Trends in Mathematics

Christopher C. Bernido
Maria Victoria Carpio-Bernido
Martin Grothaus
Tobias Kuna
Maria João Oliveira
José Luís da Silva
Editors

Stochastic and Infinite Dimensional Analysis

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Editors
Christopher C. Bernido
Research Center for Theoretical Physics
Central Visayan Institute Foundation
Jagna, Bohol, Philippines

Maria Victoria Carpio-Bernido
Research Center for Theoretical Physics
Central Visayan Institute Foundation
Jagna, Bohol, Philippines

Martin Grothaus
Fachbereich Mathematik
Technische Universität Kaiserslautern
Kaiserslautern, Germany

Tobias Kuna
Department of Mathematics and Physics
University of Reading
Reading, United Kingdom

Maria João Oliveira
Universidade Aberta
Departamento de Ciências e Tecnologia
Lisbon, Portugal

José Luís da Silva
Universidade da Madeira
Faculdade de Ciências Exatas e da Engenharia
Funchal, Madeira, Portugal

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I am an applied physicist. I apply physics to mathematics.
(S. Ulam)

Preface

This volume owes its creation to the conference "Stochastic and Infinite Dimensional Analysis" held at ZiF, Bielefeld, on June 2013 for the 75th birthday of the distinguished scientist Prof. Ludwig Streit. This event was organised to celebrate his long ongoing work in these fields, to which he contributed as a forerunner. This publication collects papers, mostly novel research, spanning the whole range of his interests and activities in the past and future. A sizeable number of the contributions do not stem from participants to the conference, and some of the contributions are only vaguely related to the presentations given during the conference.

This book stands out as it combines the many guises in which infinite dimensional analysis can occur like white noise analysis, Malliavin calculus, harmonic analysis, fractional Brownian motion and operator theory. The different guises stem from different viewpoints motivated by particular applications. Fittingly, this collection gathers applications ranging from networks, stochastic partial differential equations, superprocesses, stochastic dynamics on trees, moment problems, and polymer physics to quantum field theory. They play a prominent role as test bed for the mathematics as well as inspiration for the theory.

Prof. Ludwig Streit often recalls when he met S. Ulam and heard firsthand the citation given at the beginning of this volume. This phrase may have made a strong impression on Prof. Ludwig Streit since it actually perfectly summarises his working style. The style of this volume can be considered in this spirit.

Jagna, Bohol, Philippines — Christopher C. Bernido
Jagna, Bohol, Philippines — M. Victoria Carpio-Bernido
Kaiserslautern, Germany — Martin Grothaus
Reading, UK — Tobias Kuna
Lisbon, Portugal — Maria João Oliveira
Funchal, Madeira, Portugal — José Luís da Silva

Contents

Along Paths Inspired by Ludwig Streit: Stochastic Equations for Quantum Fields and Related Systems

Sergio Albeverio

Abstract The interaction between quantum mechanics, quantum field theory, stochastic partial differential equations and infinite dimensional analysis is briefly surveyed, referring in particular to models and techniques to which L. Streit has given outstanding contributions.

Keywords Functional integration • Feynman path integrals • Quantum field theory • Stochastic quantization • Stochastic partial differential equations • Infinite dimensional integrals

1 Introduction

It is a great pleasure to present a contribution to this volume dedicated to Ludwig Streit, on the occasion of his 75th birthday. I have written before in [3] about Ludwig's work and the strong influence it had on my own development. In the present paper I will concentrate on some aspects relating quantum theory with stochastic analysis and infinite dimensional analysis, stressing interactions between these areas and mentioning some open problems.

In Sect. 2 I shall briefly describe the relations between oscillatory and probabilistic integrals.

In Sect. 3 I shall describe canonical quantum mechanics from this point of view.

In Sect. 4 I shall discuss the complex relations between canonical quantum fields and S(P)DEs, and also relate them with Euclidean (and relativistic) quantum fields.

In Sect. 5 I shall provide some remarks on related systems.

S. Albeverio (✉)
Institut für Angewandte Mathematik, Universität Bonn, Endenicher Allee 60, 53115, Bonn, Germany

HCM, Bonn, Germany

BIBOS, Bielefeld, Bonn, Germany

IZKS, Bonn, Germany

CERFIM, Locarno, Switzerland
e-mail: albeverio@iam.uni-bonn.de

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2 Oscillatory and Probabilistic Integrals

Since the work of Feynman (preceded in part by Wentzell and Dirac), see, e.g., [2, 107–110], a very fruitful approach to quantum mechanics and quantum field theory is based on the consideration of heuristic complex-valued measures of the form

$$\mu_F(\mathrm{d}\gamma) = \text{“}Z^{-1}e^{iS(\gamma)}\,\mathrm{d}\gamma\text{”} \tag{1}$$

on a “state space” Γ, hence $\gamma \in \Gamma$, with an “action functional” $S(\gamma) : \Gamma \to \mathbb{R}$ associated with an underlying “classical system”, $\mathrm{d}\gamma$ a “flat measure on Γ”, i the imaginary unit and Z a normalization constant.

Physical quantities of interest are then computed as “averages” (linear functionals, integrals)

$$\int_\Gamma f(\gamma)\mu_F(\mathrm{d}\gamma) \tag{2}$$

of suitable “observable functionals” $f : \Gamma \to \mathbb{C}$.

For example, to solve the Schrödinger equation for a non relativistic quantum mechanical particle moving for a time from the interval $[0, t]$, $t > 0$ on a D-dimensional manifold M one takes as Γ a space of paths from $[0, t]$ into M.

For a quantum (scalar) field, vibrating for a time from the interval $[0, t]$ and in a spatial $(d-1)$-dimensional domain $\Lambda \subset \mathbb{R}^{d-1}$ (d being then the space-time-dimension) one takes Γ as a space of paths from $[0, t]$ into a space of real-valued (generalized) functions depending on a space variable $x \in \Lambda$.

Analogous choices are made, e.g., for quantum gauge fields (with Γ a space of connection 1-forms in a principal fibre bundle over a Lorentzian manifold) and for quantum gravity (with Γ a space of locally Lorentzian space-time metrics).

In the case of scalar quantum fields, f could be a product of $n \in \mathbb{N}$ field operators $\prod_{i=1}^n \gamma(t_i, x_i)$, $t_i \in \mathbb{R}$, $x_i \in \mathbb{R}^{d-1}$, in which case above integrals would yield “correlation functions” (Wightman functions) associated with the quantum field $\gamma(t, x) \in \mathbb{R}$, $t \in \mathbb{R}$, $x \in \mathbb{R}^{d-1}$. Similar choices of relevant observable functions can be given in the other cases alluded above. See, e.g., [1, 2, 9, 33, 48, 52, 78, 80, 107, 109, 110], and references therein.

The choice of the action functional S depends on the problem at hand. In above examples, S has a typical Lagrangian form, e.g., in the case of a non relativistic particle (of unit mass) moving during the time interval $[0, t]$ in the D-dimensional Euclidean space $\mathbb{R}^D$ under the force given by a (continuous) potential (function) $v : \mathbb{R}^D \to \mathbb{R}$ one has:

$$S(\gamma) = S_{QM}(\gamma) = \frac{1}{2}\int_0^t |\dot{\gamma}(s)|^2\,\mathrm{d}s - \int_0^t v(\gamma(s))\,\mathrm{d}s, \tag{3}$$

and for scalar quantum fields moving at arbitrary times $s \in \mathbb{R}$ over the space $\mathbb{R}^{d-1}$ one has

$$S(\gamma) = S_{QF}(\gamma) = \frac{1}{2}\int_{\mathbb{R}^d} \dot{\gamma}(s,\vec{x})^2 \, \mathrm{d}s \, \mathrm{d}\vec{x} - \frac{1}{2}\int_{\mathbb{R}^d} \left|\nabla\gamma(s,\vec{x})\right|^2 \, \mathrm{d}s \, \mathrm{d}\vec{x} \tag{4}$$
$$- \frac{m^2}{2}\int_{\mathbb{R}^d} \left|\gamma(s,\vec{x})\right|^2 \, \mathrm{d}s \, \mathrm{d}\vec{x} - \int_{\mathbb{R}^d} v(\gamma(s,\vec{x})) \, \mathrm{d}s \, \mathrm{d}\vec{x},$$

$(s,\vec{x}) \in \mathbb{R} \times \mathbb{R}^{d-1}$, $m \geq 0$.

From the quantum description given in terms of (1), (2), (3), and (4) one obtains heuristically the classical (particle resp. field) mechanical one by inserting the (reduced) Planck constant $\hbar$ at the right place, i.e. replacing S by $\frac{1}{\hbar}S$ and making corresponding changes in the observable f in (2), and considering $\hbar$ to be small.

Heuristically then from (2) with such replacements one should be able to derive from Feynman's heuristic quantum description (1) and (2) the corresponding classical description in the limit $\hbar \downarrow 0$, with its corresponding "small $\hbar$-corrections". In the case of relativistic models, the velocity of light c appears as a parameter. Then one should be able to recover the non relativistic limit of the relativistic quantum description (1), (2), (3), and (4) by letting the velocity of light c go to $+\infty$ (c occurs implicitly in S and f). In principle one could proceed in similar ways to describe the limiting dependence of the quantum averages (2) on other parameters occurring in the action functionals and observables occurring in the examples mentioned above.

There are well known difficulties in trying to transform this heuristic approach into a rigorous one. E.g., even in the case $v \equiv 0$ (the "free field" case), in the computation of (2), the covariance of the "complex Gaussian measure" given by the covariance $S_{QF}(\gamma)|_{v=0}$ appears. It is, for $m^2 = 1$, the fundamental solution $(\Box - 1)^{-1}(s,\vec{x};s';\vec{x}')$, which has a singularity on the submanifold $(s-s')^2-(\vec{x}-\vec{x}')^2 = 1$, indicating that it should be interpreted as a generalized function, which then means that the relevant γ's in (2) also are generalized functions. This creates difficulties in giving mathematical meaning to the complex-valued non linear function $f(\gamma)$ appearing in (2). In the linear case where $v \equiv 0$, taking e.g. f to be of the Wick product type, a sense can easily be given to (2). However, for $v \not\equiv 0$ and neither linear nor quadratic, $v(\gamma)$ is ill defined for γ which are typical relative to the complex Gaussian measure μ_F for the case $v \equiv 0$.

There is a well known trick (going back to Nagumo, Schwinger, and Symanzik) of analytically continuing μ_F to a corresponding "Euclidean" probability measure (or functional) μ_E heuristically written as

$$\mu_E(\mathrm{d}\gamma) = \text{“}Z^{-1}e^{-S_E(\gamma)}\mathrm{d}\gamma\text{”} \tag{5}$$

with $S_E(\gamma)$ the "Euclidean" action (in contrast to the above relativistic or "Minkowskian" action (4))

$$S_E(\gamma) = \frac{1}{2}\iint \left[\left|\nabla_{s,\vec{x}}\gamma(s,\vec{x})\right|^2 + \frac{m^2}{2}\iint \left|\gamma(s,\vec{x})\right|^2\right] \mathrm{d}s\,\mathrm{d}\vec{x} + \iint v(\gamma(s,\vec{x}))\,\mathrm{d}s\,\mathrm{d}\vec{x}, \tag{6}$$

in which case the typical γ's in (5) become still heuristically generalized random fields but at least μ_E would look as a "positive measure". This however, only really solves the problem for $v \equiv 0$ and arbitrary d, or special $v \not\equiv 0$ when $d = 2, 3$. In this case one interprets μ_E as a probabilistic (σ-additive) Gaussian measure, e.g., with support on the Schwartz tempered distributions space $S'(\mathbb{R}^d)$. For the mentioned special cases of $v \not\equiv 0$ and $d = 2, 3$, one manages, in fact, to "renormalize" the nonsensical $v(\gamma(s,\vec{x}))$ to give it a sense as a genuine generalized random field, obtaining non trivial quantum averages (2) (heuristically $\mu_F \neq \mu_F|_{v=0}$, that is, in particular, states which are typically with respect to one of the measures are atypical with respect to the other measure). Moreover from such averages one recovers by "analytic continuation" in the t variable a solution of the original problem (1) and (2).

This was achieved in connection with the programme of constructive quantum field theory [9, 71, 76, 78, 98, 106], to which Ludwig Streit contributed substantially and in various ways, see, e.g., [16–18, 65, 78, 79, 81, 101, 102, 107]. Independently of the proper methods of constructive quantum field theory, the original programme of giving directly a meaning to (1) and (2) has also been solved in some cases. E.g., μ_F and μ_E can be defined for various classes of (regularized) v in low space-time dimension d. The integral $\int f(\gamma)\,\mathrm{d}\mu_F(\gamma)$ is then realized as

$$_{(S)}\langle\langle f, \Phi_{\mu_F}\rangle\rangle_{(S)'} \tag{7}$$

in the framework of the infinite dimensional distributional setting

$$(S) \subset L^2(\mu_G) \subset (S)', \tag{8}$$

with pairing $\langle\langle\ ,\ \rangle\rangle$ and $(S), (S)'$ infinite dimensional analogues of the test functions space $S(\mathbb{R}^d)$ resp. tempered distributions space $S'(\mathbb{R}^d)$. μ_G is the Gaussian white noise measure on $\mathcal{S}'(\mathbb{R}^d)$, defined by its Fourier transform

$$\hat{\mu}_G(g) := \int_{\mathcal{S}'(\mathbb{R}^d)} e^{i\langle g,\gamma\rangle}\,\mathrm{d}\mu_G(\gamma) = e^{-\frac{1}{2}\|g\|^2_{L^2(\mathbb{R}^d)}}, \tag{9}$$

with $\langle g, \gamma\rangle$ the distributional pairing between $g \in \mathcal{S}(\mathbb{R}^d)$ and $\gamma \in \mathcal{S}'(\mathbb{R}^d)$.

Heuristically thus

$$\mu_G(\mathrm{d}\gamma) = \text{"}Z^{-1}e^{-\frac{1}{2}\int_{\mathbb{R}^d}|\gamma(x)|^2\,\mathrm{d}x}\,\mathrm{d}\gamma\text{"}, \tag{10}$$

and, e.g.,

$$\Phi_{\mu_F}(\gamma) = e^{iS(\gamma)} e^{\frac{1}{2}\int_{\mathbb{R}^d} |\gamma(x)|^2 \, \mathrm{d}x} \mu_G(\mathrm{d}\gamma). \tag{11}$$

For $d = 1$, i.e. for quantum mechanics (anharmonic oscillator for $m > 0$), the functional Φ_{μ_F} in (7) and (11) is well defined for a large class of continuous v and works for solving e.g. the problem of the Schrödinger equation with potential v and with smooth resp. δ-initial conditions (Green's function) by work by L. Streit and coworkers, see e.g. [74, 75] and, for a related approach [94].

Another approach to the rigorous construction of (1) and (2) (for $d = 1$, and also for $d \geq 2$, but the latter with regularized $v(\gamma)$-term in (4) resp. (6)) is presented in [26].

In the latter reference also work on the detailed expansion of (2) in fractional powers of $\hbar$ around $\hbar = 0$ by a rigorous method of stationary phase is described (for the case $d = 1$).

The relations between the white noise and other approaches are discussed, e.g., in [26, 39, 93, 94].

The analogues of Wightman functions in the Euclidean setting, called Schwinger functions (they are the moment functions to μ_E), for $d = 1$, i.e. related to quantum mechanics, have also been described in terms of white noise functionals, see [74, 75, 94]. Corresponding results for the case $v \equiv 0$ and all d, or for some $v \not\equiv 0$ and $d = 2, 3$ will be discussed in the next Sects. 3 and 4.

For characterization of interesting probability measures as white noise functionals (like μ_E and related measures) see, e.g., [88, 101, 102].

3 Canonical Quantum Mechanics

In the canonical approach to quantum mechanics (and resp. the theory of quantum fields) one takes the "Schrödinger representation" of the Hilbert space of states and operators acting in $L^2(\mathbb{R}^D, \mu)$ resp. $L^2(S'(\mathbb{R}^d), \mu)$, for some probability measures μ.

By work of Heisenberg, Coester, Haag, Araki from the early 1960s one uses, e.g., for the D-dimensional harmonic oscillators, that $L^2(\mathbb{R}^D)$ is isomorphic to $L^2(\mathbb{R}^D, \mu)$, where $\mu(\mathrm{d}x) = N(0; \mathbb{1})(\mathrm{d}x) = (\sqrt{2\pi})^{-D} e^{-\frac{1}{2}|x|^2} \, \mathrm{d}x$ is the canonical Gaussian measure on $\mathbb{R}^D$. E.g., for $D = 1$ the Hamiltonian H given on smooth functions by $H = -\frac{1}{2}\Delta + \frac{1}{2}x^2 - \frac{1}{2}$ acting in $L^2(\mathbb{R})$ is then unitarily equivalent to the operator $H_\mu = -L_\mu$ given on smooth functions by $H_\mu = -\frac{1}{2}\Delta + x \cdot \nabla$ in $L^2(\mathbb{R}, \mu)$.

L_μ can be interpreted probabilistically as the restriction to smooth functions of the Ornstein-Uhlenbeck operator associated with the classical Dirichlet form $\frac{1}{2}\int \nabla u \cdot \nabla v \, \mathrm{d}\mu$, for u, v in a suitable dense subset of $L^2(\mathbb{R}, \mu)$. For classical Dirichlet forms (on $\mathbb{R}^D$ and also on infinite dimensional spaces) see, e.g., [4, 7, 8, 10, 28, 34, 37, 49, 57, 59, 66, 69, 72, 92]. Through the replacement of $N(0; \mathbb{1})$ by a more general, not necessarily Gaussian probability measure μ, one can set up a corresponding transformation for the generator L_μ (called Dirichlet operator) associated with the

classical Dirichlet form $\frac{1}{2}\int_{\mathbb{R}^D} \nabla u \cdot \nabla v \, \mathrm{d}\mu$ in $L^2(\mathrm{R}^D, \mu)$ to a generator $-H$, $H \geq 0$ in $L^2(\mathbb{R}^D)$.

This "ground state transformation" was first studied in details in [27], where a general and powerful approach to singular interactions in quantum mechanics on $\mathbb{R}^D$ via Dirichlet forms has been initiated. E.g., 3 nucleons interacting via 2-particle δ-functions in $\mathbb{R}^3$ can be rigorously defined and discussed in this approach. This Dirichlet form approach yields, more generally, a unified picture of quantum mechanics suited both for singular interactions and infinite dimensional extensions (the analogues of above classical Dirichlet forms being naturally also defined on infinite dimensional spaces; the latter forms describe namely quantum fields, see Sect. 4).

Remark 3.1 The probabilistic technique of subordination permits to treat quantum systems with relativistic kinematics in a way similar to those with nonrelativistic kinematics, see [6, 44–46, 50].

To general classical Dirichlet forms, there are (properly) associated good Markov processes $X = (X_t)$, $t \geq 0$, see [69]. Intuitively these can be seen as Brownian motions distorted by a drift term given by the logarithmic derivative of μ, μ itself constitutes then an invariant measure for X_t. In particular X_t can be extended to a μ-symmetric process for all $t \in \mathbb{R}$.

In the quantum mechanical situation corresponding to (4) with $d = 1$, $n = 1$, and $D = 1$, the path space measure μ_E for X_t, $t \in \mathbb{R}$ (giving the joint distribution of $(X_{t_1}, \ldots, X_{t_n})$, $t_i \in \mathbb{R}$, $i = 1, \ldots, n$) is heuristically given by μ_E as specified in (5) and (6) with a suitable v. If we write $S^0(\gamma) := \frac{1}{2}\int \left[|\dot{\gamma}|^2(s) + |\gamma(s)|^2\right] \mathrm{d}s$, then

$$\mu_E(\mathrm{d}\gamma) = Z^{-1} e^{-S^0(\gamma)} e^{-\int v(\gamma(s))\,\mathrm{d}s}\, \mathrm{d}\gamma. \tag{12}$$

This can be rigorously defined for suitable v, e.g. as a probability measure on $\mathcal{S}'(\mathbb{R}^d)$. An analytic continuation in time of the (time ordered) moment functions given by μ_E ("Schwinger functions") permits to go over to the corresponding quantities in terms of μ_F ("Wightman functions"), e.g. for v resp. a polynomial or exponential function. This yields the full information on the dynamical quantum mechanical "$P(\varphi)_1$" resp. "$\exp(\varphi)_1$"-"models". Such models can also be expressed conveniently in terms of the white noise functionals mentioned in Section 2 ([74]).

One proves that both quantum mechanical Schwinger and Wightman functions can be reformulated as limits of quantities defined in the canonical Hilbert space $L^2(\mathbb{R}, N(0,1))$, since for $v = 0$ the restriction of μ_E to the σ-algebra generated by X_0 is just $\mu = N(0,1)$ (X_t acts just in the same L^2-space $L^2(\mathbb{R}, N(0,1))$ where also H_μ and the CCR are realized) and the inclusion of the v-term can be handled by "perturbation and passage to the limit", see, e.g., [22, 23, 27, 55, 111].

Let us summarize the situation in quantum mechanics for a particle moving in $\mathbb{R}^D$. As a zero step ("Level 0") we have a (fixed time) Hilbert space, say $L^2(\mathbb{R}^D)$, an Hamiltonian H, as well as position and momentum operators, with the relative canonical commutation relations (CCR), and a fixed time distribution μ on $\mathbb{R}^D$ (that

exists if the lower end of the spectrum of H is an isolated simple eigenvalue) which yields the natural Hilbert space $L^2(\mathbb{R}^D, \mu)$. At a first step ("Level 1") one has a Markov process X_t (diffusion) with values in $\mathbb{R}^D$, t being the time parameter, its path space measure μ_E (on, say, $\mathcal{S}'(\mathbb{R}^D)$), and its moments functions (Schwinger functions). This process has μ as invariant measure. In the case $v \equiv 0$, $m = 1$, the path measure is $\mu_E = N\left(0; C^{-1}\right)$, with C the operator $\left(-\frac{d^2}{dt^2} + 1\right) \mathbb{1}_D$ (on $\mathcal{S}'(\mathbb{R}, \mathbb{R}^D)$), X_t is the $\mathbb{R}^D$-valued Ornstein-Uhlenbeck process satisfying $\mathrm{d}X_t = -X_t\,\mathrm{d}t + \mathrm{d}W_t$, with W_t a D-dimensional Brownian motion. It is associated with the classical Dirichlet form $\frac{1}{2}\int_{\mathbb{R}^D} \nabla u \cdot \nabla v\,\mathrm{d}\mu$. For $D = 1$ this coincides with the measure μ_E given by (5) and (6), for $d = 1$ and $m = 1$. For $v \equiv 0$ one has $\mu_E = N(0; (-\Delta + 1)^{-1})$ with Δ the Laplacian on $\mathbb{R}$.

At "Level 2" one has another Markov process (diffusion) Y_τ, $\tau \geq 0$. For $D = 1$ this has μ_E (as just described at level 1 given by the $D = 1$, $m = 1$ version of (5) and (6)), as invariant measure. The Markov process is given by the stationary solution of the SDE $\mathrm{d}Y_\tau(t) = \left(\frac{\mathrm{d}^2}{\mathrm{d}t^2} - 1\right) Y_\tau(t)\,\mathrm{d}\tau - v'(Y_\tau(t))\,\mathrm{d}\tau + \mathrm{d}W_\tau(t)$, $\tau \geq 0$, with $\mathrm{d}W_\tau(t)$ a (τ, t)-Gaussian white noise, $\tau \in \mathbb{R}_+$, $t \in \mathbb{R}$.

τ can be interpreted as a "computer time" (t is the "time" in the Euclidean version of quantum mechanics; it will be replaced by a space-time variable in $\mathbb{R}^d$, $d \geq 2$, in a quantum field interpretation, see Sect. 4, the quantum (particle) mechanics corresponding thus to the case $d = 1$. The equation for Y_τ is called "stochastic quantization equation". It is a particular case of Parisi-Wu's approach [100] for computing invariant measures of the type of μ_E.

Note that Y_τ can be looked upon (as a modification of) the standard diffusion process associated with the classical Dirichlet form $\frac{1}{2}\int_{S'(\mathbb{R}^D)} \nabla u \nabla v\,\mathrm{d}\mu_E = \frac{1}{2}\,{}_{(S)}\langle\langle \nabla u \nabla v, \mu_E\rangle\rangle_{(S)'}$ given by μ_E.

The determination of the associated generator on smooth cylinder functions has been given in [31, 32, 87] (based on previous results in [84, 85]).

We shall now briefly go over to describe similar Level 0–2 structures for quantum fields, i.e. associated with (5) and (6) (with non trivial dependence on the space variable $\vec{x} \in \mathbb{R}^{d-1}$, $d \geq 2$).

4 Canonical Quantum Fields and S(P)DEs

We shall only discuss, for simplicity, scalar fields.

At Level 0 we have as the analogue of the position operators resp. momentum operators in quantum mechanics, the time zero quantum field $\varphi(\vec{x})$, $\vec{x} \in \mathbb{R}^{d-1}$ resp. the time zero momentum field $\Pi(\vec{x})$, satisfying the canonical commutation relations (CCR)

$$[\Pi(\vec{y}), \varphi(\vec{x})] = \frac{1}{i}\delta(\vec{x} - \vec{y}), \quad \vec{x}, \vec{y} \in \mathbb{R}^{d-1}, \tag{13}$$

on some suitable dense domain in some Hilbert space.

Since the situation for the case $v \not\equiv 0$ is quite complicated, because of the well known problem of divergences, let us first consider the case where $v \equiv 0$, i.e. the case of free fields describing first Level 0–2 for this case. If $v \equiv 0$ in S_{QF} as given by (4), then the natural Hilbert space for the CCR representation is $L^2(\mathcal{S}'(\mathbb{R}^{d-1}), \mu_E^{0,0})$, with $\mu_E^{0,0} = N(0; (-\Delta_{d-1} + 1)^{-\frac{1}{2}})$, the free time zero field measure (of mass 1), which can be realized on $\mathcal{S}'(\mathbb{R}^{d-1})$. One shows that $\mu_E^{0,0}$ is the restriction to the σ-algebra generated by the time zero fields of the measure μ_E^0, described heuristically as $\mu_E^0 = Z^{-1} e^{-S_E^0(\gamma)}\, \mathrm{d}\gamma$ with

$$S^0(\gamma) := \frac{1}{2} \int_{\mathbb{R}} \int_{\mathbb{R}^{d-1}} \left(\left| \dot{\gamma}(s, \vec{x}) \right|^2 + \left| \nabla \gamma(s, \vec{x}) \right|^2 + \left| \gamma(s, \vec{x}) \right|^2 \right) \mathrm{d}s\, \mathrm{d}\vec{x}. \tag{14}$$

μ_E^0 is realized rigorously as $N(0; (-\Delta_d + 1)^{-1})$ on $\mathcal{S}'(\mathbb{R}^d)$. It is called the Euclidean free field measure, see [98].

The above $L^2(\mathcal{S}'(\mathbb{R}^{d-1}), \mu_E^{0,0})$ is naturally isomorphic to the Fock space ("second quantization"), see [78].

Consider the classical Dirichlet form $\mathcal{E}(u, v) = \frac{1}{2} \int \nabla u \nabla v\, \mathrm{d}\mu_E^{0,0}$, so that $\mathcal{E}(u, v) = \left(u, -L_{\mu_E^{0,0}} v \right)$ for u, v in the relevant domains, in $L^2\left(\mu_E^{0,0}\right) := L^2(\mathcal{S}'(\mathbb{R}^{d-1}), \mu_E^{0,0})$ with $L_{\mu_E^{0,0}}$ the associated Dirichlet operator. One has that $H^0 := -L_{\mu_E^{0,0}}$ is self-adjoint (on its natural domain) and is a realization of the Hamiltonian for the free relativistic quantum field. In an analogous way one can consider the generators of the whole Poincaré group on space-time $\mathbb{R} \times \mathbb{R}^{d-1}$.

The generators of the Lorentz group are not positive, but can be shown to be essentially self-adjoint on smooth cylinder functions (by using the isomorphism of $L^2(\mu_E^{0,0})$ with Fock space, i.e. second quantization).

Then one has a rigorous full implementation of canonical relativistic free quantum fields in $L^2(\mu_E^{0,0})$, see [48].

Note that $L_{\mu_E^{0,0}}$ generates a diffusion process $X_t(\vec{x})$, $t \geq 0$, $\vec{x} \in \mathbb{R}^{d-1}$ with state space $\mathcal{S}'(\mathbb{R}^{d-1})$ satisfying the stochastic differential equation

$$\mathrm{d}X_t(\vec{x}) = -\left[(-\Delta_{d-1} + 1)^{\frac{1}{2}} X_t(\vec{x}) \right] \mathrm{d}t + \mathrm{d}w_t(\vec{x}), \quad t \geq 0, \vec{x} \in \mathbb{R}^{d-1}. \tag{15}$$

$\mathrm{d}w_t(\vec{x})$ denotes the Gaussian white noise in the t- and $\vec{x}$-variables.

This was first discussed in [23] and [81]. Note also that $\mu_E^{0,0}$ is the unique stationary measure for $X_t(\vec{x})$.

The path space distribution of $X_t(\vec{x})$ is the Euclidean free field measure $\mu_E^0 = N\left(0; (-\Delta_{\mathbb{R}^d} + 1)^{-1}\right)$ on $\mathcal{S}'(\mathbb{R}^d)$, as described above.

This has been discussed originally by K. Symanzik [112] and E. Nelson [98] (and, in connection with statistics, by L. Pitt, [103]).

That the restriction of μ_E^0 to the σ-algebra $\sigma(X_0)$ generated by the time zero fields $X_0(\cdot)$ can be identified with $\mu_E^{0,0}$ due to the global Markov property of the Euclidean free field [29, 38, 98, 104].

The Level 2 is described by the SDE (SPDE)

$$dX_\tau(y) = (\Delta_d - 1)X_\tau(y) + dW_\tau(y), \tag{16}$$

$y \in \mathbb{R}^d$, $\tau \geq 0$ (τ is a "computer time", y the space-time variable). $dW_\tau(y)$ denotes the Gaussian white noise in the τ- and y-variables.

The invariant measure to $X_\tau(y)$ is μ_E^0. The SPDE (16) is called stochastic quantisation equation (SQE) associated with the Euclidean free field (over $\mathbb{R}^d$).

Already for $d = 2$, in the case $v \not\equiv 0$ the construction of Levels 0–2 is much more complicated.

Levels 0 and 1 have been achieved first in models with exponential interaction (for which v is of the form $v(u) = e^{\alpha u}$, $|\alpha| < \alpha_0$, for suitable $\alpha_0 > 0$, $u \in \mathbb{R}$) with renormalization, in [82] resp. [20] (see also [11, 21, 89]).

In the same period the case of v of polynomial type, with renormalization, was achieved, see [71, 106], and references therein.

The model with v of trigonometric type was first discussed in [19] (with regularization, see also [14]) and solved (with renormalizations) in [68] (see also [14, 67]).

All models are covered and unified by the white noise calculus approach [16–18].

Let us give a short summary of these constructions. At Level 0 one constructs a non Gaussian $\mu^{v,0}$ on $\mathcal{S}'(\mathbb{R}^{d-1})$. At Level 1 one constructs the analogue of (12) for quantum fields, i.e.

$$\mu_E^v(d\gamma) = \text{“}Z^{-1}e^{-S(\gamma)}d\gamma'', \tag{17}$$

with $S(\gamma) = S^0(\gamma) + \iint v(\gamma(s,\vec{x}))\,ds\,d\vec{x}$. (Thus μ_E^v coincides with the expression given by (5) and (6)). At Level 2 the measure μ_E^v appears as invariant measure for the solution of the stochastic quantization equation (also called, in other contexts, Allen-Cahn equation, see, e.g., [99], also related to the Ginzburg-Landau equation), associated to Euclidean fields with interaction given by v:

$$dX_\tau(y) = (\Delta_d - 1)X_\tau(y)\,d\tau - v'(X_\tau(y))\,d\tau + dw_\tau(y), \quad \tau \geq 0,\ y \in \mathbb{R}^d. \tag{18}$$

The associated classical Dirichlet forms given by the restriction $\mu_E^{v,0}$ of μ_E^v to the σ-algebra of the zero fields, which is thus a measure on $S'(\mathbb{R}^{d-1})$, (coinciding with the level 0 measure $\mu^{v,0}$) resp. by μ_E^v itself, yield in turn generators of Markov processes (diffusions) $X_t(\vec{x})$ resp. $X_\tau(y)$, $t, \tau \geq 0$, $\vec{x} \in \mathbb{R}^{d-1}$, $y \in \mathbb{R}^d$, the latter solving (18).

The generator of $X_t(\vec{x})$ is identifiable (via a natural isomorphism) on smooth cylinder functions with the Hamiltonian acting in $L^2\left(\mu_E^{v,0}\right)$, of the interacting quantum fields, given the global Markov property of the Euclidean fields [29]. The generators of the Poincaré group are also realizable as self-adjoint operators on $L^2(\mu_E^{v,0})$ [21, 47].

Whether all generators are already determined on smooth cylinder functions is a hard problem, only solved for the case $X_\tau(y)$ in a bounded region when $d =$

2 [61, 90] (it has been solved in bounded and unbounded regions for $d = 1$ in [31, 32, 87]).

For recent work on Level 2 for $d = 2$ with exponential interaction see [30, 31].

Remark 4.1 The SQE has also been studied intensively with noise regularized in the y-variable and corresponding modified drift coefficient, so as to heuristically maintain the same invariant measure.

See [41–43, 56, 60, 61, 64, 70, 83–86, 95–97, 99, 100, 105], and also e.g. [58] for related problems.

For $d = 3$ partial results on Level 0–2 have been achieved for v which are of the form of a 4-th power (with renormalization), see, e.g. the references in [36].

Recently solutions of the SQE of Level 2 has been constructed by different methods in [77]. However the Markov character of the solutions (a property included if one uses processes associated with Dirichlet forms) has not yet been discussed.

The difficulties in constructing solutions is related to the expected singularity of μ_E^v with respect to μ_E^0 even in bounded regions (this has been proved rigorously in [35] only for the restriction of these measure to the σ-algebra generated by the time zero fields).

Other types of relativistic models however also exist for all d including $d = 4$, provided one relaxes the axioms to the ones which have been introduced (by Strocchi-Wightman and Morchio-Strocchi) for gauge fields, see the work [73] (in white noise analysis) and [12, 13] (and references therein).

For the construction of gauge fields for $d = 2$ see [1, 24, 25, 47, 48] (and references therein).

For $d = 3$ in the Euclidean case a model of gauge fields has been constructed using μ_F (Chern-Simons model) [15, 47, 91], again using methods from white noise analysis (to which Ludwig has fundamentally contributed).

5 Some Remarks on Related Systems

Methods related to the ones discussed in the preceding Sections can also be used in other areas.

E.g., in recent years equations for neuronal dynamics of the FitzHugh-Nagumo type have been discussed in [5, 6].

In the simplest version they describe a signal propagating along a single neuron under the influence of external noise and of certain salts concentrations. They are of the form of 2 coupled random variables, the components of a vector $X \in L^2([0,1]) \times L^2([0,1])$ satisfying a SDE of the form $\mathrm{d}X_t = AX_t\,\mathrm{d}t + F(X_t)\,\mathrm{d}t + \varepsilon\,\mathrm{d}w_t$, $t \geq 0$, with w_t space-time Gaussian white noise and $\varepsilon > 0$ a (small diffusion) parameter.

A is a diffusion operator, $F(x)$ is a non linear term, e.g., of the Fitz-Hugh-Nagumo type $F(x) = \begin{pmatrix} -x(x-1)(x-\theta), & 0 < \theta < 1 \\ 0 \end{pmatrix}$, $x \in \mathbb{R}$.

Using dissipativity, in [5, 54] the existence, uniqueness of solutions and the uniqueness of the invariant measure have been discussed, as well as the $\varepsilon \downarrow 0$ behaviour in terms of detailed asymptotic expansions, with L^p-control, $1 \leq p < +\infty$, on remainders.

The invariant measure is exhibited, as being of Gibbsian type with a density e^{-G} with respect to μ_A, and $G' = -F$, where μ_A is the invariant Gaussian measure associated to the linear stochastic equation for $F \equiv 0$.

It is interesting that in the case of Gaussian white noise replaced by Lévy noise also an invariant measure has been found in [6]. Its character is presently under discussion.

In the finite dimensional case explicit invariant measures of related systems can be constructed via an analogue of the general ground state transformation discussed early in [27], see [6, 50]. Andrisani and Cufaro-Petroni [50] have interesting applications, e.g. to the study of halo formation in intense beams of charged particles in accelerators.

Stochastic pde's of the form of those we have discussed in connection with quantum field theory and neuronal dynamics also occur in many other areas, including, e.g., hydrodynamics and polymer physics, to which Ludwig Streit has given outstanding contributions. Let us mention, in particular, his work on the Burgers equation [51] and his work on polymer-type measures, a prototype for the latter being given by the Edwards' model described heuristically by the invariant measure

$$\mu(\mathrm{d}\gamma) = \text{“}Z^{-1} e^{-\lambda \int_0^t \int_0^t \delta(\omega(s)-\omega(s'))\,\mathrm{d}s\,\mathrm{d}s'} \mu_0(\mathrm{d}\omega)\text{”} \tag{19}$$

μ_0 being Wiener measure for Brownian motion on $\mathbb{R}^d$, δ the Dirac distribution, λ a (positive) constant, $t > 0$. The Gibbs factor inhibits self-intersection of paths. For such measures and related ones see, e.g., [9, 40, 62, 63].

Varadhan showed in [113] that setting $L_\varepsilon = \int_0^t \int_0^t \delta_\varepsilon(\omega(s) - \omega(s'))\,\mathrm{d}s\,\mathrm{d}s'$ with δ_ε a natural ε-regularization of δ one has that $L_\varepsilon - E(L_\varepsilon)$ converges as $\varepsilon \downarrow 0$ in $L^2(\mu_0)$ to a limit $\tilde{L}$, in such a way that

$$\|\tilde{L} - [L_\varepsilon - E(L_\varepsilon)]\|_{L^2(\mu_0)} \leq C\varepsilon^\alpha \tag{20}$$

for some constant $C > 0$, for all $\alpha < \frac{1}{2}$.

This implies in particular the existence of the polymer measure μ, understood as weak limit of μ_ε as $\varepsilon \downarrow 0$ defined by (19) with

$$L := \int_0^t \int_0^t \delta(\omega(s) - \omega(s'))\,\mathrm{d}s\,\mathrm{d}s' \tag{21}$$

replaced by $L_\varepsilon - E(L_\varepsilon)$.

The above estimate (20) has been improved to $\alpha < 1$ in a recent publication by Ludwig and coworkers [53].

6 Conclusions

We have just been able to discuss a few of the many important developments inspired, initiated and rigorously pursued by Ludwig Streit. I am very grateful to Ludwig for having been a constant source of inspiration for me and many coworkers since many years. I wish him many more years of good health, happiness, "frohes Schaffen".

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Detecting Hierarchical Communities in Networks: A New Approach

Michael J. Barber

Abstract Agglomerative clustering is a well established strategy for identifying communities in networks. Communities are successively merged into larger communities, coarsening a network of actors into a more manageable network of communities. The order in which merges should occur is not in general clear, necessitating heuristics for selecting pairs of communities to merge. We describe a hierarchical clustering algorithm based on a local optimality property. For each edge in the network, we associate the modularity change for merging the communities it links. For each community vertex, we call the preferred edge that edge for which the modularity change is maximal. When an edge is preferred by both vertices that it links, it appears to be the optimal choice from the local viewpoint. We use the locally optimal edges to define the algorithm: simultaneously merge all pairs of communities that are connected by locally optimal edges that would increase the modularity, redetermining the locally optimal edges after each step and continuing so long as the modularity can be further increased. We apply the algorithm to model and empirical networks, demonstrating that it can efficiently produce high-quality community solutions. We relate the performance and implementation details to the structure of the resulting community hierarchies. We additionally consider a complementary local clustering algorithm, describing how to identify overlapping communities based on the local optimality condition.

Keywords Complex networks • Communities • Agglomerative clustering

1 Introduction

A prominent theme in the investigation of networks is the identification of their community structure. Informally stated, network communities are subnetworks whose constituent vertices are strongly affiliated to other community members and

M.J. Barber (✉)
Innovation Systems Department, AIT Austrian Institute of Technology GmbH,
Donau-City-Str. 1, 1220 Vienna, Austria
e-mail: michael.barber@ait.ac.at

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comparatively weakly affiliated with vertices outside the community; several formalizations of this concept have been explored (for useful reviews, see Refs. [1, 2]). The strong internal connections of community members is often accompanied by greater homogeneity of the members, e.g., communities in the World Wide Web as sets of topically related web pages or communities in scientific collaboration networks as scientists working in similar research areas. Identification of the network communities thus can facilitate qualitative and quantitative investigation of relevant subnetworks whose properties may differ from the aggregate properties of the network as a whole.

Agglomerative clustering is a well established strategy for identifying a hierarchy of communities in networks. Communities are successively merged into larger communities, coarsening a network of actors into a more manageable network of communities. The order in which merges should occur is not in general clear, necessitating heuristics for selecting pairs of communities to merge.

A key approach to community identification in networks is from Newman [3], who used a greedy agglomerative clustering algorithm to search for communities with high modularity [4]. In this algorithm, pairs of communities are successively merged based on a global optimality condition, so that the modularity increases as much as possible with each merge. The pairwise merging ultimately produces a community hierarchy that is structured as a binary tree. The structure of the hierarchy closely relates to both the quality of the solution and the efficiency of its calculation; modularity is favored by uniform community sizes [5, 6] while rapid computation is favored by shorter trees [7], so both are favored when the community hierarchy has a well-balanced binary tree structure, where the sub-trees at any node are similar in size. But the greedy algorithm may produce unbalanced community hierarchies—the hierarchy may even be dominated by a single large community that absorbs single vertices one-by-one [8], causing the hierarchy to be unbalanced at all levels.

In this chapter, we describe a new agglomerative clustering strategy for identifying community hierarchies in networks. We replace the global optimality condition for the greedy algorithm with a local optimality condition. The global optimality condition holds for communities c and c' when no other pair of communities could be merged so as to increase the modularity more than would merging c and c'. The local optimality condition weakens the global condition, holding when no pair of communities, one of which is either c or c', could be merged to increase the modularity more than would merging c and c'. The essentials of the clustering strategy follow directly: concurrently merge communities that satisfy the local optimality condition so as to increase the modularity, re-establishing the local optimality conditions and repeating until no further modularity increase is possible. The concurrent formation of communities encourages development of a cluster hierarchy with properties favorable both to rapid computation and to the quality of the resulting community solutions.

