 0 & A_T \end{bmatrix}, \tag{2.47}$$

the self-adjointness of L_E implies

$$\mathbf{Z} = \mathbf{Q}^{-1}\mathbf{A} - \mathbf{A}^*\mathbf{Q}^{-1} \tag{2.48a}$$

with

$$\mathbf{Z} \triangleq \frac{1}{2}\begin{bmatrix} (Q^{-1}G - G^*Q^{-1})(0) & 0 \\ 0 & -(Q^{-1}G - G^*Q^{-1})(T) \end{bmatrix}. \tag{2.48b}$$

Consider now the problem of constructing a factorization

$$L = M^*Q^{-1}M \tag{2.49}$$

with

$$M = I_n\frac{d}{dt} - A(t) \tag{2.50a}$$

for the formal operator L, where $A(t)$ denotes a $n \times n$ matrix function, and

$$M^* = -I_n \frac{d}{dt} - A^*(t) \tag{2.50b}$$

represents the formal adjoint of M. Matching coefficients of the derivatives on both sides of (2.49), we find $A(t)$ must satisfy the Riccati equation

$$\dot{A} + A^2 = F + GA \tag{2.51}$$

as well as the algebraic constraint

$$(Q^{-1}A - A^*Q^{-1})(t) = \frac{1}{2}(Q^{-1}G - G^*Q^{-1})(t). \tag{2.52}$$

Let

$$S(t) \triangleq \left[(Q^{-1}A - A^*Q^{-1}) - \frac{1}{2}(Q^{-1}G - G^*Q^{-1})\right]. \tag{2.53}$$

If $A(t)$ satisfies the Riccati equation (2.51), by taking into account the self-adjointness relations (2.6a)–(2.6b), one gets

$$\dot{S} = -A^*S - SA. \tag{2.54}$$

so that

$$S(t) = \phi^*(T, t)S(T)\phi(T, t), \tag{2.55}$$

where $\phi(t, s)$ denotes the transition matrix of A. Consequently, if A satisfies the Riccati equation (2.51) and $S(T) = 0$, the constraint $S(t) = 0$ is satisfied for all t. To ensure $S(T) = 0$, we need only to select $A(T) = A_T$ as initial condition for the Riccati equation (2.51), where A_T is the matrix appearing in the BC (2.46b), since the self-adjointness condition (2.48a) guarantees $S(T) = 0$. For this choice of initial condition, the existence of a solution $A(t)$ to the Riccati equation (2.51) over the interval $(0, T]$ is proved in Lemma 2.2 below.

Given the resulting solution $A(t)$ to (2.51), we can define

$$H(t, s) \triangleq \frac{\partial R}{\partial t}(t, s) - A(t)R(t, s). \tag{2.56}$$

The boundary condition (2.46b) gives $H(T, s) = 0$, which in combination with the differential equation

$$LR(t, s) = M^*Q^{-1}(t)H(t, s) = 0 \tag{2.57}$$

for $t > s$, implies $H(t, s) = 0$ for $t > s$. Thus, $x(t)$ is a Markov process with forward state-space model $(A(t), Q(t))$. □

Remark Comparing (2.46a)–(2.46b) to the BC (2.9) for general GRD, and using the fact that the matrix α in (2.2b) which parametrizes the BC of a positive Sturm–Liouville operator is unique up to left multiplication by an invertible matrix, we can conclude that if $x(t)$ is a *GMD*, its boundary covariance matrix $\mathbf{P}$ is such that $\mathbf{P}^{-1} + \mathbf{Q}^{-1}\mathbf{\Psi}$ is block diagonal, which in light of the identity (2.15) for K implies $\mathbf{P}^{-1}$ has the structure

$$\mathbf{P}^{-1} = \begin{bmatrix} * & -K^{-1} \\ -K^{-*} & * \end{bmatrix}, \tag{2.58}$$

where $*$ denotes an unspecified entry, which was used in [4] to characterize the GMDs with fixed reciprocal dynamics.

Our proof of the existence of a solution over $[0, T]$ to the Riccati equation (2.51) with initial condition $A(T) = A_T$ relies on a variational characterization of the smallest eigenvalue of L_E. First, observe by using the self-adjointness conditions (2.6a)–(2.6b) that L can be expressed[2] as

$$Lu = -\frac{d}{dt}\left[Q^{-1}\frac{du}{dt} - Su\right] - S^*\frac{du}{dt} + Wu \tag{2.59}$$

with

$$S(t) \triangleq \frac{1}{4}(Q^{-1}G - G^*Q^{-1})(t) \tag{2.60a}$$

$$W(t) \triangleq \frac{1}{2}(Q^{-1}F + F^*Q^{-1})(t). \tag{2.60b}$$

Then, integrating by parts, it is easy to verify that for all $u \in E$, where E is the space defined by the boundary conditions (2.46a)–(2.46b), we have $\langle u, Lu \rangle = J(u)$ with

$$J(u) \triangleq \int_0^T [\dot{u}^* \;\; u^*]\begin{bmatrix} Q^{-1} & -S \\ -S^* & W \end{bmatrix}\begin{bmatrix} \dot{u} \\ u \end{bmatrix} dt + [u^*(0) \;\; u^*(T)](\mathbf{Q}^{-1}\mathbf{A} + \mathbf{A}^*\mathbf{Q}^{-1})\begin{bmatrix} u(0) \\ u(T) \end{bmatrix}, \tag{2.61}$$

where A is the matrix defined in (2.47). Furthermore, as shown in [28], section 6.3, the smallest eigenvalue λ_0 of L_E admits the variational characterization

$$\lambda_0 = \min_{u \in U} \frac{J(u)}{\|u\|^2} \tag{2.62}$$

where the minimization is performed over the space U of piecewise C^1 n-vector functions over $[0, T]$, which contains E as a subspace. We can now prove the following result.

[2] Note that for this representation of L, the matrix function Q needs only to be C^1, whereas S and W must be C^1 and C^0, respectively.

LEMMA 2.2 *Let L_E be a positive definite Sturm–Liouville operator with separable boundary conditions* (2.46a)–(2.46b). *Then, if A_T is the matrix appearing in the* BC (2.46b), *the Riccati equation* (2.51) *with initial condition $A(T) = A_T$ admits a solution over* $(0, T]$.

Proof Consider the system

$$\begin{bmatrix} \dot{X} \\ \dot{Y} \end{bmatrix} = \begin{bmatrix} 0 & I_n \\ F & G \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix} \tag{2.63a}$$

with initial conditions

$$X(T) = I_n \quad Y(T) = A_T. \tag{2.63b}$$

Then, as long as $X(t)$ is nonsingular, the matrix $A(t) = Y(t)X^{-1}(t)$ solves the Riccati equation (2.51). But $X(t)$ must be nonsingular over $(0, T]$. To see this, note that it satisfies $LX = 0$ with the boundary condition (2.46b). Suppose there exists a time $t_0 > 0$ and a nonzero vector $c \in \mathbb{R}^n$ such that $X(t_0)c = 0$. We can always extend $u(t) \triangleq X(t)c$ to the left of t_0 by an identically zero function. The resulting function is piecewise C^1 and

$$J(u) = \int_{t_0}^{T} [\dot{u}^* \ u^*] \begin{bmatrix} Q^{-1} & -S \\ -S^* & W \end{bmatrix} \begin{bmatrix} \dot{u} \\ u \end{bmatrix} dt - u^*(T)Q^{-1}(T)A_T u(T). \tag{2.64}$$

Integrating by parts gives

$$J(u) = \int_{t_0}^{T} u^*(t)Lu(t)dt - u^*(t_0)Q^{-1}\dot{u}(t_0) + u^*(T)Q^{-1}(\dot{u}(T) - A_T u(T)) = 0, \tag{2.65}$$

so that we have constructed a nonzero function $u \in U$ such that $J(u) = 0$, which violates the positive definiteness assumption for L_E. Thus $X(t)$ is invertible over $(0, T]$, and $A(t)$ exists over $(0, T]$.

3 GRDS AS WEAK SOLUTIONS OF STURM–LIOUVILLE BVPs

Consider a continuous time GRD $x(t)$ over $[0, T]$. By analogy with the discrete-time case considered in [21], we now proceed to demonstrate that $x(t)$ satisfies a stochastic BVP with "cyclic" BCs, i.e conditions which couple together first order differences of the process $x(\cdot)$ at $t = 0, T$, and $x(0), x(T)$. In addition to the forward and backward first-order differences defined in (2.40a)–(2.40b), the zeroth, first, and second-order centered differences of $x(\cdot)$ are written as

$$d^0x(t, h) = \frac{1}{2}(x(t + h) + x(t - h)) \tag{3.1a}$$

$$d^1x(t, h) = \frac{1}{2}(d^+x(t, h) + d^-x(t, h)) = \frac{1}{2}(x(t + h) - x(t - h)) \tag{3.1b}$$

$$d^2x(t,h) = d^+x(t,h) - d^-x(t,h) = x(t+h) - 2x(t) + x(t-h)). \tag{3.1c}$$

When using this notation we will usually supress the h argument, as in $d^2x(t)$.

It is shown in [17] (see also [20], [22]) that

$$E\{d^2x(t)|x(t-h), x(t+h)\} = G(t)d^1x(t)h + F(t)d^0x(t)h^2 + o(h^2) \tag{3.2a}$$

$$E\{d^2x(t)d^2x^*(t)|x(t-h), x(t+h)\} = 2Q(t)h + o(h^2), \tag{3.2b}$$

where $Q(t), G(t)$ and $F(t)$ are expressed in terms of the covariance $R(t,s)$ of $x(\cdot)$ as indicated in (2.20a)–(2.20c). Consequently, the normalized residual

$$e(t,h) \triangleq -Q^{-1}(t)[d^2x(t) - E\{d^2x(t)|x(t-h), x(t+h)\}] \tag{3.3}$$

satisfies

$$\frac{e(t,h)}{h^2} = Q^{-1}(t)\left[-\frac{d^2x}{h^2}(t) + G(t)\frac{d^1(x)}{h}(t) + F(t)d^0x(t)\right] + o(h^0) \tag{3.4a}$$

with

$$E\{e(t,h)e^*(t,h)\} = 2Q^{-1}(t)h + o(h^2). \tag{3.4b}$$

Furthermore, the reciprocity property of $x(t)$ and definition (3.3) of the residual $e(t,h)$ imply $e(t,h)$ is uncorrelated with the process $x(\cdot)$ outside the interval $(t-h, t+h)$, i.e

$$E\{e(t,h)x^*(s)\} = 0 \quad \text{for} \quad |s-t| \geq h. \tag{3.5}$$

THEOREM 3.1 *If $x(t)$ is a* GRD *over $[0,T]$, it satisfies the discretized stochastic* BVP

$$L_hx(t) = \xi(t,h) \tag{3.6a}$$

$$B_hx = b(h), \tag{3.6b}$$

with

$$L_hx(t) \triangleq Q^{-1}(t)\left[-\frac{d^2x}{h^2}(t) + G(t)\frac{d^1x}{h}(t) + F(t)d^0x(t)\right] \tag{3.7}$$

and

$$B_hx \triangleq -\mathbf{PQ}^{-1}\frac{1}{h}\begin{bmatrix} d^+x(0) \\ d^-x(T) \end{bmatrix} + (\mathbf{I} + \mathbf{PQ}^{-1}\mathbf{\Psi})\begin{bmatrix} x(0) \\ x(T) \end{bmatrix}, \tag{3.8}$$

where $\xi(t,h)$ *and* $b(h)$ *represent respectively the discretized conjugate process of* $x(t)$ *in the interior and on the boundary of* $[0,T]$, *which satisfies*

$$E\{\xi(t,h)x^*(s)\} = o(h^0) \quad for \quad [t-s| > h \tag{3.9a}$$

$$E\{b(h)x^*(s)\} = o(h^0) \quad for \quad s \in [h, T-h]. \tag{3.9b}$$

Proof The expression (3.4a) implies $\xi(t,h) = e(t,h)/h^2 + o(h^0)$, so that (3.9a) is a consequence of (3.5). Employing a simple projection argument, we find

$$E\{d^+x(0)|x(h), x(T)\} = [S_{11}x(h) + S_{12}x(T)]h + o(h) \tag{3.10a}$$

$$E\{d^-x(T)|x(0), x(T-h)\} = [S_{21}x(0) + S_{22}x(T-h)]h + o(h), \tag{3.10b}$$

where

$$\mathbf{S} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \tag{3.11}$$

satisfies

$$\mathbf{SP} = \begin{bmatrix} \frac{\partial R}{\partial t}(0,0^+) & \frac{\partial R}{\partial t}(0,T) \\ \frac{\partial R}{\partial t}(T,0) & \frac{\partial R}{\partial t}(T,T^-) \end{bmatrix}. \tag{3.12}$$

Since the end-point covariance matrix $\mathbf{P}$ is not necessarily invertible, the equation (3.12) does not specify $\mathbf{S}$ uniquely. However, consider now the scaled boundary residual

$$r(h) \triangleq -\mathbf{PQ}^{-1} \begin{bmatrix} d^+x(0) - E\{d^+x(0)|x(h), x(T)\} \\ d^-x(T) - E\{d^-x(T)|x(0), x(T-h)\} \end{bmatrix}. \tag{3.13}$$

From (3.10a)–(3.10b)), we deduce it admits the expansion

$$\frac{r(h)}{h} = -\mathbf{PQ}^{-1}\frac{1}{h}\begin{bmatrix} d^+x(0) \\ d^-x(T) \end{bmatrix} + \mathbf{T}\begin{bmatrix} x(0) \\ x(T) \end{bmatrix} + o(h^o), \tag{3.14}$$

where by combining (3.12) and (2.12) we find $\mathbf{T}$ obeys

$$\mathbf{TP} = (\mathbf{I} + \mathbf{PQ}^{-1}\mathbf{\Psi})\mathbf{P}. \tag{3.15}$$

This implies

$$\mathbf{T} = \mathbf{I} + \mathbf{PQ}^{-1}\mathbf{\Psi} + \mathbf{YP}^{\perp} \tag{3.16}$$

where $\mathbf{P}^{\perp}$ is a basis of the left null space of $\mathbf{P}$, and $\mathbf{Y}$ is an arbitrary matrix of appropriate dimensions. However, since

$$\mathbf{P}^{\perp}\begin{bmatrix} x(0) \\ x(T) \end{bmatrix} = 0, \tag{3.17}$$

we can replace $\mathbf{T}$ by $\mathbf{I}+\mathbf{P}\mathbf{Q}^{-1}\mathbf{\Psi}$ in the residual expression (3.14). Again, the reciprocity property of $x(\cdot)$ and construction (3.13) of the residual $r(h)$ imply it is uncorrelated with the process $x(\cdot)$ over $[h, T-h]$, i.e.

$$E\{r(h)x^*(s)\}=0 \quad \text{for} \quad s \in [h, T-h]. \tag{3.18}$$

Observing that $b(h)=r(h)/h+o(h^0)$, this implies (3.9b). □

As $h \downarrow 0$, neither $\xi(t,h)$ nor $b(h)$ converge in a classical sense, which is to be expected from the nonsmooth nature of the sample paths of $x(t)$. $\xi(t,h)$ does converge in the sense of generalized functions to a random generalized function $\xi(t)$ defined in [20]. The limit of the boundary vector $b(h)$ as $h \downarrow 0$ cannot be defined as a separate entity, since $b(h)$ contains components proportional to $d^+x(0)/h$ and $d^-x(T)/h$ whose limits as $h \downarrow 0$ do not exist. However, the following lemma provides some information about the statistical behaviour of $b(h)$ as h tends to zero.