2 Agglomerative Clustering

2.1 Greedy Algorithms

Agglomerative clustering [9, 10] is an approach long used [11] for classifying data into a useful hierarchy. The approach is based on assigning the individual observations of the data to clusters, which are fused or merged, pairwise, into successively larger clusters. The merging process is frequently illustrated with a dendrogram, a tree diagram showing the hierarchical relationships between clusters; an example dendrogram is shown in Fig. 1. In this work, we will also refer to the binary tree defined by the merging process as a dendrogram, regardless of whether it is actually drawn.

Specific clustering algorithms depend on defining a measure of the similarity of a pair of clusters, with different measures corresponding to different concepts of clusters. Additionally, a rule must be provided for selecting which merges to make based on their similarity. Commonly, merges are selected with a greedy strategy, where the single best merge is made and the similarity recalculated for the new cluster configuration, making successive merges until only a single cluster remains. The greedy heuristic will not generally identify the optimal configuration, but can often find a good one.

2.2 Modularity

Agglomerative clustering has seen much recent use for investigating the community structure of complex networks (for a survey of agglomerative clustering and other community identification approaches, see Refs. [1, 2]). The dominant approaches follow Newman [3] in searching for communities (i.e., clusters) with high modularity Q. Modularity assesses community strength for a partition of the n network

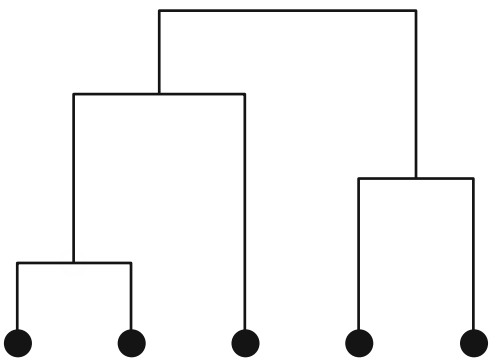

Fig. 1 Dendrogram representation of a cluster hierarchy. Clusters of data are pairwise merged into larger clusters, with all data eventually in the same cluster

vertices into disjoint sets, and is defined [4] as

$$Q = \frac{1}{2m} \sum_c \sum_{i,j \in c} \left(A_{ij} - \frac{k_i k_j}{2m} \right) \quad , \tag{1}$$

where the A_{ij} are elements of the adjacency matrix for the graph, m is the number of edges in the graph, and k_i is the degree of vertex i, i.e., $k_i = \sum_j A_{ij}$. The outer sum is over all clusters c, the inner over all pairs of vertices (i, j) within c.

With some modest manipulation, Eq. (1) can be written in terms of cluster-level properties and in a form suitable as well for use with weighted graphs:

$$Q = \lambda \sum_c \left(W_c - \lambda K_c^2 \right) \quad , \tag{2}$$

where

$$W_c = \sum_{i,j \in c} A_{ij} \tag{3}$$

$$K_c = \sum_{i \in c} k_i \tag{4}$$

$$\lambda = \left(\sum_c K_c \right)^{-1} \quad . \tag{5}$$

Here, W_c is a weight of edges internal to cluster c, measuring the self-affinity of the cluster constituents; K_c is a form of volume for cluster c, analogous to the graph volume; and λ is a scaling factor equal to $1/2m$ for an unweighted graph. Other choices for λ may also be suitable [6], but we will not consider them further.

Edges between vertices in different clusters c and c' may also be described at the cluster level; denote this edge by (c, c'). Edge (c, c') has a corresponding symmetric inter-cluster weight $w_{cc'}$, defined by

$$w_{cc'} = \sum_{i \in c} \sum_{j \in c'} A_{ij} \quad . \tag{6}$$

Using $w_{cc'}$, we can describe the merge process entirely in terms of cluster properties. When two clusters u and v are merged into a new cluster x, it will have

$$W_x = W_u + W_v + 2w_{uv} \tag{7}$$

$$K_x = K_u + K_v \quad . \tag{8}$$

The inter-cluster weights for the new cluster x will be

$$w_{xy} = w_{uy} + w_{vy} \tag{9}$$

for each existing cluster y, excluding u and v. The modularity change ΔQ_{uv} is

$$\Delta Q_{uv} = 2\lambda \left(w_{uv} - \lambda K_u K_v\right) \quad . \tag{10}$$

From Eq. (10), it is clear that modularity can only increase when $w_{uv} > 0$ and, thus, when there are edges between vertices in u and v.

With the above, we can view a partition of the vertices as an equivalent graph of clusters or communities; merging two clusters equates to edge contraction. The cluster graph is readily constructed from a network of interest by mapping the original vertices to vertices representing singleton clusters and edges between the vertices to edges between the corresponding clusters. For a cluster c derived from a vertex i, we initialize $W_c = 0$ and $K_c = k_i$.

2.3 Modularity-Based Greedy Algorithms

Newman [3] applied a greedy algorithm to finding a high modularity partition of network vertices by taking the similarity measure to be the change in modularity ΔQ_{uv}. In this approach, ΔQ_{uv} is evaluated for each inter-cluster edge, and a linked pair of clusters leading to maximal increase in modularity is selected for the merge. A naive implementation of this greedy algorithm constructs the community hierarchy and identifies the level in it with greatest modularity in worst-case time $O\left((m+n)n\right)$, where m and n are, respectively, the numbers of edges and vertices in the network.

Finding a partition giving the global maximum in Q is a formally hard, NP-complete problem, equivalent to finding the ground state of an infinite-range spin glass [12]. We should thus expect the greedy approach only to identify a high modularity partition in a reasonable amount of time, rather than to provide us with the global maximum. Variations on the basic greedy algorithm may be developed focusing on increasing the community quality, reducing the time taken, or both.

Likely the most prominent such variation is the implementation described by Clauset et al. [7]. While neither the greedy strategy nor the modularity similarity measure is altered, the possible merges are tracked with a priority queue implemented using a binary heap, allowing rapid determination of the best choice at each step. This results in a worst-case time of $O\left(mh \log n\right)$, where h is the height of the resulting dendrogram. Thus, the re-implementation is beneficial when, as for many empirical networks of interest, the dendrogram is short, ideally forming a balanced binary tree with height equal to $\lfloor \log_2 n \rfloor$, where $\lfloor x \rfloor$ denotes the integer part of x. But the dendrogram need not be short—it may be a degenerate tree of height n, formed

when all singleton clusters are merged one-by-one into the same cluster. Such a dendrogram results in $O(mn \log n)$ time, worse than for the naive implementation.

Numerous variations on the use of the change in modularity have been proposed for use with greedy algorithms, with some explicitly intended to provide a shorter, better balanced dendrogram. We note two in particular. First, Danon et al. [5] consider the impact that heterogeneity in community size has on the performance of clustering algorithms, proposing an altered modularity as the similarity measure for greedy agglomerative clustering. Second, Wakita and Tsurumi [8] report encountering poor scaling behavior for the algorithm of Clauset et al., caused by merging communities in an unbalanced manner; they too propose several modifications to the modularity to encourage more well-balanced dendrograms. In both papers, the authors report an improvement in the (unmodified) modularity found, even though they were no longer directly using modularity to select merges—promoting short, well-balanced dendrograms can promote better performance both in terms of time taken and in the quality of the resulting communities.

Alternatively, the strategy by which merges are selected may be changed, while keeping the modularity as the similarity measure, giving rise to the multistep greedy (MSG) algorithm [13, 14]. In the MSG approach, multiple merges are made at each step, instead of just the single merge with greatest increase in the modularity. The potential merges are sorted by the change in modularity ΔQ_{uv} they produce; merges are made in descending order of ΔQ_{uv}, so long as (1) the merge will increase modularity and (2) neither cluster to be merged has already been selected for a merge with greater ΔQ_{uv}. The MSG algorithm promotes building several communities concurrently, avoiding early formation of a few large communities. Again, this leads to shorter, better balanced dendrograms with improved performance both in terms of time and community quality.

When required for clarity, we will refer to the original greedy strategy as single-step greedy (SSG). Additionally, we will restrict our attention to an implementation following Clauset et al. [7].

3 Clustering with Local Optimality

3.1 Local Optimality

The SSG and MSG algorithms are global in scope, pooling information from across the entire network to identify the clusters to merge that would lead to the greatest increase in modularity. In contrast, the potential modularity change ΔQ_{uv} is local in scope and can be calculated (Eq. 10) using only properties of the clusters u and v. It is thus instructive to consider what else can be said on a local scale about the possible merges, particularly those selected in the SSG algorithm.

Let us assume that, at some stage in the SSG algorithm, clusters u and v are identified as those to merge. As noted in Sect. 2.2, there must be an edge between

the two clusters. Restricting our attention to the edges incident on u, the edge (u, v) is distinguished from the edge to any other linked cluster x by leading to a greater modularity change, so that

$$\Delta Q_{uv} \geq \Delta Q_{ux} \qquad \forall x \quad . \tag{11}$$

Considering the edges incident on v leads to a similar preference for the edge (u, v) over that to another linked cluster y, with

$$\Delta Q_{uv} \geq \Delta Q_{yv} \qquad \forall y \quad . \tag{12}$$

Informally, the two clusters each have the other as the best choice of merge.

For any cluster with incident edges, at least one edge will satisfy a condition analogous to those in Eqs. 11 and 12. Call these the *preferred* edges for the vertex; similarly, refer to the corresponding merge as the preferred merge. If an edge is preferred for both vertices on which it is incident, call it and the corresponding merge *locally optimal*. We illustrate preferred and locally optimal edges in Fig. 2.

The local optimality condition is based on softening the global optimality condition used in the SSG algorithm, replacing a network-wide comparison of potential merges with an assessment of how clusters relate to their neighbors. As we will see, locally optimal edges occur frequently and can be used as the basis for an agglomerative clustering algorithm.

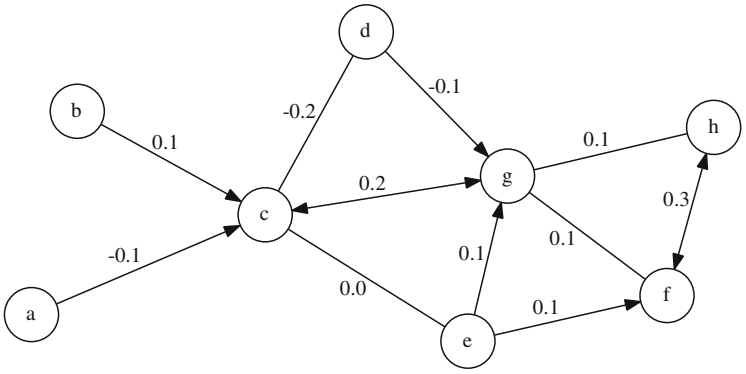

Fig. 2 Preferred and locally optimal edges. Each edge is labeled with its modularity change ΔQ_{uv}, which is the basis for determining the merge preferences shown with arrows. Edges with a single arrowhead are preferred edges for the vertex at the tail of the arrow, but not for the vertex at the head of the arrow. Edges with arrowheads at each end are preferred for both vertices; these are locally optimal edges. Those edges without arrowheads are not preferred by either of the linked vertices

3.2 Greedy Clustering Using Local Optimality

We can base an agglomerative clustering algorithm on merging along the locally optimal edges in the network, determining whether any edges become locally optimal as a consequence, and repeating this until no locally optimal edges remain. With such an approach, we discourage the formation of unbalanced dendrograms by allowing multiple merges to occur concurrently, thus favoring shorter dendrograms and—given a suitable implementation—more efficient computation. The approach lies somewhere between SSG and MSG clustering, featuring concurrent formation of clusters like MSG, but selecting merges with a generalization of the condition in SSG.

For the most part, it is straightforward to define a precise algorithm from this idea. One complication is the presence of vertices with multiple locally optimal edges incident upon them. These edges can lead to, for example, a state where edges (u, v) and (u, w) are locally optimal, but (v, w) is not locally optimal. Thus, if we make both locally optimal merges, we produce a combined cluster of $\{u, v, w\}$ which also includes the locally suboptimal merge. But to exclude merging v and w, we must then only make one of the locally optimal merges. In this work, we adopt the latter approach, arbitrarily selecting one of the locally optimal merges.

The resulting algorithm is:

1. For each edge (u, v), evaluate ΔQ_{uv}.
2. For each vertex v, identify the maximum modularity change $\Delta Q_v^{\max}$ from all incident edges.
3. For each edge (u, v), determine if it is locally optimal by testing $\Delta Q_{uv} = \Delta Q_u^{\max} = \Delta Q_v^{\max}$. If, in addition, $\Delta Q_{uv} > 0$, edge (u, v) is a candidate merge.
4. If there are no candidate merges, stop. Otherwise, for each candidate, merge the corresponding clusters, so long as neither cluster has so far been changed in the current iteration.
5. Begin a new iteration from step 1.

The order of iteration in step 4 will have an effect on the resulting community hierarchy when vertices have multiple locally optimal edges. In the implementation used in this work, we iterate through the edges in an arbitrary order that is uncorrelated with the modularity changes ΔQ_{uv}. As the algorithm greedily selects edges based on local optimality, we call it GLO clustering—greedy, local optimality clustering.

When the GLO algorithm terminates, no remaining edge will support a positive change in modularity; otherwise, one or more edges (u, v) would have $\Delta Q_{uv} > 0$, and thus there would be at least one candidate merge—that edge with the greatest ΔQ_{uv}. The clusters at termination have greater modularity than at any earlier iteration in the algorithm, since merges are only made when they increase the modularity.

Note that the GLO algorithm generally terminates only having formed the subtrees of the dendrogram for each cluster rather than the full dendrogram with single

root. If the full dendrogram is needed, additional cluster merges can be made by using an alternate greedy algorithm. Here, we follow the above steps for GLO clustering, but drop the requirement that $\Delta Q_{uv} > 0$—all locally optimal edges become candidate merges. This laxer condition is always satisfied by at least at least the edge with greatest ΔQ_{uv}, so the merge process continues until all edges have been eliminated and only a single cluster remains.

Implementing the GLO algorithm presents no special difficulties. The needed properties of the clusters (W_v, K_v, and w_{uv}) can be handled as vertex and edge attributes of a graph data structure. Straightforward implementation of the above steps can be done simply by iterating through the m edges, leading to $O(m)$ worst-case time complexity for each of the p iterations of the merge process, or $O(mp)$ overall worst-case time complexity. A simple optimization of this basic implementation strategy is to keep track of the $\Delta Q_v^{\max}$ values and a list of corresponding preferred edges, recalculating these only when merges could lead to changes; this does not change the worst case time complexity from $O(mp)$, but does notably improve the execution speed in practice.

The above estimates of time complexity have the shortcoming that they are given not just in terms of the size of the network, but also in terms of an outcome of the algorithm—the number of iterations p. There is no clear a priori relation between p and the network size, but we may place bounds on p. First, the algorithm merges at least one pair of clusters in each iteration, so p is bounded above by n. Second, the algorithm involves any cluster in at most one merge in an iteration, so p must be at least the height h of the dendrogram. This gives

$$n > p \geq h \geq \lfloor \log_2 n \rfloor \quad . \tag{13}$$

Runtime of the algorithm is thus seen to be dependent on the structure of the cluster hierarchy found, with better performance requiring a well-balanced dendrogram. We do have reason to be optimistic that p will be relatively small in this case: a well-balanced dendrogram results when multiple clusters are constructed concurrently, which also requires fewer iterations of the algorithm.

3.3 Local Clustering Using Local Optimality

Although all merging decisions in GLO clustering are made using only local information, the algorithm is nonetheless a global algorithm—the clusters possible at one point in the graph are influenced by merges concurrently made elsewhere in the network. Yet we may specify a local clustering algorithm: starting from a single vertex, successively merge along any modularity-increasing, locally optimal edges incident upon it, stopping only when no such locally optimal edges remain. In this fashion, the modularity—an assessment of a partition of the vertices—may be used to identify overlapping communities.

This local algorithm functions by absorbing vertices one-by-one into a single cluster. Unfortunately, this is exactly the behavior corresponding to the worst case behavior for the SSG and GLO algorithms, producing a degenerate binary tree as the dendrogram whose height is one less than the number of vertices in the community and conceivably is one less than the number of vertices in the graph. The expected time complexity is thus quadratic in the resulting community size. Worse still, characterizing all local clusters for the graph may require a sizable fraction of the vertices to be so investigated, giving a worst-case time complexity that is cubic in the number of vertices of the graph. Such an approach is thus suited for networks of only the most modest size.

A compromise approach is possible using a hybrid of the agglomerative and local approaches. First, determine an initial set of clusters using the GLO algorithm. Second, for each community, expand it using local clustering, treating all other vertices as belonging to distinct singleton clusters. The hybrid algorithm is still quite slow (and leaves the worst-case time complexity unchanged), but fast enough to provide some insight into the overlapping community structure of networks with tens of thousands of vertices.

4 Results

4.1 Model Networks

To begin, we confirm that the GLO clustering algorithm is able to identify network communities by applying it to randomly generated graphs with known community structure. We make use of the model graphs proposed and implemented by Lancichinetti et al. [15]. We generate 1000 random graphs using the default parameter settings, where each random graph instance has 1000 vertices with an average degree of 15.

In Table 1, we show some characteristics of the results of clustering algorithm, comparing the results to those for SSG and MSG clustering. For the model networks, GLO produces community solutions that have a greater number of communities, on average, than either SSG or MSG. The average modularity is greatest with SSG, with GLO second and MSG lowest. Modularity values are sufficiently high to indicate that GLO clustering is able to recognize the presence of communities in the model networks.

While modularity characterizes clustering, it does not directly measure the accuracy of the clusters. We instead assess accuracy using the normalized mutual information I_{norm}. For the joint probability distribution $P(X, Y)$ over random variables X and Y, $I_{\text{norm}}(X, Y)$ is

$$I_{\text{norm}}(X, Y) = \frac{2I(X, Y)}{H(X) + H(Y)} \quad , \tag{14}$$

Table 1 Algorithm performance with model networks. Values are computed by averaging over clustering results from 1000 realizations of the random graphs proposed by Lancichinetti et al. [15], with default parameter settings. Results shown are for the highest modularity clusters in the generated hierarchies, with the number of clusters in the partition, the corresponding modularity Q, the normalized mutual information I_{norm} comparing the algorithm output to the known community assignments, and the height h of the dendrogram (optimal height would be 9). Uncertainties for the final significant digits are shown parenthetically. All values in each column differ significantly ($p < 0.001$)

Algorithm	Clusters	Q	I_{norm}	h
SSG	16.16(5)	0.7155(2)	0.8481(6)	124.1(5)
GLO	25.55(5)	0.6904(2)	0.8379(5)	38.3(1)
MSG	15.70(5)	0.5673(5)	0.6457(8)	11.94(2)

where the mutual information $I(X, Y)$ and entropies $H(X)$ and $H(Y)$ are defined

$$I(X, Y) = \sum_{x,y} P(X, Y) \log \frac{P(X, Y)}{P(X) P(Y)} \tag{15}$$

$$H(X) = -\sum_{x} P(X) \log P(X) \tag{16}$$

$$H(Y) = -\sum_{y} P(Y) \log P(Y) \quad . \tag{17}$$

In Eqs. (14), (15), (16), and (17), we use the typical abbreviations $P(X = x, Y = y) = P(X, Y)$, $P(X = x) = P(X)$, and $P(Y = y) = P(Y)$. The base of the logarithms in Eqs. (15), (16), and (17) is arbitrary, as the computed measures only appear in the ratio in Eq. (14).

To assess clustering algorithms with $I_{\text{norm}}(X, Y)$, we treat the actual community membership for a vertex as a realization of a random variable X and the community membership algorithmically assigned to the vertex as a realization of a second random variable Y. The joint probability $P(X, Y)$ is defined by the distribution of paired community membership over all vertices in the graph. We can then evaluate $I_{\text{norm}}(X, Y)$, finding a result that parallels the modularity: SSG on average obtains the greatest normalized mutual information, with GLO second and MSG the lowest. The high value for $I_{\text{norm}}(X, Y)$ indicates that GLO clustering assigns most vertices to the correct communities.

As GLO clustering attempts to improve performance by favoring well-balanced dendrograms, we also assess the balance of the dendrograms using their height. Since a dendrogram is a binary tree, the optimal height for a graph with n vertices is just the integer part of $\log_2 n$; the extent to which the dendrogram height exceeds this value is then indicative of performance shortcomings of the algorithm. The random graphs considered in this section have 1000 vertices, and therefore the optimal height is 9. The results are essentially what one would expect: SSG, which does not attempt to favor merges leading to balanced dendrograms, produces

the tallest dendrograms on average; MSG, which aggressively makes concurrent merges, produces the shortest dendrograms; and GLO, which makes concurrent merges more selectively than MSG, produces dendrograms with heights on average between those resulting from SSG and MSG.

4.2 Empirical Networks

Based on the model networks considered in the preceding section, it appears that SSG produces the best community solutions of the three clustering algorithms considered. But we are ultimately not interested in model networks—it is in the application to real networks that we are concerned. In this section, we consider algorithm performance with several commonly used empirical networks.

The networks considered are a network of friendships between members of a university karate club [16]; a network of frequent associations between dolphins living near Doubtful Sound, New Zealand [17]; a network of character co-appearances in the novel *Les Misérables* [18]; a network of related purchases of political books during the 2004 U.S. presidential election [19]; a network of word adjacency in the novel *David Copperfield* [20]; a network of American college football games played during the Fall 2000 season[21]; a network of collaborations between jazz musicians [22]; a network of the neural connections in the *C. elegans* nematode worm [23]; a network of co-authorships for scientific papers concerning networks [20]; a network of metabolic processes in the *C. elegans* nematode worm [24]; a network of university e-mail interactions [25]; a network of links between political blogs during the 2004 U.S. presidential election[26]; a network of the western U.S. power grid [23]; a network of co-authorships for scientific preprints posted to the high-energy theory archive (hep-th) [27]; a network of cryptographic keys shared among PGP users [28]; a network of co-authorships for scientific preprints posted to the astrophysics archive (astro-ph) [27]; a network of the structure of the internet, at the level of autonomous systems [29]; and three networks of co-authorships for scientific preprints posted to the condensed matter archive (cond-mat), based on submissions beginning in 1995 and continuing through 1999, 2003, and 2005 [27]. Several networks feature weighted or directed edges; we ignore these, treating all networks as unweighted, undirected simple graphs. Not all of the networks are connected; we consider only the largest connected component from each network. The networks vary considerably in size, with the number of vertices n and number of edges m spanning several orders of magnitude (Table 2).

We apply SSG, MSG, and GLO clustering algorithms to each of the empirical networks. In Table 3, we show properties of the clusterings produced by each of the algorithms. The properties of the community solutions differ notably from those for the random model networks. The number of clusters produced by GLO

Table 2 Empirical networks under consideration. The number of vertices n and edges m in each network are shown

Network	n	m
Karate club	34	78
Dolphins	62	159
Les Misérables	77	254
Political books	105	441
Word adjacency	112	425
Football	115	615
Jazz	198	2742
C. elegans neural	297	2148
Network science	379	914
C. elegans metabolic	453	2040
Email	1133	5452
Political blogs	1222	16,717
Power grid	4941	6594
hep-th	5835	13,815
PGP users	10,680	24,316
cond-mat 1999	13,861	44,619
astro-ph	14,845	119,652
Internet	22,963	48,436
cond-mat 2003	27,519	116,181
cond-mat 2005	36,458	171,735

clustering no longer exceeds those for SSG and MSG clustering. Instead, the three algorithms produce similar numbers of clusters for the smaller networks, with the SSG algorithm yielding solutions with the greatest number of clusters for the largest networks. As well, the GLO algorithm tends to produce the greatest modularity values, exceeding the other approaches for 15 of the 20 empirical networks considered, including all of the larger networks.

The dendrograms produced for the empirical networks parallel those for the random networks. The dendrograms resulting from the SSG algorithm are the tallest, those from the GLO algorithm are second, and those from MSG the shortest. The SSG algorithm often produces dendrograms far taller than the ideal for a graph with a given number n of vertices.

The differences between the dendrograms suggests the abundant presence of locally optimal edges in the empirical networks. We verify this by counting the number of candidate merges in the network for each iteration of the GLO and SSG algorithms. In Fig. 3, we show the number of candidate merges for the astro-ph network; the other empirical networks show similar trends.

Table 3 Comparative performance of agglomerative clustering algorithms. For each network and each algorithm, shown are the number of clusters found, the modularity Q, and the dendrogram height h. Additionally shown for h is the minimum height for a dendrogram for the network

Network	Clusters			Q			h			
	SSG	GLO	MSG	SSG	GLO	MSG	SSG	GLO	MSG	min
Karate club	3	4	4	0.381	**0.387**	0.381	9	10	8	6
Dolphins	4	3	4	**0.495**	0.491	0.492	18	10	7	6
Les Misérables	5	6	6	0.501	**0.556**	0.536	21	13	11	7
Political books	4	5	4	0.502	**0.524**	0.506	48	18	8	7
Word adjacency	7	7	8	**0.295**	0.289	0.252	23	13	8	7
Football	7	8	5	**0.577**	0.564	0.487	27	14	8	7
Jazz	4	4	4	**0.439**	0.424	0.363	65	33	10	8
C. elegans neural	5	6	5	0.372	**0.388**	0.333	110	35	17	9
Network science	19	18	16	0.838	**0.843**	0.836	47	18	13	9
C. elegans metabolic	11	10	9	0.404	**0.428**	0.400	121	43	13	9
Email	14	11	10	0.510	**0.553**	0.487	333	60	16	11
Political blogs	11	7	10	**0.427**	0.420	0.406	631	316	77	11
Power grid	40	41	39	0.934	**0.935**	0.930	79	35	27	13
hep-th	76	56	51	0.791	**0.815**	0.794	816	82	28	13
PGP users	176	120	95	0.855	**0.874**	0.860	904	181	139	14
cond-mat 1999	165	77	71	0.764	**0.827**	0.801	2005	115	40	14
astro-ph	138	51	38	0.622	**0.708**	0.642	3576	279	60	14
Internet	43	32	28	0.630	**0.653**	0.644	3517	1635	1209	15
cond-mat 2003	316	81	67	0.671	**0.740**	0.690	5893	297	90	15
cond-mat 2005	472	77	70	0.646	**0.704**	0.645	6857	570	119	16

We additionally applied the local clustering scheme described in Sect. 3.3, expanding the clusters found for the empirical network. In each case, some or all of the clusters are expanded (Table 4), leading to overlapping communities. As a measure of the degree of cluster expansion, we define a size ratio R as

$$R = \frac{1}{n} \sum_c n_c \quad , \tag{18}$$

where n_c is the number of vertices in the expanded cluster c. The size ratio equals the expected number of clusters in which a vertex is found. Values of R for the empirical networks are given in the final column of Table 4.

The clusters do not expand uniformly. We illustrate this in Fig. 4 using the astro-ph network. In this representative example, numerous clusters expand only minimally or not at all, while others increase in size dramatically.

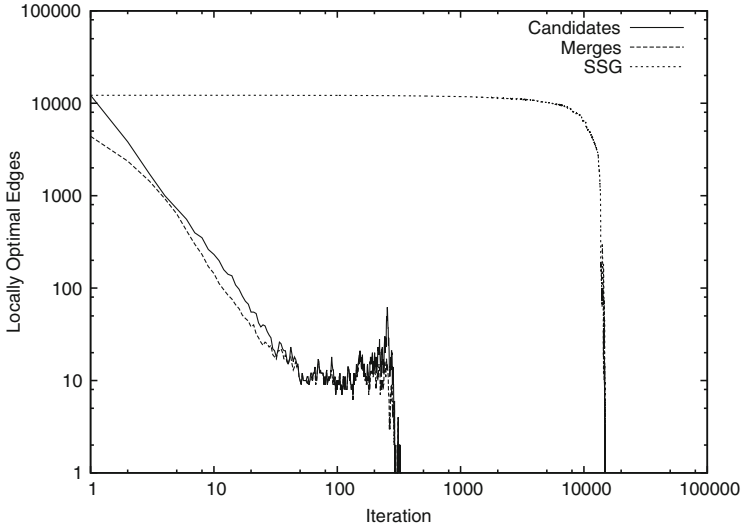

Fig. 3 Number of locally optimal edges. For the astro-ph network, we show the number of locally optimal edges that are candidate merges at each iteration of the algorithm. As the algorithm is not always able to merge all the candidates, also shown are the actual number of merges made at each iteration. For comparison, we also show, for the SSG algorithm, the number of locally optimal edges that would be candidate merges in GLO clustering

Table 4 Cluster expansion using hybrid algorithm, consisting of the GLO clustering algorithm followed by expansion using the local clustering algorithm. Shown are the number of clusters found in the GLO stage, the number of those clusters that increase in size in the local clustering stage, and the size ratio R showing an average expansion

Network	Clusters	Expanded	R
Karate club	4	1	1.18
Dolphins	3	1	1.02
Les Misérables	6	4	1.38
Political books	5	5	1.97
Word adjacency	7	6	1.31
Football	8	7	1.43
Jazz	4	4	1.51
C. elegans neural	6	6	2.33
Network science	18	11	1.33
C. elegans metabolic	10	9	1.96
Email	11	11	2.64
Political blogs	7	3	1.01
Power grid	41	23	1.01
hep-th	56	45	4.48
PGP users	120	43	2.37
cond-mat 1999	77	61	6.83
astro-ph	51	45	8.20
Internet	32	22	2.45
cond-mat 2003	81	63	9.39
cond-mat 2005	77	58	8.31

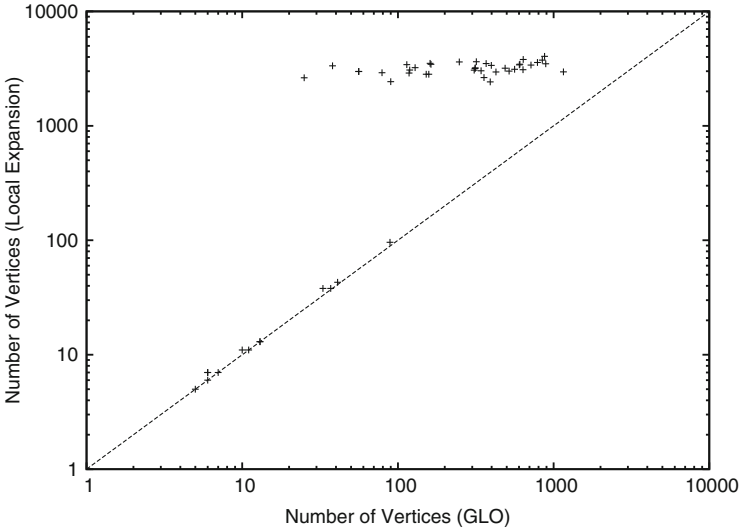

Fig. 4 Expansion of astro-ph communities with hybrid algorithm, consisting of the GLO clustering algorithm followed by expansion using the local clustering algorithm. Each point corresponds to a single cluster, with the location showing the number of vertices in the cluster as determined in the GLO stage and after the local clustering stage. The line shown indicates no expansion; all points necessarily lie on or above the line

5 Conclusion

We have described a new agglomerative hierarchical clustering strategy for detecting high-modularity community partitions in networks; we call this GLO clustering, for greedy, local optimality clustering. At the core of the approach is a locally optimality criterion, where merging two communities c and c' is locally optimal when no better merge is available to either c or c'. The cluster hierarchy is then formed by concurrently merging locally optimal community pairs that increase modularity, repeating this until no further modularity increases are possible. As all decisions on which communities to merge are based on purely local information, a natural counterpart strategy exists for local clustering.

The motivation for GLO clustering was to improve the computational performance and result quality of community identification by favoring the formation of a better hierarchy. The performance improvements have been largely achieved. The hierarchical structure, as encoded in the dendrogram, is considerably better balanced than that produced by SSG clustering, with corresponding improvements in computational performance observed for both model and empirical networks. The hierarchies produced by GLO clustering are moderately worse than those produced by MSG clustering, which is far more aggressive about making merges.

In terms of the modularity of the community solutions, the best results are found for the model networks using SSG clustering. But the results with the model are not

borne out in reality—the highest modularity solution is found with GLO clustering for 15 of the 20 empirical networks considered, including the eight largest networks.

Overall, the local optimality condition proposed in this paper appears to be a good basis for forming clusters. We can gain some insight into this from the local clustering algorithm. For each of the empirical networks considered here, there is some overlap of the communities, with several networks showing a great deal of community overlap. The borders between communities are then not entirely well defined, with the membership of particular vertices depending on the details of the sequence of merges performed in partitioning the vertices. The concurrent building of communities in GLO clustering seems to allow suitable cores of communities to form, with the local optimality condition providing a useful basis for identifying those cores.

Several directions for future work seem promising. First, the local clustering algorithm described in Sect. 3.3 has worst-case time complexity $O\left(n^3\right)$ and is thus unsuited to investigation of large networks; a reconsideration of the local algorithm may lead to a method suited to a broader class of networks. Second, we observe that nothing about GLO clustering requires that it be used with modularity, so application of GLO clustering to community quality measures for specialized classes of networks, such as bipartite networks [30], may prove beneficial. Finally, we note that GLO clustering need not be used with networks at all; application to broader classes of data analysis could thus be explored, developing GLO clustering into a general tool for classifying data into an informative hierarchy of clusters.

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Transition Probabilities for Processes with Memory on Topological Non-trivial Spaces

Christopher C. Bernido and M. Victoria Carpio-Bernido

Dedicated to Ludwig Streit on his 75th birthday.

Abstract Stochastic processes with memory subjected to a periodic boundary condition are investigated. The transition probability function for some types of memory behavior is calculated by summing over all possible paths within a white noise functional integral framework. Specific examples such as processes in spaces with circular topology and wedges are discussed.

Keywords Stochastic processes with memory • Circular topology • Wedge boundary

1 Introduction

In modeling natural phenomena, we often encounter physical systems which exhibit topological constraints. An illustrative example would be diffusion on a plane with a point singularity, or spaces with circular geometry, where the direction of diffusion can be clockwise or counterclockwise generating topologically inequivalent paths with periodic boundary condition [1, 2]. Similarly, a particle diffusing in a regular lattice could encounter a repetition of events at each lattice point. These types of paths have previously been treated as a path integral for Markov processes and for quantum systems [1–6]. In this paper, we incorporate memory which modifies the stochastic process using a memory function for more realistic applications as a system evolves from an initial time $t = 0$ to a final time τ. Specifically, we consider

C.C. Bernido (✉) • M.V. Carpio-Bernido
Research Center for Theoretical Physics, Central Visayan Institute Foundation, Jagna, Bohol 6308, Philippines
e-mail: cbernido.cvif@gmail.com

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a randomly fluctuating variable parametrized as,

$$x(\tau) = x_0 + \int_0^\tau f(\tau - t)\ h(t)\ \omega(t)\, dt\,, \tag{1}$$

where, $f(\tau - t)$ is a memory function, $h(t)$ a function of time, and $\omega(t)$ a Gaussian white noise. The calculus of white noise as "velocity" of the Brownian motion, i.e., $\omega(t) = dB(t)/dt$, has been extensively developed [7–9]. In the special case where, $f(\tau - t) = h(t) = 1$, Eq. (1) becomes, $x(\tau) = x_0 + B(\tau)$, where $B(\tau)$ is ordinary Brownian motion. This parametrization by Brownian paths $B(t)$ has been successfully applied in discussing the Feynman integral in quantum mechanics [7, 10–13] including those with boundaries [5, 14].

We show in the next section that the conditional probability density function for random variables parametrized as Eq. (1) may be evaluated as a sum over paths where $f(\tau - t)$ and $h(t)$ are chosen to suit a given physical system one wants to model [15, 16]. We shall discuss, in particular, a topologically constrained process in a circle and, in Sect. 5, in a space with a wedge-shaped boundary. We begin in the next section by discussing systems endowed with memory in spaces with circular geometry.

2 Stochastic Process with Memory on a Circle

In analogy to Eq. (1), let us consider the angular variable, $0 \leq \varphi < 2\pi$,

$$\varphi(\tau) = \varphi_0 + \int_0^\tau f(\tau - t)\ h(t)\ \omega(t)\ dt, \tag{2}$$

where, φ_0 is the initial point, $f(\tau - t)$ is a memory function, and $\omega(t)$ the Gaussian white noise [7]. For a process which starts at φ_0 and ends at φ_1, there are actually numerous possible routes since it may go clockwise or counterclockwise, as well as go around the circle n times before ending at φ_1. Given Eq. (2) we, therefore, look at all paths which satisfy the delta function constraint which pins $\varphi(\tau)$ at the endpoint φ_1, i.e.,

$$\delta(\varphi(\tau) - \varphi_1) = \delta\left(\varphi_0 - \varphi_1 + \int_0^\tau f(\tau - t)\ h(t)\ \omega(t)\ dt\right). \tag{3}$$

To evaluate the probability density function, given that there are topologically inequivalent paths on a circle, we sum Eq. (3) over all histories or all possible paths with endpoints φ_0 and φ_1, i.e.,

$$\sum_{n=-\infty}^{+\infty} \delta(\varphi(\tau) - \varphi_1 + 2\pi n) \quad ; \quad n = 0, \pm 1, \pm 2, \ldots\,. \tag{4}$$

where n is a winding number. Note that, Eq. (4) is the version of Eq. (3) on the covering space, i.e., one considers $\mathbb{R}$ as built up from infinite repetitions of the interval $[0, 2\pi)$ coding the winding number n in this way. We can then evaluate the expectation value of Eq. (4) and get the probability that indeed $\varphi(\tau)$ ends at φ_1 at time τ, if it started at φ_0. We have,

$$\begin{aligned} P(\varphi_1, \tau; \varphi_0, 0) &= \mathbb{E}\left(\sum_{n=-\infty}^{+\infty} \delta(\varphi(\tau) - \varphi_1 + 2\pi n)\right) \\ &= \int \left(\sum_{n=-\infty}^{+\infty} \delta(\varphi(\tau) - \varphi_1 + 2\pi n)\right) d\mu \\ &= \sum_{n=-\infty}^{+\infty} \int \delta(\varphi(\tau) - \varphi_1 + 2\pi n)\ d\mu. \end{aligned} \tag{5}$$

We express the delta function in terms of its Fourier representation such that,

$$\begin{aligned} P(\varphi_1, \tau; \varphi_0, 0) &= \sum_{n=-\infty}^{+\infty} \int \frac{1}{2\pi} \int_{-\infty}^{+\infty} \exp\left[ik(\varphi(\tau) - \varphi_1 + 2\pi n)\right] dk\, d\mu \\ &= \sum_{n=-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{dk}{2\pi} \exp\left[ik(\varphi_0 - \varphi_1 + 2\pi n)\right] \\ &\quad \times \int \exp\left[ik \int_0^{\tau} f(\tau - t)\ h(t)\ \omega(t)\ dt\right] d\mu, \end{aligned} \tag{6}$$

where we used Eq. (2) for $\varphi(\tau)$. The integration over $d\mu$ is done by applying [7],

$$\int \exp\left(i \int \omega(t)\, \xi(t)\, dt\right) d\mu(\omega) = \exp\left(-\frac{1}{2} \int \xi^2(t)\, dt\right), \tag{7}$$

for the characteristic functional, where $\xi(t) = k\, \chi_{[0,\tau]}(t)\, f(\tau - t)\, h(t)$, with $\chi_{[A]}(t)$ denoting the characteristic function of the set A. Hence, we obtain,

$$\begin{aligned} P(\varphi_1, \tau; \varphi_0, 0) &= \sum_{n=-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{dk}{2\pi} \exp\left[ik(\varphi_0 - \varphi_1 + 2\pi n)\right] \\ &\quad \times \exp\left(-\frac{k^2}{2} \int_0^{\tau} \left[f(\tau - t)\, h(t)\right]^2\ dt\right). \end{aligned} \tag{8}$$

The remaining integral over k is a Gaussian integral which could be evaluated to yield,

$$P(\varphi_1, \tau; \varphi_0, 0) = \sum_{n=-\infty}^{+\infty} P_n(\varphi_1, \tau; \varphi_0, 0) \tag{9}$$

with n indicating the number of times a path winds around the circle for the partial probability density,

$$P_n(\varphi_1, \tau; \varphi_0, 0) = \left(2\pi \int_0^\tau [f(\tau - t)\, h(t)]^2 \, dt\right)^{-\frac{1}{2}} \times \exp\left(-\frac{(\varphi_0 - \varphi_1 + 2\pi n)^2}{2\int_0^\tau [f(\tau - t)\, h(t)]^2 \, dt}\right). \tag{10}$$

Alternatively, from Eq. (8), we can apply the Poisson sum formula [17],

$$\frac{1}{2\pi} \sum_{n=-\infty}^{+\infty} \exp(in\phi) = \sum_{m=-\infty}^{+\infty} \delta(\phi + 2\pi m) \tag{11}$$

to obtain the expression,

$$P(\varphi_1, \tau; \varphi_0, 0) = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \int_{-\infty}^{+\infty} \delta(k + m) \exp[ik(\varphi_0 - \varphi_1)] \times \exp\left(-\frac{k^2}{2} \int_0^\tau [f(\tau - t)\, h(t)]^2 \, dt\right) dk\,. \tag{12}$$

The integration in Eq. (12) is facilitated by the delta function to yield,

$$P(\varphi_1, \tau; \varphi_0, 0) = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} \exp[-im(\varphi_0 - \varphi_1)] \times \exp\left(-\frac{m^2}{2} \int_0^\tau [f(\tau - t)\, h(t)]^2 \, dt\right). \tag{13}$$

The probability density function Eq. (13) can be expressed as,

$$P(\varphi_1, \tau; \varphi_0, 0) = \frac{1}{2\pi} \sum_{m=-\infty}^{+\infty} q^{m^2} \exp(i2mu)$$
$$= \frac{1}{2\pi} \Theta_3(u, q) \tag{14}$$

where $\Theta_3(u, q)$ is a Theta function [19], $q = \exp\left[-\frac{1}{2}\int_0^\tau [f(\tau - t)\, h(t)]^2 \, dt\right]$, and, $u = -(\varphi_0 - \varphi_1)/2$. Note that, we could also write,

$$\Theta_3(u, q) = 1 + 2 \sum_{m=1}^{\infty} q^{m^2} \cos(2mu) \ . \tag{15}$$

3 Winding Probabilities

One can also evaluate the winding probability W_n from Eqs. (10) and (14), i.e. [15, 16],

$$W_n = \frac{P_n(\varphi_1, \tau; \varphi_0, 0)}{P(\varphi_1, \tau; \varphi_0, 0)}$$
$$= \sqrt{\frac{2\pi}{\int_0^\tau [f(\tau - t)\, h(t)]^2 \, dt}} \exp\left(-\frac{(\varphi_0 - \varphi_1 + 2\pi n)^2}{2\int_0^\tau [f(\tau - t)\, h(t)]^2 \, dt}\right)$$
$$\times [\Theta_3(u, q)]^{-1} \ . \tag{16}$$

Note that the winding probability W_n depends on the memory function $f(\tau - t)$ and function $h(t)$ one chooses to model a given system.

4 Memory Functions

Further simplification of the probability density function Eq. (13), or the winding probability Eq. (16) would now depend on the explicit choice of $f(\tau - t)$ and $h(t)$. There are many possible choices and we now consider a few examples.

4.1 Fractional Brownian Motion

A familiar case of a memory function is,

$$f(\tau - t) = \frac{(\tau - t)^{H-1/2}}{\Gamma(H + 1/2)}, \tag{17}$$

with $h(t) = 1$ such that Eq. (2) becomes,

$$\varphi(\tau) = \varphi_0 + \int_0^\tau \frac{(\tau - t)^{H-1/2}}{\Gamma(H + 1/2)} \omega(t)\, dt, \tag{18}$$

where H is the Hurst exponent characterizing sub-diffusion for, $0 < H < 1/2$, and super-diffusion for $1/2 < H < 1$. Note that, for $H = 1/2$, Eq. (18) becomes that of ordinary Brownian motion. With this choice, the probability density function for n-times winding, Eq. (10), becomes,

$$P_n(\varphi_1, \tau; \varphi_0, 0) = \sqrt{\frac{H\,\Gamma^2\left(H + \frac{1}{2}\right)}{\pi \tau^{2H}}} \times \exp\left\{-\frac{H\,\Gamma^2\left(H + \frac{1}{2}\right)(\varphi_0 - \varphi_1 + 2\pi n)^2}{\tau^{2H}}\right\}. \tag{19}$$

This $P_n(\varphi_1, \tau; \varphi_0, 0)$ when used in Eq. (9) gives the conditional probability function for $\varphi(\tau)$ ending at φ_1, given that at time $t = 0$ it was at φ_0. Note that Eq. (17) allows us to write the path parametrization Eq. (18) as, $\varphi(\tau) = \varphi_0 + B^H(\tau)$, where $B^H(t)$ is a fractional Brownian motion in the Riemann-Liouville fractional integral representation defined by [18],

$$B^H(\tau) = \frac{1}{\Gamma\left(H + \frac{1}{2}\right)} \int_0^\tau (\tau - t)^{H-1/2}\, dB(t). \tag{20}$$

4.2 Bessel-Modified Brownian Motion

For memory function $f(\tau - t)$ and multiplication function $h(t)$, oscillatory functions can also be considered such as,

$$f(\tau - t) = \cos^{\frac{1}{2}}(\tau - t) \quad ; \quad h(t) = \sqrt{J_0(t)} \tag{21}$$

where $J_\nu(t)$ is a Bessel function of the first kind and, for simplicity, we take, $0 < (\tau - t) < \pi/2$. For this case, the random path representation Eq. (2) becomes,

$$\begin{aligned}\varphi(\tau) &= \varphi_0 + B^J(\tau) \\ &= \varphi_0 + \int_0^\tau \cos^{\frac{1}{2}}(\tau - t)\sqrt{J_0(t)}\,\omega(t)\,dt.\end{aligned}$$

With Eq. (6.674.8) of Ref. [19], this yields for Eq. (10) the probability density function for n-times winding,

$$P_n(\vartheta_1, \tau; \varphi_0, 0) = \frac{1}{\sqrt{2\pi\tau J_0(\tau)}} \exp\left(-\frac{(\varphi_0 - \varphi_1 + 2\pi n)^2}{2\tau J_0(\tau)}\right). \tag{22}$$

Using this in Eq. (9) gives the transition probability function for random paths with endpoints φ_0 and φ_1.

4.3 Exponentially-Modified Brownian Motion

Other examples are memory functions of the form,

$$f(\tau - t) = (\tau - t)^{(\mu-1)/2}, \tag{23}$$

and multiplication factors,

$$h(t) = \frac{e^{-\beta/2t}}{t^{(\mu+1)/2}}. \tag{24}$$

The path parametrization of Eq. (2) acquires the form,

$$\begin{aligned}\varphi(\tau) &= \varphi_0 + B^{\mu,\beta}(\tau) \\ &= \varphi_0 + \int_0^\tau \frac{(\tau - t)^{(\mu-1)/2} e^{-\beta/2t}}{t^{(\mu+1)/2}}\omega(t)\,dt.\end{aligned} \tag{25}$$

The process has short-memory behavior for $0 < \mu < 1$, and long-memory for $1 < \mu$. Using Eq. (3.471.3) of Ref. [19], the probability density function Eq. (9) has a partial probability density $P_n(\varphi_1, \tau; \varphi_0, 0)$ given by,

$$P_n(\varphi_1, \tau; \varphi_0, 0) = \frac{\beta^{\mu/2} e^{\beta/2\tau}}{\sqrt{2\pi\Gamma(\mu)\,\tau^{\mu-1}}} \exp\left(-\frac{\beta^\mu e^{\beta/\tau}(\varphi_0 - \varphi_1 + 2\pi n)^2}{2\,\Gamma(\mu)\,\tau^{\mu-1}}\right) \tag{26}$$

where $\mu > 0$, and $\Gamma(\mu)$ is the Gamma function.

5 Wedge Boundary

Consider a wedge with an angular opening of $\bar{\varphi}$ (see, Fig. 1).

As shown in Fig. 1, a particle from φ_0 can go directly to φ_1. Alternatively, the particle from φ_0 can bounce off the walls before ending at φ_1, traveling an extra $2\bar{\varphi}n$ ($n = 0, \pm 1, \pm 2, \ldots$) distance. The different possible paths may be described by the delta function constraint,

$$\delta\left(\varphi\left(\tau\right) - \varphi_1 + 2\bar{\varphi}n\right). \tag{27}$$

Using Eq. (27), consider the linear combination,

$$C_n = \delta\left(\varphi\left(\tau\right) - \varphi_1 + 2\bar{\varphi}n\right) - \delta\left(\varphi\left(\tau\right) + \varphi_1 + 2\bar{\varphi}n\right). \tag{28}$$

We can sum over all possible values of n, i.e., $\sum_n C_n$, and evaluate the expectation value as,

$$P_w\left(\varphi_1, \tau; \varphi_0, 0\right) = \int \left(\sum_{n=-\infty}^{+\infty} C_n\right) d\mu\,. \tag{29}$$

Equation (29) can further be written as,

$$P_w\left(\varphi_1, \tau; \varphi_0, 0\right) = \frac{\pi}{\bar{\varphi}} \int \sum_{n=-\infty}^{+\infty} \left[\delta\left(\frac{\pi}{\bar{\varphi}}\left(\varphi\left(\tau\right) - \varphi_1\right) + 2\pi n\right)\right.$$
$$\left. -\delta\left(\frac{\pi}{\bar{\varphi}}\left(\varphi\left(\tau\right) + \varphi_1\right) + 2\pi n\right)\right] d\mu, \tag{30}$$

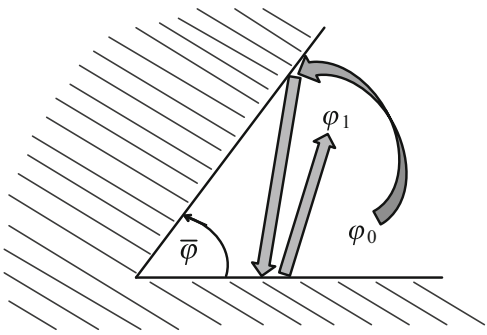

Fig. 1 The angular opening $\bar{\varphi}$ is a constant characterizing the wedge. There are many paths for a particle to go from φ_0 to φ_1

for which we apply the Poisson sum formula, Eq. (11) to get,

$$P_w(\varphi_1,\tau;\varphi_0,0)=\frac{1}{2\bar{\varphi}}\int\sum_{m=-\infty}^{+\infty}\left\{\exp\left[\frac{im\pi}{\bar{\varphi}}\left(\varphi(\tau)-\varphi_1\right)\right]-\exp\left[\frac{im\pi}{\bar{\varphi}}\left(\varphi(\tau)+\varphi_1\right)\right]\right\}d\mu. \tag{31}$$

Using the path parametrization of Eq. (2) for $\varphi(\tau)$, Eq. (31) gives,

$$\begin{aligned}P_w(\varphi_1,\tau;\varphi_0,0)=\frac{1}{2\bar{\varphi}}\int\sum_{m=-\infty}^{+\infty}&\left\{\exp\left[\frac{im\pi}{\bar{\varphi}}\left(\varphi_0-\varphi_1\right)\right]\right.\\&\left.-\exp\left[\frac{im\pi}{\bar{\varphi}}\left(\varphi_0+\varphi_1\right)\right]\right\}\\&\times\exp\left(\frac{im\pi}{\bar{\varphi}}\int_0^{\tau}f(\tau-t)\;h(t)\;\omega(t)\;dt\right)d\mu.\end{aligned} \tag{32}$$

We can further write,

$$\begin{aligned}&\sum_{m=-\infty}^{+\infty}\left\{\exp\left[\frac{im\pi}{\bar{\varphi}}\left(\varphi_0-\varphi_1\right)\right]-\exp\left[\frac{im\pi}{\bar{\varphi}}\left(\varphi_0+\varphi_1\right)\right]\right\}\\&=2\sum_{m=-\infty}^{+\infty}\sin\left(\frac{m\pi}{\bar{\varphi}}\varphi_0\right)\sin\left(\frac{m\pi}{\bar{\varphi}}\varphi_1\right).\end{aligned} \tag{33}$$

Hence, we have,

$$\begin{aligned}P_w(\varphi_1,\tau;\varphi_0,0)=\frac{1}{\bar{\varphi}}\sum_{m=-\infty}^{+\infty}&\sin\left(\frac{m\pi}{\bar{\varphi}}\varphi_0\right)\sin\left(\frac{m\pi}{\bar{\varphi}}\varphi_1\right)\\&\times\int\exp\left(\frac{im\pi}{\bar{\varphi}}\int_0^{\tau}f(\tau-t)\;h(t)\;\omega(t)\;dt\right)d\mu.\end{aligned} \tag{34}$$

The integral over the white noise measure $d\mu$ can be carried out using Eq. (7) where, $\xi(t)=\left(m\pi/\bar{\varphi}\right)\chi_{[0,\tau]}(t)\,f(\tau-t)\,h(t)$ to yield,

$$\begin{aligned}P_w(\varphi_1,\tau;\varphi_0,0)=\frac{1}{\bar{\varphi}}\sum_{m=-\infty}^{+\infty}&\sin\left(\frac{m\pi}{\bar{\varphi}}\varphi_0\right)\sin\left(\frac{m\pi}{\bar{\varphi}}\varphi_1\right)\\&\times\exp\left[-\frac{m^2\pi^2}{2\bar{\varphi}^2}\int_0^{\tau}\left[f(\tau-t)\,h(t)\right]^2dt\right],\end{aligned} \tag{35}$$

or,

$$P_w(\varphi_1,\tau;\varphi_0,0) = \sum_{m=-\infty}^{+\infty} \Phi_m(\varphi_0)\ \Phi_m(\varphi_1) \times \exp\left[-\frac{m^2\pi^2}{2\bar{\varphi}^2}\int_0^\tau [f(\tau-t)\,h(t)]^2\,dt\right]. \tag{36}$$

In Eq. (36), $\Phi_m(\varphi) = 1/\sqrt{\bar{\varphi}}\sin\left(m\pi\varphi/\bar{\varphi}\right)$, are solutions vanishing at the walls of the wedge, $\varphi = 0$ and $\varphi = \bar{\varphi}$, and hence satisfying the Dirichlet boundary condition.

6 Conclusion

Studies involving stochastic processes with memory [20], as exemplified by fractional Brownian motion, can be extended to more realistic applications by putting boundaries and topological constraints. In particular, we have shown that spaces with topological constraints could be efficiently dealt with using Feynman's sum-over-all-possible paths or histories [2, 3]. Moreover, we have demonstrated in this paper that white noise analysis appears to be an effective tool for carrying out path summation to obtain the transition probability function even for stochastic processes with varying memory behavior. Since one is able to choose the type of memory function $f(\tau - t)$ and $h(t)$ to realistically model an event, the approach is versatile enough to contribute in the description of various natural and social phenomena.

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Generalized Scaling Operators in White Noise Analysis and Applications to Hamiltonian Path Integrals with Quadratic Action

Wolfgang Bock

On the occasion of the 75th birthday of Ludwig Streit

Abstract We give an outlook, how to realize the ideas of complex scaling from [15–17] to phase space path integrals in the framework of White Noise Analysis. The idea of this scaling method goes back to [9]. Therefore we extend the concept complex scaling to scaling with suitable bounded operators.

Keywords Hamiltonian path integrals • White noise analysis • Scaling operators

Mathematics Subject Classification (2010) Primary 60H40; Secondary 81Q30

1 Introduction

As an alternative approach to quantum mechanics Feynman introduced the concept of path integrals [10–12], which was developed into an extremely useful tool in many branches of theoretical physics. The phase space Feynman integral, or Hamiltonian path integral, for a particle moving from y_0 at time 0 to y at time t under the potential V is given by

$$\mathrm{N}\int_{x(0)=y_0,x(t)=y}\int \exp\left(\frac{i}{\hbar}\int_0^t\left[p\dot{x}-\frac{p^2}{2}-V(x,p)\right]d\tau\right)\prod_{0<\tau<t}dp(\tau)dx(\tau),$$

$$\hbar=\frac{h}{2\pi}. \qquad (1)$$

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W. Bock (✉)
CMAF Avenida Prof. Gama Pinto 2, 1649-009, Lisboa, Portugal
e-mail: bock@campus.ul.pt

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Here h is Planck's constant, and the integral is thought of being over all position paths with $x(0) = y_0$ and $x(t) = y$ and all momentum paths. The missing restriction on the momentum variable at time 0 and time t is an immediate consequence of the Heisenberg uncertainty relation, i.e. the fact that one can not measure momentum and space variable at the same time. The path integral to the phase space has several advantages. Firstly the semi-classical approximation can be validated easier in a phase space formulation and secondly that quantum mechanics are founded on the phase space, i.e. every quantum mechanical observable can be expressed as a function of the space and momentum. A discussion about phase space path integrals can be found in the monograph [3] and in the references therein.

There are many attempts to give a meaning to the Hamiltonian path integral as a mathematical rigorous object. Among these are analytic continuation of probabilistic integrals via coherent states [22, 23] and infinite dimensional distributions e.g. [8]. Most recently also an approach using time-slicing was developed by Naoto Kumano-Go [27] and also by Albeverio et al. using Fresnel integrals [1–3]. As a guide to the literature on many attempts to formulate these ideas we point out the list in [3]. Here we choose a white noise approach. White noise analysis is a mathematical framework which offers generalizations of concepts from finite-dimensional analysis, like differential operators and Fourier transform to an infinite-dimensional setting. We give a brief introduction to White Noise Analysis in Sect. 2, for more details see [4, 18, 20, 28, 32]. Of special importance in White Noise Analysis are spaces of generalized functions and their characterizations. In this article we choose the space of Hida distributions, see Sect. 2.

The idea of realizing Feynman integrals within the white noise framework goes back to [19]. There the authors used exponentials of quadratic (generalized) functions in order to give meaning to the Feynman integral in configuration space representation

$$\mathrm{N}\int_{x(0)=y_0,x(t)=y} \exp\left(\frac{i}{\hbar}S(x)\right)\prod_{0<\tau<t} dx(\tau), \quad \hbar = \frac{h}{2\pi},$$

with the classical action $S(x) = \int_0^t \left[\frac{1}{2}m\dot{x}^2 - V(x)\right] d\tau$. In [5, 6] and [7] concepts of quadratic actions in White Noise Analysis, see [14] were used to give a rigorous meaning to the Feynman integrand

$$I_V = \mathrm{Nexp}\left(\frac{i}{\hbar}\int_0^t \left[p(\tau)\dot{x}(\tau) - \frac{p(\tau)^2}{2m}\right] d\tau + \frac{1}{2}\int_0^t \left[\dot{x}(\tau)^2 + p(\tau)^2\right] d\tau\right) \qquad (2)$$
$$\cdot \exp\left(-\frac{i}{\hbar}\int_0^t V(x(\tau), p(\tau), \tau)\, d\tau\right) \cdot \delta(x(t) - y)$$

as a Hida distribution. In this expression the sum of the first and the third integral in the exponential is the action $S(x, p)$, and the (Donsker's) delta function serves to pin trajectories to y at time t. The second integral is introduced to simulate the Lebesgue

integral by a local compensation of the fall-off of the Gaussian reference measure μ. Furthermore a Brownian motion starting in y_0 is used to model the space variable when the momentum variable is modeled by white noise, i.e.

$$x(\tau) = y(0) + \sqrt{\frac{\hbar}{m}} B(\tau), \quad p(\tau) = \omega(\tau), \quad 0 \leq \tau \leq t. \tag{3}$$

For the integrand we have thus the following ansatz

$$I_V = \mathrm{Nexp}\big(-\frac{1}{2}\langle(\omega_x, \omega_p), K(\omega_x, \omega_p)\rangle\big) \cdot \exp\big(-\frac{1}{2}\langle(\omega_x, \omega_p), L(\omega_x, \omega_p)\rangle\big) \cdot \delta\big(\langle(\omega_x, \omega_p), (\mathbf{1}_{[0,t)}, 0)\rangle - y\big),$$

where K is given by

$$K = \begin{pmatrix} -\mathbf{1}_{[0,t)} & -i\mathbf{1}_{[0,t)} \\ -i\mathbf{1}_{[0,t)} & -(1-i)\mathbf{1}_{[0,t)} \end{pmatrix}. \tag{4}$$

Here the operator $\mathbf{1}_{[0,t)}$ denotes the multiplication with $\mathbf{1}_{[0,t)}$. And the operator L, fulfilling the assumptions of Lemma 2.14 is used to model the quadratic potential. For sake of simplicity we consider in this article path integrals with one degree of freedom, i.e. the underlying space is the space $S_2'(\mathbb{R})$.

In the euclidean configuration space a solution to the heat equation is given by the Feynman-Kac formula with its corresponding heat kernel. In White Noise Analysis one constructs the integral kernel by inserting Donsker's delta function to pin the final point $x \in \mathbb{R}$ and taking the expectation, i.e.,

$$K_V(x, t, x_0, t_0) = \mathbb{E}\left(\exp\Big(\int_{t_0}^{t} V(x_0 + \langle \mathbf{1}_{[t_0,r)}, \cdot\rangle)\, dr\Big)\delta(x_0 + \langle \mathbf{1}_{[t_0,t)}, \cdot\rangle - x)\right),$$

where the integrand is a suitable distribution in White Noise Analysis (e.g. a Hida distribution).

A complementary strategy to construct Feynman integrals in the configuration space with White Noise methods was inspired by [9], see also [16, 36, 37] and also [30] and [24] . Here for suitable potentials V a complex-scaled Feynman-Kac kernel can be rigorously justified by giving a meaning to

$$K(x, t, x_0, t_0) = \mathbb{E}\left(\exp\left(\frac{1}{z^2}\int_{t_0}^{t} V(x + zB_s)\, ds\right)\sigma_z\delta(B_t - (x - x_0))\right). \tag{5}$$

In the configuration space, this has been done in [37] and [16, 36]. Note that if $z = \sqrt{i}$ in (5), we have the Schrödinger kernel.

This scaling approach has several advantages e.g.

- Treatable potentials are beyond perturbation theory such as

$$V(x) = (-1)^{n+1} a_{4n+2} x^{4n+2} + \sum_{j=1}^{4n+1} a_j x^j, \quad x \in \mathbb{R}, n \in \mathbb{N},$$

  with $a_{4n+2} > 0, a_j \in \mathbb{C}$.
- Due to a Wick formula we have a convenient structure (i.e. "Brownian motion is replaced by a Brownian bridge")
- The kinetic energy "$\sigma_z \delta''$ and the potential can be treated separately, for details see e.g. [29].

We give an idea how to implement this approach to phase space for quadratic potentials. This is a first step to a scaling approach to the above potential class also for Hamiltonian path integrands.

2 Preliminaries

2.1 Gel'fand Triples

Starting point is the Gel'fand triple $S_d(\mathbb{R}) \subset L^2_d(\mathbb{R}) \subset S'_d(\mathbb{R})$ of the $\mathbb{R}^d$-valued, $d \in \mathbb{N}$, Schwartz test functions and tempered distributions with the Hilbert space of (equivalence classes of) $\mathbb{R}^d$-valued square integrable functions w.r.t. the Lebesgue measure as central space (equipped with its canonical inner product $(\cdot, \cdot)$ and norm $\|\cdot\|$), see e.g. [18, 28]. Since $S_d(\mathbb{R})$ is a nuclear space, represented as projective limit of a decreasing chain of Hilbert spaces $(H_p)_{p\in\mathbb{N}}$, see e.g. [34, Chap. 2] and [13], i.e.

$$S_d(\mathbb{R}) = \bigcap_{p\in\mathbb{N}} H_p,$$

we have that $S_d(\mathbb{R})$ is a countably Hilbert space in the sense of Gel'fand and Vilenkin [13]. We denote the inner product and the corresponding norm on H_p by $(\cdot, \cdot)_p$ and $\|\cdot\|_p$, respectively, with the convention $H_0 = L^2_d(\mathbb{R})$. Let H_{-p} be the dual space of H_p and let $\langle \cdot, \cdot \rangle$ denote the dual pairing on $H_p \times H_{-p}$. H_p is continuously embedded into $L^2_d(\mathbb{R})$. By identifying $L^2_d(\mathbb{R})$ with its dual $L^2_d(\mathbb{R})'$, via the Riesz isomorphism, we obtain the chain $H_p \subset L^2_d(\mathbb{R}) \subset H_{-p}$. Note that $S'_d(\mathbb{R}) = \bigcup_{p\in\mathbb{N}} H_{-p}$, i.e. $S'_d(\mathbb{R})$ is the inductive limit of the increasing chain of Hilbert spaces $(H_{-p})_{p\in\mathbb{N}}$, see e.g. [13]. We denote the dual pairing of $S_d(\mathbb{R})$ and $S'_d(\mathbb{R})$ also by $\langle \cdot, \cdot \rangle$. Note that its restriction on $S_d(\mathbb{R}) \times L^2_d(\mathbb{R})$ is given by $(\cdot, \cdot)$. We also use the complexifications of these spaces denoted with the sub-index $\mathbb{C}$ (as well as their

inner products and norms). The dual pairing we extend in a bilinear way. Hence we have the relation

$$\langle g,f\rangle = (\mathbf{g},\bar{\mathbf{f}}), \quad \mathbf{f},\mathbf{g}\in L^2_d(\mathbb{R})_{\mathbb{C}},$$

where the overline denotes the complex conjugation.

2.2 White Noise Spaces

We consider on $S'_d(\mathbb{R})$ the σ-algebra $\mathcal{C}_\sigma(S'_d(\mathbb{R}))$ generated by the cylinder sets $\{\omega \in S'_d(\mathbb{R})|\langle\xi_1,\omega\rangle \in F_1,\ldots,\langle\xi_n,\omega\rangle \in F_n\}$, $\xi_i \in S_d(\mathbb{R})$, $F_i \in \mathcal{B}(\mathbb{R})$, $1 \le i \le n$, $n \in \mathbb{N}$, where $\mathcal{B}(\mathbb{R})$ denotes the Borel σ-algebra on $\mathbb{R}$.

The canonical Gaussian measure μ on $C_\sigma(S'_d(\mathbb{R}))$ is given via its characteristic function

$$\int_{S'_d(\mathbb{R})} \exp(i\langle\mathbf{f},\boldsymbol{\omega}\rangle)d\mu(\boldsymbol{\omega}) = \exp(-\tfrac{1}{2}\|\mathbf{f}\|^2), \quad \mathbf{f}\in S_d(\mathbb{R}),$$

by the theorem of Bochner and Minlos, see e.g. [31], [4, Chap. 2 Theo. 1. 11]. The space $(S'_d(\mathbb{R}),\mathcal{C}_\sigma(S'_d(\mathbb{R})),\mu)$ is the basic probability space in our setup. The central Gaussian spaces in our framework are the Hilbert spaces $(L^2) := L^2(S'_d(\mathbb{R}),\ \mathcal{C}_\sigma(S'_d(\mathbb{R})),\mu)$ of complex-valued square integrable functions w.r.t. the Gaussian measure μ.

Within this formalism a representation of a d-dimensional Brownian motion is given by

$$\mathbf{B}_t(\boldsymbol{\omega}) := (B_t(\omega_1),\ldots,B_t(\omega_d)) := (\langle\mathbf{1}_{[0,t)},\omega_1\rangle,\ldots\langle\mathbf{1}_{[0,t)},\omega_d\rangle), \tag{6}$$

with $\boldsymbol{\omega} = (\omega_1,\ldots,\omega_d) \in S'_d(\mathbb{R}), \quad t \ge 0$, in the sense of an (L^2)-limit. Here $\mathbf{1}_A$ denotes the indicator function of a set A.

2.3 The Hida Triple

Let us now consider the Hilbert space (L^2) and the corresponding Gel'fand triple

$$(S) \subset (L^2) \subset (S)'.$$

Here (S) denotes the space of Hida test functions and $(S)'$ the space of Hida distributions. In the following we denote the dual pairing between elements of (S) and $(S)'$ by $\langle\langle\cdot,\cdot\rangle\rangle$. Instead of reproducing the construction of $(S)'$ here we give its characterization in terms of the T-transform.

Definition 2.1 We define the T-transform of $\Phi \in (S)'$ by

$$T\Phi(\mathbf{f}) := \langle\langle \exp(i\langle \mathbf{f}, \cdot \rangle), \Phi \rangle\rangle, \quad \mathbf{f} := (f_1, \ldots, f_d) \in S_d(\mathbb{R}).$$

Remark 2.2 (i) Since $\exp(i\langle \mathbf{f}, \cdot \rangle) \in (S)$ for all $\mathbf{f} \in S_d(\mathbb{R})$, the T-transform of a Hida distribution is well-defined.

(ii) For $\mathbf{f} = 0$ the above expression yields $\langle\langle \Phi, 1 \rangle\rangle$, therefore $T\Phi(0)$ is called the generalized expectation of $\Phi \in (S)'$

(iii) Another important examples of Hida test functions are the so-called coherent states or Wick exponentials

$$:\exp(\langle \mathbf{f}, \cdot \rangle): = \exp(-\frac{1}{2}\langle \mathbf{f}, \mathbf{f} \rangle) \cdot \exp(\langle \mathbf{f}, \cdot \rangle), \quad \mathbf{f} \in S_d(\mathbb{R}).$$

In order to characterize the space $(S)'$ by the T-transform we need the following definition.

Definition 2.3 A mapping $F : S_d(\mathbb{R}) \to \mathbb{C}$ is called a U-functional if it satisfies the following conditions:

U1. For all $\mathbf{f}, \mathbf{g} \in S_d(\mathbb{R})$ the mapping $\mathbb{R} \ni \lambda \mapsto F(\lambda \mathbf{f} + \mathbf{g}) \in \mathbb{C}$ has an analytic continuation to $\lambda \in \mathbb{C}$ (**ray analyticity**).

U2. There exist constants $0 < C, D < \infty$ and a $p \in \mathbb{N}_0$ such that

$$|F(z\mathbf{f})| \leq C \exp(D|z|^2 \|\mathbf{f}\|_p^2),$$

for all $z \in \mathbb{C}$ and $\mathbf{f} \in S_d(\mathbb{R})$ (**growth condition**).

This is the basis of the following characterization theorem. For the proof we refer to [18, 25, 26, 33].

Theorem 2.4 *A mapping $F : S_d(\mathbb{R}) \to \mathbb{C}$ is the T-transform of an element in $(S)'$ if and only if it is a U-functional.*

Theorem 2.4 enables us to discuss convergence of sequences of Hida distributions by considering the corresponding T-transforms, i.e. by considering convergence on the level of U-functionals. The following corollary is proved in [18, 26, 33].

Corollary 2.5 *Let $(\Phi_n)_{n\in\mathbb{N}}$ denote a sequence in $(S)'$ such that:*

(i) *For all $\mathbf{f} \in S_d(\mathbb{R})$, $((T\Phi_n)(\mathbf{f}))_{n\in\mathbb{N}}$ is a Cauchy sequence in $\mathbb{C}$.*

(ii) *There exist constants $0 < C, D < \infty$ such that for some $p \in \mathbb{N}_0$ one has*

$$|(T\Phi_n)(z\mathbf{f})| \leq C \exp(D|z|^2 \|\mathbf{f}\|_p^2)$$

for all $\mathbf{f} \in S_d(\mathbb{R})$, $z \in \mathbb{C}$, $n \in \mathbb{N}$.

Then $(\Phi_n)_{n\in\mathbb{N}}$ converges strongly in $(S)'$ to a unique Hida distribution.

Example 2.6 (Vector valued white noise) Let $\mathbf{B}(t)$, $t \geq 0$, be the d-dimensional Brownian motion as in (6). Consider

$$\frac{\mathbf{B}(t+h,\boldsymbol{\omega}) - \mathbf{B}(t,\boldsymbol{\omega})}{h} = (\langle \frac{\mathbf{1}_{[t,t+h)}}{h}, \omega_1\rangle, \dots (\langle \frac{\mathbf{1}_{[t,t+h)}}{h}, \omega_d\rangle), \quad h > 0.$$

Then in the sense of Corollary 2.5 it exists

$$\langle \boldsymbol{\delta}_t, \boldsymbol{\omega}\rangle := (\langle \delta_t, \omega_1\rangle, \dots, \langle \delta_t, \omega_d\rangle) := \lim_{h\searrow 0} \frac{\mathbf{B}(t+h,\boldsymbol{\omega}) - \mathbf{B}(t,\boldsymbol{\omega})}{h}.$$

Of course for the left derivative we get the same limit. Hence it is natural to call the generalized process $\langle \boldsymbol{\delta}_t, \boldsymbol{\omega}\rangle$, $t \geq 0$ in $(S)'$ vector valued white noise. One also uses the notation $\boldsymbol{\omega}(t) = \langle \boldsymbol{\delta}_t, \boldsymbol{\omega}\rangle$, $t \geq 0$.

Another useful corollary of Theorem 2.4 concerns integration of a family of generalized functions, see [18, 26, 33].

Corollary 2.7 *Let $(\Lambda, \mathcal{A}, \nu)$ be a measure space and $\Lambda \ni \lambda \mapsto \Phi(\lambda) \in (S)'$ a mapping. We assume that its T–transform $T\Phi$ satisfies the following conditions:*

(i) *The mapping $\Lambda \ni \lambda \mapsto T(\Phi(\lambda))(\mathbf{f}) \in \mathbb{C}$ is measurable for all $\mathbf{f} \in S_d(\mathbb{R})$.*
(ii) *There exists a $p \in \mathbb{N}_0$ and functions $D \in L^\infty(\Lambda, \nu)$ and $C \in L^1(\Lambda, \nu)$ such that*

$$|T(\Phi(\lambda))(z\mathbf{f})| \leq C(\lambda) \exp(D(\lambda)\, |z|^2\, \|\mathbf{f}\|^2),$$

for a.e. $\lambda \in \Lambda$ and for all $\mathbf{f} \in S_d(\mathbb{R})$, $z \in \mathbb{C}$.

Then, in the sense of Bochner integration in $H_{-q} \subset (S)'$ for a suitable $q \in \mathbb{N}_0$, the integral of the family of Hida distributions is itself a Hida distribution, i.e. $\int_\Lambda \Phi(\lambda)\, d\nu(\lambda) \in (S)'$ and the T–transform interchanges with integration, i.e.

$$T\left(\int_\Lambda \Phi(\lambda) d\nu(\lambda)\right)(\mathbf{f}) = \int_\Lambda T(\Phi(\lambda))(\mathbf{f})\, d\nu(\lambda), \quad \mathbf{f} \in S_d(\mathbb{R}).$$

Based on the above theorem, we introduce the following Hida distribution.

Definition 2.8 We define Donsker's delta at $x \in \mathbb{R}$ corresponding to $0 \neq \boldsymbol{\eta} \in L^2_d(\mathbb{R})$ by

$$\delta_0(\langle \boldsymbol{\eta}, \cdot\rangle - x) := \frac{1}{2\pi} \int_{\mathbb{R}} \exp(i\lambda(\langle \boldsymbol{\eta}, \cdot\rangle - x))\, d\lambda$$

in the sense of Bochner integration, see e.g. [18, 29, 37]. Its T–transform in $\mathbf{f} \in S_d(\mathbb{R})$ is given by

$$T(\delta_0(\langle \boldsymbol{\eta}, \cdot \rangle - x)(\mathbf{f}) = \frac{1}{\sqrt{2\pi \langle \boldsymbol{\eta}, \boldsymbol{\eta} \rangle}} \exp\left(-\frac{1}{2\langle \boldsymbol{\eta}, \boldsymbol{\eta} \rangle} (i\langle \boldsymbol{\eta}, \mathbf{f} \rangle - x)^2 - \frac{1}{2} \langle \mathbf{f}, \mathbf{f} \rangle \right), \ \mathbf{f} \in S_d(\mathbb{R}).$$

2.4 Generalized Gauss Kernels

Here we review a special class of Hida distributions which are defined by their T-transform, see e.g. [14]. Let $\mathcal{B}$ be the set of all continuous bilinear mappings $B : S_d(\mathbb{R}) \times S_d(\mathbb{R}) \to \mathbb{C}$. Then the functions

$$S_d(\mathbb{R}) \ni f \mapsto \exp\left(-\frac{1}{2} B(\mathbf{f}, \mathbf{f}) \right) \in \mathbb{C}$$

for all $B \in \mathcal{B}$ are U-functionals. Therefore, by using the characterization of Hida distributions in Theorem 2.4, the inverse T-transform of these functions

$$\Phi_B := T^{-1} \exp\left(-\frac{1}{2} B \right)$$

are elements of $(S)'$.

Definition 2.9 The set of **generalized Gauss kernels** is defined by

$$GGK := \{ \Phi_B, \ B \in \mathcal{B} \}.$$

Definition 2.10 Let K be a symmetric trace class operator on $L^2_d(\mathbb{R})$. We define for $\boldsymbol{\omega} \in S'_d(\mathbb{R})$

$$\langle \boldsymbol{\omega}, \mathbf{K}\boldsymbol{\omega} \rangle := \lim_{N \to \infty} \sum_{n=1}^{N} \langle \mathbf{e}_n, \boldsymbol{\omega} \rangle (k_n) \langle \mathbf{e}_n, \boldsymbol{\omega} \rangle,$$

where $(\mathbf{e}_n)_{n \in \mathbb{N}}$ denotes an eigenbasis of the corresponding eigenvalues $(k_n)_{n \in \mathbb{N}}$.

Example 2.11 ([14]) We consider a symmetric trace class operator K on $L^2_d(\mathbb{R})$ such that $-\frac{1}{2} < K \leq 0$, then

$$\int_{S'_d(\mathbb{R})} \exp\left(-\langle \omega, K\omega \rangle \right) d\mu(\boldsymbol{\omega}) = (\det(Id + 2K))^{-\frac{1}{2}} < \infty.$$

Here Id denotes the identity operator on the Hilbert space $L^2_d(\mathbb{R})$, and $\det(A)$ of a symmetric trace class operator A on $L^2_d(\mathbb{R})$ denotes the infinite product of its eigenvalues, if it exists. In the present situation we have $\det(Id + 2K) \neq 0$. Therefore we obtain that the exponential $g = \exp(-\frac{1}{2}\langle \cdot, K\cdot\rangle)$ is square-integrable and its T-transform is given by

$$Tg(\mathbf{f}) = (\det(Id + K))^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\mathbf{f}, (Id + K)^{-1}\mathbf{f})\right), \quad \mathbf{f} \in S_d(\mathbb{R}).$$

Therefore $(\det(Id + K))^{\frac{1}{2}}\, g$ is a generalized Gauss kernel.

Definition 2.12 Let $K : L^2_{d,\mathbb{C}}(\mathbb{R}, dx) \to L^2_{d,\mathbb{C}}(\mathbb{R}, dx)$ be linear and continuous such that

(i) $Id + K$ is injective,
(ii) there exists $p \in \mathbb{N}_0$ such that $(Id + K)(L^2_{d,\mathbb{C}}(\mathbb{R}, dx)) \subset H_{p,\mathbb{C}}$ is dense,
(iii) there exist $q \in \mathbb{N}_0$ such that $(Id + K)^{-1} : H_{p,\mathbb{C}} \to H_{-q,\mathbb{C}}$ is continuous with p as in (ii).

Then we define the normalized exponential

$$\mathrm{Nexp}(-\frac{1}{2}\langle \cdot, K\cdot\rangle) \tag{7}$$

by

$$T(\mathrm{Nexp}(-\frac{1}{2}\langle \cdot, K\cdot\rangle))(\mathbf{f}) := \exp(-\frac{1}{2}\langle \mathbf{f}, (Id + K)^{-1}\mathbf{f}\rangle), \quad \mathbf{f} \in S_d(\mathbb{R}).$$

Remark 2.13 The "normalization" of the exponential in the above definition can be regarded as a division of a divergent factor. In an informal way one can write

$$T(\mathrm{Nexp}(-\frac{1}{2}\langle \cdot, K\cdot\rangle))(\mathbf{f}) = \frac{T(\exp(-\frac{1}{2}\langle \cdot, K\cdot\rangle))(\mathbf{f})}{T(\exp(-\frac{1}{2}\langle \cdot, K\cdot\rangle))(0)}$$
$$= \frac{T(\exp(-\frac{1}{2}\langle \cdot, K\cdot\rangle))(\mathbf{f})}{\sqrt{\det(Id + K)}}, \quad \mathbf{f} \in S_d(\mathbb{R}),$$

i.e. we can still define the normalized exponential by the T-transform even if the determinant is not defined.

Lemma 2.14 ([6]) *Let L be a $d \times d$ block operator matrix on $L^2_d(\mathbb{R})_{\mathbb{C}}$ acting component-wise such that all entries are bounded operators on $L^2(\mathbb{R})_{\mathbb{C}}$. Let K be a $d \times d$ block operator matrix on $L^2_d(\mathbb{R})_{\mathbb{C}}$, such that $Id + K$ and $N = Id + K + L$ are bounded with bounded inverse. Furthermore assume that* $\det(Id + L(Id + K)^{-1})$ *exists and is different from zero (this is e.g. the case if L is trace class and -1 in*

the resolvent set of $L(Id+K)^{-1}$*). Let* $M_{N^{-1}}$ *be the matrix given by an orthogonal system* $(\boldsymbol{\eta}_k)_{k=1,\dots,J}$ *of non–zero functions from* $L^2_d(\mathbb{R})$*,* $J \in \mathbb{N}$*, under the bilinear form* $\big(\cdot, N^{-1}\cdot\big)$*, i.e.* $(M_{N^{-1}})_{i,j} = \big(\boldsymbol{\eta}_i, N^{-1}\boldsymbol{\eta}_j\big)$*,* $1 \le i,j \le J$*. Under the assumption that either*

$$\Re(M_{\mathbf{N}^{-1}}) > 0 \quad \text{or} \quad \Re(M_{\mathbf{N}^{-1}}) = 0 \text{ and } \Im(M_{\mathbf{N}^{-1}}) \neq 0,$$

where $M_{\mathbf{N}^{-1}} = \Re(M_{\mathbf{N}^{-1}}) + i\Im(M_{\mathbf{N}^{-1}})$ *with real matrices* $\Re(M_{\mathbf{N}^{-1}})$ *and* $\Im(M_{\mathbf{N}^{-1}})$*, then*

$$\Phi_{K,L} := \mathrm{Nexp}\Big(-\frac{1}{2}\langle\cdot, K\cdot\rangle\Big)\cdot\exp\Big(-\frac{1}{2}\langle\cdot, L\cdot\rangle\Big)\cdot\exp(i\langle\cdot,\mathbf{g}\rangle)\cdot\prod_{i=1}^{J}\delta_0(\langle\cdot,\boldsymbol{\eta}_k\rangle - y_k),$$

for $\mathbf{g} \in L^2_d(\mathbb{R},\mathbb{C})$*,* $t>0$*,* $y_k \in \mathbb{R}$*,* $k = 1\dots,J$*, exists as a Hida distribution. Moreover for* $\mathbf{f} \in S_d(\mathbb{R})$

$$T\Phi_{K,L}(\mathbf{f}) = \frac{1}{\sqrt{(2\pi)^J\det((M_{N^{-1}}))}}\sqrt{\frac{1}{\det(Id+L(Id+K)^{-1})}}$$
$$\times\exp\bigg(-\frac{1}{2}\Big((\mathbf{f}+\mathbf{g}), N^{-1}(\mathbf{f}+\mathbf{g})\Big)\bigg)\exp\bigg(-\frac{1}{2}(u,(M_{N^{-1}})^{-1}u)\bigg), \tag{8}$$

where

$$u = \Big(\big(iy_1 + (\boldsymbol{\eta}_1, N^{-1}(\mathbf{f}+\mathbf{g}))\big),\dots,\big(iy_J + (\boldsymbol{\eta}_J, N^{-1}(\mathbf{f}+\mathbf{g}))\big)\Big).$$

2.5 Scaling Operator

First note, that every test function $\varphi \in (S)$ can be extended to $S_d(\mathbb{R})'_{\mathbb{C}}$, see e.g. [28]. Thus the following definition makes sense.

Definition 2.15 Let φ be the continuous version of an element of (S). Then for $0 \neq z \in \mathbb{C}$ we define the scaling operator σ_z by

$$(\sigma_z\varphi)(\omega) = \varphi(z\omega), \quad \omega \in S'_d(\mathbb{R}).$$

Proposition 2.16 (i) *For all* $0 \neq z \in \mathbb{C}$ *we have* $\sigma_z \in L((S),(S))$*,*
(ii) *for* $\varphi,\psi \in (S)$ *we have*

$$\sigma_z(\varphi\cdot\psi) = (\sigma_z\varphi)(\sigma_z\psi).$$

Proof (*i*) is proved in [37]

For (*ii*), first note that (S) is an algebra under pointwise multiplication. Since the scaling operator is continuous from (S) to itself by (*i*), it suffices to show the assumption for the set of Wick ordered exponentials. Since this set is total the rest follows by a density argument. We have for $\xi, \eta \in S_d(\mathbb{R})$,

$$\begin{aligned}\sigma_z(:\exp(\langle\xi,\cdot\rangle):\cdot:\exp(\langle\eta,\cdot\rangle):) &= \\ \sigma_z(\exp\left(-\frac{1}{2}(\langle\xi,\xi\rangle+\langle\eta,\eta\rangle)\right)\exp(\langle\xi+\eta,\omega\rangle)&\\ = \exp\left(-\frac{1}{2}(\langle\xi,\xi\rangle+\langle\eta,\eta\rangle)\right)\exp(\langle\xi+\eta,z\omega\rangle)&\\ = \exp\left(-\frac{1}{2}(\langle\xi,\xi\rangle+\langle\eta,\eta\rangle)\right)\exp(\langle z\xi,\omega\rangle)\exp(\langle z\eta,\omega\rangle)&\end{aligned}$$

on the other hand

$$\begin{aligned}\sigma_z(:\exp(\langle\xi,\cdot\rangle):)\cdot\sigma_z(:\exp(\langle\eta,\cdot\rangle):) &= \\ \exp(-\frac{1}{2}\langle\xi,\xi\rangle)\exp(\langle\xi,z\omega\rangle)\exp(-\frac{1}{2}\langle\eta,\eta\rangle)\exp(\langle\eta,z\omega\rangle),&\end{aligned}$$

which proves the assumption. □

More precisely we have, compare to [36] and [37] the following proposition.