LEMMA 3.1 *If $x(t)$ is a* GRD *over* $[0,T]$ *with covariance $R(t,s)$ the boundary vector $b(h)$ specified by* (3.6b) *satisfies*

$$\lim_{h\downarrow 0} E\{x(s)b^*(h)\} = \begin{cases} [R(0,0) \quad R(0,T)] & s=0 \\ 0 & 0<s<T \\ [R(T,0) \quad R(T,T)] & s=T. \end{cases} \tag{3.19}$$

Proof For $0<s<T$, (3.19) follows from (3.9b). For $s=0$ and $s=T$, we can recover (3.19) by evaluating the LHS of (2.18) at these two values of s, and being careful to interpret $\frac{\partial G}{dt}(0,s)$ at $s=0$ as $\frac{\partial G}{dt}(0^+,0)$, $\frac{\partial G}{dt}(T,s)$ at $s=T$ as $\frac{\partial G}{dt}(T^-,T)$. □

Note that the BVP (3.6a)–(3.6b) can be formulated for any stochastic process $x(\cdot)$ on $[0,T]$, in particular for any zero-mean Gaussian process with continuous sample paths, regardless of reciprocality. However, in this case the driving noise $\xi(t,h)$ and boundary vector $b(h)$ do not correspond any longer to the discretized conjugate process of $x(\cdot)$, and do not satisfy the properties (3.9a)–(3.9b). Our goal for the remainder of this section is twofold:

(1) Given a zero mean Gaussian process with continuous sample paths a.s., but not necessarily reciprocal, give a precise definition of what it means for $x(t)$ to solve the BVP

$$Lx(t)=\xi(t) \tag{3.20a}$$

$$Bx=b, \tag{3.20b}$$

which is obtained by formally letting $h \downarrow 0$ in (3.6a)–(3.6b), where B is the linear boundary functional defined in (2.9).

(2) Once a precise definition of (3.20a)–(3.20b) is obtained, use it to characterize those zero mean Gaussian processes with continuous sample paths a.s. that are reciprocal.

We use the following result to motivate our proposed definiton for the solution of (3.20a)–(3.20b).

LEMMA 3.2 *Let $u(t) \in L_n^2[0, T]$ with $\ddot{u} \in L_n^2[0, T]$ be a solution of the deterministic BVP*

$$Lu(t) = f(t) \tag{3.21a}$$

$$Bu = b, \tag{3.21b}$$

where $f(t) \in L_n^2[0, T]$ and $b \in \mathbb{R}^n$. Then, for all $\phi \in E$, where E is the subspace defined by (2.9), *we have*

$$\langle L\phi, u\rangle = \langle \phi, f\rangle + \bar{\phi}^* \begin{bmatrix} -\mathbf{\Psi}^* \\ \mathbf{I} \end{bmatrix} \mathbf{Q}^{-1} b, \tag{3.22}$$

where $\bar{\phi}^*$ denotes the boundary vector

$$\bar{\phi}^* = \begin{bmatrix} \phi^*(0) & \phi^*(T) & \dot{\phi}^*(0) & \dot{\phi}^*(T) \end{bmatrix}. \tag{3.23}$$

Proof It is immediate from superposition that

$$u(t) = \int_0^T R(t,s) f(s) ds + [\psi_1(t)\psi_2(t)]b, \tag{3.24}$$

where $R(t,s)$ is the Green's function for L_E. That the 2nd term in (3.24) does in fact satisfy the nonhomogeneous BC (3.21b) may come as a surprise but can be verified directly. For $\phi \in E$, we use the representation (3.24) of u together with integration by parts to get

$$\langle L\phi, u\rangle = \langle \phi, f\rangle + \bar{\phi}^* \begin{bmatrix} \mathbf{Z} & -\mathbf{Q}^{-1} \\ \mathbf{Q}^{-1} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{I} \\ \mathbf{\Psi} \end{bmatrix} b, \tag{3.25}$$

where $\mathbf{Z}$ is the matrix given by (2.48b). From the self-adjointness of L it can be shown that

$$\mathbf{Z} = \mathbf{Q}^{-1}\mathbf{\Psi} - \mathbf{\Psi}^*\mathbf{Q}^{-1}, \tag{3.26}$$

from which (3.22) follows. □

Now consider a zero mean Gaussian process $x(t)$, not necessarily reciprocal, and having continuous sample paths a.s.. We can always apply the discretized operator L_h to x, as well as the discretized boundary functional B_h. The results of applying these operations are denoted as $\xi(t,h)$ and $b(h)$, respectively, so that we obtain a discretized system of the form (3.6a)–(3.6b). For each $h > 0$, define the random linear functional Y_h on E by the rule $\phi \in E \rightarrow Y_h(\phi)$, where

$$Y_h(\phi) \triangleq \sum_{k=1}^{N-1} \phi^*(t_k)\xi(t_k, h)h + \bar{\phi}^* \begin{bmatrix} -\Psi^* \\ \mathbf{I} \end{bmatrix} \mathbf{Q}^{-1} b(h), \tag{3.27}$$

with $h = T/N$ and $t_k = kh$. Now define the random linear functional Y on E by the rule $\phi \in E \to Y(\phi)$, where

$$Y(\phi) \triangleq \langle L\phi, x \rangle. \tag{3.28}$$

We have the following theorem.

THEOREM 3.2 *Let $x(t)$ be a zero-mean Gaussian process on $[0, T]$ having continuous sample paths almost surely. Then, for all $\phi \in E$, $Y_h(\phi)$ converges almost surely to $Y(\phi)$ as $h \downarrow 0$, i.e.*

$$\forall \phi \in E \quad P\left[\lim_{h \downarrow 0} Y_h(\phi) = Y(\phi)\right] = 1. \tag{3.29}$$

Proof Although a fair amount of calculation is required, the basic idea is almost trivial. We simply undo, at the discrete level, the integration by parts underlying the definition of $Y_h(\phi)$. Let $\omega \in \Omega$ be such that $x(\omega) \in C[0, T]$ (the set of such ω's has P measure 1 by hypothesis). Applying summation by parts to $Y_h(\phi, \omega) = Y_h(\phi)$ gives

$$\begin{aligned}
Y_h(\phi) = \sum_{k=2}^{N-2} & \left[-\frac{d^2}{h^2}(Q^{-1}\phi) - \frac{d^1}{h}(G^*Q^{-1}\phi) + d^0(F^*Q^{-1}\phi)\right]^*(t_k)x(t_k)h && \text{(i)} \\
& + \tfrac{1}{2}\left[(G^*Q^{-1}\phi)^*(t_{N-2})x(t_{N-1}) + (G^*Q^{-1}\phi)^*(t_{N-1})x(t_N)\right] && \text{(iia)} \\
& - \tfrac{1}{2}\left[(G^*Q^{-1}\phi)^*(t_1)x(t_0) + (G^*Q^{-1}\phi)^*(t_2)x(t_1)\right] && \text{(iib)} \\
& + \frac{d^-}{h}(Q^{-1}\phi)^*(t_{N-1})x(t_{N-1}) - \frac{d^+}{h}(Q^{-1}\phi)^*(t_1)x(t_1) && \text{(iii)} \\
& - (Q^{-1}\phi)^*(t_{N-1})\frac{d^-}{h}x(t_N) + (Q^{-1}\phi)^*(t_1)\frac{d^+}{h}x(t_0) && \text{(iva)} \\
& + \bar{\phi}^*\begin{bmatrix} -\mathbf{\Psi}^* \\ \mathbf{I} \end{bmatrix}\mathbf{Q}^{-1}b(h). && \text{(ivb)}
\end{aligned} \tag{3.30}$$