Proposition 2.17 *Let $\varphi \in (S)$, $z \in \mathbb{C}$, then*

$$\sigma_z\varphi = \sum_{n=0}^{\infty}\langle\varphi_z^{(n)}, :\cdot^n:\rangle,$$

with kernels

$$\varphi_z^{(n)} = z^n\sum_{k=0}^{\infty}\frac{(n+2k)!}{k!n!}\left(\frac{z^2-1}{2}\right)^k\cdot tr^k\varphi^{(n+2k)}.$$

Definition 2.18 Since σ_z is a continuous mapping from (S) to itself we can define its dual operator $\sigma_z^\dagger : (S)^* \to (S)^*$ by

$$\langle\!\langle\varphi, \sigma_z^\dagger\Phi\rangle\!\rangle = \langle\!\langle\sigma_z\varphi, \Phi\rangle\!\rangle,$$

for $\Phi \in (S)^*$ and $\varphi \in (S)$.

The following proposition can be found in [37] and [36].

Proposition 2.19 *Let $\Phi \in (S)^*$, $\varphi, \psi \in (S)$ and $z \in \mathbb{C}$ then we have*

(i)

$$\sigma_z^\dagger \Phi = J_z \diamond \Gamma_z \Phi,$$

where Γ_z is defined by

$$S(\Gamma_z \Phi)(\xi) = S(\Phi)(z\xi), \quad \xi \in S_d(\mathbb{R}),$$

and $J_z = \mathrm{Nexp}(-\frac{1}{2}z^2\langle \cdot, \cdot \rangle)$. In particular we have

$$\sigma_z^\dagger \mathbf{1} = J_z.$$

(ii) $J_z \varphi = \sigma_z^\dagger(\sigma_z \varphi)$.

3 Generalized Scaling Operators

In a view to the previous section we want to generalize the notion of scaling to bounded operators. More precisely we investigate for which kind of linear mappings $B \in L(S_d(\mathbb{R})', S_d(\mathbb{R})')$ there exists some operator $\sigma_B : (S) \to (S)$ such that

$$\Phi_{(BB^*)} \cdot \varphi := \sigma_B^\dagger \sigma_B \varphi.$$

Further we state a generalization of the Wick formula to Gauss kernels. We start with the definition of σ_B.

Definition 3.1 Let $B \in L(S_d(\mathbb{R})_\mathbb{C}, S_d'(\mathbb{R})_\mathbb{C})$. By tr_B we denote the element in $S_d'(\mathbb{R})_\mathbb{C} \otimes S_d'(\mathbb{R})_\mathbb{C}$, which is defined by

$$\forall \xi,\ \eta \in S_d(\mathbb{R})_\mathbb{C} :\ tr_B(\xi \otimes \eta) := \langle \xi, B\eta \rangle .$$

Note that tr_B is not symmetric. Further there exists a $q \in \mathbb{Z}$ such that $tr_B \in H_{q,\mathbb{C}} \otimes H_{q,\mathbb{C}}$.

Proposition 3.2 *Let $B \in L(L_d^2(R, \mathbb{C}), L_d^2(R, \mathbb{C}))$ be a Hilbert-Schmidt operator. Then $tr_B \in L_d^2(R, \mathbb{C}) \otimes L_d^2(R, \mathbb{C})$. Furthermore for each orthonormal basis $(e_j)_{j \in \mathbb{N}}$ of $L_d^2(R, \mathbb{C})$ we have:*

$$tr_B = \sum_{i=0}^{\infty} Be_i \otimes e_i.$$

Proof We have

$$\left|\sum_{i,j=0}^{\infty}\left\langle e_i, Be_j\right\rangle e_i\otimes e_j\right|_0^2=\sum_{i,j=0}^{\infty}\left|\left\langle e_i, Be_j\right\rangle\right|^2=\sum_{j=0}^{\infty}|Be_j|_0^2$$
$$=\|B\|_{HS}^2<\infty.$$

Hence the sum is a well-defined element in $L_d^2(R,\mathbb{C})\otimes L_d^2(R,\mathbb{C})$. The identity follows by verifying the formula for $\{e_k\otimes e_l\}_{k,l\in\mathbb{N}}$:

$$\left\langle e_k\otimes e_l,\sum_{i=0}^{\infty}Be_i\otimes e_i\right\rangle=(e_k,\overline{Be_l})_{\mathcal{H}}(e_l,\overline{e_l})_{L_d^2(R,\mathbb{C})}=(e_k,\overline{Be_l})_{L_d^2(R,\mathbb{C})}=\langle e_k,Be_l\rangle.$$

□

Proposition 3.3 *In the case $S_d(\mathbb{R})=S_d(\mathbb{R})$ and $B\in L(S_d(\mathbb{R})_{\mathbb{C}},S_d'(\mathbb{R})_{\mathbb{C}})$ we have*

$$tr_B=\sum_{i=0}^{\infty}Bh_i\otimes h_i$$

Proof By the continuity of the bilinear form $\langle\cdot,B\cdot\rangle$ on $S_d(\mathbb{R})_{\mathbb{C}}\times S_d(\mathbb{R})_{\mathbb{C}}$ there exists $p\geq 0$ such that $B\in L(H_{p,\mathbb{C}},H_{-p,\mathbb{C}})$. Let $q>p+1$. Then

$$|\sum_{n=0}^{\infty}Bh_n\otimes h_n|_{-q}^2=\sum_{n=0}^{\infty}|Bh_n|_{-q}^2\cdot|h_n|_{-q}^2\leq K\sum_{n=0}^{\infty}|h_n|_p^2\cdot|h_n|_{-q}^2,$$

for some $K>0$. For the last expression we have

$$K\sum_{n=0}^{\infty}|h_n|_p^2\cdot|h_n|_{-q}^2\leq K\sum_{n=0}^{\infty}\left(\frac{1}{2n+2}\right)^2<\infty.$$

Then as in the proof of Proposition 3.2 we obtain

$$tr_B=\sum_{n=0}^{\infty}Bh_n\otimes h_n,$$

since

$$\overline{\operatorname{span}\{h_n\otimes h_l\}_{n,l}}^{S(\mathbb{R})\otimes S_d(\mathbb{R})}=S_d(\mathbb{R})\otimes S_d(\mathbb{R}).$$

□

Definition 3.4 For $B \in L(S'_d(\mathbb{R})_{\mathbb{C}}, S'_d(\mathbb{R})_{\mathbb{C}})$ we define $\sigma_B\varphi$, $\varphi \in (S)$, via its chaos decomposition, which is given by

$$\sigma_B\varphi = \sum_{n=0}^{\infty} \left\langle \varphi_B^{(n)}, :\cdot^{\otimes n}: \right\rangle, \tag{9}$$

with kernels

$$\varphi_B^{(n)} = \sum_{k=0}^{\infty} \frac{(n+2k)!}{k!n!} \left(-\frac{1}{2}\right)^k (B^*)^{\otimes n} (\mathrm{tr}^k_{(Id-BB^*)} \varphi^{(n+2k)}).$$

Here, B^* means the dual operator of B with respect to $\langle \cdot, \cdot \rangle$. Further for $A \in L(S_d(\mathbb{R})_{\mathbb{C}}, S'_d(\mathbb{R})_{\mathbb{C}})$, the expression $\mathrm{tr}^k_A \varphi^{(n+2k)}$ is defined by

$$\mathrm{tr}^k_A \varphi^{(n+2k)} := \left\langle \mathrm{tr}_A^{\otimes k}, \varphi^{(n+2k)} \right\rangle \in S_d(\mathbb{R})^{\hat{\otimes} n},$$

where the generalized trace kernel tr_A is defined in (3.1).

Proposition 3.5 *Let $B \in L(S_d(\mathbb{R})_{\mathbb{C}}, S_d(\mathbb{R})_{\mathbb{C}})$ and $n \in \mathbb{N},\ n > 0$. Then for all $p \in \mathbb{N}$ there exists a $K > 0$ and $q_1, q_2 \in \mathbb{N}$, with $p < q_1 < q_2$ such that for all $\theta \in S_d(\mathbb{R})^{\otimes n}_{\mathbb{C}}$ we have*

$$\left|B^{\otimes n}\theta\right|_p \leq \left(K \left\|B\right\|_{q_2,q_1} \left\|i_{q_1,p}\right\|_{HS}\right)^n \cdot |\theta|_{q_2}.$$

Proof Choose $q_1,\ q_2 \in \mathbb{N}$ with $q_2 > q_1 > p$ and

$$B \in L(H_{q_1,\mathbb{C}}, H_{p,\mathbb{C}}) \text{ and } B \in L(H_{q_2,\mathbb{C}}, H_{q_1,\mathbb{C}},).$$

For a shorter notation we write e_J for $e_{j_1} \otimes \cdots \otimes e_{j_n}$. Now let $(e_J)_J$ be an orthonormal basis of $H_p^{\otimes n}$. Further let $\mathcal{I}_p :\ (H_{p,\mathbb{C}}^{\otimes n})' \to H_{p,\mathbb{C}}^{\otimes n}$ be the Riesz isomorphism. Then for $\theta \in S_d(\mathbb{R})^{\otimes n}_{\mathbb{C}}$

$$\begin{aligned}
\left|B^{\otimes n}\theta\right|_p^2 &= \sum_J \left|(B^{\otimes n}\theta, e_J)_p\right|^2 = \sum_J \left|\left\langle B^{\otimes n}\theta, \overline{\mathcal{I}_p^{-1}(e_J)} \right\rangle\right|^2 \\
&= \sum_J \left|\left\langle B^{\otimes n}\theta, \mathcal{I}_p^{-1}(e_J) \right\rangle\right|^2 = \sum_J \left|\left\langle \theta, (B^*)^{\otimes n}\mathcal{I}_p^{-1}(e_J) \right\rangle\right|^2 \\
&\leq |\theta|_{q_2}^2 \cdot \sum_J \left|(B^*)^{\otimes n}\mathcal{I}_p^{-1}(e_J)\right|_{-q_2}^2,
\end{aligned}$$

We can estimate this with the norm of $B^* : H_{-q_1,\mathbb{C}} \to H_{-q_2,\mathbb{C}}$, denoted by $\|B^*\|_{-q_1,-q_2}$. Then for a $K > 0$ we have

$$|\theta|_{q_2}^2 \cdot \sum_J \left|(B^*)^{\otimes n}\mathcal{I}_p^{-1}(e_J)\right|_{-q_2}^2 \leq |\theta|_{q_2}^2 \cdot K^{2n} \|B^*\|_{-q_1,-q_2}^{2n} \sum_J \left|\mathcal{I}_p^{-1}(e_J)\right|_{-q_1}^2,$$
$$= |\theta|_{q_2}^2 \cdot K^{2n} \|B\|_{q_1,q_2}^{2n} \left\|i_{q_1,p}\right\|_{HS}^{2n},$$

where the last equation is due to [35, Theorem 4.10(2), p. 93] □

Next we show the continuity of the generalized scaling operator.

Proposition 3.6 *Let $B : S_d'(\mathbb{R})_{\mathbb{C}} \to S_d'(\mathbb{R})_{\mathbb{C}}$ a bounded operator. Then $\varphi \mapsto \sigma_B\varphi$ is continuous from (S) into itself.*

Proof Let $\varphi_B^{(n)}$ as in Definition 9.

First choose $q_1 > 0$, such that $|tr_{Id-BB^*}|_{-q_1}^k < \infty$. Then, by (3.5), there exist $C(B) > 0$, $q_2 > q1$ such that

$$|\varphi_B^{(n)}|_p = |\sum_{k=0}^{\infty} \frac{(n+2k)!}{k!n!}\left(-\frac{1}{2}\right)^k (B^*)^{\otimes n}(\mathrm{tr}_{Id-BB^*}^k \varphi^{(n+2k)})|_p$$
$$\leq \frac{1}{\sqrt{n!}} C(B)^n \sum_{k=0}^{\infty} \sqrt{\binom{n+2k}{2k}} \frac{\sqrt{(2k)!}}{k!2^k} \sqrt{(n+2k)!} |tr_{Id-BB^*}|_{-q_2}^k |\varphi^{n+2k}|_{q_2}$$

Since $\frac{\sqrt{(2k)!}}{k!2^k} < 1$, see [37], we have

$$\frac{1}{\sqrt{n!}} C(B)^n \sum_{k=0}^{\infty} \sqrt{\binom{n+2k}{2k}} \frac{\sqrt{(2k)!}}{k!2^k} \sqrt{(n+2k)!} |tr_{Id-BB^*}|_{-q_2}^k |\varphi^{n+2k}|_{q_2}$$
$$\leq \frac{1}{\sqrt{n!}} C(B)^n \sum_{k=0}^{\infty} \sqrt{\binom{n+k}{k}} \sqrt{(n+k)!} |tr_{Id-BB^*}|_{-q_2}^{\frac{k}{2}} |\varphi^{n+k}|_{q_2}$$
$$\leq \frac{1}{\sqrt{n!}} C(B)^n 2^{-n\frac{q'}{2}} \left(\sum_{k=0}^{\infty} \binom{n+k}{k} 2^{-q'k} |tr_{Id-BB^*}|_{-q_2}^k\right)^{\frac{1}{2}}$$
$$\times \left(\sum_{k=0}^{\infty} (n+k)! 2^{q'(n+k)} |\varphi^{(n+k)}|_{q_2}^2\right)^{\frac{1}{2}}$$
$$\leq \|\varphi\|_{q_2,q'} \frac{1}{\sqrt{n!}} 2^{-n\frac{q'}{2}} C(B)^n \left(1 - 2^{-q'} |tr_{Id-BB^*}|_{-q_2}\right)^{-\frac{n+1}{2}}.$$

If q' fulfills

$$2^{-q'}|tr_{Id-BB^*}|_{-q_2} < 1,$$

we obtain

$$\|\sigma_B\varphi\|^2_{q_2,q} \leq \|\varphi\|^2_{q_2,q'} \cdot \sum_{n=0}^{\infty} 2^{n(q-q')} C(B)^{2n} \left(1 - 2^{-q'}|tr_{Id-BB^*}|_{-q_2}\right)^{-(n+1)},$$

where the right hand side converges if $q' - q$ is large enough. □

Proposition 3.7 *Let $\varphi \in (S)$ given by its continuous version. Then it holds*

$$\sigma_B\varphi(\omega) = \varphi(B\omega),$$

if $B \in L(S'_d(\mathbb{R}), S'_d(\mathbb{R}))$, $\omega \in S'_d(\mathbb{R})$.

This can be proved directly by an explicit calculation on the the set of Wick exponentials, a density argument and a verifying of pointwise convergence, compare [32, Proposition 4.6.7, p. 104], last paragraph.

In the same manner the following statement is proved.

Proposition 3.8 *Let $B : S(\mathbb{R})' \to S(\mathbb{R})'$ be a bounded operator. For $\varphi, \psi \in (\mathcal{N})$ the following equation holds*

$$\sigma_B(\varphi\psi) = (\sigma_B\varphi)(\sigma_B\psi).$$

Since we consider a continuous mapping from $(\mathcal{N})$ into itself one can define the dual scaling operator with respect to $\langle\cdot,\cdot\rangle$, $\sigma_B^\dagger : (\mathcal{N})' \to (\mathcal{N})'$ by

$$\left\langle\!\left\langle \sigma_B^\dagger\Phi, \psi \right\rangle\!\right\rangle = \left\langle\!\left\langle \Phi, \sigma_B\psi \right\rangle\!\right\rangle.$$

The Wick formula as stated in [16, 36] for Donsker's delta function can be extended to Generalized Gauss kernels.

Proposition 3.9 (Generalized Wick formula) *Let $\Phi \in (S)'$, $\varphi, \psi \in (S)$ and $B \in L(S'_d(\mathbb{R}), S'_d(\mathbb{R}))$. then we have*

(i)

$$\sigma_B^\dagger = \Phi_{BB^*} \diamond \Gamma_B{}^*\Phi,$$

where $\Gamma_B{}^*$ is defined by

$$S(\Gamma_B{}^*\Phi)(\xi) = S(\Phi)(B^*\xi), \quad \xi \in S_d(\mathbb{R}).$$

In particular we have

$$\sigma_B^\dagger \mathbf{1} = \Phi_{BB^*}.$$

(ii) $\Phi_{BB^*} \cdot \varphi = \sigma_B^\dagger(\sigma_B \varphi)$.
(iii) $\Phi_{BB^*} \cdot \varphi = \Phi_{BB^*} \diamond (\Gamma_{B^*} \circ \sigma_B(\varphi))$.

Proof Proof of (i): Let $\Phi \in (S)'$ and $\xi \in S_d(\mathbb{R})_{\mathbb{C}}$ then we have

$$\begin{aligned} S(\sigma_B^\dagger \Phi)(\xi) &= \langle\!\langle : \exp(\langle \xi, \cdot \rangle) :, \sigma_B^\dagger \Phi \rangle\!\rangle \\ &= \langle\!\langle \sigma_B : \exp(\langle \xi, \cdot \rangle) :, \Phi \rangle\!\rangle = \exp(-\frac{1}{2}\langle \xi, \xi \rangle) \langle\!\langle \exp(\langle B^* \xi, \cdot \rangle), \Phi \rangle\!\rangle \\ &= \exp(-\frac{1}{2}\langle \xi, (Id - BB^*)\xi \rangle) S(\Phi)(B^* \xi) = S(\Phi_{BB^*})(\xi) \cdot S(\Gamma_{B^*}\Phi)(\xi) \end{aligned}$$

Proof of (ii): First we have $\sigma_B^\dagger \mathbf{1} = \Phi_{BB^*} \diamond \Gamma_{B^*} \mathbf{1} = \Phi_{BB^*}$. Thus for all $\varphi, \psi \in (S)$

$$\begin{aligned} \langle\!\langle \Phi_{BB^*} \varphi, \psi \rangle\!\rangle &= \langle\!\langle \sigma^\dagger \mathbf{1}, \varphi \cdot \psi \rangle\!\rangle = \\ &\langle\!\langle \mathbf{1}, (\sigma_B \varphi)(\sigma_B \psi) \rangle\!\rangle = \langle\!\langle (\sigma_B \varphi), (\sigma_B \psi) \rangle\!\rangle = \langle\!\langle \sigma_B^\dagger (\sigma_B \varphi), \psi \rangle\!\rangle \end{aligned}$$

Proof of (iii): Immediate from (i) and (ii). □

Remark 3.10 The scaling operator can be considered as a linear measure transform. Let $\varphi \in S - d(\mathbb{R})$ and B a real bounded operator on $S_d(\mathbb{R})'$. Then we have

$$\int_{S(\mathbb{R})'} \sigma_B \varphi(\omega)\, d\mu(\omega) = \int_{S(\mathbb{R})'} \varphi(B\omega)\, d\mu(\omega) = \int_{S(\mathbb{R})'} \varphi(\omega)\, d\mu(B^{-1}\omega)$$

Moreover we have

$$\int_{S(\mathbb{R})'} \exp(i\langle \xi, \omega)\, d\mu(B^{-1}\omega) = \exp(-\frac{1}{2}\langle B^* \xi, B^* \xi \rangle,$$

which is a characteristic function of a probability measure by the Theorem of Bochner and Minlos [31]. Furthermore

$$\int_{S(\mathbb{R})'} \exp(i\langle \xi, \omega)\, d\mu(B^{-1}\omega) = T(\sigma^\dagger \mathbf{1})(\xi),$$

such that Φ_{BB^*} is represented by the positive Hida measure $\mu \circ B^{-1}$.

4 Construction of Hamiltonian Path Integrand via Generalized Scaling

We construct in this section by a suitable generalized scaling the Hamiltonian path integral as an expectation based on the formula above as in (5).

In phase space however the arguments are multidimensional, since we consider momentum and space variables as independent variables. For simplicity we consider $t_0 = 0$ and furthermore $\hbar = m = 1$. Indeed we have the following

Proposition 4.1 *Let* $N^{-1} = \begin{pmatrix} \mathbf{1}_{[0,t)^c} & 0 \\ 0 & \mathbf{1}_{[0,t)^c} \end{pmatrix} + i \begin{pmatrix} \mathbf{1}_{[0,t)} & \mathbf{1}_{[0,t)} \\ \mathbf{1}_{[0,t)} & 0 \end{pmatrix}$ *as in the case of the free Hamiltonian integrand* I_0 *(i.e.* $V = 0$*). Let* R *be a symmetric operator (w.r.t. the dual pairing) with* $R^2 = N^{-1}$*. Indeed we have:*

$$R = \begin{pmatrix} \mathbf{1}_{[0,t)^c} & 0 \\ 0 & \mathbf{1}_{[0,t)^c} \end{pmatrix} + \frac{\sqrt{i}}{1 + (\frac{\sqrt{5}+1}{2})^2} U^T \begin{pmatrix} \frac{1+\sqrt{5}}{2}\mathbf{1}_{[0,t)} & 0 \\ 0 & \frac{1-\sqrt{5}}{2}\mathbf{1}_{[0,t)} \end{pmatrix} U,$$

with

$$U = \begin{pmatrix} -\frac{\sqrt{5}+1}{2} & 1 \\ -1 & -\frac{\sqrt{5}+1}{2} \end{pmatrix}$$

Then under the assumption that $\sigma_R \delta(\langle(\mathbf{1}_{[0,t)}, 0), \cdot\rangle) = \delta(\langle R(\mathbf{1}_{[0,t)}, 0), \cdot\rangle) \in (S)'$*, we have*

$$I_0 = \sigma_R^\dagger \sigma_R \delta(\langle(\mathbf{1}_{[0,t)}, 0), \cdot\rangle).$$

Consequently the Hamiltonian path integrand for an arbitrary space dependent potential V, can be informally written as

$$\begin{aligned} I_V &= \mathrm{Nexp}\left(-\frac{1}{2}\langle \cdot, K\cdot\rangle\right) \exp\left(-i\int_0^t V(x_0 + \langle(\mathbf{1}_{[0,r)}, 0), \cdot\rangle)\, dr\right) \\ &\qquad \times \delta(x_0 + \langle(\mathbf{1}_{[t_0,t)}, 0), \cdot\rangle - x) \\ &= \sigma_R^\dagger\Big(\sigma_R\Big(\exp\left(-i\int_0^t V(x_0 + \langle(\mathbf{1}_{[0,r)}, 0), \cdot\rangle)\, dr\right)\Big) \\ &\qquad \times \sigma_R \delta(x_0 + \langle(\mathbf{1}_{[t_0,t)}, 0), \cdot\rangle - x)\Big), \end{aligned} \tag{10}$$

for $x, x_0 \in \mathbb{R}$ and $0 < t_0 < t < \infty$.

In the following we give some ideas to give a mathematical meaning to the expression in (10). First we consider a quadratic potential, i.e. we consider

$$\exp(-\frac{1}{2}\langle \cdot L \cdot \rangle)\delta(\langle(\mathbf{1}_{[t_0,t)},0),\cdot\rangle - x).$$

Definition 4.2 For L fulfilling the assumption of Lemma 2.14 and

$$\delta(\langle(\mathbf{1}_{[t_0,t)},0),\cdot\rangle - x)$$

we define

$$\sigma_R\left(\exp(-\frac{1}{2}\langle \cdot L \cdot \rangle)\delta(\langle(\mathbf{1}_{[t_0,t)},0),\cdot\rangle - x)\right)$$
$$:= \exp(-\frac{1}{2}\langle \cdot RLR \cdot \rangle)\delta(\langle R(\mathbf{1}_{[t_0,t)},0),\cdot\rangle - x).$$

We now take a look at the T-transform of this expression in $\mathbf{f} \in S_2(\mathbb{R})$. We have

$$\begin{aligned}
&T(\sigma_R^\dagger \sigma_R\left(\exp(-\frac{1}{2}\langle \cdot L \cdot \rangle)\delta(\langle(\mathbf{1}_{[t_0,t)},0),\cdot\rangle - y)\right))(\mathbf{f})\\
&\quad = T(\sigma_R\left(\exp(-\frac{1}{2}\langle \cdot L \cdot \rangle)\delta(\langle(\mathbf{1}_{[t_0,t)},0),\cdot\rangle - y)\right))(R\mathbf{f})\\
&\quad = \frac{1}{\sqrt{2\pi\det(Id+RLR)}}\exp(-\frac{1}{2}\langle R\mathbf{f},(Id+RLR)^{-1}R\mathbf{f}\rangle)\\
&\qquad \times \exp\big(\frac{(iy-\langle R\mathbf{f},(Id+RLR)^{-1}R(\mathbf{1}_{[t_0,t)},0)\rangle)^2}{2\langle R(\mathbf{1}_{[t_0,t)},0),(Id+RLR)^{-1}R(\mathbf{1}_{[t_0,t)},0)\rangle}\big).
\end{aligned}$$

Now with $R^2 = N^{-1}$ and since R is invertible with $R^{-1}R^{-1} = N$, we have

$$Id + RLR = RR^{-1}R^{-1}R + RLR = R(Id + K + L)R$$

and

$$(Id + RLR)^{-1} = R^{-1}(Id + K + L)^{-1}R^{-1}.$$

Thus

$$T(\sigma_R^\dagger \sigma_R \left(\exp(-\frac{1}{2}\langle \cdot L \cdot \rangle)\delta(\langle (\mathbf{1}_{[t_0,t)},0),\cdot\rangle - y)\right))(\xi)$$
$$= \frac{1}{\sqrt{2\pi \det((N+L)N^{-1})}} \exp(-\frac{1}{2}\langle \xi, (N+L)^{-1}\xi\rangle)$$
$$\exp\big(\frac{1}{2\langle (\mathbf{1}_{[t_0,t)},0),(N+L)^{-1}(\mathbf{1}_{[t_0,t)},0)\rangle}(iy - \langle \xi,(N+L)^{-1}(\mathbf{1}_{[t_0,t)},0)\rangle)^2\big),$$

which equals the expression from Lemma 2.14. Hence we have that for a suitable quadratic potential

$$\sigma_R^\dagger \sigma_R \left(\exp(-\frac{1}{2}\langle \cdot L \cdot \rangle)\delta(\langle (\mathbf{1}_{[t_0,t)},0),\cdot\rangle - y)\right),$$

exists as a Hida distribution. Moreover for all quadratic potentials from the previous chapter, the T-transform obtained via scaling gives the generating functional as in chapter "38 Years with Professor Ludwig Streit". Since the T-transforms coincide, also the distributions are the same.

For the case of quadratic potentials we obtained the correct physics also by the scaling approach.

Example 4.3 We construct the Feynman integrand for the harmonic oscillator in phase space via the generalized scaling. I.e. the potential is given by $x \mapsto V(x) = \frac{1}{2}kx^2$, $0 \le k < \infty$.

Thus the matrix L which includes the information about the potential, is given by

$$L = \begin{pmatrix} ikA & 0 \\ 0 & 0 \end{pmatrix},\ y \in \mathbb{R},\ t > 0,$$

where $Af(s) = \mathbf{1}_{[0,t)}(s)\int_s^t \int_0^\tau f(r)\,dr\,d\tau, f \in L^2(\mathbb{R},\mathbb{C}), s \in \mathbb{R}$, then for $\mathbf{f} \in S_2(\mathbb{R})_{\mathbb{C}}$, see also [6] and [14] we have

$$T\left(\sigma_R^\dagger \sigma_R \left(\exp(-\frac{1}{2}\langle \cdot L \cdot \rangle)\delta(\langle (\mathbf{1}_{[t_0,t)},0),\cdot\rangle - y)\right)\right)(\mathbf{f})$$
$$= \sqrt{\left(\frac{\sqrt{k}}{2\pi i \sin(\sqrt{k}t)}\right)} \exp\left(\frac{1}{2}\frac{\sqrt{k}}{i\tan(\sqrt{k}t)}\Big(iy + (\boldsymbol{\eta}, \mathbf{f}+\mathbf{g})\Big)^2\right)$$

$$\times \exp\left(-\frac{1}{2}\left((\mathbf{f}+\mathbf{g}), \begin{pmatrix} \mathbf{1}_{[0,t)^c} & 0 \\ 0 & \mathbf{1}_{[0,t)^c} \end{pmatrix} (\mathbf{f}+\mathbf{g}) \right) \right)$$

$$\times \exp\left(-\frac{1}{2}\left((\mathbf{f}+\mathbf{g}), \frac{t}{i}\mathbf{1}_{[0,t)} \begin{pmatrix} \frac{1}{t}(kA-\mathbf{1}_{[0,t)})^{-1} & (kA-\mathbf{1}_{[0,t)})^{-1} \\ (kA-\mathbf{1}_{[0,t)})^{-1} & ktA(kA-\mathbf{1}_{[0,t)})^{-1} \end{pmatrix} (\mathbf{f}+\mathbf{g}) \right) \right),$$

which is identically equal to the generating functional of the Feynman integrand for the harmonic oscillator in phase space, see e.g.[6].

Moreover its generalized expectation

$$\mathbb{E}(I_{HO}) = T(I_{HO})(0) = \sqrt{\left(\frac{\sqrt{k}}{2\pi i \sin(\sqrt{k}t)} \right)} \exp\left(i \frac{\sqrt{k}}{2\tan(\sqrt{k}t)} y^2 \right)$$

is the Greens function to the Schrödinger equation for the harmonic oscillator, compare e.g. with [21].

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Computer Simulations of Self-repelling Fractional Brownian Motion

Jinky Bornales, Cresente Cabahug, Roel Baybayon, Sim Bantayan, and Beverly Gemao

Abstract Self-repelling fractional Brownian motion (fBm) has been constructed, generalizing the Edwards model for the conformations of chain polymers. In this context of particular interest is the predicted scaling behaviour of their end-to-end length, i.e. the anomalous diffusion of self-repelling fBm. We briefly present the model and a heuristic formula of the scaling behaviour for general dimension and Hurst index, and then our computer simulations of self-repelling fBm paths, their method and first results.

Keyword Fractional Brownian motion

Mathematics Subject Classification (2010) 60G22

1 Self-Repelling Brownian Motion

The field of self-avoiding or self-repelling random paths has been widely studied in combinatorics, stochastic analysis, statistical mechanics, numerically using Monte Carlo methods, and in the chemistry of polymers. It is thus highly interdisciplinary: while the motivation came from chemistry and the modelling of polymer conformations [9], physics provided structural intuition and far-reaching predictions. The mathematical results are less far-reaching but have the higher reliability characteristic of the mathematical approach. Large scale computer simulations back up the theoretical arguments. For reviews of recent results in the mathematics and physics communities see [11] and [17].

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J. Bornales (✉) • C. Cabahug • R. Baybayon • S. Bantayan • B. Gemao
Physics Department, Mindanao State University – Iligan Institute of Technology,
9200 Iligan City, Philippines
e-mail: jinky.bornales@g.msuiit.edu.ph

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2 The Edwards Model

Self-repelling paths were introduced by Edwards [8] to avoid the combinatorial complications of strictly self-avoiding random walks. For Brownian trajectories this can be done via a "Boltzmann factor" which suppresses the probability of self-intersections, informally

$$G = \frac{1}{Z} \exp\left(-g \int_0^N ds \int_0^N dt \delta\left(B(s) - B(t)\right)\right).$$

Mathematically, the self-intersection local time in the exponent is increasingly singular for increasing spatial dimension d of the Brownian motion; for $d = 2$ it requires centering [19] to be finite, in higher dimension a multiplicative renormalization is required [20].

3 The Flory Formula

A characteristic observable is the (mean square) end-to-end distance R of paths $B = x$:

$$R^2(N) = E\left((x(N) - x(0))^2\right).$$

When the time N (the number of monomers) becomes large one expects a scaling behavior

$$R(N) \sim N^{\nu}.$$

For Brownian motion the root-mean-square length R is scaling with $\nu = 1/2$. But self avoidance, "the excluded volume effect", makes the polymers swell: the end-to-end length increases; there is the famous Flory formula [9]

$$\nu = \frac{3}{d+2},$$

derived on the basis of heuristic arguments. The following table summarizes what is known about the Flory index.

	Flory	*Theory*	*Exp.*
$d = 1$:	1	1	
$d = 2$:	0.75	0.75	0.79
$d = 3$:	0.60	0.588	0.59
$d = 4$:	0.5	0.5	

The theoretical values are of a different nature: for $d = 1$ there exists a mathematical proof, see e.g. [11], and for $d \geq 4$ there are no self-intersections of Brownian paths, hence no anomalous scaling. For $d = 2$ there exists an often quoted justification for $\nu = 3/4$ using arguments from quantum field theory [16].

4 Generalization to Fractional Brownian Motion

Fractional Brownian motion in $\mathbb{R}^d$, $d \geq 1$, with "Hurst parameter" $H \in (0, 1)$ is a d-dimensional centered Gaussian process [2, 15] $B^H = \{B_t^H : t \geq 0\}$ with covariance function

$$\mathbb{E}(B_t^H B_s^H) = \frac{\delta_{ij}}{2}\left(t^{2H} + s^{2H} - |t-s|^{2H}\right), \quad i,j = 1,\ldots,d,\ s,t \geq 0,$$

and, by the Kolmogorov-Chentsov argument, has continuous trajectories. $H = 1/2$ is ordinary Brownian motion. So increments are uncorrelated for $H = 1/2$, and positively correlated ("persistent" paths) for $H > 1/2$, and negatively correlated for $H < 1/2$ so that for larger resp. smaller H the paths are smoother resp. curlier than those of Brownian motion.

5 Extension of the Edwards Model and of the Flory Formula

The Varadhan existence proof of the Edwards model has been extended to fractional Brownian motion in [10]. If $Hd < 1$, the fBm Edwards model is well defined. Starting from a smooth approximation

$$\delta_\varepsilon(x) := \frac{1}{(2\pi\varepsilon)^{d/2}} e^{-\frac{|x|^2}{2\varepsilon}}, \quad \varepsilon > 0,$$

of the Dirac $\delta-$function we get that

$$L := \lim_{\varepsilon \to 0^+} \int_0^N dt \int_0^t ds\, \delta_\varepsilon(B^H(t) - B^H(s)) \tag{1}$$

exists in L^2 [12] so that

$$G := \frac{1}{Z} \exp\left(-g \int_0^N ds \int_0^N dt \delta\left(B^H(s) - B^H(t)\right)\right)$$

is integrable for $g \geq 0$. For $H = 1/d$, and g sufficiently small

$$G = \lim_{\varepsilon \searrow 0} \frac{1}{Z_\varepsilon} \exp\left(-g \int_0^N ds \int_0^N dt \delta_\varepsilon \left(B^H(s) - B^H(t) \right) \right) ,$$

with

$$Z_\varepsilon \equiv \mathbb{E}\left(\exp\left(-g \int_0^N ds \int_0^N dt \delta_\varepsilon \left(B^H(s) - B^H(t) \right) \right) \right)$$

is well-defined [10].

As is to be expected from the Brownian case, no such mathematical rigorous result exists (yet) for the Flory index. Heuristic physical arguments [5] suggest

$$\nu_H = \begin{cases} 1 & if \quad 2H \geq d \\ H & if \quad Hd \geq 2 \\ \frac{2H+2}{d+2} & otherwise \end{cases} \tag{2}$$

The first case pertains to $d = 1$ and $H > 1/2$ where the repulsion produces linear scaling, the second comes from the fact that for $Hd \geq 2$ there are no more self-intersections [18].

More generally [4],

$$\upsilon_H = \frac{2H + k + 1}{kd + 2} \tag{3}$$

if up to k-fold intersections are tolerated [6, 7].

The heuristic derivation calls for validation. Analytic arguments do not easily carry over from the Brownian case insofar as they are typically based on the Markov property which is not available in the fractional case. This makes numerical simulations particularly interesting.

6 Numerical Computation

As a starting point for our computational simulations we have focused on the one-dimensional case. While this would be unphysical as a polymer model it is the best studied case in mathematical terms [11], and there exists a recursion relation linking it to the Flory index in higher dimensions [4, 5], see also [13] for the Brownian case.

6.1 Off-lattice Discretization

Approximations of fBm by random walks on a lattice are notoriously difficult. By contrast an off-lattice N step discretization, with

$$x_k = B^H(k), \quad k = 0, 1, 2, \ldots, N-1$$

is easy. Physically this would correspond to the positions of N consecutive monomers.

We introduce $N-1$ "bond vectors"

$$y_k = B^H(k+1) - B^H(k)$$

and invert the covariance $A_{kl} = \mathbb{E}(y_k y_l)$ to get their probability density

$$\varrho_0(y) = \frac{1}{\sqrt{(2\pi)^{N-1} \det A}} \exp\left(-\frac{1}{2}(y, A^{-1}y)\right).$$

To discretize the self-intersection local time one expresses it by the local time at points x as follows:

$$L = \int_{-\infty}^{+\infty} dx L_x^2 \tag{4}$$

where

$$L_x = \int_0^N ds \delta\left(B^H(s) - x\right) \quad -\infty < x < \infty.$$

is the local time of Fractional Brownian motion, see for e.g. [1] (the relation (6.1) is in fact rigorous for the approximate local time with the δ_ϵ instead of δ). One discretizes this by decomposing the real line into cells I_n of equal length l, and replaces L_x by the number of positions $x_k = B^H(k)$ that fall into the cell with number n:

$$L_n = \#\{x_k : x_k \in I_n\} \quad n = 0, \pm 1, \pm 2, \ldots.$$

Likewise we replace the self-intersection local time of (4) by

$$L = \sum_{n=-\infty}^{\infty} L_n^2$$

so that the unnormalized probability density becomes

$$\rho(y) \sim \exp\left(-\frac{1}{2}\left(y, A^{-1}y\right) - gL(y)\right).$$

Given this density, the Metropolis algorithm [14] can now be invoked to produce updates of configurations by updating a randomly chosen $y_{k.} \to y'_{k.}$ so that

$$y^{(0)} = (y_1, \ldots, y_k, \ldots, y_{N-1})$$

becomes

$$y^{(1)} = \left(y_1, \ldots, y'_k, \ldots, y_{N-1}\right)$$

and so on by iteration, generating asymptotically an equilibrium distribution of conformations. In practice, for polymers of a length N between 200 and 450, we have performed 4×10^7 relaxation updates before starting the sampling during another 10^7 updates.

In these computations one has to set various parameters on which however the final outcome should depend as little as possible; we mention the relaxation time, the sample size, updating range, incidence cell size, and in particular the coupling g. Asymptotically for large N, scaling should be independent of the value of $g > 0$. For finite N we expect a steep rise of the scaling exponent to its asymptotic value as g increases from zero. In Fig. 1 we show the behaviour found in the Brownian case. After the initial steep rise there is first an overshoot, but unexpectedly the scaling index then does not settle to the asymptotic value but drops down further.

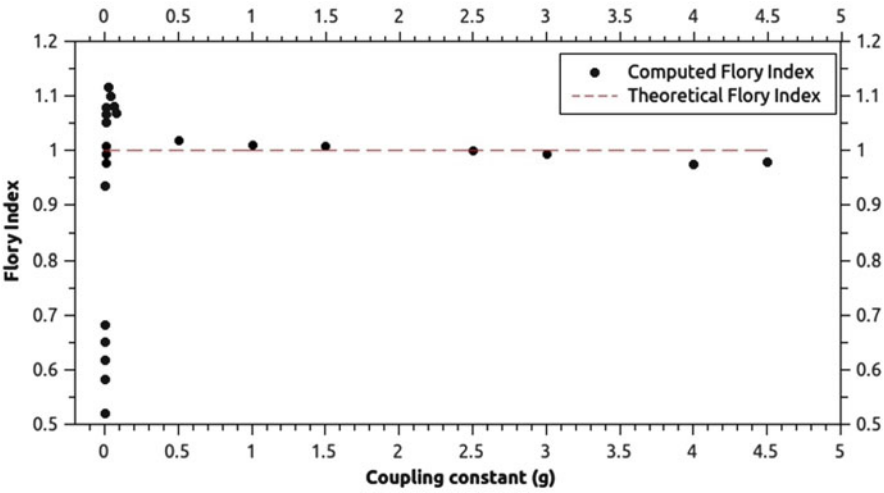

Fig. 1 Computation of the Flory index for $H = 1/2$ as a function of the coupling constant

	N=200	N=250	N=300	N=350	N=400	N=450
1	148.561384	185.806757	223.251292	3.448908	297.20476	331.017782
2	148.652515	185.72289	222.974883	70.237671	297.43551	334.692323
3	148.586736	185.779066	222.867817	260.452468	297.619368	334.650762
4	148.639374	185.817225	223.000005	259.749553	56.303116	334.420879
5	148.55003	185.86164	222.859288	260.067569	297.109958	5.103747
6	148.577061	185.841825	222.884541	260.544606	297.673914	39.028559
7	148.581016	185.698062	223.126486	260.057698	297.24476	334.641647
8	148.615485	185.858159	21.789704	260.265199	63.775105	42.701186
9	148.533144	185.725278	196.492051	257.004769	297.639218	334.28078
10	148.534548	185.837531	223.024658	85.857103	45.0312	92.201333
11	148.576327	185.901009	222.783749	260.357831	297.392041	32.10668
12	148.662716	185.816336	223.064216	260.213159	297.463301	92.7516
13	148.587298	185.827205	222.746137	260.277839	11.691363	119.339916
14	148.62341	185.922296	18.333827	15.130467	297.675597	72.621415
15	148.557851	185.721584	223.084027	260.526415	164.260284	182.796229
16	148.600935	185.699077	223.134297	222.626352	1.610342	68.209445
17	148.603842	185.969839	188.739957	260.404777	297.540813	43.970589
18	148.549373	185.744266	168.512637	260.395694	215.65133	333.182499
19	148.62828	185.897628	222.922391	260.398273	87.128402	10.22831
20	148.542545	185.801928	222.898458	259.82197	297.33094	149.353809
21	148.64334	185.693459	103.821578	259.987072	297.480941	146.287636
22	148.69905	185.882721	222.93866	260.227582	67.058627	139.531098
23	148.539749	185.750587	223.059164	260.117636	297.578633	173.411716
24	148.533786	185.598232	222.907012	260.334485	297.679209	111.216881
25	148.669657	185.753258	222.147937	87.399481	296.95735	81.674027
26	148.642073	185.667924	13.518397	260.05062	296.966906	34.016774
27	148.592352	185.608875	13.719802	1.472821	297.510537	334.547351
28	148.647449	185.582618	223.066872	260.263489	297.300942	31.119832
29	148.475577	185.663681	162.451293	260.286568	297.91388	67.170682
30	148.520298	185.608068	223.115845	259.970831	297.337112	334.553507
	148.5909067	185.7686341	185.6412327	215.5982969	231.952182	158.0276331

Fig. 2 Thirty simulations of the end-to-end length, exhibiting outliers

To understand this phenomenon it is useful to study the output of independent simulations undertaken in parallel, with identical parameters but different (random) initial conformations. As one sees in Fig. 2, there is remarkable agreement among them of the output end-to-end-length, except for a number of outliers (underlaid in blue). Their number increases for longer polymers as well as for decreasing Hurst parameter. To some extent one would find saturation of the Hurst index if one

neglected the outliers, but as one sees they become dominant for longer polymers so that this ad hoc method is also not practical.