As $h \downarrow 0$, (i) converges to $Y(\phi)$, and the boundary terms (ii) through (iv) converge to

$$(G^*Q^{-1}\phi)^*(t)x(t)|_0^T + \frac{d}{dt}(Q^{-1}\phi)^*(t)x(t)|_0^T + \bar{\phi}^*\begin{bmatrix} \mathbf{Q}^{-1}\mathbf{\Psi} - \mathbf{\Psi}^*\mathbf{Q}^{-1} \\ \mathbf{Q}^{-1} \end{bmatrix}\begin{bmatrix} x(0) \\ x(T) \end{bmatrix}. \tag{3.31}$$

From the identity (3.26) and the self-adjointness relation (2.6a), we can then conclude that (3.31) is zero, thus proving Theorem 3.2. □

Remark The deterministic identity (3.22) suggests that $Y(\phi)$ admits also the mnemonic representation

$$Y(\phi) = \int_0^T \phi^*(t)\xi(t)dt + \bar{\phi}^*\begin{bmatrix} -\mathbf{\Psi}^* \\ \mathbf{I} \end{bmatrix}\mathbf{Q}^{-1}b, \tag{3.32}$$

which at this point is purely formal.

We recall that for $h > 0$ a GRD satisfies the discretized BVP (3.6a)–(3.6b), or at $h = 0$ the mnemonic BVP (3.20a)–(3.20b). We can distinguish a GRD on $[0, T]$ from an arbitrary zero-mean Gaussian process having continuous sample paths a.s. by means of the following characterization of GRDs:

THEOREM 3.3 *$x(t)$ is a* GRD *on $[0, T]$ if and only if*

$$\lim_{h\downarrow 0} E\{Y_h(\phi)x^*(s)\} = E\{Y(\phi)x^*(s)\} = \phi^*(s) \tag{3.33}$$

for all $\phi \in E$ and $0 \le s \le T$.

Proof Since almost sure converges implies convergence in probability, we can deduce from Theorem 3.2 that for all $\phi \in E$, the zero mean Gaussian random variable $Y(\phi) - Y_h(\phi)$ converges to 0 in probability. From the Gaussian property it then follows that

$$\lim_{h\downarrow 0} E\{(Y(\phi) - Y_h(\phi))^2\} = 0. \tag{3.34}$$

Let (Ω, F, P) be the probability space underlying the $x(t)$ process. Then (3.34) indicates that $Y(\phi) - Y_h(\phi)$ converges to zero in the Hilbert space $L^2(\Omega, F, P)$ of scalar random variables having finite 2nd moment that are measurable with respect to F. From continuity of the inner product in a Hilbert space it follows that

$$\lim_{h\downarrow 0} E\{Y_h(\phi)x_i(s)\} = E\{Y(\phi)x_i(s)\}, \tag{3.35}$$

where $x_i(s)$ is the ith component of $x(s)$, so that the first equality in (3.33) holds.

We need to show that the second equality holds iff $x(t)$ is a GRD. Now,

$$E\{Y_h(\phi)x^*(s)\} = E\left\{\left[\int_0^T (L\phi)^*(t)x(t)dt\right]x^*(s)\right\} = \int_0^T (L\phi)^*(t)R(t,s)dt. \tag{3.36}$$

Clearly (3.36) equals $\phi^*(s)$ if and only if their transposes are equal, i.e. if and only if

$$\int_0^T R^*(t,s)(L\phi)(t)dt = \phi(s). \tag{3.37}$$

But

$$\int_0^T R^*(t,s)(L\phi)(t)dt = \int_0^T R(s,t)(L\phi)(t)dt = ((M \circ L_E)\phi)(s), \tag{3.38}$$

where M is the integral operator whose kernel is R and whose domain is $L_n^2[0, T]$. Clearly $((M \circ L_E)\phi)(s) = \phi(s)$ iff $M = L_E^{-1}$, i.e. iff R is the Green's function for L_E. But by Theorem 2.1, R is the Green's function for L_E iff $x(t)$ is a GRD on $[0, T]$. Note that $(L_E^{-1} \circ L_E)\phi$ must equal ϕ throughout $[0, T]$, not just on $(0, T)$, by the smoothness requirements of E. □

Theorem 3.3 can be used to give a more precise interpretation to the mnemonic representation (3.32) of $Y(\phi)$. Let ϕ and θ be two functions in E. Then, from (3.33) and the definition (3.28) of $Y(\theta)$, we find

$$E\{Y(\phi)Y^{*}(\theta)\} = \langle \phi, L\theta \rangle = \langle L\phi, \theta \rangle, \tag{3.39}$$

which provides an implicit description of the combined statistical properties of the generalized noise $\xi(t)$ and vector b. The statistics of $\xi(t)$ can be inferred from (3.37), since when ϕ and θ belong to the subspace $C_0^{\infty}[0, T] \subset E$, the boundary term proportional to b drops out of the mnemonic representation (3.32) for $Y(\phi)$ and $Y(\theta)$, and we can immediately deduce from (3.39) that $\xi(t)$ is a generalized Gaussian process with zero-mean and covariance

$$E\{\xi(t)\xi^{*}(s)\} = L_t \delta(t-s), \tag{3.40a}$$

which in light of (3.33) satisfies

$$E\{\xi(t)x^{*}(s)\} = I_n \delta(t-s), \tag{3.40b}$$

and thus constitutes the conjugate process of $x(\cdot)$, as was already noted in [20]. On the other hand, the boundary vector b is only a formal symbol, whose statistical properties cannot be characterized independently of those of $\xi(t)$.

4 FIRST ORDER MODEL OF GRDs WITH NEGATIVE STRESS TENSOR

The objective of this section is to recast the n-dimensional stochastic Sturm–Liouville BVP (3.20a)–(3.20b) satisfied by GRDs into a $2n$-dimensional first-order BVP of the type examined in [17, 2, 26]. It turns out this is possible only for GRDs with a negative definite stress-tensor. As background, we recall [20, 19, 22] that the kinematics and dynamics of a reciprocal diffusion $x(t)$ can be described in terms of its probability density $\rho(x, t)$, mean velocity $v(x, t)$ and stress tensor $\pi(x, t)$. For a GRD these quantities admit the parametrization

$$\rho(x, t) \sim \mathcal{N}(0, R(t, t)) \tag{4.1a}$$

$$v(x, t) = V(t)x = \frac{1}{2}\left(\frac{\partial R}{\partial t}(t^{+}, t) + \frac{\partial R}{\partial t}(t^{-}, t)\right) R^{-1}(t, t)x \tag{4.1b}$$

$$\pi(t) = \frac{1}{2}\left(\frac{\partial^2 R}{\partial t \partial s}(t^{+}, t) + \frac{\partial^2 R}{\partial r \partial s}(t^{-}, t)\right) - V(t)R(t, t)V^{*}(t), \tag{4.1c}$$

and the conservation laws can be expressed compactly as

$$\frac{d}{dt}\mathbf{\Omega} = \mathbf{\Lambda}\mathbf{\Omega} + \mathbf{\Omega}\mathbf{\Lambda}^{*}, \tag{4.2}$$

with

$$\mathbf{\Omega}(t) \triangleq \begin{bmatrix} R(t,t) & R(t,t)V^*(t) \\ V(t)R(t,t) & \pi(t) + V(t)R(t,t)V^*(t) \end{bmatrix} \tag{4.3a}$$

$$\mathbf{\Lambda}(t) \triangleq \begin{bmatrix} 0 & I_n \\ F(t) & G(t) \end{bmatrix}. \tag{4.3b}$$

The reader is referred to [10, 11] for a detailed study of the conservation laws of GRDs. It is the stress tensor $\pi(t)$ that concerns us here.