Sampling during the relaxation phase revealed that the energy relaxes very fast but there are instances where the end-to-end length does not, there are knotted conformations which "are stuck" and will not unfold even after some 10^7 updates of the bond vectors.

To remedy this we have used a different relaxation schedule where during the relaxation phase we gradually increase the coupling constant g toward its final value which will then be maintained during the sampling phase as before. And as one sees in Fig. 3, the outliers disappear completely.

Repetition	N=200	N=250	N=300	N=350	N=400	N=450
1	148.6504	185.563832	223.120711	260.237567	297.203576	334.201745
2	148.587533	185.975031	223.05208	260.146227	297.591033	333.918754
3	148.550504	185.869825	223.165109	260.172032	297.534908	334.908739
4	148.593103	185.745288	223.007484	260.366241	297.299172	334.040505
5	148.610276	185.824746	222.949928	260.112603	297.460062	334.104725
6	148.573696	185.909148	222.857897	260.348838	297.307381	334.49865
7	148.597635	185.821458	223.143498	260.041732	297.553124	334.598725
8	148.489073	185.699712	222.824836	260.21261	297.328421	334.319885
9	148.552984	185.76551	223.170691	259.924632	296.953543	334.222533
10	148.431483	185.861387	222.927253	260.258366	297.121156	334.459799
11	148.633894	185.791991	222.754894	260.260697	297.844716	334.602555
12	148.531866	185.607052	222.86885	260.299898	297.543014	334.354046
13	148.644907	185.559144	223.12939	259.832518	296.95551	334.580474
14	148.487541	185.799071	223.141509	260.179839	297.238684	334.515631
15	148.49412	185.818187	223.110507	260.340611	297.170119	334.686127
16	148.62402	185.724318	223.130467	259.989741	297.288408	334.806163
17	148.51484	185.834309	222.87394	260.065101	297.285923	334.330625
18	148.560266	185.941492	223.101371	260.272554	297.033194	335.117352
19	148.542795	185.700651	223.09496	260.258955	297.523493	334.328159
20	148.54457	185.644292	222.861689	260.20083	297.653882	334.309695
21	148.543491	185.678962	223.224613	260.513108	296.851085	334.196446
22	148.554732	185.604953	222.907663	260.263076	297.64733	334.197565
23	148.667461	185.776529	222.944079	260.10418	297.333776	334.760177
24	148.634812	185.654273	222.93497	260.167068	297.63772	334.033739
25	148.611196	185.880865	222.917895	259.876358	297.325034	333.943712
26	148.538941	185.870052	223.012433	260.02487	297.281886	334.451067
27	148.551245	185.621134	222.91257	260.255444	297.140606	334.89955
28	148.51419	185.689918	223.212625	260.277183	297.444075	335.013269
29	148.625335	185.852606	222.932698	260.199741	297.426877	333.842213
30	148.581303	185.788748	222.849463	260.235273	297.789288	334.794652
Average	148.5679404	185.7624828	223.0045358	260.1812631	297.3588999	334.4345759

Fig. 3 Thirty simulations of the end-to-end length, outliers eliminated

Preliminary results under this regime have produced Flory indices deviating no more that about 1% from the theoretical prediction of

$$\nu = \frac{2H + 2}{d + 2}$$

for $d = 1$ and Hurst indices in the range $0.1 \leq H \leq 0.5$.

A more detailed investigation, including a study of parameter dependence and error estimates, is in preparation [3].

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Principal Solutions Revisited

Stephen Clark, Fritz Gesztesy, and Roger Nichols

Dedicated with admiration to Ludwig Streit on the occasion of his 75th birthday

Abstract The main objective of this paper is to identify principal solutions associated with Sturm–Liouville operators on arbitrary open intervals $(a, b) \subseteq \mathbb{R}$, as introduced by Leighton and Morse in the scalar context in 1936 and by Hartman in the matrix-valued situation in 1957, with Weyl–Titchmarsh solutions, as long as the underlying Sturm–Liouville differential expression is nonoscillatory (resp., disconjugate or bounded from below near an endpoint) and in the limit point case at the endpoint in question. In addition, we derive an explicit formula for Weyl–Titchmarsh functions in this case (the latter appears to be new in the matrix-valued context).

Keywords Matrix-valued Schrödinger operators • Weyl–Titchmarsh solutions • principal solutions • oscillation theory

Mathematics Subject Classification (2010) Primary 34B20, 34B24, 34C10; Secondary 34B27, 34L05, 34L40, 47A10, 47E05.

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S. Clark
Department of Mathematics & Statistics, Missouri University of Science and Technology, Rolla, MO 65409, USA
e-mail: sclark@mst.edu

F. Gesztesy (✉)
Department of Mathematics, University of Missouri, Columbia, MO 65211, USA
e-mail: gesztesyf@missouri.edu

R. Nichols
Mathematics Department, The University of Tennessee at Chattanooga, 415 EMCS Building, Dept. 6956, 615 McCallie Ave, Chattanooga, TN 37403, USA
e-mail: Roger-Nichols@utc.edu

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1 Introduction

We dedicate this paper to Ludwig Streit in great appreciation of the tremendous influence he exerted on all those who were permitted a glimpse at his boundless curiosity and approach to all aspects of science. We hope this modest contribution will create some joy for him.

The main focus of this paper centers around Weyl–Titchmarsh and principal solutions for general Sturm–Liouville operators (associated with three coefficients) on arbitrary open intervals $(a, b) \subseteq \mathbb{R}$. We will discuss in great detail the case of scalar coefficients p, q, r associated with the differential expression

$$\ell = \frac{1}{r}\bigg(-\frac{d}{dx} p \frac{d}{dx} + q\bigg), \quad -\infty \leqslant a < x < b \leqslant \infty, \tag{1}$$

and corresponding operator realizations in the Hilbert space $L^2((a, b); rdx)$, as well as the case of $m \times m$ matrix-valued coefficients P, Q, R, $m \in \mathbb{N}$, associated with the differential expression

$$L = R^{-1}\bigg(-\frac{d}{dx} P \frac{d}{dx} + Q\bigg), \quad -\infty \leqslant a < x < b \leqslant \infty, \tag{2}$$

and operator realizations of L in the Hilbert space $L^2((a, b); Rdx; \mathbb{C}^m)$.

Focusing in this introduction for reasons of brevity exclusively on the right end point b, if ℓ is nonoscillatory at b, (real-valued) *principal solutions* $u_b(\lambda, \cdot)$ of $\ell u = \lambda u$, $\lambda \in \mathbb{R}$, are characterized by the condition that $u_b(\lambda, \cdot)$ does not vanish in a neighborhood $[c, b)$ of b (with $c \in (a, b)$) and that

$$\int_c^b dx\, p(x)^{-1} u_b(\lambda, x)^{-2} = \infty. \tag{3}$$

As discussed in Lemma 2.7, $u_b(\lambda, \cdot)$ is unique up to constant (possibly, λ-dependent) multiples and, in a certain sense (made precise in Lemma 2.7), also characterized as the smallest (minimal) possible solution of $\ell u = \lambda u$ near the endpoint b.

In contrast to (3), if ℓ is in the limit point case at b, *Weyl–Titchmarsh solutions* $\psi_+(z, \cdot)$ of $\ell u = zu$, $z \in \mathbb{C}\backslash\mathbb{R}$, are characterized by the condition that for some (and hence for all) $c \in (a, b)$,

$$\psi_+(z, \cdot) \in L^2((c, b); rdx) \quad z \in \mathbb{C}\backslash\mathbb{R}. \tag{4}$$

Again, $\psi_+(z, \cdot)$ is unique up to constant (generally, z-dependent) multiples.

Our main result, Theorem 2.13 in Sect. 2, then proves equality of these solutions (up to constant, possibly spectral parameter dependent multiples) under appropriate assumptions. More precisely, assuming ℓ to be nonoscillatory and in the limit point

case at b, there exists $\lambda_b \in \mathbb{R}$, such that for all $\lambda < \lambda_b$, $x, x_0 \in (a,b)$, with x, x_0 beyond the last zero of $\psi_+(\lambda,\cdot), u_b(\lambda,\cdot)$ (if any),

$$\psi_+(\lambda,x)\psi_+(\lambda,x_0)^{-1} = u_b(\lambda,x)u_b(\lambda,x_0)^{-1}. \tag{5}$$

Here, $\psi_+(\lambda,\cdot)$, $\lambda < \lambda_b$, denotes the extension of $\psi_+(z,\cdot)$, defined initially only for $z \in \mathbb{C}\backslash\mathbb{R}$, to real values $z < \lambda_b$. This extension is permitted on the basis that ℓ is assumed to be nonoscillatory and in the limit point case at b (cf. Remark 2.12).

We also recall Green's function formulas in terms of principal solutions and an explicit formula for the Weyl–Titchmarsh function at the end of Sect. 2, supposing the underlying limit point assumptions on ℓ.

In Sect. 3, the main new section in this paper, we prove the analogous results in the matrix-valued setting. We will be primarily concerned with self-conjugate solutions $U(\lambda,\cdot)$ of $LU = \lambda U$, $\lambda \in \mathbb{R}$, defined by the vanishing of the underlying $m \times m$ matrix-valued Wronskian,

$$W(U(\lambda,\cdot)^*, U(\lambda,\cdot)) = 0, \quad \lambda \in \mathbb{R}. \tag{6}$$

Focusing again exclusively on the endpoint b, a self-conjugate solution $U_b(\lambda,\cdot)$ of $LU = \lambda U$ that is invertible on $[c,b)$ for some $c \in (a,b)$ is called a *principal solution* of $LU = \lambda U$ at b if

$$\lim_{x\uparrow b}\bigg[\int_c^x dx'\, U_b(\lambda,x')^{-1}P(x')^{-1}\big[U_b(\lambda,x')^{-1}\big]^*\bigg]^{-1} = 0. \tag{7}$$

Again, by Lemma 3.6, $U_b(\lambda,\cdot)$ is unique up to right multiplication by invertible (possibly, λ-dependent) constant $m \times m$ matrices, and in a certain sense (detailed in Lemma 3.7) it represents the smallest (minimal) solution of $LU = \lambda U$ near the endpoint b.

In analogy to (4), if L is in the limit point case at b, *Weyl–Titchmarsh solutions* $\Psi_+(z,\cdot)$ of $LU = zU$, $z \in \mathbb{C}\backslash\mathbb{R}$, are then characterized by the condition that for some (and hence for all) $c \in (a,b)$, there exists an invertible $m \times m$ matrix-valued solution $\Psi_+(z,\cdot)$ of $LU = zU$ such that the $m \times m$ matrices

$$\int_c^b dx\, \Psi_+(z,x)^* R(x) \Psi_+(z,x), \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{8}$$

exist. As in the context of principal solutions, $\Psi_+(z,\cdot)$ is unique up to right multiplication by (generally, z-dependent) invertible $m \times m$ matrices and it can be shown that $\Psi_+(z,\cdot)$ is self-conjugate.

Our main result, Theorem 3.11 in Sect. 3, once again proves equality of these solutions (up to right multiplication by possibly, spectral parameter dependent invertible $m \times m$ matrices) under appropriate assumptions. More precisely, assuming the existence of $\lambda_b \in \mathbb{R}$, such that $L - \lambda_b I$ is disconjugate on $[c,b)$ for all $c \in (a,b)$, and supposing L to be in the limit point case at b, then for all $\lambda < \lambda_b$, $x, x_0 \in (a,b)$,

with x, x_0 beyond the last zero of $\det_{\mathbb{C}^m}(\Psi_+(\lambda,\cdot))$, $\det_{\mathbb{C}^m}(U_b(\lambda,\cdot))$ (if any),

$$\Psi_+(\lambda,x)\Psi_+(\lambda,x_0)^{-1} = U_b(\lambda,x)U_b(\lambda,x_0)^{-1}. \tag{9}$$

Moreover, with the normalized $m\times m$ matrix-valued solutions $\Theta(z,\cdot,x_0)$ of $LU = zU$ defined by

$$\Theta(z,x_0,x_0) = I_m, \quad [P(x)\Theta'(z,x,x_0)](x_0)|_{x=x_0} = 0, \tag{10}$$

we will show the following formula for the $m \times m$ matrix-valued Weyl–Titchmarsh function associated with L,

$$M_+(z,x_0) = -\lim_{x\uparrow b}\left[\int_{x_0}^{x} dx'\,\Theta(z,x',x_0)^{-1}P(x')^{-1}\big[\Theta(\bar{z},x',x_0)^{-1}\big]^*\right]^{-1}, \quad z\in\mathbb{C}\backslash\mathbb{R}, \tag{11}$$

assuming L to be in the limit point case at b. If in addition, $Lu = \lambda_b u$ is disconjugate for some $\lambda_b \in \mathbb{R}$, then also

$$M_+(\lambda,x_0) = -\left[\int_{x_0}^{b} dx'\,\Theta(\lambda,x',x_0)^{-1}P(x')^{-1}\big[\Theta(\lambda,x',x_0)^{-1}\big]^*\right]^{-1}, \quad \lambda<\lambda_b, \tag{12}$$

holds, and

$$\begin{aligned}&\big(\xi, M_+(\lambda,x_0)^{-1}\eta\big)_{\mathbb{C}^m}\\ &\quad = -\int_{x_0}^{b} dx'\,\big(\xi,\Theta(\lambda,x',x_0)^{-1}P(x')^{-1}\big[\Theta(\lambda,x',x_0)^{-1}\big]^*\eta\big)_{\mathbb{C}^m}, \quad \lambda<\lambda_b,\ \xi,\eta\in\mathbb{C}^m,\end{aligned} \tag{13}$$

exists as a Lebesgue integral. Both formulas, (11) and (12), are of independent interest and we know of no previous source that recorded them.

Concluding this introduction, we briefly summarize some of the notation used in this paper. If $\mathcal{H}$ is a separable complex Hilbert space the symbol $(\cdot,\cdot)_{\mathcal{H}}$ denotes the scalar product in $\mathcal{H}$ (linear in the second entry). If T is a linear operator mapping (a subspace of) a Hilbert space into another, $\mathrm{dom}(T)$ denotes the domain of T. The spectrum and resolvent set of a closed linear operator in $\mathcal{H}$ will be denoted by $\sigma(\cdot)$ and $\rho(\cdot)$, respectively. The closure of a closable operator S in $\mathcal{H}$ is denoted by $\overline{S}$.

The Banach spaces of bounded and compact linear operators on $\mathcal{H}$ are denoted by $\mathcal{B}(\mathcal{H})$ and $\mathcal{B}_\infty(\mathcal{H})$, respectively.

The symbol I_m, $m \in \mathbb{N}$, represents the identity operator in $\mathbb{C}^m$. The set of $m \times m$ matrices with complex-valued (resp., real-valued) entries is abbreviated by $\mathbb{C}^{m\times m}$ (resp., $\mathbb{R}^{m\times m}$), and similarly, $L^s((c,d);dx)^{m\times m}$ (resp., $L^s_{loc}((c,d);dx)^{m\times m}$)

denotes the set of $m \times m$ matrices with entries belonging to $L^s((c,d);dx)$ (resp., $L^s_{loc}((c,d);dx)$), where $s > 0$ and $a \leqslant c < d \leqslant b$. For notational simplicity, I represents the identity operator in $L^2((a,b);rdx)$ and also in $L^2((a,b);rdx;\mathbb{C}^m)$.

Finally, $\mathbb{C}_+$ (resp., $\mathbb{C}_-$) denotes the open complex upper (resp., lower) half-plane, and we will use the abbreviation "a.e." for "Lebesgue almost everywhere."

2 Basic Facts on Scalar Principal Solutions

In this preparatory section we recall some of the basic facts on oscillation theory with particular emphasis on principal solutions, a notion originally due to Leighton and Morse [68], in connection with scalar Sturm–Liouville operators on arbitrary open intervals $(a,b) \subseteq \mathbb{R}$.

We start by summarizing a few key results in the one-dimensional scalar case, whose extension to the matrix-valued context we are particularly interested in.

Our basic hypothesis in this section will be the following (however, we emphasize that all results in this section have been proved under more general conditions on the coefficients p, q, and for more general differential expressions ℓ, in [16]).

Hypothesis 2.1 *Let $-\infty \leqslant a < b \leqslant \infty$ and suppose that p, q, r are (Lebesgue) measurable on (a,b), and that*

$$\begin{aligned} &p > 0, r > 0 \text{ a.e. on } (a,b), \, q \text{ is real-valued}, \\ &1/p, q, r \in L^1_{loc}((a,b);dx). \end{aligned} \tag{14}$$

Given Hypothesis 2.1, we consider the differential expression

$$\ell = \frac{1}{r}\bigg(-\frac{d}{dx} p \frac{d}{dx} + q \bigg), \quad -\infty \leqslant a < x < b \leqslant \infty, \tag{15}$$

and define the minimal operator T_{min} and maximal operator T_{max} in the Hilbert space $L^2((a,b);rdx)$ associated with ℓ by

$$\begin{aligned} &T_{min} u = \ell u, \\ &u \in \operatorname{dom}(T_{min}) = \big\{ v \in L^2((a,b);rdx) \,\big|\, v, pv' \in AC_{loc}((a,b)); \\ &\qquad\qquad \operatorname{supp}(v) \subset (a,b) \text{ compact}; \, \ell v \in L^2((a,b);rdx) \big\}, \end{aligned} \tag{16}$$

$$\begin{aligned} &T_{max} u = \ell u, \\ &u \in \operatorname{dom}(T_{max}) = \big\{ v \in L^2((a,b);rdx) \,\big|\, v, pv' \in AC_{loc}((a,b)); \\ &\qquad\qquad \ell v \in L^2((a,b);rdx) \big\}, \end{aligned} \tag{17}$$

respectively. Here $AC_{loc}((a,b))$ denotes the set of locally absolutely continuous functions on (a,b).

Then T_{min} is densely defined and [73, p. 64, 88]

$$T_{min}{}^* = T_{max}, \quad T_{max}^* = \overline{T_{min}}. \tag{18}$$

Remark 2.2 (*i*) In obvious notation, we will occasionally write $[p(x_0)u'(x_0)]$ for the quasi-derivative $pu'|_{x=x_0}$.

(*ii*) In the following we will frequently invoke solutions $u(z,\cdot)$ of $\ell u = zu$ for some $z \in \mathbb{C}$. Such solutions are always assumed to be distributional solutions, that is, we tacitly assume

$$u(z,\cdot),\, p(\cdot)u'(z,\cdot) \in AC_{loc}((a,b)) \tag{19}$$

in such a case.

Lemma 2.3 (cf., e.g., [33]) *Assume Hypothesis 2.1.*

(*i*) *Suppose $\ell u = \lambda u$ for some $\lambda \in \mathbb{R}$ with $u(\lambda,\cdot) \geqslant 0$ ($u(\lambda,\cdot) \not\equiv 0$) on (a,b). Then $u(\lambda,\cdot) > 0$ on (a,b).*

(*ii*) *(Harnack's inequality). Let $\mathcal{K} \subset (a,b)$ be compact and $\lambda \in \mathbb{R}$. Then there exists a $C_{\mathcal{K},\lambda} > 0$ such that for all solutions $u(\lambda,\cdot) \geqslant 0$ satisfying $\ell u = \lambda u$, one has*

$$\sup_{x\in\mathcal{K}}(u(\lambda,x)) \leqslant C_{\mathcal{K},\lambda} \inf_{x\in\mathcal{K}}(u(\lambda,x)). \tag{20}$$

Definition 2.4 Assume Hypothesis 2.1.

(*i*) Fix $c \in (a,b)$. Then ℓ is called *nonoscillatory* near a (resp., b) for some $\lambda \in \mathbb{R}$ if and only if every solution $u(\lambda,\cdot)$ of $\ell u = \lambda u$ has finitely many zeros in (a,c) (resp., (c,b)). Otherwise, ℓ is called *oscillatory* near a (resp., b).

(*ii*) Let $\lambda_0 \in \mathbb{R}$. Then T_{min} is bounded from below by λ_0, and one writes $T_{min} \geqslant \lambda_0 I$, if

$$(u, [T_{min} - \lambda_0 I]u)_{L^2((a,b);rdx)} \geqslant 0, \quad u \in \operatorname{dom}(T_{min}). \tag{21}$$

The following is a key result.

Theorem 2.5 ([39, 55, 80, 90]) *Assume Hypothesis 2.1. Then the following assertions are equivalent:*

(*i*) *T_{min} (and hence any symmetric extension of T_{min}) is bounded from below.*

(*ii*) *There exists a $\lambda_0 \in \mathbb{R}$ such that ℓ is nonoscillatory near a and b for all $\lambda < \lambda_0$.*

(*iii*) *For fixed $c \in (a,b)$, there exists a $\lambda_0 \in \mathbb{R}$ such that for all $\lambda < \lambda_0$, $\ell u = \lambda u$ has solutions $u_a(\lambda,\cdot) > 0$, $\hat{u}_a(\lambda,\cdot) > 0$ in a neighborhood $(a,c]$ of a, and solutions $u_b(\lambda,\cdot) > 0$, $\hat{u}_b(\lambda,\cdot) > 0$ in a neighborhood $[c,b)$ of b, such that*

$$W(u_a(\lambda,\cdot), \hat{u}_a(\lambda,\cdot)) = 1, \quad u_a(\lambda,x) = o(\hat{u}_a(\lambda,x)) \text{ as } x \downarrow a, \tag{22}$$

$$W(u_b(\lambda,\cdot),\hat{u}_b(\lambda,\cdot)) = 1, \quad u_b(\lambda,x) = o(\hat{u}_b(\lambda,x)) \text{ as } x \uparrow b, \tag{23}$$

$$\int_a^c dx\, p(x)^{-1} u_a(\lambda,x)^{-2} = \int_c^b dx\, p(x)^{-1} u_b(\lambda,x)^{-2} = \infty, \tag{24}$$

$$\int_a^c dx\, p(x)^{-1} \hat{u}_a(\lambda,x)^{-2} < \infty, \quad \int_c^b dx\, p(x)^{-1} \hat{u}_b(\lambda,x)^{-2} < \infty. \tag{25}$$

Here

$$W(u,v)(x) = u(x)(pv')(x) - (pu')(x)v(x), \quad x \in (a,b), \tag{26}$$

denotes the Wronskian of u and v, assuming $u, (pu'), v, (pv') \in C((a,b))$. In particular, if $\ell u_j = z_j u_j$, $z_j \in \mathbb{C}$, then

$$\frac{d}{dx} W(u_1(z_1,x), u_2(z_2,x)) = (z_1 - z_2) r(x) u_1(z_1,x) u_2(z_2,x), \quad x \in (a,b). \tag{27}$$

Definition 2.6 Assume Hypothesis 2.1 and let $\lambda \in \mathbb{R}$. Then $u_a(\lambda,\cdot)$ (resp., $u_b(\lambda,\cdot)$) in Theorem 2.5 (*iii*) is called a *principal* (or *minimal*) solution of $\ell u = \lambda u$ at a (resp., b). A solution $\tilde{u}_a(\lambda,\cdot)$ (resp., $\tilde{u}_b(\lambda,\cdot)$) of $\ell u = \lambda u$ linearly independent of $u_a(\lambda,\cdot)$ (resp., $u_b(\lambda,\cdot)$) is called *nonprincipal* at a (resp., b).

Principal and nonprincipal solutions are well-defined due to Lemma 2.7 (i) below.

Lemma 2.7 ([39]) *Assume Hypothesis 2.1.*

(*i*) *$u_a(\lambda,\cdot)$ and $u_b(\lambda,\cdot)$ in Theorem 2.5 (iii) are unique up to constant multiples. Moreover, $u_a(\lambda,\cdot)$ and $u_b(\lambda,\cdot)$ are minimal solutions of $\ell u = \lambda u$ in the sense that*

$$u(\lambda,x)^{-1} u_a(\lambda,x) = o(1) \text{ as } x \downarrow a, \tag{28}$$

$$u(\lambda,x)^{-1} u_b(\lambda,x) = o(1) \text{ as } x \uparrow b, \tag{29}$$

for any other solution $u(\lambda,\cdot)$ of $\ell u = \lambda u$ (which is positive near a, resp., b) with $W(u_a(\lambda,\cdot), u(\lambda,\cdot)) \neq 0$, respectively, $W(u_b(\lambda,\cdot), u(\lambda,\cdot)) \neq 0$.

(*ii*) *Let $u(\lambda,\cdot)$ be any positive solution of $\ell u = \lambda u$ near a (resp., b). Then for $c_1 > a$ (resp., $c_2 < b$) sufficiently close to a (resp., b),*

$$\hat{u}_a(\lambda,x) = u(\lambda,x) \int_x^{c_1} dx'\, p(x')^{-1} u(\lambda,x')^{-2} \tag{30}$$

$$\left(\text{resp., } \hat{u}_b(\lambda,x) = u(\lambda,x) \int_{c_2}^x dx'\, p(x')^{-1} u(\lambda,x')^{-2} \right) \tag{31}$$

is a nonprincipal solution of $\ell u = \lambda u$ at a (resp., b). If $\hat{u}_a(\lambda, \cdot)$ (resp., $\hat{u}_b(\lambda, \cdot)$) is a nonprincipal solution of $\ell u = \lambda u$ at a (resp., b) then

$$u_a(\lambda, x) = \hat{u}_a(\lambda, x) \int_a^x dx'\, p(x')^{-1} \hat{u}_a(\lambda, x')^{-2} \tag{32}$$

$$\left(\text{resp., } u_b(\lambda, x) = \hat{u}_b(\lambda, x) \int_x^b dx'\, p(x')^{-1} \hat{u}_b(\lambda, x')^{-2} \right) \tag{33}$$

is principal at a (resp., b).

The following two theorems describe a fundamental link between spectral theory and non-oscillation results.

Theorem 2.8 ([39]) *Assume Hypothesis 2.1 and let $\lambda_0 \in \mathbb{R}$. Then the following assertions are equivalent:*

(*i*) $T_{min} \geqslant \lambda_0 I$.
(*ii*) *There exists a positive (distributional) solution $u > 0$ of $\ell v = \lambda_0 v$ on (a, b).*

For the proof of Theorem 2.8 one notes that Theorems XI.6.1 and XI.6.2 and Corollary XI.6.1 in Hartman's monograph [39] extend to our more general hypotheses on p, q, r without modifications. In particular, item (*ii*) implies item (*i*) by Jacobi's factorization identity

$$\begin{aligned} -(pg')' + h^{-1}(ph')'g &= -h^{-1}(ph^2(g/h)')', \\ 0 < h,\, ph' &\in AC_{loc}((a,b)),\ g \in \operatorname{dom}(T_{min}). \end{aligned} \tag{34}$$

Theorem 2.9 (Dunford–Schwartz [15], Theorem XIII.7.40, [16], Section 11) *Suppose Hypothesis 2.1. Then the following assertions hold:*

(*i*) *T_{min} is not bounded from below if and only if for all $\lambda \in \mathbb{R}$, every solution $u(\lambda, \cdot)$ of $\ell u = \lambda u$ has infinitely many zeros on (a, b).*
(*ii*) *If T_{min} is bounded from below and $\mu_0 = \inf(\sigma_{ess}(T))$ for some self-adjoint extension T of T_{min}, then, for $\lambda > \mu_0$, every solution $u(\lambda, \cdot)$ of $\ell u = \lambda u$ has infinitely many zeros on (a, b), while, for $\lambda < \mu_0$, no solution $u(\lambda, \cdot)$ of $\ell u = \lambda u$ has infinitely many zeros on (a, b).*

Thus, the existence of positive solutions on (a, b) can be used to characterize $\inf(\sigma(T))$ while the existence of nonoscillatory solutions can be used to characterize $\inf(\sigma_{ess}(T))$. Without going into further details at this point, we note that under appropriate assumptions on the coefficients, these characterizations extend to elliptic partial differential operators. We also note that eigenvalue counts in essential spectral gaps in terms of (renormalized) oscillation theory in terms of zeros of Wronskians, rather than zeros of eigenfunctions, was established in [29]. For additional work in this direction we refer to [63–65].

Next, in order to set up the connection between principal and Weyl–Titchmarsh solutions, we recall Weyl's definition of the limit point property of ℓ at the endpoint a (resp., b).

Definition 2.10 Assume Hypothesis 2.1 and let $z \in \mathbb{C}\backslash\mathbb{R}$. Then ℓ is said to be in the *limit point case* (*l.p.c.*) *at* b (*resp.*, a) if for some (and hence for all) $c \in (a, b)$, there exists a unique solution (up to constant multiples) $\psi_+(z, \cdot)$ (resp., $\psi_-(z, \cdot)$) of $\ell u = zu$ such that

$$\psi_+(z, \cdot) \in L^2((c, b); rdx) \ \big(\text{resp., } \psi_-(z, \cdot) \in L^2((a, c); rdx)\big). \tag{35}$$

The constants permitted above in Definition 2.10 (while of course x-independent) are generally z-dependent.

One notes that L^2-solutions $u_\pm(z, \cdot)$ of $\ell u = zu$ in a neighborhood of a and b always exist. What singles out the limit point case for ℓ at a or b is the uniqueness (up to constant multiples) of the L^2-solution $\psi_+(z, \cdot)$, respectively, $\psi_-(z, \cdot)$ in Definition 2.10.

Any solution of $\ell u = zu$ satisfying the square integrability in (35) in a neighborhood of b (resp., a), independent of whether it is unique up to constant multiples or not, is called a *Weyl–Titchmarsh solution* of $\ell u = zu$ near b (resp., a).

We continue with the fact that nonoscillatory behavior at one end point plus a simple condition on r/p implies the limit point property at that endpoint:

Lemma 2.11 (Hartman [37], see also [16], Section 11, [26, 75, 80]) *Assume Hypothesis 2.1, let $c \in (a, b)$, and suppose that for some $\lambda_0 \in \mathbb{R}$, $\ell - \lambda_0$ is nonoscillatory near $d \in \{a, b\}$. Then, if*

$$\left| \int_c^d dx\, [r(x)/p(x)]^{1/2} \right| = \infty, \tag{36}$$

ℓ is in the limit point case at d.

Hartman's elegant proof of Lemma 2.11 in [37] is based on an application of (non)principal solutions of $\ell u = \lambda u$.

Remark 2.12 Assuming ℓ to be nonoscillatory and in the limit point case at a (resp., b), one recalls that ψ_- (resp., ψ_+) in (35) analytically extends to $z < \lambda_a$ for some $\lambda_a \in \mathbb{R}$ (resp., $z < \lambda_b$ for some $\lambda_b \in \mathbb{R}$). In particular, for fixed $x \in (a, b)$, $\psi_-(\cdot, x)$ (resp., $\psi_+(\cdot, x)$) is analytic in $\mathbb{C}\backslash[\lambda_a, \infty)$ (resp., $\mathbb{C}\backslash[\lambda_b, \infty)$). For more details in this context we refer to the comments following [29, Proposition 1.1].

Next, we fix a reference point $x_0 \in (a, b)$, and introduce the normalized solutions $\phi(z, \cdot, x_0)$ and $\theta(z, \cdot, x_0)$ of $\ell u = zu$ by

$$\begin{aligned} &\phi(z, x_0, x_0) = 0, \quad [p(x)\phi'(z, x, x_0)]_{x=x_0} = 1, \\ &\theta(z, x_0, x_0) = 1, \quad [p(x)\theta'(z, x, x_0)]_{x=x_0} = 0, \end{aligned} \tag{37}$$

with prime $'$ denoting $\partial/\partial x$, one infers (from the z-independence of the initial conditions in (37)) that for fixed $x \in (a,b)$, $\phi(\cdot\,,x,x_0)$ and $\theta(\cdot\,,x,x_0)$ are entire with respect to $z \in \mathbb{C}$ and that

$$W(\theta(z,\cdot\,,x_0),\phi(z,\cdot\,,x_0)) = 1, \quad z \in \mathbb{C},\ x_0 \in (a,b). \tag{38}$$

Consequently, if $u_\pm(z,\cdot\,)$ denote *any* nontrivial square integrable solutions of $\ell u = zu$ in a neighborhood of a and b, that is, for some (and hence for all) $c \in (a,b)$,

$$u_+(z,\cdot\,) \in L^2((c,b);rdx), \quad u_-(z,\cdot\,) \in L^2((a,c);rdx), \tag{39}$$

one obtains $u_\pm(z,x_0) \neq 0$, and

$$\begin{aligned} u_\pm(z,x)u_\pm(z,x_0)^{-1} &= \theta(z,x,x_0) + \phi(z,x,x_0)m_\pm(z,x_0), \\ &\qquad z \in \mathbb{C}\backslash\mathbb{R},\ x,x_0 \in (a,b), \end{aligned} \tag{40}$$

for some coefficients $m_\pm(\cdot\,,x_0)$, the Weyl–Titchmarsh functions associated with ℓ.

The function $m_+(z,x_0)$ (resp., $m_-(z,x_0)$) is uniquely determined if and only if ℓ is in the limit point case at b (resp., a). In this case $u_+(z,\cdot\,)$ (resp., $u_-(z,\cdot\,)$) coincides up to z-dependent constant multiples with $\psi_+(z,\cdot\,)$ (resp., $\psi_-(z,\cdot\,)$) in (35).

Moreover, $\pm m_\pm(\cdot\,,x_0)$ are Nevanlinna–Herglotz functions, that is, for all $x_0 \in (a,b)$,

$$m_\pm(\cdot\,,x_0) \text{ are analytic in } \mathbb{C}\backslash\mathbb{R}, \tag{41}$$

and

$$\pm \operatorname{Im}(m_\pm(z,x_0)) > 0, \quad z \in \mathbb{C}_+. \tag{42}$$

In addition, for all $x_0 \in (a,b)$, $m_\pm(\cdot\,,x_0)$ satisfy

$$m_\pm(z,x_0) = \overline{m_\pm(\overline{z},x_0)}, \quad z \in \mathbb{C}_+. \tag{43}$$

Finally, one also infers for all $z \in \mathbb{C}\backslash\mathbb{R}$, $x_0 \in (a,b)$,

$$W(u_+(z,\cdot\,),u_-(z,\cdot\,)) = [m_-(z,x_0) - m_+(z,x_0)]u_+(z,x_0)u_-(z,x_0), \tag{44}$$

$$m_\pm(z,x_0) = [p(x_0)u'_\pm(z,x_0)]/u_\pm(z,x_0). \tag{45}$$

Given these preparations we can finally state the main result of this section which identifies principal and Weyl–Titchmarsh solutions at an endpoint where ℓ is nonoscillatory and in the limit point case:

Theorem 2.13 *Assume Hypothesis 2.1.*

(*i*) *If ℓ is nonoscillatory and in the limit point case at b, then there exists $\lambda_b \in \mathbb{R}$, such that for all $\lambda < \lambda_b$, $x, x_0 \in (a,b)$, with x, x_0 to the right of the last zero of $\psi_+(\lambda,\cdot), u_b(\lambda,\cdot)$ (if any),*

$$\psi_+(\lambda,x)\psi_+(\lambda,x_0)^{-1} = u_b(\lambda,x)u_b(\lambda,x_0)^{-1}, \tag{46}$$

that is, $\psi_+(\lambda,\cdot)$ and $u_b(\lambda,\cdot)$, $\lambda < \lambda_b$, are constant multiples of each other.

(*ii*) *If ℓ is nonoscillatory and in the limit point case at a, then there exists $\lambda_a \in \mathbb{R}$, such that for all $\lambda < \lambda_a$, $x, x_0 \in (a,b)$, with x, x_0 to the left of the first zero of $\psi_-(\lambda,\cdot), u_a(\lambda,\cdot)$ (if any),*

$$\psi_-(\lambda,x)\psi_-(\lambda,x_0)^{-1} = u_a(\lambda,x)u_a(\lambda,x_0)^{-1}, \tag{47}$$

that is, $\psi_-(\lambda,\cdot)$ and $u_a(\lambda,\cdot)$, $\lambda < \lambda_a$ are constant multiples of each other.

Proof It suffices to consider the case of ψ_+ and u_b. Then, if ψ_+ is a nonprincipal solution of $\ell u = \lambda u$, Lemma 2.7 (*i*) implies the existence of $C_+ > 0$ and $c \in (a,b)$, such that for all $\lambda < \lambda_b$ and for all $x \in (c,b)$,

$$|u_b(\lambda,x)| \leqslant C_+|\psi_+(\lambda,x)|. \tag{48}$$

Thus, $u_b(\lambda,\cdot) \in L^2((c,b);rdx)$. But since by hypothesis ψ_+ and u_b are linearly independent, $W(\psi_+(\lambda,\cdot), u_b(\lambda,\cdot)) \neq 0$, this contradicts the limit point hypothesis at b which yields precisely one $L^2((c,b);rdx)$-solution up to constant (generally, λ-dependent) multiples. □

In particular, if T_{min} is bounded from below by $\lambda_0 \in \mathbb{R}$ and essentially self-adjoint, then for all $\lambda < \lambda_0$, principal and Weyl–Titchmarsh solutions at an endpoint coincide up to constant (λ-dependent) multiples.

We briefly follow up with the connection between Green's functions and principal solutions for Sturm–Liouville operators, illustrating once more the relevance of principal solutions.

Lemma 2.14 *Assume Hypothesis 2.1 and suppose that $T_{min} \geqslant \lambda_0 I$ for some $\lambda_0 \in \mathbb{R}$. In addition, assume that ℓ is in the limit point case at a and b. Then*

$$\overline{T_{min}} = T_{max} := T \tag{49}$$

is the unique self-adjoint extension of T_{min} in $L^2((a,b);rdx)$ and for any $x_0 \in (a,b)$,

$$\begin{aligned} 0 < G(\lambda,x,x') = \bigg(\int_{x_0}^{b} dt\, p(t)^{-1}u_a(\lambda,t)^{-2}\bigg)u_b(\lambda,x_0)^{-1}u_a(\lambda,x_0)\times \\ \times \begin{cases} u_a(\lambda,x)u_b(\lambda,x'), & a < x \leqslant x' < b, \\ u_a(\lambda,x')u_b(\lambda,x), & a < x' \leqslant x < b, \end{cases} \quad \lambda < \lambda_0, \end{aligned} \tag{50}$$

is the positive Green's function of T. Here we abbreviated

$$G(z,x,x') = (T - zI)^{-1}(x,x'), \quad x,x' \in (a,b),\ z \in \mathbb{C}\backslash[\lambda_0,\infty). \tag{51}$$

As a consequence of Theorem 2.13, $u_a(\lambda,\cdot)$ and $u_b(\lambda,\cdot)$ in the Green's function representation (50) can be replaced by $\psi_-(z,\cdot)$ and $\psi_+(z,\cdot)$. More precisely, an additional analytic continuation with respect to $z \in \mathbb{C}\backslash[\lambda_0,\infty)$ yields

$$G(z,x,x') = \frac{1}{W(\psi_+(z,\cdot),\psi_-(z,\cdot))} \begin{cases} \psi_-(z,x)\psi_+(z,x'), & a < x \leqslant x' < b, \\ \psi_+(z,x)\psi_-(z,x'), & a < x' \leqslant x < b, \end{cases}$$
$$z \in \mathbb{C}\backslash[\lambda_0,\infty), \tag{52}$$

where for all $z \in \mathbb{C}\backslash[\lambda_0,\infty)$, $x_0 \in (a,b)$,

$$W(\psi_+(z,\cdot),\psi_-(z,\cdot)) = [m_-(z,x_0) - m_+(z,x_0)]\psi_+(z,x_0)\psi_-(z,x_0), \tag{53}$$
$$m_\pm(z,x_0) = [p(x_0)\psi'_\pm(z,x_0)]/\psi_\pm(z,x_0). \tag{54}$$

The material in Lemma 2.3–Theorem 2.9, Lemmas 2.11 and 2.14 (and considerably more) is discussed in great detail in [33] (with special emphasis on the Friedrichs extension T_F of T_{min}), and under more general conditions on ℓ and its coefficients in [16].

We conclude this section by recalling a known formula for $m_+(\cdot,x_0)$ (resp., $m_-(\cdot,x_0)$) whenever ℓ is in the limit point case and nonoscillatory at b (resp., a): Assuming the limit point case of ℓ at b (resp., at a), it is well-known that

$$\begin{aligned} &m_+(z,x_0) = -\lim_{x\uparrow b} \theta(z,x,x_0)/\phi(z,x,x_0), \quad z \in \mathbb{C}\backslash\mathbb{R}, \\ &\text{(resp., } m_-(z,x_0) = -\lim_{x\downarrow a} \theta(z,x,x_0)/\phi(z,x,x_0), \quad z \in \mathbb{C}\backslash\mathbb{R}). \end{aligned} \tag{55}$$

Next, fix $z \in \mathbb{C}$ and suppose that $v(z,\cdot,x_0)$ satisfies $\ell u = zu$ and $v(z,x) \neq 0$ for $x \in [x_0,b)$, then clearly $w(z,\cdot,x_0)$ defined by

$$w(z,x) = v(z,x,x_0)\bigg[C_1 + C_2 \int_{x_0}^{x} dx'\, p(x')^{-1} v(z,x',x_0)^{-2}\bigg], \quad x \in [x_0,b), \tag{56}$$

is a solution of $\ell u = zu$ satisfying $W(v(z,\cdot,x_0), w(z,\cdot,x_0)) = C_2$. An elementary application of these facts to $\phi(z,\cdot,x_0)$ and $\theta(z,\cdot,x_0)$, taking into account that $\theta(z,x,x_0) \neq 0$, $z \in \mathbb{C}\backslash\mathbb{R}$, $x,x_0 \in (a,b)$, yields

$$\phi(z,x,x_0) = \theta(z,x,x_0) \int_{x_0}^{x} dx'\, p(x')^{-1} \theta(z,x',x_0)^{-2}, \quad z \in \mathbb{C}\backslash\mathbb{R},\ x,x_0 \in (a,b). \tag{57}$$

Insertion of (57) into (55) yields the interesting formula,

$$m_+(z,x_0) = -\lim_{x\uparrow b}\bigg[\int_{x_0}^{x} dx'\, p(x')^{-1}\theta(z,x',x_0)^{-2}\bigg]^{-1}, \quad z\in\mathbb{C}\backslash\mathbb{R}. \tag{58}$$

If in addition, ℓ is nonoscillatory at b, analytic continuation of both sides in (58) with respect to z permits one to extend (58) to all $z\in\mathbb{C}\backslash[\lambda_b,\infty)$, with λ_b as in Theorem 2.13 (i). We also note that for $\lambda<\lambda_b$, the expression

$$\bigg[\int_{x_0}^{x} dx'\, p(x')^{-1}\theta(\lambda,x',x_0)^{-2}\bigg]^{-1}, \quad \lambda<\lambda_b, \tag{59}$$

is strictly monotonically decreasing with respect to x and hence the existence of the limit of the integral in (59) as $x\uparrow b$ is guaranteed and one obtains

$$m_+(\lambda,x_0) = -\bigg[\int_{x_0}^{b} dx'\, p(x')^{-1}\theta(\lambda,x',x_0)^{-2}\bigg]^{-1}, \quad \lambda<\lambda_b, \tag{60}$$

with $\int_{x_0}^{b} dx'\cdots$ in (60) representing a Lebesgue integral.

We first found (60) mentioned without proof in a paper by Kotani [58]. Kotani kindly alerted us to a paper by Kac and Krein [54], where such a formula is discussed near the end of their section 2, but the precise history of (60) is unknown to us at this point. We will provide a detailed derivation of (58), (60) in the matrix-valued context in Sect. 3.

Next, replacing $\phi(z,\cdot\,,x_0),\theta(z,\cdot\,,x_0)$ satisfying $\ell u = zu$ and (37) by the more general $\phi_\alpha(z,\cdot\,,x_0),\theta_\alpha(z,\cdot\,,x_0)$ satisfying $\ell u = zu$ and

$$\begin{aligned}
&\phi_\alpha(z,x_0,x_0) = -\sin(\alpha), \quad [p(x)\phi_\alpha'(z,x,x_0)]|_{x=x_0} = \cos(\alpha),\\
&\theta_\alpha(z,x_0,x_0) = \cos(\alpha), \quad [p(x)\theta_\alpha'(z,x_0,x_0)]|_{x=x_0} = \sin(\alpha),
\end{aligned} \tag{61}$$

for some $\alpha\in[0,\pi)$, and hence replacing (40) by

$$\begin{aligned}
u_{\pm,\alpha}(z,x) = \theta_\alpha(z,x,x_0) + \phi_\alpha(z,x,x_0)m_{\pm,\alpha}(z,x),\\
z\in\mathbb{C}\backslash\mathbb{R},\ x,x_0\in(a,b),
\end{aligned} \tag{62}$$

for appropriate Weyl–Titchmarsh coefficients $m_{\pm,\alpha}(\,\cdot\,,x_0)$, one obtains along the lines leading to (57) for $z\in\mathbb{C}\backslash\mathbb{R}$,

$$\begin{aligned}
\phi_\alpha(z,x,x_0) = -\tan(\alpha)\theta_\alpha(z,x,x_0) + \theta_\alpha(z,x,x_0)\int_{x_0}^{x}\frac{dx'}{p(x')\theta_\alpha(z,x',x_0)^2},\\
\alpha\in[0,\pi)\backslash\{\pi/2\},
\end{aligned} \tag{63}$$

$$\theta_\alpha(z,x,x_0) = -\cot(\alpha)\phi_\alpha(z,x,x_0) - \phi_\alpha(z,x,x_0)\int_{x_0}^{x} \frac{dx'}{p(x')\phi_\alpha(z,x',x_0)^2}, \qquad (64)$$
$$\alpha \in (0,\pi),$$

and using

$$m_{+,\alpha}(z,x_0) = -\lim_{x\uparrow b} \theta_\alpha(z,x,x_0)/\phi_\alpha(z,x,x_0), \quad z \in \mathbb{C}\backslash\mathbb{R}, \qquad (65)$$

one now obtains

$$m_{+,\alpha}(z) = \begin{cases} \left[\tan(\alpha) - \lim_{x\uparrow b}\int_{x_0}^{x} dx'\, p(x')^{-1}\theta_\alpha(z,x',x_0)^{-2}\right]^{-1}, & \alpha \in [0,\pi)\backslash\{\pi/2\}, \\ \cot(\alpha) + \lim_{x\uparrow b}\int_{x_0}^{x} dx'\, p(x')^{-1}\phi_\alpha(z,x',x_0)^{-2}, & \alpha \in (0,\pi), \end{cases}$$
$$z \in \mathbb{C}\backslash\mathbb{R}, \qquad (66)$$

whenever ℓ is in the limit point case at b (and similarly for $z < \lambda_{b,\alpha}$ for an appropriate $\lambda_{b,\alpha} \in \mathbb{R}$, and a Lebesgue integral $\int_{x_0}^{b} dx' \cdots$ if ℓ is also nonoscillatory at b).

Replacing $\lim_{x\uparrow b}\int_{x_0}^{x} dx' \cdots$ by $-\lim_{x\downarrow a}\int_{x}^{x_0} dx' \cdots$, all formulas for $m_+(\cdot,x_0)$ and $m_{+,\alpha}(\cdot,x_0)$ immediately extend to $m_-(\cdot,x_0)$ and $m_{-,\alpha}(\cdot,x_0)$, assuming ℓ to be in the limit point case at a (and analogously if ℓ is also nonoscillatory at a).

3 Matrix-Valued Principal Solutions

This section is devoted to an extension of some of the basic results on principal solutions of the previous Sect. 2 to those associated with matrix-valued singular Sturm–Liouville operators.

Matrix oscillation theory relevant to this paper originated with Hartman [38] and Reid [76]. The literature on oscillation theory for systems of differential equations is so rich by now that we cannot possibly offer a comprehensive list of references. Hence, we restrict ourselves primarily to a number of monographs by Coppel [14, Ch. 2], Hartman [39, Sects. X.10, X.11], Hille [41, Sect. 9.6], [42], Kratz [62, Chs. 4, 7], Reid [78, Ch. VII], [79, Ch. V], Rofe-Beketov and Kholkin [84, Chs. 1–4], and a few additional such as [4, 6, 9, 17, 21–24, 36, 51, 77, 83], and [95].

Basic Weyl–Titchmarsh theory and general spectral theory for matrix-valued singular Sturm–Liouville operators as well as the more general case of singular Hamiltonian systems has been derived in detail by Hinton and Shaw [46–50] (we also refer to [8, Ch. 10], [10–13, 22, 27, 30], [41, Sect. 10.7], [43–45, 52, 53, 57, 59–61, 69, 74, 81, 89, 94] for pertinent spectral results in this connection).

In the following we take these developments for granted and only focus on the required changes in Sect. 2 in connection with principal solutions which are implied by inherent noncommutativity issues due to the matrix-valued setting.

The basic assumptions for this section then read as follows:

Hypothesis 3.1 *Let $-\infty \leqslant a < b \leqslant \infty$ and suppose that $P, Q, R \in \mathbb{C}^{m\times m}$, $m \in \mathbb{N}$, have (Lebesgue) measurable entries on (a, b), and that*

$$\begin{aligned} &P > 0, R > 0 \text{ a.e. on } (a, b),\ Q = Q^* \text{ is self-adjoint},\\ &P^{-1}, Q, R \in L^1_{loc}((a, b); dx)^{m\times m}. \end{aligned} \tag{67}$$

In addition, we introduce the Hilbert space of $\mathbb{C}^m$-valued elements,

$$\begin{aligned} L^2((a, b); Rdx; \mathbb{C}^m) = \Big\{ &U = (U_1, \dots, U_m)^\top, U_k \text{ (Lebesgue) measurable},\\ &1 \leqslant k \leqslant m \,\Big|\, \int_{(a,b)} dx\, (U(x), R(x)U(x))_{\mathbb{C}^m} < \infty \Big\}, \end{aligned} \tag{68}$$

with associated scalar product

$$\begin{aligned} (U, V)_{L^2((a,b);Rdx;\mathbb{C}^m)} = \int_{(a,b)} &dx\, (U(x), R(x)V(x))_{\mathbb{C}^m},\\ &U, V \in L^2((a, b); Rdx; \mathbb{C}^m). \end{aligned} \tag{69}$$

Here $(\dots)^\top$ indicates a column vector in $\mathbb{C}^m$ and $(\cdot, \cdot)_{\mathbb{C}^m}$ represents the standard scalar product in $\mathbb{C}^m$, that is,

$$(w_1, w_2)_{\mathbb{C}^m} = \sum_{k=1}^m \overline{w_{1,k}} w_{2,k}, \quad w_j = (w_{j,1}, \dots, w_{j,m})^\top \in \mathbb{C}^m,\ j = 1, 2. \tag{70}$$

Given Hypothesis 3.1, we consider the differential expression

$$L = R^{-1}\Big(-\frac{d}{dx} P \frac{d}{dx} + Q \Big), \quad -\infty \leqslant a < x < b \leqslant \infty, \tag{71}$$

and once more define the minimal operator T_{min} and maximal operator T_{max} in $L^2((a, b); Rdx; \mathbb{C}^m)$ associated with L by

$$\begin{aligned} &T_{min} u = Lu,\\ &u \in \mathrm{dom}(T_{min}) = \big\{ v \in L^2((a, b); Rdx; \mathbb{C}^m) \,\big|\, v, Pv' \in AC_{loc}((a, b))^{m\times 1};\\ &\qquad \mathrm{supp}\,(v) \subset (a, b) \text{ compact}; \ Lv \in L^2((a, b); Rdx; \mathbb{C}^m) \big\}, \end{aligned} \tag{72}$$

$$T_{max}u = Lu,$$
$$u \in \mathrm{dom}(T_{max}) = \big\{v \in L^2((a,b);Rdx;\mathbb{C}^m) \,\big|\, v, Pv' \in AC_{loc}((a,b))^{m\times 1}; \quad Lv \in L^2((a,b);Rdx;\mathbb{C}^m)\big\}, \tag{73}$$

respectively. Here $AC_{loc}((a,b))^{m\times n}$ denotes the set of $m \times n$ matrices, $m, n \in \mathbb{N}$, with locally absolutely continuous entries on (a,b) (we will use the analogous in connection with $C((a,b))^{m\times n}$ below).

Again, T_{min} is densely defined and

$$T_{min}{}^* = T_{max}, \quad T_{max}^* = \overline{T_{min}}. \tag{74}$$

In the following, matrix-valued solutions $U(z,\cdot)$ of $LU = zU$ for some $z \in \mathbb{C}$, are always assumed to be distributional solutions, in addition, we either assume the vector-valued

$$u(z,\cdot),\, Pu'(z,\cdot) \in AC_{loc}((a,b))^{m\times 1}, \tag{75}$$

or the $m \times m$ matrix-valued case

$$U(z,\cdot),\, PU'(z,\cdot) \in AC_{loc}((a,b))^{m\times m}, \tag{76}$$

in this context. In fact, assuming $U, (PU'), V, (PV') \in C((a,b))^{m\times m}$, one introduces the matrix-valued Wronskian of u and v by

$$W(U,V)(x) = U(x)(PV')(x) - (PU')(x)V(x), \quad x \in (a,b), \tag{77}$$

and if U_j are $m \times m$ matrix solutions of $LU_j = z_jU_j$, $z_j \in \mathbb{C}$, then

$$\frac{d}{dx}W(U_1(\overline{z_1},x)^*, U_2(z_2,x)) = (z_1 - z_2)U_1(\overline{z_1},x)^*R(x)U_2(z_2,x), \quad x \in (a,b). \tag{78}$$

Definition 3.2 Assume Hypothesis 3.1 and let $z \in \mathbb{C}\backslash\mathbb{R}$. Then L is said to be in the *limit point case* (*l.p.c.*) *at* b (*resp., a*) if for some (and hence for all) $c \in (a,b)$, there exists a unique invertible $m \times m$ matrix-valued solution (up to constant multiples by right multiplication with invertible $m \times m$ matrices) $\Psi_+(z,\cdot)$ (resp., $\Psi_-(z,\cdot)$) of $LU = zU$ such that the $m \times m$ matrices

$$\int_c^b dx\, \Psi_+(z,x)^*R(x)\Psi_+(z,x) \ \left(\text{resp.}, \int_a^c dx\, \Psi_-(z,x)^*R(x)\Psi_-(z,x)\right) \tag{79}$$

exist.

Again, the constant invertible $m \times m$ matrices permitted in connection with right multiplication in Definition 3.2 (while of course x-independent) are generally z-dependent.

Given the analogy to the scalar case $m = 1$, any solution of $LU = zU$ satisfying the square integrability condition (79) in a neighborhood of b (resp., a), independent of uniqueness up to right multiplication by constant invertible matrices, will be called a ($m \times m$ matrix-valued) Weyl–Titchmarsh solution of $LU = zU$ near b (resp., a).

Remark 3.3 Assuming there exists a $\lambda_a \in \mathbb{R}$ (resp., $\lambda_b \in \mathbb{R}$) for which $(u, [T_{min} - \lambda_a I]u)_{L^2((a,b);Rdx;\mathbb{C}^m)} \geqslant 0$ for all $u \in \operatorname{dom}(T_{min})$ with $u = 0$ in a neighborhood of b (resp., $(u, [T_{min} - \lambda_b I]u)_{L^2((a,b);Rdx;\mathbb{C}^m)} \geqslant 0$ for all $u \in \operatorname{dom}(T_{min})$ with $u = 0$ in a neighborhood of a) and that L is in the limit point case at a (resp., b), then Ψ_- (resp., Ψ_+) in (79) analytically extends to $z < \lambda_a$ (resp., $z < \lambda_b$). In particular, for fixed $x \in (a, b)$, $\Psi_-(\cdot\,, x)$ (resp., $\Psi_+(\cdot\,, x)$) is analytic in $\mathbb{C}\backslash[\lambda_a, \infty)$ (resp., $\mathbb{C}\backslash[\lambda_b, \infty)$) (cf. the analogous Remark 2.12 in the scalar context).

We shall now turn to a brief summary of the principal facts of Weyl–Titchmarsh theory in the present matrix-valued context. Again, we fix a reference point $x_0 \in (a, b)$, and introduce the normalized $m \times m$ matrix-valued solutions $\Phi(z, \cdot\,, x_0)$ and $\Theta(z, \cdot\,, x_0)$ of $LU = zU$ by

$$\begin{aligned} &\Phi(z, x_0, x_0) = 0, \quad [P(x)\Phi'(z, x, x_0)]|_{x=x_0} = I_m, \\ &\Theta(z, x_0, x_0) = I_m, \quad [P(x)\Theta'(z, x, x_0)]|_{x=x_0} = 0, \end{aligned} \tag{80}$$

and note again that for fixed $x \in (a, b)$, $\Phi(\cdot\,, x, x_0)$ and $\Theta(\cdot\,, x, x_0)$ are entire with respect to $z \in \mathbb{C}$. Moreover, one verifies (cf., e.g., [11, Sect. 2], [31, Sect. 2]) that for any $z \in \mathbb{C}$, $x_0 \in (a, b)$,

$$W(\Theta(\overline{z}, \cdot\,, x_0)^*, \Phi(z, \cdot\,, x_0)) = I_m, \tag{81}$$

$$W(\Phi(\overline{z}, \cdot\,, x_0)^*, \Theta(z, \cdot\,, x_0)) = I_m, \tag{82}$$

$$W(\Phi(\overline{z}, \cdot\,, x_0)^*, \Phi(z, \cdot\,, x_0)) = 0, \tag{83}$$

$$W(\Theta(\overline{z}, \cdot\,, x_0)^*, \Theta(z, \cdot\,, x_0)) = 0, \tag{84}$$

as well as,

$$\Phi(z, x, x_0)\Theta(\overline{z}, x, x_0)^* - \Theta(z, x, x_0)\Phi(\overline{z}, x, x_0)^* = 0, \tag{85}$$

$$\begin{aligned} &[P(x)\Phi'(z, x, x_0)][P(x)\Theta'(\overline{z}, x, x_0)]^* \\ &\quad - [P(x)\Theta'(z, x, x_0)][P(x)\Phi'(\overline{z}, x, x_0)]^* = 0, \end{aligned} \tag{86}$$

$$[P(x)\Phi'(z, x, x_0)]\Theta(\overline{z}, x, x_0)^* - [P(x)\Theta'(z, x, x_0)]\Phi(\overline{z}, x, x_0)^* = I_m, \tag{87}$$

$$\Theta(z, x, x_0)[P(x)\Phi'(\overline{z}, x, x_0)]^* - \Phi(z, x, x_0)[P(x)\Theta'(\overline{z}, x, x_0)]^* = I_m. \tag{88}$$

Consequently, if $U_\pm(z,\cdot)$ denote *any* invertible square integrable $m\times m$ matrix-valued solutions of $LU = zU$ in a neighborhood of a and b in the sense that for some (and hence for all) $c\in(a,b)$, the $m\times m$ matrices

$$\int_c^b dx\, U_+(z,x)^* R(x) U_+(z,x), \quad \int_a^c dx\, U_-(z,x)^* R(x) U_-(z,x), \tag{89}$$

exist, one obtains

$$\begin{aligned} U_\pm(z,x)U_\pm(z,x_0)^{-1} = \Theta(z,x,x_0) + \Phi(z,x,x_0)M_\pm(z,x_0), \\ z\in\mathbb{C}\backslash\mathbb{R},\ x,x_0\in(a,b), \end{aligned} \tag{90}$$

for some $m\times m$ matrix-valued coefficients $M_\pm(z,x_0)\in\mathbb{C}^{m\times m}$, the Weyl–Titchmarsh matrices associated with L.

Again, the matrix $M_+(z,x_0)$ (resp., $M_-(z,x_0)$) is uniquely determined if and only if L is in the limit point case at b (resp., a). In this case $U_+(z,\cdot)$ (resp., $U_-(z,\cdot)$) coincides up to right multiplication by z-dependent constant matrices with $\Psi_+(z,\cdot)$ (resp., $\Psi_-(z,x_0)$) in (79).

Moreover, $\pm M_\pm(\cdot\,,x_0)$ are $m\times m$ Nevanlinna–Herglotz matrices, that is, for all $x_0\in(a,b)$,

$$M_\pm(\cdot\,,x_0) \text{ are analytic in } \mathbb{C}\backslash\mathbb{R}, \quad \operatorname{rank}\big(M_\pm(z,x_0)\big) = m,\ z\in\mathbb{C}_+, \tag{91}$$

and

$$\pm\operatorname{Im}(M_\pm(z,x_0)) > 0, \quad z\in\mathbb{C}_+. \tag{92}$$

(Here, in obvious notation, $\operatorname{Im}(M) = (2i)^{-1}(M-M^*)$, $M\in\mathbb{C}^{m\times m}$.) In addition, for all $x_0\in(a,b)$, $M_\pm(\cdot\,,x_0)$ satisfy

$$M_\pm(z,x_0) = M_\pm(\bar z,x_0)^*, \quad z\in\mathbb{C}_+. \tag{93}$$

Finally, one also infers for all $z\in\mathbb{C}\backslash\mathbb{R}$, $x_0\in(a,b)$,

$$W(U_+(\bar z,\cdot)^*, U_-(z,\cdot)) = U_+(\bar z,x_0)^*[M_-(z,x_0) - M_+(z,x_0)]U_-(z,x_0), \tag{94}$$

$$M_\pm(z,x_0) = P(x_0)U'_\pm(z,x_0)U_\pm(z,x_0)^{-1}. \tag{95}$$

Unraveling the crucial identities (93) and (95) results in the fundamental fact

$$U_\pm(\bar z,x)^*[P(x)U'_\pm(z,x)] = [P(x)U'_\pm(\bar z,x)]^* U_\pm(z,x), \quad z\in\mathbb{C}\backslash\mathbb{R}, \tag{96}$$

for $x\in(a,b)$. In particular,

$$W(U_\pm(\bar z,\cdot)^*, U_\pm(z,\cdot)) = 0. \tag{97}$$

In other words, invertible square integrable $m \times m$ matrix-valued solutions of $LU = zU$ in the sense of (89) closely resemble *prepared* solutions in the sense of Hartman [38]. We use the term "closely resemble" as Hartman avoids the use of a complex spectral parameter and focuses on $z = 0$ instead. The term "prepared" did not stick as one finds also the notions of *conjoined, isotropic*, and *self-conjugate* solutions in the literature in connection with the property (96) (resp., (97)). Be that as it may, isolating property (96) was definitely a crucial step in the spectral analysis of systems of differential equations as the following observations will demonstrate.

Definition 3.4 Assume Hypothesis 3.1, let $\lambda \in \mathbb{R}$, and suppose that $U(\lambda, \cdot)$ is an $m \times m$ matrix-valued solution of $LU = \lambda U$. Then $U(\lambda, \cdot)$ is called *self-conjugate* if

$$W(U(\lambda, \cdot)^*, U(\lambda, \cdot)) = 0, \tag{98}$$

equivalently, if

$$U(\lambda, x)^*[P(x)U'(\lambda, x)] = [P(x)U'(\lambda, x)]^* U(\lambda, x), \quad x \in (a, b). \tag{99}$$

That is, $U(\lambda, x)^*[P(x)U'(\lambda, x)]$ is self-adjoint in (99) for all $x \in (a, b)$, and this is why we thought it most natural to follow those who adopted the term "self-conjugate" in connection with Definition 3.4. While we could have extended Definition 3.4 immediately to $\lambda \in \mathbb{C}$ along the lines of (96), (97), we are eventually aiming at principal matrix-valued solutions which are typically considered for $\lambda \in \mathbb{R}$.

Next, let $V_+(z, \cdot, c)$ (resp., $V_-(z, \cdot, c)$) be $m \times m$ matrix-valued solutions of $LU = zU$, invertible on the interval $[c, b)$ (resp., $(a, c]$) for some $c \in (a, b)$, satisfying property (96) on $[c, b)$ (resp., $(a, c]$). In particular,

$$W(V_\pm(\overline{z}, \cdot, c)^*, V_\pm(z, \cdot, c)) = 0. \tag{100}$$

We introduce

$$\begin{aligned} W_+(z, x, c) &= V_+(z, x, c)\bigg[C_{+,1} \\ &\quad + \int_c^x dx' V_+(z, x', c)^{-1} P(x')^{-1} \big[V_+(\overline{z}, x', c)^{-1}\big]^* C_{+,2}\bigg], \quad x \in [c, b), \end{aligned} \tag{101}$$

and

$$\begin{aligned} W_-(z, x, c) &= V_-(z, x, c)\bigg[C_{-,1} \\ &\quad - \int_x^c dx' V_+(z, x', c)^{-1} P(x')^{-1} \big[V_+(\overline{z}, x', c)^{-1}\big]^* C_{-,2}\bigg], \quad x \in (a, c], \end{aligned} \tag{102}$$

where $C_{\pm,j} \in \mathbb{C}^{m\times m}$, $j = 1, 2$. Then straightforward computations yield

$$LW_+(z,\cdot\,,c) = zW_+(z,\cdot\,,c) \text{ on } [c,b), \tag{103}$$

$$LW_-(z,\cdot\,,c) = zW_-(z,\cdot\,,c) \text{ on } (a,c], \tag{104}$$

$$W(V_\pm(\overline{z},\cdot\,,c)^*, W_\pm(z,\cdot\,,c)) = C_{\pm,2}, \tag{105}$$

$$W(W_\pm(\overline{z},\cdot\,,c)^*, W_\pm(z,\cdot\,,c)) = C_{\pm,1}^* C_{\pm,2} - C_{\pm,2}^* C_{\pm,1}. \tag{106}$$

At this point we introduce the notion of matrix-valued principal solutions of $LU = \lambda U$, $\lambda \in \mathbb{R}$.

Definition 3.5 Assume Hypothesis 3.1 and let $\lambda \in \mathbb{R}$.

(*i*) Suppose that $U_b(\lambda,\cdot\,)$ is a self-conjugate solution of $LU = \lambda U$ that is invertible on $[c,b)$ for some $c \in (a,b)$. Then $U_b(\lambda,\cdot\,)$ is called a *principal solution* of $LU = \lambda U$ at b if

$$\lim_{x\uparrow b}\left[\int_c^x dx'\, U_b(\lambda,x')^{-1}P(x')^{-1}\big[U_b(\lambda,x')^{-1}\big]^*\right]^{-1} = 0. \tag{107}$$

(*ii*) Suppose that $U_a(\lambda,\cdot\,)$ is a self-conjugate solution of $LU = \lambda U$ that is invertible on $(a,c]$ for some $c \in (a,b)$. Then $U_a(\lambda,\cdot\,)$ is called a *principal solution* of $LU = \lambda U$ at a if

$$\lim_{x\downarrow a}\left[\int_x^c dx'\, U_a(\lambda,x')^{-1}P(x')^{-1}\big[U_a(\lambda,x')^{-1}\big]^*\right]^{-1} = 0. \tag{108}$$

Principal solutions, if they exist, are unique up to right multiplication with invertible constant $m \times m$ matrices:

Lemma 3.6 *Assume Hypothesis 3.1 and let $\lambda \in \mathbb{R}$. Then if a principal solution $U_b(\lambda,\cdot\,)$ at b (resp., $U_a(\lambda,\cdot\,)$ at a) of $LU = \lambda U$ exists, it is unique up to right multiplication with an invertible (generally, λ-dependent) constant $m \times m$ matrix.*

This follows from [14, Theorem 2.3], or [39, Theorem 10.5 (*ii*)].

Lemma 3.7 *Assume Hypothesis 3.1 and let $\lambda \in \mathbb{R}$. Suppose that $U_0(\lambda,\cdot\,)$ is a self-conjugate solution of $LU = \lambda U$ that is invertible on $[c,b)$ (resp., $(a,c]$) and let $V(\lambda,\cdot\,)$ be any $m \times m$ matrix-valued solution of $LU = \lambda U$. Then $U_0(\lambda,\cdot\,)$ is a principal solution at b (resp., a) and*

$$W(U_0(\lambda,\cdot\,)^*, V(\lambda,\cdot\,)) \text{ is invertible,} \tag{109}$$

if and only if $V(\lambda,\cdot\,)$ is invertible near b (resp., a) and

$$\lim_{x\uparrow b} V(\lambda,x)^{-1}U_0(\lambda,x) = 0 \ \ (\text{resp., } \lim_{x\downarrow a} V(\lambda,x)^{-1}U_0(\lambda,x) = 0). \tag{110}$$

If (110) *holds, then, for appropriate* $c_b, c_a \in (a,b)$,

$$\lim_{x\uparrow b}\bigg[\int_{c_b}^{x} dx'\, V(\lambda,x')^{-1}P(x')^{-1}\big[V(\lambda,x')^{-1}\big]^*\bigg]^{-1} \text{ exists and is invertible} \tag{111}$$

$$\bigg(\text{resp., } \bigg[\lim_{x\downarrow a}\int_{x}^{c_a} dx'\, V(\lambda,x')^{-1}P(x')^{-1}\big[V(\lambda,x')^{-1}\big]^*\bigg]^{-1} \text{ exists and is invertible}\bigg).$$

Again, this follows from [14, Proposition 2.4], or [39, Theorem 10.5 (*iii*)].

Definition 3.8 Assume Hypothesis 3.1. The equation $Lu = zu$, $z \in \mathbb{C}$, is called *disconjugate* on the interval $J \subseteq (a,b)$ if every nontrivial (i.e., not identically vanishing) solution v of $Lu = zu$ vanishes at most once on J.

It is well known (cf., e.g., [14, Sect. 2.1], [39, Theorem XI.10.1]) that $Lu = zu$, $z \in \mathbb{C}$, is disconjugate on $J \subseteq (a,b)$ if and only if

$$\begin{aligned}&\text{for any } x_j \in J \text{ and any } \eta_j \in \mathbb{C}^m,\ Lu = zu \text{ has a unique solution } v(z,\cdot)\\ &\quad \text{satisfying } v(z,x_j) = \eta_j,\ j = 1,2.\end{aligned} \tag{112}$$

Equivalently, $Lu = zu$, $z \in \mathbb{C}$, is disconjugate on $J \subseteq (a,b)$ if and only if

$$\begin{aligned}&\text{for any } x_j \in J,\ j = 1,2,\ x_1 \neq x_2,\ Lu = zu \text{ has a no nontrivial solution}\\ &\quad v(z,\cdot) \text{ satisfying } v(z,x_j) = 0,\ j = 1,2.\end{aligned} \tag{113}$$

We also recall the following useful result:

Theorem 3.9 ([14], Sect. 2.1–2.2, [39], Theorem XI.10.2) *Assume Hypothesis 3.1.*

(*i*) *If J is a closed half-line (i.e., $J = [c,b)$ or $J = (a,c]$ for some $c \in (a,b)$), then $Lu = zu$, $z \in \mathbb{C}$, is disconjugate on J if and only if there exists a self-conjugate solution $U(z,\cdot)$ of $LU = zU$ such that $U(z,\cdot)$ is invertible on the interior of J.*

(*ii*) *If J is a closed bounded subinterval of (a,b) or $J \subseteq (a,b)$ is an open interval, then $Lu = zu$, $z \in \mathbb{C}$, is disconjugate on J if and only if there exists a self-conjugate solution $U(z,\cdot)$ of $LU = zU$ such that $U(z,\cdot)$ is invertible on J.*

Next, we derive the analog of (57)–(60) in the present matrix-valued context. Combining (80)–(84) and (100)–(102) yields the analog of (57),

$$\Phi(z,x,x_0) = \Theta(z,x,x_0)\int_{x_0}^{x} dx'\, \Theta(z,x',x_0)^{-1}P(x')^{-1}\big[\Theta(\overline{z},x',x_0)^{-1}\big]^*,$$
$$z \in \mathbb{C}\backslash\mathbb{R},\ x, x_0 \in (a,b). \tag{114}$$

Moreover, assuming that L is in the limit point case at b (resp., at a), it is known (cf., [46]) that the analog of (55) also holds in the form,

$$\begin{aligned} &M_+(z,x_0) = -\lim_{x\uparrow b} \Phi(z,x,x_0)^{-1}\Theta(z,x,x_0), \quad z\in\mathbb{C}\backslash\mathbb{R}, \\ &\big(\text{resp., } M_-(z,x_0) = -\lim_{x\downarrow a} \Phi(z,x,x_0)^{-1}\Theta(z,x,x_0), \quad z\in\mathbb{C}\backslash\mathbb{R}\big). \end{aligned} \tag{115}$$

Hence, we obtain the following formulas for $M_\pm(\,\cdot\,,x_0)$, the analogs of (58) and (60):

Theorem 3.10 *Assume Hypothesis 3.1 and suppose that L is in the limit point case at b (resp., at a). Then*

$$M_+(z,x_0) = -\lim_{x\uparrow b}\bigg[\int_{x_0}^{x} dx'\,\Theta(z,x',x_0)^{-1}P(x')^{-1}\big[\Theta(\overline{z},x',x_0)^{-1}\big]^*\bigg]^{-1}, \quad z\in\mathbb{C}\backslash\mathbb{R}, \tag{116}$$

$$\begin{aligned} \Big(\textit{resp., } M_-(z,x_0) = \lim_{x\downarrow a}\bigg[\int_{x}^{x_0} dx'\,\Theta(z,x',x_0)^{-1} \\ \times P(x')^{-1}\big[\Theta(\overline{z},x',x_0)^{-1}\big]^*\bigg]^{-1}, \quad z\in\mathbb{C}\backslash\mathbb{R}\Big). \end{aligned} \tag{117}$$

If, in addition, $Lu=\lambda_b u$ is disconjugate on $[x_0,b)$ (resp., $(a,x_0]$) for some $\lambda_b\in\mathbb{R}$ (resp., $\lambda_a\in\mathbb{R}$), then

$$M_+(\lambda,x_0) = -\bigg[\int_{x_0}^{b} dx'\,\Theta(\lambda,x',x_0)^{-1}P(x')^{-1}\big[\Theta(\lambda,x',x_0)^{-1}\big]^*\bigg]^{-1}, \quad \lambda<\lambda_b, \tag{118}$$

$$\begin{aligned} \Big(\textit{resp., } M_-(\lambda,x_0) = \bigg[\int_{a}^{x_0} dx'\,\Theta(\lambda,x',x_0)^{-1} \\ \times P(x')^{-1}\big[\Theta(\lambda,x',x_0)^{-1}\big]^*\bigg]^{-1}, \quad \lambda<\lambda_a\Big), \end{aligned} \tag{119}$$

and

$$\begin{aligned} \big(\xi, M_+(\lambda,x_0)^{-1}\eta\big)_{\mathbb{C}^m} = -\int_{x_0}^{b} dx'\,\big(\xi,\Theta(\lambda,x',x_0)^{-1} \\ \times P(x')^{-1}\big[\Theta(\lambda,x',x_0)^{-1}\big]^*\eta\big)_{\mathbb{C}^m}, \\ \lambda<\lambda_b,\ \xi,\eta\in\mathbb{C}^m, \end{aligned} \tag{120}$$

$$\Big(\textit{resp.,}\ \big(\xi, M_-(\lambda, x_0)^{-1}\eta\big)_{\mathbb{C}^m} = \int_a^{x_0} dx'\, \big(\xi, \Theta(\lambda, x', x_0)^{-1} \times P(x')^{-1}\big[\Theta(\lambda, x', x_0)^{-1}\big]^*\eta\big)_{\mathbb{C}^m}, \quad \lambda < \lambda_a,\ \xi, \eta \in \mathbb{C}^m\Big), \tag{121}$$

exists as a Lebesgue integral.

Proof It suffices to focus on the endpoint b. Combining (114) and (115) (employing that L is l.p.c. at b) yields relation (116).

For the remainder of this proof we thus assume that $Lu = \lambda_b u$ is disconjugate on $[x_0, b)$ for some $\lambda_b \in \mathbb{R}$ (in addition to L being l.p.c. at b). Then,

$$\int_{x_0}^{x} dx'\, \Theta(\lambda, x', x_0)^{-1} P(x')^{-1}\big[\Theta(\lambda, x', x_0)^{-1}\big]^*, \quad \lambda < \lambda_b, \tag{122}$$

is strictly monotone increasing with respect to $x > x_0$. Recalling the well-known fact (cf. [7, Lemma 2.1]),

$$\begin{aligned} &\text{If } 0 \leqslant C_1 \leqslant C_2 \leqslant \cdots \leqslant C_\infty, \text{ with } C_n, C_\infty \in \mathcal{B}_\infty(\mathcal{H}),\ n \in \mathbb{N}, \\ &\quad \text{then } \lim_{n\to\infty} \|C_n - C\|_{\mathcal{B}(\mathcal{H})} = 0 \text{ for some } C \in \mathcal{B}_\infty(\mathcal{H}), \end{aligned} \tag{123}$$

one infers convergence of the $m \times m$ matrix $-\int_{x_0}^{x} dx' \cdots$ to $-\int_{x_0}^{b} dx' \cdots$ on the right-hand-side in (118) as $x \uparrow b$. In addition, the monotone convergence theorem implies the existence of

$$\int_{x_0}^{b} dx'\, \big(\xi, \Theta(\lambda, x', x_0)^{-1} P(x')^{-1}\big[\Theta(\lambda, x', x_0)^{-1}\big]^*\xi\big)_{\mathbb{C}^m}, \quad \lambda < \lambda_b,\ \xi \in \mathbb{C}^m, \tag{124}$$

as a Lebesgue integral. The general case depicted in (120) for $\xi, \eta \in \mathbb{C}^m$ then follows by polarization.

It remains to prove equality of $M_+(\lambda, x_0)$ with the right-hand side of (118) for $\lambda < \lambda_b$. We start by noting that disconjugacy of $Lu = \lambda_b u$ implies analyticity of $M_+(\cdot, x_0)$ on $\mathbb{C}\backslash[\lambda_b, \infty)$ and hence the fact that the $m \times m$ matrix-valued measure $\Omega(\cdot, x_0)$ in the Nevanlinna–Herglotz representation for $M_+(\cdot, x_0)$ is supported on $[\lambda_b, \infty)$, that is, one infers the representation,

$$\begin{aligned} M_+(z, x_0) &= A + \int_{[\lambda_b,\infty)} d\Omega(\lambda, x_0)\big[(\lambda - z)^{-1} - \lambda(1 + \lambda^2)^{-1}\big], \\ &\qquad\qquad z \in \mathbb{C}\backslash[\lambda_b, \infty), \\ A = A^* \in \mathbb{C}^{m\times m}, &\quad \int_{[\lambda_b,\infty)} d(\xi, \Omega(\lambda, x_0)\xi)_{\mathbb{C}^m}(1 + \lambda^2)^{-1} < \infty,\ \xi \in \mathbb{C}^m. \end{aligned} \tag{125}$$

Similarly, one infers that for each $x \in [x_0, b)$ the $m \times m$ matrix-valued function, $M_{+,x}(\cdot, x_0)$, defined by

$$\begin{aligned} M_{+,x}(z, x_0) &:= -\Phi(z, x, x_0)^{-1}\Theta(z, x, x_0) \\ &= -\bigg[\int_{x_0}^{x} dx'\, \Theta(z, x', x_0)^{-1} P(x')^{-1}\big[\Theta(\overline{z}, x', x_0)^{-1}\big]^*\bigg]^{-1}, \\ &\qquad\qquad z \in \mathbb{C}\backslash[\lambda_b, \infty),\ x \in (x_0, b), \end{aligned} \tag{126}$$

is meromorphic on $\mathbb{C}$ and analytic on $\mathbb{C}\backslash[\lambda_b, \infty)$. General Weyl–Titchmarsh theory in connection with the interval $[x_0, x]$, $x \in (x_0, b)$, where x_0, x are regular endpoints for L, yields that for fixed $x_0, y \in (a, b)$, $M_{+,y}(\cdot, x_0)$, and hence the $m \times m$ matrix-valued integral in (126), represents a matrix-valued meromorphic Herglotz–Nevanlinna function (cf. [46]). Indeed, employing (85) yields

$$M_{+,y}(z, x_0)^* = M_{+,y}(\overline{z}, x_0), \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{127}$$

and introducing

$$\begin{aligned} U_y(z, x, x_0) = \Theta(z, x, x_0) + \Phi(z, x, x_0)[-\Phi(z, y, x_0)^{-1}\Theta(z, y, x_0)], \\ z \in \mathbb{C}\backslash\mathbb{R},\ x \in [x_0, y], y \in (x_0, b), \end{aligned} \tag{128}$$

a combination of (78) (for $z = \overline{z}_1 = z_2$), $U_y(z, y, x_0) = 0$, (81), (82), (83), and (84) imply the identity

$$\begin{aligned} \operatorname{Im}(M_{+,y}(z, x_0)) &= \operatorname{Im}\big(-\Phi(z, y, x_0)^{-1}\Theta(z, y, x_0)\big) \\ &= \operatorname{Im}(z)\int_{x_0}^{y} dx'\, U_y(z, x', x_0)^* R(x') U_y(z, x', x_0), \quad z \in \mathbb{C}\backslash\mathbb{R},\ y \in (x_0, b). \end{aligned} \tag{129}$$

Again, disconjugacy of $Lu = \lambda_b u$ implies that the $m \times m$ matrix-valued measure Ω_x associated with $M_{+,x}(\cdot, x_0)$ in (126), is again supported on $[\lambda_b, \infty)$, that is, for each $x \in (x_0, b)$,

$$\begin{aligned} M_{+,x}(z, x_0) &= -\Phi(z, x, x_0)^{-1}\Theta(z, x, x_0) \\ &\quad = -\bigg[\int_{x_0}^{x} dx'\, \Theta(z, x', x_0)^{-1} P(x')^{-1}\big[\Theta(\overline{z}, x', x_0)^{-1}\big]^*\bigg]^{-1} \\ &= A_x + \int_{[\lambda_b, \infty)} d\Omega_x(\lambda, x_0)\big[(\lambda - z)^{-1} - \lambda(1 + \lambda^2)^{-1}\big], \quad z \in \mathbb{C}\backslash[\lambda_b, \infty), \end{aligned} \tag{130}$$

$$A_x = A_x^* \in \mathbb{C}^{m\times m}, \quad \int_{[\lambda_b, \infty)} d(\xi, \Omega_x(\lambda, x_0)\xi)_{\mathbb{C}^m}(1 + \lambda^2)^{-1} < \infty,\ \xi \in \mathbb{C}^m.$$

In accordance with the limiting relation (115), the finite measures $d\Omega_x(\lambda, x_0)(1 + \lambda^2)^{-1}$ converge to $d\Omega(\lambda, x_0)(1 + \lambda^2)^{-1}$ as $x \uparrow b$ in the weak-* sense (cf. also [66]), that is,

$$\lim_{x\uparrow b} \int_{[\lambda_b,\infty)} d\Omega_x(\lambda, x_0)\,(1+\lambda^2)^{-1} f(\lambda) = \int_{[\lambda_b,\infty)} d\Omega(\lambda, x_0)(1+\lambda^2)^{-1} f(\lambda) \tag{131}$$

for all $f \in C(\mathbb{R}) \cap L^\infty(\mathbb{R}; d\lambda)$. The Nevanlinna–Herglotz representation (130) for $M_{+,x}(\cdot, x_0)$ demonstrates that for any compact $K \subset \mathbb{C}\backslash[\lambda_b, \infty)$, there exists a constant $C(K) > 0$ such that $\|M_{+,x}(z, x_0)\|_{\mathcal{B}(\mathbb{C}^m)} \leqslant C(K)$ uniformly with respect to $z \in K$ and $x \in (x_0, b)$. An application of Vitali's Theorem (see, e.g., [82, Sect. 7.3]) then proves that the convergence in (115) extends to

$$M_+(z, x_0) = -\lim_{x\uparrow b} \Phi(z, x, x_0)^{-1}\Theta(z, x, x_0), \quad z \in \mathbb{C}\backslash[\lambda_b, \infty), \tag{132}$$

in particular, it applies to $z < \lambda_b$ and hence yields (118). □

We are not aware of any source containing formulas of the type (116), (117), (118), (119), (120), and (121). Naturally, these formulas can be extended to the more general self-adjoint boundary conditions at the regular endpoint $x_0 \in (a, b)$ discussed in detail in [46] (cf. also [10, 11]) in the matrix-valued context, extending the scalar case described in (61), (62), and (66). We omit further details at this point.

The main result of this section then reads as follows.