Consider a GRD $x(t)$ over $[0, T]$ and the mnemonic BVP (3.20a)–(3.20b) it satisfies. Let also $L = M^*Q^{-1}M$ be a factorization of L, where M has the form (2.50a). As was shown in Section 2, the matrix $A(t)$ specifying M must satisfy the Riccati equation (2.51) and algebraic constraint (2.52), which as noted earlier holds throughout $[0, T]$ provided it holds for one t. The existence of a matrix funtion $A(t)$ satisfying both (2.51) and (2.52) over $[0, T]$ can be established by noting that L_D is positive definite, and adapting the argument of Lemma 2.2 to the case of Dirichlet conditions (see p. 46 of [20] for a brief proof).

In [20], it was shown that for an arbitrary factor M, the generalized noise process $\xi(t)$ admits the representation

$$\xi(t) = M^*Q^{-1}(t)\frac{dw}{dt}, \tag{4.4}$$

where $w(t)$ is a zero-mean Gaussian independent increments process taking values in $\mathbb{R}^n$, of intensity $Q(t)$, i.e.

$$E\{w(t)w^*(s)\} = \int_0^{t\wedge s} Q(\tau)d\tau, \tag{4.5}$$

with continuous sample paths a.s. Here $t \wedge s = \min(t, s)$. Let

$$\mathbf{A} \triangleq \begin{bmatrix} A(0) & 0 \\ 0 & A(T) \end{bmatrix}. \tag{4.6}$$

For the case when

$$\mathbf{C} \triangleq \mathbf{P} + \mathbf{P}\mathbf{Q}^{-1}(\mathbf{\Psi} - \mathbf{A})\mathbf{P} \tag{4.7}$$

is a covariance matrix, we now demonstrate that the counterpart of the representation (4.4) for the boundary vector b takes the form

$$b = -\mathbf{P}\mathbf{Q}^{-1}\begin{bmatrix} \dot{w}(0) \\ \dot{w}(T) \end{bmatrix} + c, \tag{4.8}$$

where c is a zero-mean Gaussian random vector independent of w with covariance $\mathbf{C}$.

To give a precise interpretation to the formal expressions (4.4) and (4.8), note that if we integrate by parts the formal representation

$$x(t) = \int_0^T R(t,s)\xi(s)ds + [\psi_1(t)\ \psi_2(t)]b \tag{4.9}$$

of the solution of the mnemonic BVP (3.20a)–(3.20b), and substitute (4.4) and (4.8), we obtain the alternate expression

$$x(t) = \int_0^T (M_s R(s,t))^* Q^{-1}(s)dw(s) + [\psi_1(t)\ \psi_2(t)]c, \tag{4.10}$$

which is now well defined, since the first term corresponds to a standard Wiener integral, and the second term depends only on the Gaussian vector c. In obtaining (4.10), we have used to identity

$$[R(t,0)\ R(t,T)] = [\psi_1(t)\ \psi_2(t)]\mathbf{P} \tag{4.11}$$

which is a direct consequence of the decomposition (2.17) for R, where $\hat{R}$ and $\tilde{R}$ admit the representations (2.13) and (2.16), respectively. We then have the following result, which constitutes the justification of (4.4) and (4.8).

THEOREM 4.1 *Let $x(t)$ be a* GRD *with covariance $R(t,s)$. If its corresponding second-order differential operator admits a factorization $L = M^* Q^{-1} M$ such that the matrix* $\mathbf{C}$ *given by* (4.7) *is symmetric nonnegative definite, the zero-mean Gaussian process specified by the* RHS *of* (4.9) *has covariance $R(t,s)$, so that it constitutes a realization of $x(t)$.*

Proof Let $y(t)$ be the process defined by the RHS of (4.10). It covariance can be expressed as

$$E\{y(t)y^*(s)\} = \int_0^T (M_u R(u,t))^* Q^{-1}(u) M_u R(u,s)du + [\psi_1(t)\quad \psi_2(t)]\ \mathbf{C} \begin{bmatrix} \psi_1^*(s) \\ \psi_2^*(s) \end{bmatrix}. \tag{4.12}$$

Integrating by parts, and taking into account (4.7), (4.11), and the boundary condition (2.23), we find

$$\begin{aligned} E\{y(t)y^*(s)\} &= R(t,s) + [\psi_1(t)\quad \psi_2(t)] \left\{ (\mathbf{I} + \mathbf{PQ}^{-1}\mathbf{\Psi}) \begin{bmatrix} R(0,s) \\ R(T,s) \end{bmatrix} - \mathbf{PQ}^{-1} \begin{bmatrix} \frac{\partial R}{\partial t}\ (0,s) \\ \frac{\partial R}{\partial t}\ (T,s) \end{bmatrix} \right\} \\ &= R(t,s), \end{aligned} \tag{4.13}$$

as desired. □

The only issue left unresolved by Theorem 4.1 is whether we can always find a factor M, or equivalently a solution $A(\cdot)$ of the Riccati equation (2.51) with side constraint (2.52), such that the matrix $\mathbf{C}$ given by (4.7) is symmetric nonnegative definite. It turns out that $\mathbf{C}$ is always symmetric, since

$$\begin{aligned}\mathbf{C}-\mathbf{C}^* &= \mathbf{P}\big[(\mathbf{Q}^{-1}\boldsymbol{\Psi}-\boldsymbol{\Psi}^*\mathbf{Q}^{-1})-(\mathbf{Q}^{-1}\mathbf{A}-\mathbf{A}^*\mathbf{Q}^{-1})\big]\mathbf{P}\\ &= \mathbf{P}\big[\mathbf{Z}-(\mathbf{Q}^{-1}\mathbf{A}-\mathbf{A}^*\mathbf{Q}^{-1})\big]\mathbf{P}=0,\end{aligned} \tag{4.14}$$

where we have the identity (3.26) and the side contraint (2.52) satisfied by $A(\cdot)$. Unfortunately, as we shall see below, it is not always possible to select $A(\cdot)$ such that $\mathbf{C}$ is nonnegative. Specifically, such a construction can be accomplished only for the class of GRDs with a negative definite stress tensor.

However, before establishing this result, we present an alternative construction of the process $x(t)$ obtained in (4.10) for the case when $\mathbf{C}$ is nonnegative. As starting point, note that when the formal identities (4.4) and (4.8) are substituted inside the mnemonic BVP (3.20)–(3.20b) for $x(t)$, we obtain

$$M^*Q^{-1}\left(Mx(t)-\frac{dw}{dt}\right)=0 \tag{4.15a}$$

$$(\mathbf{I}+\mathbf{PQ}^{-1}\boldsymbol{\Psi})\begin{bmatrix}x(0)\\x(T)\end{bmatrix}-\mathbf{PQ}^{-1}\begin{bmatrix}\frac{d}{dt}(x-w)\ (0)\\ \frac{d}{dt}(x-w)\ (T)\end{bmatrix}=c. \tag{4.15b}$$