Theorem 3.11 *Assume Hypothesis 3.1.*

(*i*) *Suppose that for some* $\lambda_b \in \mathbb{R}$, $(u, [T_{min} - \lambda_b I]u)_{L^2((a,b);Rdx;\mathbb{C}^m)} \geqslant 0$ *for all* $u \in \mathrm{dom}(T_{min})$ *with* $u = 0$ *in a neighborhood of a. In addition, assume that L is in the limit point case at b. Then for all* $\lambda < \lambda_b$, *the Weyl–Titchmarsh solution* $\Psi_+(\lambda, \cdot)$ *is also a principal solution of* $LU = \lambda U$ *at b, that is, for* x, x_0 *to the right of the last zero of* $\det_{\mathbb{C}^m}(\Psi_+(\lambda, \cdot))$, $\det_{\mathbb{C}^m}(U_b(\lambda, \cdot))$ *(if any),*

$$\Psi_+(\lambda, x)\Psi_+(\lambda, x_0)^{-1} = U_b(\lambda, x)U_b(\lambda, x_0)^{-1}. \tag{133}$$

(*ii*) *Suppose that for some* $\lambda_a \in \mathbb{R}$, $(u, [T_{min} - \lambda_a I]u)_{L^2((a,b);Rdx;\mathbb{C}^m)} \geqslant 0$ *for all* $u \in \mathrm{dom}(T_{min})$ *with* $u = 0$ *in a neighborhood of b. In addition, assume that L is in the limit point case at a. Then for all* $\lambda < \lambda_a$, *the Weyl–Titchmarsh solution* $\Psi_-(\lambda, \cdot)$ *is also a principal solution of* $LU = \lambda U$ *at a, that is, for* x, x_0 *to the left of the first zero of* $\det_{\mathbb{C}^m}(\Psi_-(\lambda, \cdot))$, $\det_{\mathbb{C}^m}(U_a(\lambda, \cdot))$ *(if any),*

$$\Psi_-(\lambda, x)\Psi_-(\lambda, x_0)^{-1} = U_a(\lambda, x)U_a(\lambda, x_0)^{-1}. \tag{134}$$

Proof It suffices to consider item (*i*). By [39, Theorem XI.10.3], the assumption on $T_{min} - \lambda_b I$ implies that for all $\lambda < \lambda_b$ and all $c \in (a, b)$, $Lu = \lambda u$ is disconjugate on $[c, b)$. By [14, Theorem 2.3] or [39, Theorem XI.10.5], $LU = \lambda U$ has a principal solution $U_b(\lambda, \cdot)$ for all $\lambda < \lambda_b$. Without loss of generality we may uniquely

determine $U_b(\lambda, \cdot, x_0)$ by demanding the normalization $U_b(\lambda, x_0; x_0) = I_m$. As proved in [14, p. 44–45], it is possible to approximate $U_b(\lambda, \cdot, x_0)$ as follows: For $y \in (x_0, b)$, consider the unique solution $U_y(\lambda, \cdot; x_0)$, of $LU = \lambda U$, $\lambda < \lambda_b$, satisfying

$$U_y(\lambda, x_0, x_0) = I_m, \quad U_y(\lambda, y, x_0) = 0. \tag{135}$$

Then

$$U_b(\lambda, \cdot, x_0) = \lim_{y \uparrow b} U_y(\lambda, \cdot, x_0), \quad \lambda < \lambda_b. \tag{136}$$

In addition, one obtains that

$$U_y(\lambda, \cdot, x_0) = \Theta(\lambda, \cdot, x_0) + \Phi(\lambda, \cdot, x_0) M_{+,y}(\lambda; x_0), \tag{137}$$

with $M_{+,y}(\lambda; x_0)$ introduced in (126). Employing the convergence result (118), that is, $\lim_{y \uparrow b} M_{+,y}(\lambda, x_0) = M_+(\lambda, x_0)$, $\lambda < \lambda_b$, in (137) thus also yields

$$\lim_{y \uparrow b} U_y(\lambda, \cdot, x_0) = \Psi_+(\lambda, x) \Psi_+(\lambda, x_0)^{-1}, \quad \lambda < \lambda_b. \tag{138}$$

A comparison of (136) and (138) then proves

$$U_b(\lambda, \cdot, x_0) = \Psi_+(\lambda, x) \Psi_+(\lambda, x_0)^{-1}, \quad \lambda < \lambda_b, \tag{139}$$

completing the proof. □

We emphasize that the continuity assumptions on the coefficients in L made in the context of oscillation theory in [14, Sect. 2.1], [39, Sect. XI.10] are not necessary and the quoted results in this section all extend to our current Hypothesis 3.1.

We also note that while we focused on Sturm–Liouville operators with matrix-valued coefficients, a treatment of more general singular Hamiltonian systems (along the lines of [11], [14, Ch. 2], [43–50, 76, 77], [78, Ch. VII], [79, Chs. V, VI], is clearly possible.

Emboldened by the results in Theorem 3.11 in the matrix context, one might guess that if $T_{min} \geqslant \lambda_0 I$ for some $\lambda_0 \in \mathbb{R}$, positivity of the solution $u(\lambda_0, \cdot)$ of $\ell u = \lambda_0 u$, or alternatively, $u \neq 0$ in Theorem 2.8 could be translated to the matrix-valued case in a multitude of different ways. Let $U(\lambda_0, \cdot) \in \mathbb{C}^{m \times m}$ denote a matrix-valued solution of $LU = \lambda_0 U$, then here is a possible list of "positivity results" one could imagine in the matrix context from the outset:

(*I*) $U \in \mathbb{C}^{m \times m}$ is invertible.
(*II*) $U \in \mathbb{C}^{m \times m}$ is positive definite.
(*III*) $U \in \mathbb{C}^{m \times m}$ is positivity preserving.
(*IV*) $U \in \mathbb{C}^{m \times m}$ is positivity improving.

For completeness we briefly recall the notions of positivity preserving (resp., improving) matrices:

Definition 3.12 Let $A = \big(A_{j,k}\big)_{1\leqslant j,k\leqslant m} \in \mathbb{R}^{m\times m}$ for some $m \in \mathbb{N}$.

(*i*) A is called *positivity preserving* if $A_{j,k} \geqslant 0$ for all $1 \leqslant j, k \leqslant m$.
(*ii*) A is called *positivity improving* if $A_{j,k} > 0$ for all $1 \leqslant j, k \leqslant m$.

However, item (*II*) implies self-adjointness of $U(\lambda_0, \cdot)$ and hence upon invoking the equation adjoint to $LU = \lambda_0 U$, commutativity of $U(\lambda_0, \cdot)$ and $Q(\cdot)$. Our next example, a matrix-valued Schrödinger operator (i.e., $P(\cdot) = R(\cdot) = I_m$ in L), provides a simple counter-example to positive definiteness.

Example 3.13 Let $m = 2$, $(a, b) = \mathbb{R}$, $P(\cdot) = R(\cdot) = I_2$ a.e. on $\mathbb{R}$, and

$$Q(x) = \begin{pmatrix} 0 & 1 \\ 1 & 2 \end{pmatrix} \tag{140}$$

in L. One verifies that

$$T_{min} \geqslant -2. \tag{141}$$

Taking $E = -2$, the general solution to $LU = -2U$ has the form

$$U(x) = \begin{pmatrix} U_{1,1}(x) & U_{1,2}(x) \\ U_{2,1}(x) & U_{2,2}(x) \end{pmatrix}, \quad x \in \mathbb{R}, \tag{142}$$

where

$$U_{1,1}(x) = c_1 e^{\sqrt{2}x} + c_2 e^{-\sqrt{2}x}, \tag{143}$$

$$U_{2,1}(x) = \tilde{c}_1 e^{2x} + \tilde{c}_2 e^{-2x} - (c_1/2)e^{\sqrt{2}x} - (c_2/2)e^{-\sqrt{2}x}, \tag{144}$$

$$U_{2,2}(x) = d_1 \cos(x) + d_2 \sin(x) + d_3 e^{\sqrt{7}x} + d_4 e^{-\sqrt{7}x}, \tag{145}$$

$$U_{1,2}(x) = \tilde{d}_1 e^{\sqrt{2}x} + \tilde{d}_2 e^{-\sqrt{2}x} - (d_1/3)\cos(x) - (d_2/3)\sin(x) \tag{146}$$

$$+ (d_3/5)e^{\sqrt{7}x} + (d_4/5)e^{-\sqrt{7}x}, \tag{147}$$

and $c_j, \tilde{c}_j, \tilde{d}_j, j \in \{1, 2\}$, and $d_k, k \in \{1, 2, 3, 4\}$ are arbitrary parameters. No solution of the form (142), (143), (144), (145), (146), and (147) is positive definite for all $x \in \mathbb{R}$. If such a solution were positive definite, it would commute with Q, so it suffices to show that solutions that commute with Q are not positive definite. By writing out $UQ = QU$, and equating corresponding matrix entries, one infers that U commutes with Q if and only if

$$\tilde{c}_1 = \tilde{c}_2 = d_1 = d_2 = d_3 = d_4 = 0,\ c_1 = -2\tilde{d}_1,\ c_2 = -2\tilde{d}_2, \tag{148}$$

with $\tilde{d}_1$ and $\tilde{d}_2$ arbitrary. (One could just as well arrive at (148) using self-adjointness of $U(x)$.) Taking (148) for granted, for a fixed choice of constants $\tilde{d}_1$ and $\tilde{d}_2$, $U(x)$ has the form

$$U(x) = \begin{pmatrix} -2A(x) & A(x) \\ A(x) & 0 \end{pmatrix}, \quad x \in \mathbb{R}, \tag{149}$$

where we have set

$$A(x) = \tilde{d}_1 e^{\sqrt{2}x} + \tilde{d}_2 e^{-\sqrt{2}x}, \quad x \in \mathbb{R}. \tag{150}$$

One then computes the eigenvalues of $U(x)$ in (149) to be

$$\lambda_\pm(x) = -A(x) \pm \sqrt{2}|A(x)|, \quad x \in \mathbb{R}. \tag{151}$$

Since $\lambda_-(x) \leqslant 0$ for all $x \in \mathbb{R}$, $U(x)$ is not positive definite for any value of x, let alone for all $x \in \mathbb{R}$.

In addition, items (*III*) and (*IV*) are ruled out by the following elementary constant coefficient example:

Example 3.14 Let $m = 2$, $(a, b) = \mathbb{R}$, $P(\cdot) = R(\cdot) = I_2$ a.e. on $\mathbb{R}$, $q_0 \in \mathbb{R}\backslash\{0\}$, and

$$Q(x) = \begin{pmatrix} 0 & q_0 \\ q_0 & 0 \end{pmatrix}. \tag{152}$$

One verifies that

$$T_{min} \geqslant -|q_0|. \tag{153}$$

Assuming that $E \leqslant -|q_0| < 0$, let

$$\delta_\pm(E) = \sqrt{|E \pm q_0|}. \tag{154}$$

We claim that $U_\infty(E, \cdot)$, defined by

$$U_\infty(E, x) = \begin{pmatrix} e^{-\delta_-(E)x} & -e^{-\delta_+(E)x} \\ e^{-\delta_-(E)x} & e^{-\delta_+(E)x} \end{pmatrix}, \quad E \leqslant -|q_0| < 0, \ x \in \mathbb{R}, \tag{155}$$

is a principal solution of $LU = EU$ at ∞. That $U_\infty(E, \cdot)$ is self-conjugate follows from the observation that

$$(U_\infty(E, x)')^* U_\infty(E, x) = \begin{pmatrix} -2\delta_-(E)e^{-\delta_-(E)x} & 0 \\ 0 & -2\delta_+(E)e^{-\delta_+(E)x} \end{pmatrix}. \tag{156}$$

Since $\det(U_\infty(E,x)) = 2e^{-(\delta_-(E)+\delta_+(E))x}$, one infers that $U_\infty(E,\cdot)$ is invertible on $\mathbb{R}$. That this particular solution is principal at ∞ follows from the fact that

$$\begin{aligned}&\bigg[\int_0^x dx'\, U_\infty(E,x')^{-1}\big[U_\infty(E,x')^{-1}\big]^*\bigg]^{-1}\\ &\quad = \begin{pmatrix} 4\delta_-(E)/(e^{2\delta_-(E)x}-1) & 0\\ 0 & 4\delta_+(E)/(e^{2\delta_+(E)x}-1)\end{pmatrix} \underset{x\uparrow\infty}{\to} 0.\end{aligned} \tag{157}$$

Next, we turn to all principal solutions of this example and hence consider

$$\begin{aligned}\tilde U_\infty(E,x) &= \begin{pmatrix} e^{-\delta_-(E)x} & -e^{-\delta_+(E)x}\\ e^{-\delta_-(E)x} & e^{-\delta_+(E)x}\end{pmatrix}\begin{pmatrix}\alpha & \beta\\ \gamma & \epsilon\end{pmatrix}\\ &= \begin{pmatrix} \alpha e^{-\delta_-(E)x} - \gamma e^{-\delta_+(E)x} & \beta e^{-\delta(E)x} - \epsilon e^{-\delta_+(E)x}\\ \alpha e^{-\delta_-(E)x} + \gamma e^{-\delta_+(E)x} & \beta e^{-\delta(E)x} + \epsilon e^{-\delta_+(E)x}\end{pmatrix}\end{aligned} \tag{158}$$

with $\left(\begin{smallmatrix}\alpha & \beta\\ \gamma & \epsilon\end{smallmatrix}\right) \in \mathbb{C}^{2\times 2}$ a nonsingular constant matrix.
By inspection, $\widetilde U_\infty(-|q_0|,\cdot)$ is never positivity preserving (let alone, improving).

The question of positive vector solutions of $Lu = \lambda_0 u$ has been studied in the literature and we refer, for instance to [1–3, 5, 25, 91].

We conclude with the remark that the results presented in this section extend from the case of $m \times m$ matrix-valued coefficients to the situation of operator-valued coefficients in an infinite-dimensional, complex, separable Hilbert space. For instance, basic Weyl–Titchmarsh theory for the infinite-dimensional case has been derived by Gorbachuk [34], Gesztesy, Weikard, and Zinchenko [31, 32], Saito [85–88] (see also [28], [35, Chs. 3, 4], [70–72], [84, Chs. 1–4], [92, 93]). For oscillation theoretic results in the infinite-dimensional context we refer, for example, to [18–20, 40, 56, 67]. A detailed treatment of this circle of ideas will appear elsewhere.

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Laplace Operators in Gamma Analysis

Dennis Hagedorn, Yuri Kondratiev, Eugene Lytvynov, and Anatoly Vershik

Abstract Let $\mathbb{K}(\mathbb{R}^d)$ denote the cone of discrete Radon measures on $\mathbb{R}^d$. The gamma measure $\mathcal{G}$ is the probability measure on $\mathbb{K}(\mathbb{R}^d)$ which is a measure-valued Lévy process with intensity measure $s^{-1}e^{-s}\,ds$ on $(0,\infty)$. We study a class of Laplace-type operators in $L^2(\mathbb{K}(\mathbb{R}^d),\mathcal{G})$. These operators are defined as generators of certain (local) Dirichlet forms. The main result of the paper is the essential self-adjointness of these operators on a set of 'test' cylinder functions on $\mathbb{K}(\mathbb{R}^d)$.

Keywords Dirichlet form • Gamma measure • Measure-valued Lévy process • Laplace operator

Mathematics Subject Classification (2010) Primary 60G51, 60G55, 60G57; Secondary 60G20, 60H40

1 Introduction

Handling and modeling complex systems have become an essential part of modern science. For a long time, complex systems have been treated in physics, where e.g. methods of probability theory are used to determine their macroscopic behavior by their microscopic properties. Nowadays, complex systems, including ecosystems, biological populations, societies, and financial markets, play an important role in various fields, like biology, chemistry, robotics, computer science, and social science.

D. Hagedorn • Y. Kondratiev
Fakultät für Mathematik, Universität Bielefeld, Postfach 10 01 31, D-33501 Bielefeld , Germany
e-mail: dhagedor@math.uni-bielefeld.de; kondrat@mathematik.uni-bielefeld.de

E. Lytvynov (✉)
Department of Mathematics, Swansea University, Singleton Park, Swansea SA2 8PP, UK
e-mail: e.lytvynov@swansea.ac.uk

A. Vershik
Laboratory of Representation Theory and Computational Mathematics, St.Petersburg Department of Steklov Institute of Mathematics, 27 Fontanka, St.Petersburg 19102, Russia
e-mail: vershik@pdmi.ras.ru

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A mathematical tool to study complex systems is infinite dimensional analysis. Such studies are often related to a probability measure μ defined on an infinite dimensional state space. The most 'traditional' example of a measure μ is the Gaussian (white noise) measure, which is defined on the Schwartz space of tempered distributions, $\mathcal{S}'(\mathbb{R}^d)$, see e.g. [3, 4, 9]. Another example of measure μ is the Poisson random measure on $\mathbb{R}^d$. This is a probability measure on the configuration space $\Gamma(\mathbb{R}^d)$ consisting of all locally finite subsets of $\mathbb{R}^d$. A configuration $\gamma = \{x_i\} \in \Gamma(\mathbb{R}^d)$ may be interpreted either as a collection of indistinguishable physical particles located at points x_i, or as a population of a species whose individuals occupy points x_i, or otherwise depending on the type of the problem. The Poisson measure corresponds to a system without interaction between its entities. In order to describe an interaction, one introduces Gibbs perturbations of the Poisson measure, i.e., Gibbs measures on $\Gamma(\mathbb{R}^d)$.

In papers [1, 2], some elements of analysis and geometry on the configuration space $\Gamma(\mathbb{R}^d)$ were introduced. In particular, for each $\gamma = \{x_i\} \in \Gamma(\mathbb{R}^d)$, a tangent space to $\Gamma(\mathbb{R}^d)$ at point γ was defined as

$$T_\gamma(\Gamma) := L^2(\mathbb{R}^d \to \mathbb{R}^d, \gamma),$$

where we identified γ with the Radon measure $\sum_i \delta_{x_i}$. A gradient of a differentiable function $F : \Gamma(\mathbb{R}^d) \to \mathbb{R}$ was explicitly identified as a function

$$\Gamma(\mathbb{R}^d) \ni \gamma \mapsto (\nabla^\Gamma F)(\gamma) \in T_\gamma(\Gamma).$$

This, in turn, led to a Dirichlet form

$$\mathcal{E}^\Gamma(F, G) = \int_{\Gamma(\mathbb{R}^d)} \langle (\nabla^\Gamma F)(\gamma), (\nabla^\Gamma G)(\gamma) \rangle_{T_\gamma(\Gamma)} \, d\mu(\gamma),$$

where μ is either Poisson measure or a Gibbs measure. Denote by $-L^\Gamma$ the generator of the Dirichlet form $\mathcal{E}^\Gamma$. Then, in the case where μ is Poisson measure, the operator L^Γ can be understood as a Laplace operator on the configuration space $\Gamma(\mathbb{R}^d)$.

Assume that the dimension d of the underlying space $\mathbb{R}^d$ is ≥ 2. By using the theory of Dirichlet forms, it was shown that there exists a diffusion process on $\Gamma(\mathbb{R}^d)$ which has generator L^Γ, see [1, 2, 19, 22, 31]. In particular, this diffusion process has μ as an invariant measure. (For $d = 1$, in order to construct an associated diffusion process an extension of $\Gamma(\mathbb{R}^d)$ is required.)

A further fundamental example of a probability measure on an infinite dimensional space is given by the gamma measure [6, 27, 29, 30]. This measure, denoted in this paper by $\mathcal{G}$, was initially defined through its Fourier transform as a probability measure on the Schwartz space of tempered distributions, $\mathcal{S}'(\mathbb{R}^d)$. White noise analysis related to the gamma measure was initiated by Kondratiev, da Silva, Streit, and Us in [14], and further developed in [12, 16, 17]. Note that the gamma measure belongs to the class of five Meixner-type Lévy measures (this class also includes Gaussian and Poisson measures). Each measure μ from this Meixner-type class

admits a 'nice' orthogonal decomposition of $L^2(\mu)$ in orthogonal polynomials of infinitely many variables. In particular, in the case of the gamma measure $\mathcal{G}$, these orthogonal polynomials are an infinite dimensional counterpart of the Laguerre polynomials on the real line [14].

A more delicate analysis shows that the gamma measure is concentrated on the smaller space $\mathbb{M}(\mathbb{R}^d)$ of all Radon measures on $\mathbb{R}^d$. More precisely, $\mathcal{G}$ is concentrated on the cone of discrete Radon measures on $\mathbb{R}^d$, denoted by $\mathbb{K}(\mathbb{R}^d)$. By definition, $\mathbb{K}(\mathbb{R}^d)$ consists of all Radon measures of the form $\eta = \sum_i s_i \delta_{x_i}$. It should be stressed that, with $\mathcal{G}$-probability one, the countable set of positions, $\{x_i\}$, is dense in $\mathbb{R}^d$. As for the weights s_i, with $\mathcal{G}$-probability one, we have $\eta(\mathbb{R}^d) = \sum_i s_i = \infty$, but for each compact set $A \subset \mathbb{R}^d$, $\eta(A) = \sum_{i:\, x_i \in A} s_i < \infty$. Elements $\eta \in \mathbb{K}(\mathbb{R}^d)$ may model, for example, biological systems, so that the points x_i represent location of some organisms, and the values s_i are a certain attribute attached to these organisms, like their weight or height.

A very important property of the gamma measure is that it is quasi-invariant with respect to a natural group of transformations of the weights s_i [27], see also [15]. Note also that an infinite dimensional analog of the Lebesgue measure is absolutely continuous with respect to the gamma measure [27, 28].

In paper [13], which is currently in preparation, we introduce elements of differential structure on the space of Radon measures, $\mathbb{M}(\mathbb{R}^d)$. More precisely, for a differentiable function $F : \mathbb{M}(\mathbb{R}^d) \to \mathbb{R}$, we define its gradient $(\nabla^{\mathbb{M}} F)(\eta)$ as a function of $\eta \in \mathbb{M}(\mathbb{R}^d)$ taking value in a tangent space $T_\eta(\mathbb{M})$ to $\mathbb{M}(\mathbb{R}^d)$ at point η. Furthermore, we identify a class of measure-valued Lévy processes μ which are probability measures on $\mathbb{K}(\mathbb{R}^d)$ and which admit an integration by parts formula. This class of measures μ includes the gamma measure $\mathcal{G}$ as an important example. We introduce and study the corresponding Dirichlet form

$$\mathcal{E}^{\mathbb{M}}(F, G) = \int_{\mathbb{K}(\mathbb{R}^d)} \langle (\nabla^{\mathbb{M}} F)(\eta), (\nabla^{\mathbb{M}} G)(\eta) \rangle_{T_\eta(\mathbb{M})} \, d\mu(\eta).$$

In particular, we find an explicit form of the generator $-L^{\mathbb{M}}$ of this Dirichlet form on a proper set of 'test' functions on $\mathbb{K}(\mathbb{R}^d)$. Note that the operator $L^{\mathbb{M}}$ can, in a certain sense, be thought of as a Laplace operator on $\mathbb{K}(\mathbb{R}^d)$, associated with the measure μ.

In this paper, we will discuss a class of Laplace-type operators associated with the gamma measure $\mathcal{G}$. More precisely, we will consider a Dirichlet form

$$\mathcal{E}^{\mathbb{M}}(F, G) = \int_{\mathbb{K}(\mathbb{R}^d)} \langle (\nabla^{\mathbb{M}} F)(\eta), c(\eta)(\nabla^{\mathbb{M}} G)(\eta) \rangle_{T_\eta(\mathbb{M})} \, d\mathcal{G}(\eta),$$

where $c(\eta)$ is a certain coefficient (possibly equal identically to one). We prove that this bilinear form is closable, its closure is a Dirichlet form and derive the generator $-L^{\mathbb{M}}$ of this form. The main result of the paper is that, under some assumption on the coefficient $c(\eta)$, the operator $L^{\mathbb{M}}$ is essentially self-adjoint on a proper set of 'test' functions on $\mathbb{K}(\mathbb{R}^d)$.

Unfortunately, our result does not yet cover the case where $c(\eta)$ is identically equal to one. The open problem here is to prove the essential self-adjointness of a certain differential operator on $\mathbb{R}^d \times (0, \infty)$.

Let us briefly discuss the structure of the paper. In Sect. 2, we recall basic notions from [13] related to differentiation on $\mathbb{M}(\mathbb{R}^d)$, like a tangent space and a gradient of a function on $\mathbb{M}(X)$. As intuitively clear, we have two types of such objects: one related to transformations of the support of a Radon measure, which we call intrinsic transformations, and one related to transformations of masses, which we call extrinsic transformations. We also combine the two types of tangent spaces/gradients into a full tangent space/gradient.

In Sect. 3, we explicitly construct the gamma measure $\mathcal{G}$ on $\mathbb{K}(\mathbb{R}^d)$. In Sect. 4, we construct and study the respective Dirichlet forms on the space $L^2(\mathbb{K}(\mathbb{R}^d), \mathcal{G})$. These Dirichlet forms are related to the intrinsic, extrinsic, and full gradients. We carry out the integration by parts with respect to the measure $\mathcal{G}$ and derive the generators of these bilinear forms.

Finally, in Sect. 5, we prove the essential self-adjointness in $L^2(\mathbb{K}(\mathbb{R}^d), \mathcal{G})$ of the generators of the Dirichlet forms on a proper set of 'test' functions on $\mathbb{K}(\mathbb{R}^d)$. To this end, we construct a unitary isomorphism between $L^2(\mathbb{K}(\mathbb{R}^d), \mathcal{G})$ and the symmetric Fock space $\mathcal{F}(\mathcal{H})$ over the space

$$\mathcal{H} = L^2(\mathbb{R}^d \times (0, \infty), dx\, s^{-1} e^{-s}\, ds).$$

We show that the semigroup $(\mathbf{T}_t)_{t \geq 0}$ in $L^2(\mathbb{K}(\mathbb{R}^d), \mathcal{G})$ which corresponds to the Dirichlet form is unitary isomorphic to the second quantization of a respective semigroup $(T_t)_{t \geq 0}$ in $\mathcal{H}$. It can be shown that this semigroup $(T_t)_{t \geq 0}$ generates a diffusion on $\mathbb{R}^d \times (0, \infty)$. In particular, in the extrinsic case, the respective diffusion on $\mathbb{R}^d \times (0, \infty)$ is related to a simple space-time transformation of the square of the 0-dimensional Bessel process on $[0, \infty)$.

In the forthcoming paper [5], by using the theory of Dirichlet forms, we will prove the existence of a diffusion on $\mathbb{K}(\mathbb{R}^d)$ with generator $L^{\mathbb{M}}$. We will also explicitly construct the Markov semigroup of kernels on $\mathbb{K}(\mathbb{R}^d)$ which corresponds to this diffusion. Furthermore, we plan to study equilibrium dynamics on $\mathbb{K}(\mathbb{R}^d)$ for which a Gibbs perturbation of the gamma measure (see [8]) is a symmetrizing (and hence invariant) measure.

2 Differentiation on the Space of Radon Measures

In this section, we present some definitions from [13].

Let X denote the Euclidean space $\mathbb{R}^d$, $d \in \mathbb{N}$, and let $\mathcal{B}(X)$ denote the Borel σ-algebra on X. Let $\mathbb{M}(X)$ denote the space of all (nonnegative) Radon measures on $(X, \mathcal{B}(X))$. The space $\mathbb{M}(X)$ is equipped with the vague topology, i.e., the coarsest

topology making all mappings

$$\mathbb{M}(X) \ni \eta \mapsto \langle \varphi, \eta \rangle := \int_X \varphi \, d\eta, \quad \varphi \in C_0(X),$$

continuous. Here $C_0(X)$ is the space of all continuous functions on X with compact support. It is well known (see e.g. [11, 15.7.7]) that $\mathbb{M}(X)$ is a Polish space. Let $\mathcal{B}(\mathbb{M}(X))$ denote the Borel σ-algebra on $\mathbb{M}(X)$.

Let us now introduce an appropriate notion of a gradient $\nabla^{\mathbb{M}}$ of a differentiable function $F : \mathbb{M}(X) \to \mathbb{R}$. We start with transformations of the support, which we call intrinsic transformations. We fix any $v \in C_0^\infty(X \to X)$, a smooth, compactly supported vector field over X. Let $(\phi_t^v)_{t\in\mathbb{R}}$ be the corresponding one-parameter group of diffeomorphisms of X which are equal to the identity outside a compact set in X. More precisely, $(\phi_t^v)_{t\in\mathbb{R}}$ is the unique solution of the Cauchy problem

$$\begin{cases} \dfrac{d}{dt}\, \phi_t^v(x) = v(\phi_t^v(x)), \\ \phi_0^v(x) = x. \end{cases} \tag{1}$$

We naturally lift the action of this group to the space $\mathbb{M}(X)$. For each $\eta \in \mathbb{M}(X)$, we define $\phi_t^v(\eta) \in \mathbb{M}(X)$ as the pushforward of η under the mapping ϕ_t^v. Hence, for each $f \in L^1(X, \eta)$,

$$\langle f, \phi_t^v(\eta) \rangle = \langle f \circ \phi_t^v, \eta \rangle. \tag{2}$$

For a function $F : \mathbb{M}(X) \to \mathbb{R}$, we define the intrinsic derivative of F in direction v by

$$(\nabla_v^{\mathrm{int}} F)(\eta) := \frac{d}{dt}\Big|_{t=0} F(\phi_t^v(\eta)), \quad \eta \in \mathbb{M}(X), \tag{3}$$

provided the derivative on the right hand side of formula (3) exists. As an intrinsic tangent space to $\mathbb{M}(X)$ at point $\eta \in \mathbb{M}(X)$ we choose the space

$$T_\eta^{\mathrm{int}}(\mathbb{M}) := L^2(X \to X, \eta),$$

i.e., the space of X-valued functions on X which are square integrable with respect to the measure η. The intrinsic gradient of F at point η is, by definition, the element $(\nabla^{\mathrm{int}} F)(\eta)$ in $T_\eta^{\mathrm{int}}(\mathbb{M})$ satisfying

$$\begin{aligned} (\nabla_v^{\mathrm{int}} F)(\eta) &= ((\nabla^{\mathrm{int}} F)(\eta), v)_{T_\eta^{\mathrm{int}}(\mathbb{M})} \\ &= \int_X \langle (\nabla^{\mathrm{int}} F)(\eta, x), v(x) \rangle_X \, d\eta(x), \quad v \in C_0^\infty(X \to X). \end{aligned} \tag{4}$$

(In the above formula, $\langle \cdot, \cdot \rangle_X$ denotes the usual scalar product in X.)

We will now introduce transformations of the masses, which we call extrinsic transformations. We fix any $h \in C_0(X)$. We consider the one-parameter group of transformations of $\mathbb{M}(X)$ given through multiplication of each measure $\eta \in \mathbb{M}(X)$ by the function $e^{th(x)}$, $t \in \mathbb{R}$. Thus, for each $\eta \in \mathbb{M}(X)$, we define $M_{th}(\eta) \in \mathbb{M}(X)$ by

$$dM_{th}(\eta)(x) := e^{th(x)}\, d\eta(x). \tag{5}$$

The extrinsic derivative of a function $F : \mathbb{M}(X) \to \mathbb{R}$ in direction h is defined by

$$(\nabla_h^{\text{ext}} F)(\eta) := \frac{d}{dt}\Big|_{t=0} F(M_{th}(\eta)), \quad \eta \in \mathbb{M}(X), \tag{6}$$

provided the derivative on the right hand side of (6) exists. As an extrinsic tangent space to $\mathbb{M}(X)$ at point $\eta \in \mathbb{M}(X)$ we choose

$$T_\eta^{\text{ext}}(\mathbb{M}) := L^2(X, \eta).$$

The extrinsic gradient of F at point η is defined to be the element $(\nabla^{\text{ext}} F)(\eta)$ in $T_\eta^{\text{ext}}(\mathbb{M})$ satisfying

$$\begin{aligned}(\nabla_h^{\text{ext}} F)(\eta) &= ((\nabla^{\text{ext}} F)(\eta), h)_{T_\eta^{\text{ext}}(\mathbb{M})} \\ &= \int_X (\nabla^{\text{ext}} F)(\eta, x) h(x)\, d\eta(x), \quad h \in C_0(X).\end{aligned} \tag{7}$$

We finally combine the intrinsic and extrinsic differentiation. For any $\eta \in \mathbb{M}(X)$, the full tangent space to $\mathbb{M}(X)$ at point η is defined by

$$T_\eta(\mathbb{M}) := T_\eta^{\text{int}}(\mathbb{M}) \oplus T_\eta^{\text{ext}}(\mathbb{M}).$$

We define the full gradient $\nabla^{\mathbb{M}} := (\nabla^{\text{int}}, \nabla^{\text{ext}})$.

For example, let us consider the set $\mathcal{FC}_b^\infty(\mathcal{D}(X), \mathbb{M}(X))$ of all functions $F : \mathbb{M}(X) \to \mathbb{R}$ of the form

$$F(\eta) = g(\langle f_1, \eta\rangle, \ldots, \langle f_N, \eta\rangle), \tag{8}$$

where $g \in C_b^\infty(\mathbb{R}^N)$ (an infinitely differentiable function on $\mathbb{R}^N$ which, together with all its derivatives, is bounded), $f_1 \ldots, f_N \in \mathcal{D}(X)$, and $N \in \mathbb{N}$. Here $\mathcal{D}(X) := C_0^\infty(X)$ is the space of all smooth, compactly supported functions on X. An easy calculation shows that

$$(\nabla^{\text{int}} F)(\eta, x) = \sum_{i=1}^N (\partial_i g)(\langle f_1, \eta\rangle, \ldots, \langle f_N, \eta\rangle) \nabla f_i(x), \tag{9}$$

$$(\nabla^{\mathrm{ext}}F)(\eta,x)=\sum_{i=1}^{N}(\partial_i g)(\langle f_1,\eta\rangle,\dots,\langle f_N,\eta\rangle)f_i(x), \tag{10}$$

so that

$$(\nabla^{\mathbb{M}}F)(\eta,x)=\sum_{i=1}^{N}(\partial_i g)(\langle f_1,\eta\rangle,\dots,\langle f_N,\eta\rangle)(\nabla f_i,f_i).$$

Here $\partial_i g$ denotes the partial derivative of g in the i-th variable.

3 Gamma Measure

In this section, following [13, 27], we will recall a construction of the gamma measure. Recall that we denote by $\mathbb{K}(X)$ the cone of discrete Radon measures on X:

$$\mathbb{K}(X):=\left\{\eta=\sum_i s_i\delta_{x_i}\in\mathbb{M}(X)\mid s_i>0,\ x_i\in X\right\}.$$

Here, δ_{x_i} is the Dirac measure with mass at x_i, the atoms x_i are assumed to be distinct and their total number is at most countable. By convention, the cone $\mathbb{K}(X)$ contains the null mass $\eta=0$, which is represented by the sum over the empty set of indices i. We denote $\tau(\eta):=\{x_i\}$, i.e., the set on which the measure η is concentrated. For $\eta\in\mathbb{K}(X)$ and $x\in\tau(\eta)$, we denote by $s(x)$ the mass of η at point x, i.e., $s(x):=\eta(\{x\})$. Thus, each $\eta\in\mathbb{K}(X)$ can be written in the form $\eta=\sum_{x\in\tau(\eta)}s(x)\delta_x$.

As shown in [8], $\mathbb{K}(X)\in\mathcal{B}(\mathbb{M}(X))$. We denote by $\mathcal{B}(\mathbb{K}(X))$ the trace σ-algebra of $\mathcal{B}(\mathbb{M}(X))$ on $\mathbb{K}(X)$.

Proposition 3.1 *There exists a unique probability measure $\mathcal{G}$ on $(\mathbb{K}(X),\mathcal{B}(\mathbb{K}(X)))$, called the gamma measure, which has Laplace transform*

$$\int_{\mathbb{K}(X)}e^{\langle\varphi,\eta\rangle}\,d\mathcal{G}(\eta)=\exp\left[-\int_X\log(1-\varphi(x))\,dx\right],\quad\varphi\in C_0(X),\ \varphi<1. \tag{11}$$

We will present a constructive proof of this statement, as it will be used throughout the paper.

Proof of Proposition 3.1 Denote $\mathbb{R}_+^*:=(0,\infty)$ and define a metric on $\mathbb{R}_+^*$ by

$$d_{\mathbb{R}_+^*}(s_1,s_2):=\left|\log(s_1)-\log(s_2)\right|,\quad s_1,s_2\in\mathbb{R}_+^*.$$

Then $\mathbb{R}_+^*$ becomes a locally compact Polish space, and any set of the form $[a,b]$, with $0<a<b<\infty$, is compact. We denote $\widehat{X}:=X\times\mathbb{R}_+^*$ and define the

configuration space over $\widehat{X}$ by

$$\Gamma(\widehat{X}) := \big\{\gamma \subset \widehat{X} \mid |\gamma \cap \Lambda| < \infty \text{ for each compact } \Lambda \subset \widehat{X}\big\}.$$

Here $|\gamma \cap \Lambda|$ denotes the number of points in the set $\gamma \cap \Lambda$. One can identify a configuration $\gamma \in \Gamma(\widehat{X})$ with the Radon measure $\sum_{(x,s)\in\gamma} \delta_{(x,s)}$ from $\mathbb{M}(\widehat{X})$. The space $\Gamma(\widehat{X})$ is endowed with the vague topology, i.e., the weakest topology on $\Gamma(\widehat{X})$ with respect to which all maps

$$\Gamma(\widehat{X}) \mapsto \langle f, \gamma\rangle := \int_{\widehat{X}} f(x,s)\, d\gamma(x,s) = \sum_{(x,s)\in\gamma} f(x,s), \quad f \in C_0(\widehat{X}),$$

are continuous. Let $\mathcal{B}(\Gamma(\widehat{X}))$ denote the Borel σ-algebra on $\Gamma(\widehat{X})$. We denote by π the Poisson measure on $(\Gamma(\widehat{X}), \mathcal{B}(\Gamma(\widehat{X})))$ with intensity measure

$$d\varkappa(x,s) := dx\, d\lambda(s), \tag{12}$$

where

$$d\lambda(s) := \frac{1}{s}\, e^{-s}\, ds. \tag{13}$$

The measure π can be characterized as the unique probability measure on $\Gamma(\widehat{X})$ which satisfies the Mecke identity: for each measurable function $F : \Gamma(\widehat{X}) \times \widehat{X} \to [0, \infty]$, we have

$$\int_{\Gamma(\widehat{X})} d\pi(\gamma) \int_{\widehat{X}} d\gamma(x,s)\, F(\gamma, x, s) = \int_{\Gamma(\widehat{X})} d\pi(\gamma) \int_{\widehat{X}} d\varkappa(x,s)\, F(\gamma \cup \{(x,s)\}, x, s). \tag{14}$$

Denote by $\Gamma_p(\widehat{X})$ the set of so-called pinpointing configurations in $\widehat{X}$. By definition, $\Gamma_p(\widehat{X})$ consists of all configurations $\gamma \in \Gamma(\widehat{X})$ such that if $(x_1, s_1), (x_2, s_2) \in \gamma$ and $(x_1, s_1) \neq (x_2, s_2)$, then $x_1 \neq x_2$. Thus, a configuration $\gamma \in \Gamma_p(\widehat{X})$ can not contain two points (x, s_1) and (x, s_2) with $s_1 \neq s_2$. As easily seen, $\Gamma_p(\widehat{X}) \in \mathcal{B}(\Gamma(\widehat{X}))$. Since the Lebesgue measure dx is non-atomic, the set

$$\big\{(x_1, s_1, x_2, s_2) \in \widehat{X}^2 \mid x_1 = x_2\big\}$$

is of zero $\varkappa^{\otimes 2}$-measure. Denote by $\mathcal{B}_c(\widehat{X})$ the set of all Borel measurable sets in $\widehat{X}$ which have compact closure. Fix any $\Lambda \in \mathcal{B}_c(\widehat{X})$. Using the distribution of the configuration $\gamma \cap \Lambda$ under π (see e.g. [11]), we conclude that

$$\pi\big(\gamma \in \Gamma(\widehat{X}) \mid \exists (x_1, s_1), (x_2, s_2) \in \gamma \cap \Lambda : x_1 = x_2,\, s_1 \neq s_2\big) = 0.$$

Hence, $\pi(\Gamma_p(\widehat{X})) = 1$.

For each $\gamma \in \Gamma_p(\widehat{X})$ and $A \in \mathcal{B}_c(X)$, we define a local mass by

$$\mathfrak{M}_A(\gamma) := \int_{\widehat{X}} \chi_A(x)s\, d\gamma(x,s) = \sum_{(x,s)\in\gamma} \chi_A(x)s \in [0,\infty]. \tag{15}$$

Here χ_A denotes the indicator function of the set A. The set of pinpointing configurations with finite local mass is defined by

$$\Gamma_{pf}(\widehat{X}) := \big\{\gamma \in \Gamma_p(\widehat{X}) \mid \mathfrak{M}_A(\gamma) < \infty \text{ for each } A \in \mathcal{B}_c(X)\big\}.$$

As easily seen, $\Gamma_{pf}(\widehat{X}) \in \mathcal{B}(\Gamma(\widehat{X}))$ and we denote by $\mathcal{B}(\Gamma_{pf}(\widehat{X}))$ the trace σ-algebra of $\mathcal{B}(\Gamma(\widehat{X}))$ on $\Gamma_{pf}(\widehat{X})$. For each $A \in \mathcal{B}_c(X)$, using the Mecke identity (14), we get

$$\int_{\Gamma_p(\widehat{X})} \mathfrak{M}_A(\gamma)\, d\pi(\gamma) = \int_{\Gamma_p(\widehat{X})} d\pi(\gamma) \int_A d\varkappa(x,s)\, s = \int_A dx < \infty.$$

Therefore, $\pi(\Gamma_{pf}(\widehat{X})) = 1$ and we can consider π as a probability measure on $(\Gamma_{pf}(\widehat{X}), \mathcal{B}(\Gamma_{pf}(\widehat{X})))$.