This new problem is also formal, but if we introduce the auxiliary variable

$$z(t)=Q^{-1}(t)\left(Mx(t)-\frac{dw}{dt}\right), \tag{4.16}$$

the problem (4.15a)–(4.15b) can be expressed as a $2n$-dimensional first-order stochastic differential equation

$$\mathbf{J}\begin{bmatrix}dx(t)\\dz(t)\end{bmatrix}=\mathbf{H}(t)\begin{bmatrix}x(t)\\z(t)\end{bmatrix}dt+\begin{bmatrix}I_n\\0\end{bmatrix}dw(t) \tag{4.17a}$$

with two-point boundary value condition

$$\beta\begin{bmatrix}x\\z\end{bmatrix}\triangleq(\mathbf{I}+\mathbf{PQ}^{-1}(\boldsymbol{\Psi}-\mathbf{A}))\begin{bmatrix}x(0)\\x(T)\end{bmatrix}-\mathbf{P}\begin{bmatrix}z(0)\\-z(T)\end{bmatrix}=c, \tag{4.17b}$$

where

$$\mathbf{J}=\begin{bmatrix}I_n & 0\\0 & -I_n\end{bmatrix},\quad \mathbf{H}(t)=\begin{bmatrix}A(t) & Q(t)\\0 & A^*(t)\end{bmatrix}. \tag{4.17c}$$

Since this stochastic BVP is of the form considered in [17, 2, 26], it is no longer formal, and its solution can be expressed as a Wiener integral plus boundary terms. The existence and uniqueness of a solution to (4.17a)–(4.17b) depends entirely on the well-posedness of the corresponding deterministic BVP, which can be established as follows.

LEMMA 4.1 *Let S be the subspace of vector functions $[u^*(t)\ v^*(t)]^* \in C^1_{2n}[0,T]$ such that*

$$\beta\begin{bmatrix} u \\ v \end{bmatrix} = 0, \tag{4.18}$$

and denote by N_S the differential operator obtained by applying

$$N \triangleq \mathbf{J}\frac{d}{dt} - \mathbf{H}(t) \tag{4.19}$$

to functions in S. Then N_S is invertible if and only if L_E is invertible, and the Green's function $\boldsymbol{\Gamma}(t,s)$ of N_S can be expressed in terms of the Green's function $R(t,s)$ of L_E as

$$\boldsymbol{\Gamma}(t,s) = \begin{bmatrix} (M_s R(s,t))^* Q^{-1}(s) & R(t,s) \\ Q^{-1}(t)M_t(M_s R(s,t))^* Q^{-1}(s) & Q^{-1}(t)M_t R(t,s) \end{bmatrix}. \tag{4.20}$$

Proof If $[u^*(t)\ v^*(t)]^*$ is a nonzero function of S such that

$$N\begin{bmatrix} u(t) \\ v(t) \end{bmatrix} = 0, \tag{4.21}$$

by observing that $v(t) = Q^{-1}Mu(t)$, we conclude that u is nonzero. Then eliminating v from (4.21) and the boundary condition (4.18), we find $Lu = 0$ and $Bu = 0$. This proves that L_E is invertible if and only if N_S is invertible. To show that the Green's function of N_S has the form (4.20), note that the Green's function must satisfy

$$N\boldsymbol{\Gamma}(t,s) = I_{2n}\delta(t-s) \tag{4.22a}$$

with

$$\beta\boldsymbol{\Gamma}(\cdot,s) = 0. \tag{4.22b}$$

From the fact that $R(t,s)$ satisfies $LR(t,s) = 0$ with the boundary condition $BR(\cdot,s) = 0$, we can immediately deduce that the kernel $\boldsymbol{\Gamma}(t,s)$ specified by (4.20) satisfies $N\boldsymbol{\Gamma}(t,s) = 0$ for $t > s$ and $t < s$, as well as the boundary condition (4.22b). Consequently, to establish it is the Green's function of N_S we only need to show that it satisfies the jump condition

$$\mathbf{J}[\boldsymbol{\Gamma}(t^+,t) - \boldsymbol{\Gamma}(t^-,t)] = I_{2n}. \tag{4.23}$$

Since its (1, 2) block is $R(t,s)$, which is continuous across the diagonal $t = s$, the (1, 2) block does not have any jump, as desired. The jump of the (2, 2) block is given by

$$-Q^{-1}(t)\left(\frac{\partial R}{\partial t}(t^+,t) - \frac{\partial R}{\partial t}(t^-,t)\right) = I_n, \tag{4.24}$$

where we have used the definition (2.20a) of Q. Proceding similarly, we also find the jump of the $(1,1)$ block is I_n. Finally, the jump of the $(1,2)$ block can be expressed as

$$\Delta_{12}(t) = -Q^{-1}(t)\left[\left(\frac{\partial^2 R}{\partial t \partial s}(t^+,t) - \frac{\partial^2 R}{\partial t \partial s}(t^-,t)\right) - A(t)\left(\frac{\partial R}{\partial s}(t^+,t) - \frac{\partial R}{\partial s}(t^-,t)\right)\right.$$
$$\left. - \left(\frac{\partial R}{\partial t}(t^+,t) - \frac{\partial R}{\partial t}(t^-,t)\right)A^*(t)\right]Q^{-1}(t). \tag{4.25}$$

From (2.20a) and (2.20b), we have

$$\frac{\partial^2 R}{\partial t \partial s}(t^+,t) - \frac{\partial^2 R}{\partial t \partial s}(t^-,t) = (\dot{Q} - GQ)(t). \tag{4.26}$$

Then substituting the definition (2.20a) of Q inside (4.25), and taking into account (2.6a), we obtain

$$-Q\Delta_{12}Q = \dot{Q} - GQ + QA^* - AQ = \frac{1}{2}(QG^* - GQ) - (QA^* - AQ) = 0, \tag{4.27}$$

where the last equality is a consequence of the side constriant (2.52) satisfied by A. This implies that $\mathbf{\Gamma}$ obeys the jump condition (4.24), so that it is the Green's function of N_S. □

To obtain a complete expression for the solution of the stochastic BVP (4.17a)–(4.17b), it is also useful to observe that

$$\eta(t) \triangleq \begin{bmatrix} \psi_1(t) & \psi_2(t) \\ Q^{-1}M\psi_1(t) & Q^{-1}M\psi_2(t) \end{bmatrix} \tag{4.28}$$

satisfies

$$N\eta(t) = 0 \tag{4.29a}$$

with the boundary condition

$$\beta\eta = I_{2n}. \tag{4.29b}$$

Then we have the following result.

THEOREM 4.2 *Let* $x(t)$ *be a* GRD *with covariance* $R(t,s)$. *If its operator* L *admits a factorization such that the matrix* $\mathbf{C}$ *given by* (4.7) *is nonnegative definite,* $x(t)$ *coincides up to law with the first component of the solution of* (4.17a)–(4.17b), *which admits the representation* (4.10).

Proof As shown in [17, 2], the solution of the stochastic BVP (4.17a)–(4.17b) can be expressed as

$$\begin{bmatrix} x(t) \\ z(t) \end{bmatrix} = \int_0^T \mathbf{\Gamma}(t,s)\begin{bmatrix} I_n \\ 0 \end{bmatrix} dw(s) + \eta(t)c. \tag{4.30}$$

Substituting the structure (4.20) and (4.28) of $\mathbf{\Gamma}(t,s)$ and $\eta(t)$, it is easy to verify that the first component of the solution admits the representation (4.10), so that it has covariance $R(t,s)$. □

Next, we derive a necessary and sufficient condition for the nonnegativity of the matrix $\mathbf{C}$ given by (4.6). Let

$$W^{-1} = \int_0^T \phi(T,s)Q(s)\phi^*(T,s)ds \tag{4.31}$$

be the reachability Gramian of the pair $(A, Q^{1/2})$, where $Q^{1/2}$ denotes an arbitrary matrix square-root of Q. Since $Q(t)$ is positive definite for all t, the Gramian W^{-1} is positive definite. Then the factor $A(\cdot)$ and $\mathbf{C}$ can both be parametrized in terms of W as shown below.

LEMMA 4.2 *We have*

$$\mathbf{Q}^{-1}(\mathbf{\Psi} - \mathbf{A}) = -\bar{\mathbf{P}}^{-1} \triangleq -\begin{bmatrix} -K^{-1} \\ W \end{bmatrix} W^{-1}[-K^{-*} \ W], \tag{4.32}$$

so that $\mathbf{C}$ *can be expressed as*

$$\mathbf{C} = \mathbf{P} - \mathbf{P}\bar{\mathbf{P}}^{-1}\mathbf{P}. \tag{4.33}$$

Furthermore, the identity (4.31) *implies*

$$A(T) = \dot{\psi}_2(T) - Q(T)W, \tag{4.34}$$

which indicates that the inverse Gramian W specifies uniquely the initial condition $A(T)$ for the Riccati equation (2.51).

Proof Substituting the factorization (2.49) into the BVP (2.7)–(2.8) satisfied by $\psi_i(t)$ with $i = 1, 2$ gives

$$Q^{-1}(t)M\psi_i(t) = \phi^*(a_i, t)W_i, \tag{4.35}$$

where a_i is a reference time, and W_i a constant matrix. Integrating this expression gives

$$\psi_i(t) = \phi(t,o)\psi_i(0) + \int_0^t \phi(t,s)Q(s)\phi^*(a_i,s)ds W_i. \tag{4.36}$$

For $i = 2$, selecting $a_2 = T$ and setting $t = T$ in (4.36) gives $W_2 = W$. Similarly, with $a_1 = 0$, one finds

$$W_1 = -\phi^*(T,0)W\phi(T,0). \tag{4.37}$$

Then, substituting these identities inside (4.35) gives (4.32), where we have used the fact that

$$K^{-1} = Q^{-1}(0)\dot{\psi}_2(0) = Q^{-1}(0)(M\psi_2)(0) = \phi^*(T,0)W. \tag{4.38}$$

Comparing (4.32) with (2.58), it is easy to verify that the matrix $\bar{\mathbf{P}}$ is the boundary covariance matrix for a Gauss–Markov process $\bar{x}(t)$ in the reciprocal class[3]. The notation $\bar{\Pi}^{-1}(0) = 0$ means that all components of the initial state $\bar{x}(0)$ have infinite variance.

Finally, the identity (4.34) corresponds to the (2, 2) block of (4.32). It satisfies the algebraic constraint (2.52), and thus provides a valid initial condition for the solution $A(\cdot)$ of the Riccati equation (2.51). This identity establishes a bijection between inverse Gramian matrices W and the solutions $A(\cdot)$ of (2.51). □

In the remainder of this section, it will be assumed that the endpoint covariance matrix $\mathbf{P}$ is invertible. Then, the above discussion indicates that the problem of finding a factor M of L such that the covariance matrix $\mathbf{C}$ of the boundary vector c is nonnegative reduces to one of finding a symmetric positive definite matrix W such that

$$\mathbf{P}^{-1}\mathbf{C}\mathbf{P}^{-1} = \mathbf{P}^{-1} - \bar{\mathbf{P}}^{-1}(W) \geq 0, \tag{4.39}$$

where the dependence of $\bar{\mathbf{P}}^{-1}$ on W is denoted explicitly. The existence of such a W can be characterized as follows.

THEOREM 4.3 *Let $x(t)$ be a* GRD *on* $[0, T]$ *with stress tensor $\pi(t)$, whose endpoint covariance matrix* $\mathbf{P}$ *is invertible. Then, there exists a positive definite matrix W such that* (4.39) *holds, or equivalently such that the matrix* $\mathbf{C}$ *in* (4.6) *is nonnegative, if and only if $\pi(t) < 0$ on* $[0, T]$.

Proof Let

$$\Sigma(W) \triangleq \begin{bmatrix} W & [-K^{-*} \quad W] \\ \begin{bmatrix} -K^{-1} \\ W \end{bmatrix} & \mathbf{P}^{-1} \end{bmatrix}. \tag{4.40}$$

Clearly $\mathbf{P}^{-1} - \bar{\mathbf{P}}^{-1}(W)$ is the Schur complement[4] of the W diagonal block in $\Sigma(W)$. Since the inverse Gramian W is positive definite, (4.39) holds if and only if

$$\Sigma(W) \geq 0. \tag{4.41}$$

It turns out that this type of linear matrix inequality has been studied extensively in the context of linear quadratic optimal control and stochastic realization theory [24]. Specifically, if $D = -I_n/2$, $R = \mathbf{P}^{-1}$ and

$$H = -\begin{bmatrix} 0 \\ I_n \end{bmatrix}, \quad \bar{H} = -\begin{bmatrix} K^{-1} \\ 0 \end{bmatrix}, \tag{4.42}$$

[3] Two GRDs are said to be in the same reciprocal class if they admit the same operator L, or following the terminology of [9], if they have the same set of local reciprocal invariants.

[4] See [16], p. 656 for a definition of the Schur complement of a matrix.

the inequality (4.41) can be rewritten as

$$\begin{bmatrix} DW + WD^* & WH^* - \bar{H}^* \\ HW - \bar{H} & -R \end{bmatrix} \leq 0, \tag{4.43}$$

which is exactly in the form considered in [24].

This means that we can characterize the solutions of (4.43) in terms of the so-called Kalman–Yakubovich–Popov positive real lemma [3]. Let

$$\mathcal{W} = \{W : W = W^*, \Sigma(W) \geq 0\}, \tag{4.44}$$

be the set of symmetric matrices satisfying the inequality (4.43). Then $\mathcal{W}$ is nonempty if and only if the s table rational matrix

$$\mathbf{\Theta}_+(s) \triangleq \frac{R}{2} + H(sI_n - D)^{-1}\bar{H} = \mathbf{P}^{-1} + \begin{bmatrix} 0 & 0 \\ \frac{K^{-*}}{s+\frac{1}{2}} & 0 \end{bmatrix} \tag{4.45}$$

is positive real, i.e. if

$$\mathbf{\Theta}(s) = \mathbf{\Theta}_+(s) + \mathbf{\Theta}_+^*(-s) = \mathbf{P}^{-1} + \begin{bmatrix} 0 & \frac{K^{-1}}{\frac{1}{2}-s} \\ \frac{K^{-*}}{\frac{1}{2}+s} & 0 \end{bmatrix} \tag{4.46}$$

is positive for all s on the imaginary axis. Furthermore, there exists a one-to-one correspondence between the elements of $\mathcal{W}$ and the classes of equivalence of minimal spectral factors

$$S(s) = \frac{HB}{s+\frac{1}{2}} + J \tag{4.47}$$

of $\mathbf{\Theta}(s)$. As a reminder $S(s)$ is a spectral factor of $\mathbf{\Theta}(s)$ if $\mathbf{\Theta}(s) = S(s)S^*(-s)$, and two spectral factors $S_1(s)$ and $S_2(s)$ of $\mathbf{\Theta}(s)$ are said to be equivalent if they are related to each other through right multiplication by a constant orthonormal matrix T, i.e., $S_2(s) = S_1(s)T$ with $T^*T = I_n$. Note that we do not restrict our attention to square spectral factors. Each factor $S(s)$ is parametrized by the matrices B and J, which in turn specify a W in $\mathcal{W}$ through the identity

$$\Sigma(W) = \begin{bmatrix} B \\ J \end{bmatrix} [B^* \ J^*], \tag{4.48}$$

which yields $W = BB^*$.

However, positivity of $\mathbf{\Theta}$ everywhere on the imaginary axis is actually equivalent to positivity of $\mathbf{\Theta}$ at the origin. To see this, let ω be real and notice that

$$\mathbf{\Theta}(i\omega) = \begin{bmatrix} I_n & 0 \\ 0 & \frac{I_n}{1+2i\omega} \end{bmatrix} \mathbf{\Theta}(0) \begin{bmatrix} I_n & 0 \\ 0 & \frac{I_n}{1-2i\omega} \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & \frac{2i\omega I_n}{1+2i\omega} \end{bmatrix} \mathbf{P}^{-1} \begin{bmatrix} 0 & 0 \\ 0 & \frac{-2i\omega I_n}{1-2i\omega} \end{bmatrix}. \tag{4.49}$$

Clearly (4.49) is positive if and only if $\mathbf{\Theta}(0)$ is.

By applying standard formulas for the inverse entries of the block matrix $\mathbf{P}$, we can explicitly calculate the block entries of $\mathbf{\Theta}(0)$. The Schur complement of the (2,2) block of $\mathbf{\Theta}(0)$ can then be calculated explicitly. Denote this Schur complement as Δ. Then

$$-\Delta = R(T,T) - \left[R(T,0) + \frac{1}{2}K\right]R^{-1}(0,0)\left[R(0,T) + \frac{1}{2}K^*\right]. \tag{4.50}$$

But $-\Delta$ is exactly the Schur complement of $R(0,0)$ in the matrix Ξ defined as

$$\Xi = \begin{bmatrix} R(0,0) & R(0,T) \\ R(T,0) & R(T,T) \end{bmatrix} + \frac{1}{2}\begin{bmatrix} 0 & K^* \\ K & 0 \end{bmatrix}. \tag{4.51}$$

It follows that $\mathbf{\Theta}(0)$ is positive if and only if Ξ has signature (n,n), i. e., it has n positive eigenvalues and n negative eigenvalues. But it is shown in [10] that

$$\begin{bmatrix} \psi_1(t) & \psi_2(t) \\ \dot{\psi}_1(t) & \dot{\psi}_2(t) \end{bmatrix} \Xi \begin{bmatrix} \psi_1(t) & \psi_2(t) \\ \dot{\psi}_1(t) & \dot{\psi}_2(t) \end{bmatrix}^* = \mathbf{\Omega}(t), \tag{4.52}$$

where $\mathbf{\Omega}(t)$ is given by (4.3a), so that Ξ has signature (n,n) if and only if $\pi(t) < 0$ on $[0,T]$. □

Remark The evolution equation (4.2) implies that the inertia of $\mathbf{\Omega}(t)$, i.e., the triple formed by its numbers of positive, zero, and negative eigenvalues, remains constant for all t. Since the Schur complement of $R(t,t)$ inside $\mathbf{\Omega}(t)$ is $\pi(t)$ and $R(t,t)$ is positive definite for all t, the inertia of $\pi(t)$ is also preserved for all t. In particular $\pi(t) < 0$ over the interval $[0,T]$ if and only if $\pi(0) < 0$.

To interpret Theorem 4.3, it is useful to use as benchmarks two important subclasses of the general class of GRDs, namely the Gaussian Markov and quantum diffusions. They are characterized [22] by the property that

$$\pi(t) = \frac{\epsilon}{4}Q(t)R^{-1}(t,t)Q(t) \tag{4.53}$$

with $\epsilon = -1$ in the Markov case, and $+1$ in the quantum case. Thus, as expected, the Markov diffusions satisfy the condition $\pi(t) < 0$, whereas the quantum diffusions, which draw their name from the equivalence existing between their conservation laws and Schrödinger's equation [22], and for which (4.53) is an expression of Heisenberg's uncertainty principle, do not meet the condition of Theorem 4.3.

As the following theorem indicates, the class of GRDs with $\pi(t) < 0$ contains in fact all diffusions obeying first-order stochastic BVPs.

THEOREM 4.4 *If $x(t)$ solves a well-posed first-order stochastic* BVP *of the form*

$$\begin{aligned} dx &= A(t)x\,dt + dw \\ u &= U_0x(0) + U_Tx(T) \end{aligned} \tag{4.54a}$$

where $w(t)$ is a zero-mean Gaussian independent increments process with intensity $Q(t)$ and u is a zero-mean Gaussian vector independent of w with variance $\Pi_u, x(t)$ is reciprocal with $\pi(t) \leq 0$.

Proof It is shown in [17] that the well-posedness of the BVP (4.54a)–(4.54b) is equivalent to the invertibility of $\chi = U_0 + U_T\phi(T,0)$, where $\phi(t,s)$ is the transition matrix of A defined in (2.43a). We can therefore assume that $\chi = I_n$, in which case the Green's function can be expressed as

$$\Gamma(t,s) = \begin{cases} \phi(t,0)U_0\phi(0,s) & t > s \\ \phi(t,0)(U_0 - I_n)\phi(0,s) & t < s. \end{cases} \tag{4.55}$$

Then, the solution of (4.54a)–(4.54b) is given by

$$x(t) = \phi(t,0)u + \int_0^T \Gamma(t,s)dw(s), \tag{4.56}$$

where the integral is a Wiener integral.

The covariance of $x(t)$ takes the form

$$R(t,s) = \phi(t,0)\Pi_u\phi^*(s,0) + \int_0^T \Gamma(t,\tau)Q(\tau)\Gamma^*(s,\tau)d\tau, \tag{4.57}$$

and it is straightforward to verify that

$$\frac{\partial}{\partial t}R(t,s) = A(t)R(t,s) + Q(t)\Gamma^*(s,t) \tag{4.58}$$

for $t \neq s$. Then, if M is defined as in (2.50a) and $L = M^*Q^{-1}M$, the identity (4.58) implies

$$L_tR(t,s) = M_t^*\Gamma^*(s,t) = I_n\delta(t-s), \tag{4.59}$$

where the last equality uses the fact that $\Gamma(t,s)$ is a Green's function for M. This proves that $x(t)$ is reciprocal.

Using (4.58) to evaluate the expression (4.1b) for $V(t)$, we find

$$V(t) = A(t) + \frac{1}{2}(QS)^*(t)R^{-1}(t,t) \tag{4.60a}$$

with

$$S(t) \triangleq \Gamma(t^+,t) + \Gamma(t^-,t) = \phi(t,0)(2U_0 - I_n)\phi(0,t). \tag{4.60b}$$

Similarly, an evaluation of the expression (4.1c) for $\pi(t)$ gives

$$\begin{aligned} \pi(t) &= A(t)R(t,t)A^*(t) + \frac{1}{2}(QS^*)(t)A^*(t) + \frac{1}{2}A(t)(SQ)(t) - V(t)R(t,t)V^*(t) \\ &= -\frac{1}{4}(QS^*)(t)R^{-1}(t,t)(SQ)(t) \leq 0 \end{aligned} \tag{4.61}$$

which proves that solutions of BVPs of the form (4.54a)–(4.54b) have a negative stress tensor. □

5 CONCLUSIONS

In this paper, we have shown that there exists a bijection between GRDs and positive definite Sturm–Liouville operators, which identifies the covariance of a GRD with the Green's function of the corresponding Sturm–Liouville operator. This bijection was used to construct GRDs as weak solutions of a stochastic Sturm–Liouville BVP. For the case of GRDs with a negative stress tensor, a realization of GRDs in terms of a $2n$-dimensional first-order stochastic BVP was given. In doing so, we focused our attention exclusively on self-adjoint boundary conditions with the same structure as the homogeneous BCs (2.23) for the covariance $R(t, s)$. However, since only GRDs with a negative stress tensor can be realized as solutions of the first-order BVP considered is Section 4, it is natural to ask whether the remaining GRDs could be realized by considering first-order problems with different BCs. For the case of initial conditions, preliminary results obtained in [18] suggest in fact that all GRDs can be realized as components of a $2n$-dimensional Markov process.

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