We construct a bijective mapping $\mathcal{R} : \Gamma_{pf}(\widehat{X}) \to \mathbb{K}(X)$ by setting, for each $\gamma = \{(x_i, s_i)\} \in \Gamma_{pf}(\widehat{X})$, $\mathcal{R}\gamma := \sum_i s_i \delta_{x_i} \in \mathbb{K}(X)$. By [8, Theorem 6.2], we have

$$\mathcal{B}(\mathbb{K}(X)) = \big\{\mathcal{R}A \mid A \in \mathcal{B}(\Gamma_{pf}(\widehat{X}))\big\}.$$

Hence, both $\mathcal{R}$ and its inverse $\mathcal{R}^{-1}$ are measurable mappings. We define $\mathcal{G}$ to be the pushforward of the measure π under $\mathcal{R}$. One can easily check that $\mathcal{G}$ has Laplace transform (11) and this Laplace transform uniquely characterizes this measure. □

Corollary 3.2 *For each measurable function $F : \mathbb{K}(X) \times X \to [0,\infty]$, we have*

$$\int_{\mathbb{K}(X)} d\mathcal{G}(\eta) \int_X d\eta(x)\, F(\eta, x) = \int_{\mathbb{K}(X)} d\mathcal{G}(\eta) \int_{\widehat{X}} dx\, ds\, e^{-s} F(\eta + s\delta_x, x). \tag{16}$$

Proof By the proof of Proposition 3.1 (in particular, using the Mecke identity), we see that the left hand side of (16) is equal to

$$\begin{aligned} &\int_{\Gamma_{pf}(\widehat{X})} d\pi(\gamma) \int_{\widehat{X}} d\gamma(x,s)\, sF(\mathcal{R}\gamma, x) \\ &\quad = \int_{\Gamma_{pf}(\widehat{X})} d\pi(\gamma) \int_{\widehat{X}} d\varkappa(x,s)\, sF(\mathcal{R}(\gamma \cup \{(x,s)\}), x), \end{aligned}$$

which is equal to the right hand side of (16). □

Remark 3.3 In fact, identity (16) uniquely characterizes the gamma measure $\mathcal{G}$, i.e., if a probability measure μ on $\mathbb{K}(X)$ satisfies identity (16) with $\mathcal{G}$ being replaced by μ, then $\mu = \mathcal{G}$. See [8, Theorem 6.3] for a proof of this statement.

Remark 3.4 By using either the Laplace transform of the gamma measure (formula (11)) or formula (16), one can easily show that the gamma measure has all moments finite, that is, for each $A \in \mathcal{B}_c(X)$ and $n \in \mathbb{N}$, we have

$$\int_{\mathbb{K}(X)} \langle \chi_A, \eta \rangle^n \, d\mathcal{G}(\eta) = \int_{\mathbb{K}(X)} \eta(A)^n \, d\mathcal{G}(\eta) < \infty. \tag{17}$$

4 Dirichlet Forms

Having arrived at notions of both a gradient and a tangent space to $\mathbb{M}(X)$, we would like to construct a corresponding Dirichlet form on the space $L^2(\mathbb{K}(X), \mathcal{G})$. This, in turn, should lead us, in future, to a diffusion process on $\mathbb{K}(X)$. In fact, we will consider different types of Dirichlet forms, corresponding to the intrinsic gradient ∇^{int}, extrinsic gradient ∇^{ext}, and the full gradient $\nabla^{\mathbb{M}}$. Furthermore, in the case of the intrinsic gradient (full gradient, respectively), we will use a coefficient in the Dirichlet form which depends on masses only. The sense of this coefficient will become clear below.

A natural candidate for the domain of these bilinear forms (before the closure) seems to be the set $\mathcal{FC}_b^\infty(\mathcal{D}(X), \mathbb{M}(X))$, see (8). However, as we learnt in [13], the gamma measure does not allow, on this set, an integration by parts formula with respect to intrinsic differentiation. In view of this, we will now introduce an alternative set of test functions on $\mathbb{K}(X)$.

Denote by $\mathcal{D}(\widehat{X})$ the space of all infinitely differentiable functions on $\widehat{X}$ which have compact support in $\widehat{X}$. In particular, the support of each $\varphi \in \mathcal{D}(\widehat{X})$ is a subset of some set $A \times [a, b]$, where $A \in \mathcal{B}_c(X)$ and $0 < a < b < \infty$. We denote by $\mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \Gamma(\widehat{X}))$ the set of all cylinder functions $F : \Gamma(\widehat{X}) \to \mathbb{R}$ of the form

$$F(\gamma) = g(\langle \varphi_1, \gamma \rangle, \ldots, \langle \varphi_N, \gamma \rangle), \quad \gamma \in \Gamma(\widehat{X}), \tag{18}$$

where $g \in C_b^\infty(\mathbb{R}^N)$, $\varphi_1 \ldots, \varphi_N \in \mathcal{D}(\widehat{X})$, and $N \in \mathbb{N}$. Next, we define

$$\mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \mathbb{K}(X)) := \left\{ F : \mathbb{K}(X) \to \mathbb{R} \mid F(\eta) = G(\mathcal{R}^{-1}\eta) \text{ for some } G \in \mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \Gamma(\widehat{X})) \right\}.$$

For $\varphi \in \mathcal{D}(\widehat{X})$ and $\eta \in \mathbb{K}(X)$, we denote

$$\langle\langle \varphi, \eta \rangle\rangle := \langle \varphi, \mathcal{R}^{-1}\eta \rangle = \sum_{x \in \tau(\eta)} \varphi(x, s(x)) = \int_X \frac{\varphi(x, s(x))}{s(x)} \, d\eta(x).$$

Then, each function $F \in \mathcal{FC}_b^{\infty}(\mathcal{D}(\widehat{X}), \mathbb{K}(X))$ has the form

$$F(\eta) = g\big(\langle\!\langle \varphi_1, \eta \rangle\!\rangle, \dots, \langle\!\langle \varphi_N, \eta \rangle\!\rangle\big), \quad \eta \in \mathbb{K}(X), \tag{19}$$

with $g, \varphi_1 \dots, \varphi_N$ and N as in (18).

We note that $\mathcal{FC}_b^{\infty}(\mathcal{D}(\widehat{X}), \Gamma(\widehat{X}))$ is a dense subset of $L^2(\Gamma(\widehat{X}), \zeta)$ for any probability measure ζ on $\Gamma(\widehat{X})$. Hence, $\mathcal{FC}_b^{\infty}(\mathcal{D}(\widehat{X}), \mathbb{K}(X))$ is a dense subset of $L^2(\mathbb{K}(X), \mu)$ for any probability measure μ on $\mathbb{K}(X)$, in particular, $\mathcal{FC}_b^{\infty}(\mathcal{D}(\widehat{X}), \mathbb{K}(X))$ is dense in $L^2(\mathbb{K}(X), \mathcal{G})$.

For a function F of the form (19), $v \in C_0^{\infty}(X \to X)$, $h \in C_0(X)$, and $\eta \in \mathbb{K}(X)$, we easily calculate:

$$\begin{aligned}
&(\nabla_v^{\mathrm{int}} F)(\eta) \\
&= \sum_{i=1}^{N} (\partial_i g)\big(\langle\!\langle \varphi_1, \eta \rangle\!\rangle, \dots, \langle\!\langle \varphi_N, \eta \rangle\!\rangle\big) \sum_{x \in \tau(\eta)} \langle \nabla_y \big|_{y=x} \varphi_i(y, s(x)), v(x) \rangle_X \\
&= \sum_{i=1}^{N} (\partial_i g)\big(\langle\!\langle \varphi_1, \eta \rangle\!\rangle, \dots, \langle\!\langle \varphi_N, \eta \rangle\!\rangle\big) \\
&\qquad \times \int_X \frac{1}{s(x)} \langle \nabla_y \big|_{y=x} \varphi_i(y, s(x)), v(x) \rangle_X \, d\eta(x), \\
&(\nabla_h^{\mathrm{ext}} F)(\eta) \\
&= \sum_{i=1}^{N} (\partial_i g)\big(\langle\!\langle \varphi_1, \eta \rangle\!\rangle, \dots, \langle\!\langle \varphi_N, \eta \rangle\!\rangle\big) \sum_{x \in \tau(\eta)} \frac{\partial}{\partial u}\Big|_{u=s(x)} \varphi(x, u) s(x) h(x) \\
&= \sum_{i=1}^{N} (\partial_i g)\big(\langle\!\langle \varphi_1, \eta \rangle\!\rangle, \dots, \langle\!\langle \varphi_N, \eta \rangle\!\rangle\big) \int_X \frac{\partial}{\partial u}\Big|_{u=s(x)} \varphi(x, u) h(x) \, d\eta(x).
\end{aligned}$$

Hence,

$$(\nabla^{\mathrm{int}} F)(\eta, x) = \sum_{i=1}^{N} (\partial_i g)\big(\langle\!\langle \varphi_1, \eta \rangle\!\rangle, \dots, \langle\!\langle \varphi_N, \eta \rangle\!\rangle\big) \frac{1}{s(x)} \nabla_y \big|_{y=x} \varphi_i(y, s(x)), \tag{20}$$

$$(\nabla^{\mathrm{ext}} F)(\eta, x) = \sum_{i=1}^{N} (\partial_i g)\big(\langle\!\langle \varphi_1, \eta \rangle\!\rangle, \dots, \langle\!\langle \varphi_N, \eta \rangle\!\rangle\big) \frac{\partial}{\partial u}\Big|_{u=s(x)} \varphi(x, u). \tag{21}$$

Let $F : \mathbb{K}(X) \to \mathbb{R}$, $\eta \in \mathbb{K}(X)$, and $x \in \tau(\eta)$. We define

$$(\nabla_x^X F)(\eta) := \nabla_y \big|_{y=x} F(\eta - s(x)\delta_x + s(x)\delta_y), \tag{22}$$

$$(\nabla_x^{\mathbb{R}_+^*})(\eta) := \frac{d}{du}\Big|_{u=s(x)} F(\eta - s(x)\delta_x + u\delta_x), \tag{23}$$

provided the derivatives on the right hand side of (22) and (23) exist. Here the variable y is from X, ∇_y is the usual gradient on X in the y variable, and the variable u is from $\mathbb{R}_+^*$. The following simple result is proven in [13].

Lemma 4.1 *For each $F \in \mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \mathbb{K}(X))$, $\eta \in \mathbb{K}(X)$, and $x \in \tau(\eta)$, we have*

$$(\nabla^{\mathrm{int}} F)(\eta, x) = \frac{1}{s(x)} (\nabla_x^X F)(\eta), \tag{24}$$

$$(\nabla^{\mathrm{ext}} F)(\eta, x) = (\nabla_x^{\mathbb{R}_+^*} F)(\eta). \tag{25}$$

We fix a measurable function $c : \mathbb{R}_+^* \to [0, \infty)$ which is locally bounded. We define the symmetric bilinear forms on $L^2(\mathbb{K}(X), \mathcal{G})$ by

$$\begin{aligned}\mathcal{E}^{\mathrm{int}}(F, G) &:= \int_{\mathbb{K}(X)} \langle (\nabla^{\mathrm{int}} F)(\eta), c(s(\cdot))(\nabla^{\mathrm{int}} G)(\eta) \rangle_{T_\eta^{\mathrm{int}}(\mathbb{M})} \, d\mathcal{G}(\eta), \\ &= \int_{\mathbb{K}(X)} d\mathcal{G}(\eta) \int_X d\eta(x) \left\langle (\nabla^{\mathrm{int}} F)(\eta, x), \, c(s(x))(\nabla^{\mathrm{int}} G)(\eta, x) \right\rangle_X , \end{aligned} \tag{26}$$

$$\mathcal{E}^{\mathrm{ext}}(F, G) := \int_{\mathbb{K}(X)} \langle (\nabla^{\mathrm{ext}} F)(\eta), (\nabla^{\mathrm{ext}} G)(\eta) \rangle_{T_\eta^{\mathrm{ext}}(\mathbb{M})} \, d\mathcal{G}(\eta), \tag{27}$$

$$\mathcal{E}^{\mathbb{M}}(F, G) := \mathcal{E}^{\mathrm{int}}(F, G) + \mathcal{E}^{\mathrm{ext}}(F, G), \tag{28}$$

where $F, G \in \mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \mathbb{K}(X))$. It follows from formulas (20) and (21) that, for each $F \in \mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \mathbb{K}(X))$, there exist a constant $C_1 > 0$, a set $A \in \mathcal{B}_c(X)$ and an interval $[a, b]$ with $0 < a < b < \infty$ such that

$$\max\{\|\nabla^{\mathrm{int}} F(\eta, x)\|_X, |\nabla^{\mathrm{ext}} F(\eta, x)|\} \le C_1 \, \chi_A(x) \, \chi_{[a,b]}(s(x)), \eta \in \mathbb{K}(X), \; x \in \tau(\eta). \tag{29}$$

Since the function c is locally bounded, there exists a constant $C_2 > 0$ such that

$$c(s(x))\chi_{[a,b]}(s(x)) \le C_2, \quad \eta \in \mathbb{K}(X), \; x \in \tau(\eta). \tag{30}$$

Therefore, by (17), (29), and (30), the integrals in (26) and (27) indeed make sense and are finite for any $F, G \in \mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \mathbb{K}(X))$.

Using Lemma 4.1, we may also give an equivalent representation of the bilinear forms $\mathcal{E}^{\mathrm{int}}$, $\mathcal{E}^{\mathrm{ext}}$.

Lemma 4.2 *For any* $F, G \in \mathcal{FC}_b^{\infty}(\mathcal{D}(\widehat{X}), \mathbb{K}(X))$,

$$\mathcal{E}^{\mathrm{int}}(F,G) = \int_{\mathbb{K}(X)} d\mathcal{G}(\eta) \int_{\widehat{X}} dx\, ds\, e^{-s}\, \frac{c(s)}{s^2} \big\langle \nabla_x F(\eta + s\delta_x), \nabla_x G(\eta + s\delta_x) \big\rangle_X , \tag{31}$$

$$\mathcal{E}^{\mathrm{ext}}(F,G) = \int_{\mathbb{K}(X)} d\mathcal{G}(\eta) \int_{\widehat{X}} dx\, ds\, e^{-s} \left(\frac{d}{ds} F(\eta + s\delta_x) \right) \left(\frac{d}{ds} G(\eta + s\delta_x) \right). \tag{32}$$

Proof Formulas (31) and (32) directly follow from Corollary 3.2, Lemma 4.1, and formulas (26) and (27). □

The lemma below shows that the introduced symmetric bilinear forms are well defined on $L^2(\mathbb{K}(X), \mathcal{G})$.

Lemma 4.3 *Let* $F, G \in \mathcal{FC}_b^{\infty}(\mathcal{D}(\widehat{X}), \mathbb{K}(X))$ *and let* $F = 0$ $\mathcal{G}$*-a.e. Then* $\mathcal{E}^{\sharp}(F,G) = 0$, $\sharp = \mathrm{int}, \mathrm{ext}, \mathbb{M}$.

Proof For each $A \in \mathcal{B}_c(X)$, making use of Corollary 3.2, we get

$$\int_{\mathbb{K}(X)} d\mathcal{G}(\eta) \int_{\widehat{X}} dx\, ds\, e^{-s} |F(\eta + s\delta_x)| \chi_A(x) = \int_{\mathbb{K}(X)} d\mathcal{G}(\eta)\, |F(\eta)|\, \eta(A) = 0.$$

Hence $F(\eta + s\delta_x) = 0$ $d\mathcal{G}(\eta)\, dx\, ds$-a.e. on $\mathbb{K}(X) \times \widehat{X}$. From here and Lemma 4.2, the statement easily follows. □

Lemma 4.4 *For* $\sharp = \mathrm{int}, \mathrm{ext}, \mathbb{M}$, *the bilinear form* $(\mathcal{E}^{\sharp}, \mathcal{FC}_b^{\infty}(\mathcal{D}(\widehat{X}), \mathbb{K}(X)))$ *is a pre-Dirichlet form on* $L^2(\mathbb{K}(X), \mathcal{G})$ *(i.e., if it is closable, then its closure is a Dirichlet form).*

Proof The assertion follows, by standard methods, directly from [18, Chap. I, Proposition 4.10] (see also [18, Chap. II, Exercise 2.7]). □

Analogously to (22) and (23), we define, for a function $F : \mathbb{K}(X) \to \mathbb{R}$, $\eta \in \mathbb{K}(X)$, and $x \in \tau(\eta)$,

$$(\Delta_x^X F)(\eta) := \Delta_y \big|_{y=x} F(\eta - s(x)\delta_x + s(x)\delta_y), \tag{33}$$

$$(\Delta_x^{\mathbb{R}_+^*} F)(\eta) := \left(\frac{d^2}{du^2} - \frac{d}{du} \right) \Big|_{u=s(x)} F(\eta - s(x)\delta_x + u\delta_x). \tag{34}$$

Here and below, Δ denotes the usual Laplacian on X (Δ_y denoting the Laplacian in the y variable). Explicitly, for a function $F \in \mathcal{FC}_b^{\infty}(\mathcal{D}(\widehat{X}), \mathbb{K}(X))$ of the form (19),

we get

$$
\begin{aligned}
(\Delta_x^X F)(\eta) &= \sum_{i,j=1}^{N} (\partial_i \partial_j g)(\langle\!\langle \varphi_1, \eta \rangle\!\rangle, \ldots, \langle\!\langle \varphi_N, \eta \rangle\!\rangle) \\
&\quad \times \langle \nabla_y \big|_{y=x} \varphi_i(y, s(\eta, \breve{a}x)), \nabla_y \big|_{y=x} \varphi_j(y, s(x)) \rangle_X \\
&\quad + \sum_{i=1}^{N} (\partial_i g)(\langle\!\langle \varphi_1, \eta \rangle\!\rangle, \ldots, \langle\!\langle \varphi_N, \eta \rangle\!\rangle) \Delta_y \big|_{y=x} \varphi_i(y, s(x)),
\end{aligned} \tag{35}
$$

and similarly, we calculate $(\Delta_x^{\mathbb{R}_+^*} F)(\eta)$.

Proposition 4.5 *For each $F \in \mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \mathbb{K}(X))$, we define*

$$
(L^{\mathrm{int}} F)(\eta) := \int_X d\eta(x) \, \frac{c(s(x))}{s(x)^2} \, (\Delta_x^X F)(\eta), \tag{36}
$$

$$
(L^{\mathrm{ext}} F)(\eta) := \int_X d\eta(x) \, (\Delta_x^{\mathbb{R}_+^*} F)(\eta), \quad \eta \in \mathbb{K}(X), \tag{37}
$$

$$
L^{\mathbb{M}} F := L_1^{\mathrm{int}} F + L_1^{\mathrm{ext}} F. \tag{38}
$$

Then, for $\sharp = \mathrm{int}, \mathrm{ext}, \mathbb{M}$, $(L^\sharp, \mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \mathbb{K}(X)))$ is a symmetric operator in $L^2(\mathbb{K}(X), \mathcal{G})$ which satisfies

$$
\mathcal{E}^\sharp(F, G) = (-L^\sharp F, G)_{L^2(\mathbb{K}(X), \mathcal{G})}, \quad F, G \in \mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \mathbb{K}(X)).
$$

The bilinear form $(\mathcal{E}^\sharp, \mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \mathbb{K}(X)))$ is closable on $L^2(\mathbb{K}(X), \mathcal{G})$ and its closure, denoted by $(\mathcal{E}^\sharp, D(\mathcal{E}^\sharp))$, is a Dirichlet form. The operator

$$
(-L^\sharp, \mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \mathbb{K}(X)))
$$

has Friedrichs' extension, which we denote by $(-L^\sharp, D(L^\sharp))$.

Proof We first note that, for a fixed $F \in \mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \mathbb{K}(X))$, there exist $A \in \mathcal{B}_c(X)$ and an interval $[a, b]$ with $0 < a < b < \infty$ such that the functions

$$
\widehat{X} \ni (x, s) \mapsto \nabla_x F(\eta + s\delta_x), \quad \widehat{X} \ni (x, s) \mapsto \frac{d}{ds} F(\eta + s\delta_x)
$$

vanish outside the set $A \times [a, b]$. Let $\sharp = \mathrm{int}$ and let $F, G \in \mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \mathbb{K}(X))$. Using Lemma 4.2 and integrating by parts in the x variable, we get

$$
\mathcal{E}^{\mathrm{int}}(F, G) = \int_{\mathbb{K}(X)} d\mathcal{G}(\eta) \int_{\widehat{X}} dx \, ds \, e^{-s} \, \frac{c(s)}{s^2} \big(- \Delta_x F(\eta + s\delta_x) \big) G(\eta + s\delta_x). \tag{39}
$$

Note that, for F of the form (19), we have

$$
\begin{aligned}
&(\Delta_x F)(\eta + s\delta_x) \\
&= \sum_{i,j=1}^{N} (\partial_i \partial_j g)\big(\langle\!\langle \varphi_1, \eta \rangle\!\rangle + \varphi_1(x,s), \ldots, \langle\!\langle \varphi_N, \eta \rangle\!\rangle + \varphi_N(x,s)\big) \qquad (40) \\
&\quad \times \langle \nabla_x \varphi_i(x,s), \nabla_x \varphi_j(x,s) \rangle_X \\
&\quad + \sum_{i=1}^{N} (\partial_i g)\big(\langle\!\langle \varphi_1, \eta \rangle\!\rangle + \varphi_1(x,s), \ldots, \langle\!\langle \varphi_N, \eta \rangle\!\rangle + \varphi_N(x,s)\big) \Delta_x \varphi_i(x,s). \qquad (41)
\end{aligned}
$$

Hence, the function under the sign of integral on the right hand side of (39) is integrable. By Corollary 3.2, (35), (36), (39), and (41), we get

$$
\begin{aligned}
\mathcal{E}^{\mathrm{int}}(F,G) &= \int_{\mathbb{K}(X)} d\mathcal{G}(\eta) \int_{\widehat{X}} d\eta(x)\, \frac{c(s(x))}{s(x)^2}\, (-\Delta_x^X F)(\eta, x) G(\eta) \\
&= \int_{\mathbb{K}(X)} (-L^{\mathrm{int}} F)(\eta) G(\eta)\, d\mathcal{G}(\eta). \qquad (42)
\end{aligned}
$$

By (35) and the local boundedness of the function c, there exist $C_3 > 0$ and $A \in \mathcal{B}_c(X)$ such that

$$
\frac{c(s(x))}{s(x)^2}\, |(\Delta_x F)(\eta)| \le C_3 \chi_A(x), \quad \eta \in \mathbb{K}(X),\ x \in \tau(\eta).
$$

Hence, by (17) and (36), we get $L^{\mathrm{int}} F \in L^2(\mathbb{K}(X), \mathcal{G})$. Thus, the bilinear form $(\mathcal{E}^{\mathrm{int}}, \mathcal{FC}_b^{\infty}(\mathcal{D}(\widehat{X}), \mathbb{K}(X)))$ has L^2-generator. Hence, the statement of the proposition regarding $\sharp = \mathrm{int}$ holds.

The proof for $\sharp = \mathrm{ext}$ (and so also for $\sharp = \mathbb{M}$) is similar. □

Remark 4.6 Let us quickly note some natural choices of the coefficient function $c(s)$. Choosing $c(s) = 1$, the intrinsic Dirichlet form becomes the closure of the bilinear form

$$
\mathcal{E}^{\mathrm{int}}(F,G) := \int_{\mathbb{K}(X)} \langle (\nabla^{\mathrm{int}} F)(\eta), (\nabla^{\mathrm{int}} G)(\eta) \rangle_{T_\eta^{\mathrm{int}}(\mathbb{K})}\, d\mathcal{G}(\eta).
$$

The choice of $c(s) = s$ yields, in fact, the Dirichlet form which is associated with a diffusion process on $\mathbb{K}(X)$ of the type $\eta(t) = \sum_{i=1}^{\infty} s_i \delta_{x_i(t)}$, where $(x_i(t))_{i=1}^{\infty}$ are independent Brownian motions on X, see [5]. When we choose $c(s) = s^2$, the generator of the intrinsic Dirichlet form becomes (see (36))

$$
(L^{\mathrm{int}} F)(\eta) = \int_X d\eta(x)\, (\Delta_x^X F)(\eta).
$$

Below we denote by $\mathcal{FC}_b^\infty(\mathcal{D}(X), \mathbb{K}(X))$ the set of the functions on $\mathbb{K}(X)$ which are restrictions of functions from $\mathcal{FC}_b^\infty(\mathcal{D}(X), \mathbb{M}(X))$ to $\mathbb{K}(X)$, i.e., they have the form (8) with $\eta \in \mathbb{K}(X)$. We note that $\mathcal{FC}_b^\infty(\mathcal{D}(X), \mathbb{K}(X))$ is a dense subset of $L^2(\mathbb{K}(X), \mu)$ for any probability measure μ on $\mathbb{K}(X)$ (see [7, Corollary 6.2.8] for a proof of this rather obvious statement). In particular, $\mathcal{FC}_b^\infty(\mathcal{D}(X), \mathbb{K}(X))$ is dense in $L^2(\mathbb{K}(X), \mathcal{G})$. We finish this section with the following proposition.

Proposition 4.7 *Assume that the function c satisfies*

$$\int_{\mathbb{R}_+^*} c(s)e^{-s}\, ds < \infty. \tag{43}$$

For $\sharp = \text{int}, \text{ext}, \mathbb{M}$*, we have*

$$\mathcal{FC}_b^\infty(\mathcal{D}(X), \mathbb{K}(X)) \subset D(\mathcal{E}^\sharp), \tag{44}$$

and for any $F, G \in \mathcal{FC}_b^\infty(\mathcal{D}(X), \mathbb{K}(X))$*,* $\mathcal{E}^\sharp(F, G)$ *is given by the respective formula in* (26)*,* (27)*, and* (28)*.*

Proof For $F \in D(\mathcal{E}^\sharp)$, denote $\mathcal{E}^\sharp(F) := \mathcal{E}^\sharp(F, F)$. On $D(\mathcal{E}^\sharp)$ we consider the norm

$$\|F\|_{D(\mathcal{E}^\sharp)} := \mathcal{E}^\sharp(F)^{1/2} + \|F\|_{L^2(\mathbb{K}(X),\mathcal{G})}\,. \tag{45}$$

Let $F \in \mathcal{FC}_b^\infty(\mathcal{D}(X), \mathbb{K}(X))$, and for simplicity of notation, assume that F is of the form $F(\eta) = g(\langle f, \eta\rangle)$, where $g \in C_b^\infty(\mathbb{R})$ and $f \in \mathcal{D}(X)$. For each $n \in \mathbb{N}$, we fix any function $u_n \in C^\infty(\mathbb{R})$ such that

$$\chi_{[1/n,\,\infty)} \le u_n \le \chi_{[1/(2n),\,\infty)} \tag{46}$$

and

$$|u_n'(t)| \le 4n\, \chi_{[1/(2n),\,1/n]}(t), \quad t \in \mathbb{R}. \tag{47}$$

For $n \in \mathbb{N}$, let $v_n \in C^\infty(\mathbb{R})$ be such that

$$\chi_{(-\infty,n+1]} \le v_n \le \chi_{(-\infty,n+2]} \tag{48}$$

and

$$|v_n'(t)| \le 2\, \chi_{[n+1,\,n+2]}(t), \quad t \in \mathbb{R}. \tag{49}$$

We define

$$h_n(s) := s u_n(s) v_n(s), \quad s \in \mathbb{R}_+^*,\ n \in \mathbb{N}, \tag{50}$$

and

$$\varphi_n(x,s) := f(x)h_n(s), \quad (x,s) \in \widehat{X},\ n \in \mathbb{N}. \tag{51}$$

Note that $h_n \in C_0^\infty(\mathbb{R}_+^*)$ and $\varphi_n \in \mathcal{D}(\widehat{X})$. Let

$$F_n(\eta) := g(\langle\!\langle \varphi_n, \eta \rangle\!\rangle), \quad \eta \in \mathbb{K}(X),\ n \in \mathbb{N}, \tag{52}$$

each F_n being an element of $\mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \mathbb{K}(X))$. For each $\eta \in \mathbb{K}(X)$,

$$\langle\!\langle \varphi_n, \eta \rangle\!\rangle = \sum_{x \in \tau(\eta)} f(x)s(x)u_n(s(x))v_n(s(x)) \to \langle f, \eta \rangle \quad \text{as } n \to \infty. \tag{53}$$

Hence, by the dominated convergence theorem, $F_n \to F$ in $L^2(\mathbb{K}(X), \mathcal{G})$. Note that

$$F_n(\eta + s\delta_x) = g(\langle\!\langle \varphi_n, \eta \rangle\!\rangle + \varphi_n(x,s)), \quad \eta \in \mathbb{K}(X),\ (x,s) \in \widehat{X}. \tag{54}$$

Using Lemma 4.2 and formulas (46), (47), (48), (49), (50), (51), (52), (53), and (54), one can easily show that

$$\mathcal{E}^\sharp(F_n - F_m) \to 0 \quad \text{as } n, m \to \infty. \tag{55}$$

Since $(\mathcal{E}^\sharp, D(\mathcal{E}^\sharp))$ is a closed bilinear form on $L^2(\mathbb{K}(X), \mathcal{G})$, we therefore have $F \in D(\mathcal{E}^\sharp)$, and furthermore $\mathcal{E}^\sharp(F_n) \to \mathcal{E}^\sharp(F)$ as $n \to \infty$. From here, analogously to the proof of (55), we conclude that $\mathcal{E}^\sharp(F)$ is given by the respective formula in (26), (27), and (28) with $G = F$.

The statement of the proposition about $\mathcal{E}^\sharp(F,G)$ for general $F, G \in \mathcal{FC}_b^\infty(\mathcal{D}(X), \mathbb{K}(X))$ follows from the above statement about $\mathcal{E}^\sharp(F)$ and the polarization identity. □

Remark 4.8 Let $\sharp = \text{int}, \text{ext}, \mathbb{M}$. For $\sharp = \text{int}, \mathbb{M}$, assume that condition (43) is satisfied and the dimension d of the underlying space X is ≥ 2. In the forthcoming paper [5], for $\sharp = \text{int}, \text{ext}, \mathbb{M}$, we will prove the existence of a conservative diffusion process on $\mathbb{K}(X)$ (i.e., a conservative strong Markov process with continuous sample paths in $\mathbb{K}(X)$) which is properly associated with the Dirichlet form $(\mathcal{E}^\sharp, D(\mathcal{E}^\sharp))$, see [18] for details on diffusion processes properly associated with a Dirichlet form. In particular, this diffusion process is $\mathcal{G}$-symmetric and has $\mathcal{G}$ as an invariant measure.

Remark 4.9 Let $\sharp = \text{int}, \text{ext}, \mathbb{M}$. Consider the Dirichlet form $(\mathcal{E}^\sharp, D_1(\mathcal{E}^\sharp))$ which is defined as the closure of the bilinear form $(\mathcal{E}^\sharp, \mathcal{FC}_b^\infty(\mathcal{D}(X), \mathbb{K}(X)))$. By Proposition 4.7, the Dirichlet form $(\mathcal{E}^\sharp, D(\mathcal{E}^\sharp))$ is an extension of the Dirichlet form $(\mathcal{E}^\sharp, D_1(\mathcal{E}^\sharp))$, i.e., $D_1(\mathcal{E}^\sharp) \subset D(\mathcal{E}^\sharp)$. So, there is a natural question whether these Dirichlet forms coincide, i.e., $D_1(\mathcal{E}^\sharp) = D(\mathcal{E}^\sharp)$, or, equivalently, whether the set $\mathcal{FC}_b^\infty(\mathcal{D}(X), \mathbb{K}(X))$ is dense in the space $D(\mathcal{E}^\sharp)$ equipped with norm (45). We do not expect a positive answer to this question. Furthermore, we do not expect the

existence of a conservative diffusion process on $\mathbb{K}(X)$ which is properly associated with the Dirichlet form $(\mathcal{E}^\sharp, D_1(\mathcal{E}^\sharp))$.

5 Essential Self-Adjointness of the Generators

In this section, for $\sharp = \mathrm{int}, \mathrm{ext}, \mathbb{M}$, we will discuss the essential self-adjointness of the operator $(L^\sharp, D(L^\sharp))$ on the domain $\mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \mathbb{K}(X))$.

Theorem 5.1 *Let $\sharp = \mathrm{int}, \mathrm{ext}, \mathbb{M}$. Let the function $c : \mathbb{R}_+^* \to [0, \infty)$ be measurable and locally bounded. For $\sharp = \mathbb{M}$, assume additionally that*

$$c(s) = a_1 s + a_2 s^2 + a_3 s^3 \tag{56}$$

for some $a_i \geq 0$, $i = 1, 2, 3$, $\max\{a_1, a_2, a_3\} > 0$. Then the operator $(L^\sharp, \mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \mathbb{K}(X)))$ is essentially self-adjoint on $L^2(\mathbb{K}(X), \mathcal{G})$.

Proof Fix any $F \in \mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \Gamma(\widehat{X}))$ and $\gamma \in \Gamma(\widehat{X})$. Consider the function

$$\widehat{X} \setminus \gamma \ni (x, s) \mapsto F(\gamma + \delta_{(x,s)}).$$

It is evident that this function admits a unique extension by continuity to the whole space $\widehat{X}$. We denote the resulting function by $F(\gamma + \delta_{(x,s)})$, although $\gamma + \delta_{(x,s)}$ is not necessarily an element of $\Gamma(\widehat{X})$. Note that $F(\gamma + \delta_{(x,s)})$ is a smooth functions of $(x, s) \in \widehat{X}$.

We preserve the notation $(\mathcal{E}^\sharp, D(\mathcal{E}^\sharp))$ for the realization of the respective Dirichlet form on $\Gamma_{pf}(\widehat{X})$. Thus, $(\mathcal{E}^\sharp, D(\mathcal{E}^\sharp))$ is the closure of the bilinear form

$$(\mathcal{E}^\sharp, \mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \Gamma(\widehat{X})))$$

on $L^2(\Gamma(\widehat{X}), \pi)$. Furthermore, by the counterpart of Lemma 4.2 for the domain $\mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \mathbb{K}(X))$, we get, for any $F, G \in \mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \Gamma(\widehat{X}))$,

$$\begin{aligned}
&\mathcal{E}^{\mathrm{int}}(F, G) \\
&\quad = \int_{\Gamma_{pf}(\widehat{X})} d\pi(\gamma) \int_{\widehat{X}} dx\, ds\, e^{-s} \frac{c(s)}{s^2} \left\langle \nabla_x F(\gamma + \delta_{(x,s)}), \nabla_x G(\gamma + \delta_{(x,s)}) \right\rangle_X, \\
&\mathcal{E}^{\mathrm{ext}}(F, G) \\
&\quad = \int_{\Gamma_{pf}(\widehat{X})} d\pi(\gamma) \int_{\widehat{X}} dx\, ds\, e^{-s} \left(\frac{d}{ds} F(\gamma + \delta_{(x,s)}) \right) \left(\frac{d}{ds} G(\gamma + \delta_{(x,s)}) \right), \\
&\mathcal{E}^{\mathbb{K}}(F, G) = \mathcal{E}^{\mathrm{int}}(F, G) + \mathcal{E}^{\mathrm{ext}}(F, G).
\end{aligned} \tag{57}$$

We keep the notation $(L^\sharp, D(L^\sharp))$ for the generator of the closed bilinear form $(\mathcal{E}^\sharp, D(\mathcal{E}^\sharp))$ on $L^2(\Gamma_{pf}, \pi)$. We easily conclude from Proposition 4.5 that

$$\mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \Gamma(\widehat{X})) \subset D(L^\sharp)$$

and for each $F \in \mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \Gamma(\widehat{X}))$ and $\gamma \in \Gamma(\widehat{X})$

$$(L^{\mathrm{int}}F)(\gamma) = \int_{\widehat{X}} d\gamma(x,s)\, \frac{c(s)}{s}\, (\Delta_x^X F)(\gamma), \tag{58}$$

$$(L^{\mathrm{ext}}F)(\gamma) = \int_{\widehat{X}} d\gamma(x,s)\, s\, (\Delta_x^{\mathbb{R}_+^*} F)(\gamma), \tag{59}$$

$$(L^{\mathbb{K}}F)(\gamma) = (L^{\mathrm{int}}F)(\gamma) + (L^{\mathrm{ext}}F)(\gamma), \tag{60}$$

with

$$(\Delta_x^X F)(\gamma) := \Delta_y\big|_{y=x} F(\gamma - \delta_{(x,s)} + \delta_{(y,s)}),$$

$$(\Delta_x^{\mathbb{R}_+^*} F)(\gamma) := \left(\frac{d^2}{du^2} - \frac{d}{du}\right)\Big|_{u=s} F(\gamma - \delta_{(x,s)} + \delta_{(x,u)}).$$

We equivalently have to prove that the symmetric operator $(L^\sharp, \mathcal{FC}_b^\infty(\mathcal{D}(\widehat{X}), \Gamma(\widehat{X})))$ is essentially self-adjoint on $L^2(\Gamma(\widehat{X}), \pi)$. Denote by $(H^\sharp, D(H^\sharp))$ the closure of this symmetric operator on $L^2(\Gamma(\widehat{X}), \pi)$. So we have to prove that the operator $(H^\sharp, D(H^\sharp))$ is self-adjoint.

It is not hard to check by approximation that, for each $\varphi \in \mathcal{D}(\widehat{X})$ and $n \in \mathbb{N}$, $F = \langle \varphi, \cdot \rangle^n \in D(H^\sharp)$ and $(H^\sharp F)(\gamma)$ is given by the right hand sides of formulas (58), (59), and (60), respectively. Hence, by the polarization identity (e.g. [3, Chap. 2, formula (2.17)]), we have

$$\langle \varphi_1, \cdot \rangle \cdots \langle \varphi_n, \cdot \rangle \in D(H^\sharp), \quad \varphi_1, \ldots, \varphi_n \in \mathcal{D}(\widehat{X}),\ n \in \mathbb{N}, \tag{61}$$

and again the action of $H^\sharp$ onto a function F as in (61) is given by the right hand side of formulas (58), (59), and (60), respectively. Let $\mathcal{P}$ denote the set of all functions on $\Gamma(\widehat{X})$ which are finite sums of functions as in (61) and constants. Thus, $\mathcal{P}$ is a set of polynomials on $\Gamma(\widehat{X})$, and $\mathcal{P} \subset D(H^\sharp)$. Furthermore,

$$(-H^\sharp F, G)_{L^2(\Gamma(\widehat{X}),\pi)} = \mathcal{E}^\sharp(F, G), \quad F, G \in \mathcal{P},\ \sharp = \mathrm{int}, \mathrm{ext}, \mathbb{M}. \tag{62}$$

In formula (62), $\mathcal{E}^\sharp(F, G)$ is given by formulas (57).

For a real separable Hilbert space $\mathcal{H}$, we denote by $\mathcal{F}(\mathcal{H})$ the symmetric Fock space over $\mathcal{H}$. Thus, $\mathcal{F}(\mathcal{H})$ is the real Hilbert space

$$\mathcal{F}(\mathcal{H}) = \bigoplus_{n=0}^{\infty} \mathcal{F}^{(n)}(\mathcal{H}),$$

where $\mathcal{F}^{(0)}(\mathcal{H}) := \mathbb{R}$, and for $n \in \mathbb{N}$, $\mathcal{F}^{(n)}(\mathcal{H})$ coincides with $\mathcal{H}^{\odot n}$ as a set, and for any $f^{(n)}, g^{(n)} \in \mathcal{F}^{(n)}(\mathcal{H})$

$$(f^{(n)}, g^{(n)})_{\mathcal{F}^{(n)}(\mathcal{H})} := (f^{(n)}, g^{(n)})_{\mathcal{H}^{\odot n}}\, n!\,.$$

Here $\odot$ stands for symmetric tensor product.

Recall the measure $\varkappa$ on $\widehat{X}$ defined by formulas (12) and (13). Let

$$I : L^2(\Gamma(\widehat{X}), \pi) \to \mathcal{F}(L^2(\widehat{X}, \varkappa)) \tag{63}$$

denote the unitary isomorphism which is derived through multiple stochastic integrals with respect to the centered Poisson random measure on $\widehat{X}$ with intensity measure $\varkappa$, see e.g. [26]. Denote by $\tilde{\mathcal{P}}$ the subset of $\mathcal{F}(L^2(\widehat{X}, \varkappa))$ which is the linear span of vectors of the form

$$\varphi_1 \odot \varphi_2 \odot \cdots \odot \varphi_n, \quad \varphi_1, \ldots, \varphi_n \in \mathcal{D}(\widehat{X}),\ n \in \mathbb{N}$$

and the vacuum vector $\Psi = (1, 0, 0, \ldots)$. For any $\varphi \in \mathcal{D}(\widehat{X})$, denote by M_φ the operator of multiplication by the function $\langle \varphi, \cdot \rangle$ in $L^2(\Gamma(\widehat{X}), \pi)$. Using the representation of the operator $IM_\varphi I^{-1}$ as a sum of creation, neutral, and annihilation operators in the Fock space (see e.g. [26]), we easily conclude that $I\mathcal{P} = \tilde{\mathcal{P}}$.

We define a bilinear form $(\tilde{\mathcal{E}}^\sharp, \tilde{\mathcal{P}})$ by

$$\tilde{\mathcal{E}}^\sharp(f, g) := \mathcal{E}^\sharp(I^{-1}f, I^{-1}g), \quad f, g \in \tilde{\mathcal{P}}$$

on $\mathcal{F}(L^2(\widehat{X}, \varkappa))$.

For each $(x, s) \in \widehat{X}$, we define an annihilation operator at (x, s) as follows:

$$\partial_{(x,s)} : \tilde{\mathcal{P}} \to \tilde{\mathcal{P}}$$

is the linear map given by

$$\partial_{(x,s)}\Psi := 0, \quad \partial_{(x,s)}\varphi_1 \odot \varphi_2 \odot \cdots \odot \varphi_n := \sum_{i=1}^{n} \varphi_i(x, s)\varphi_1 \odot \varphi_2 \odot \cdots \odot \check{\varphi}_i \odot \cdots \odot \varphi_n, \tag{64}$$

where $\check{\varphi}_i$ denotes the absence of φ_i. We will preserve the notation $\partial_{(x,s)}$ for the operator $I\partial_{(x,s)}I^{-1} : \mathcal{P} \to \mathcal{P}$. This operator admits the following explicit representation:

$$\partial_{(x,s)}F(\gamma) = F(\gamma + \delta_{(x,s)}) - F(\gamma)$$

for π-a.a. $\gamma \in \Gamma(\widehat{X})$, see e.g. [10, 20]. Note that

$$\nabla_x F(\gamma + \delta_{(x,s)}) = \nabla_x \big(F(\gamma + \delta_{(x,s)}) - F(\gamma)\big),$$
$$\frac{d}{ds} F(\gamma + \delta_{(x,s)}) = \frac{d}{ds} \big(F(\gamma + \delta_{(x,s)}) - F(\gamma)\big).$$

Hence, by (57), for any $F, G \in \mathcal{P}$,

$$\mathcal{E}^{\mathrm{int}}(F,G) = \int_{\Gamma(\widehat{X})} d\pi(\gamma) \int_{\widehat{X}} dx\, ds\, e^{-s}\, \frac{c(s)}{s^2} \big\langle \nabla_x\, \partial_{(x,s)} F(\gamma), \nabla_x\, \partial_{(x,s)} G(\gamma) \big\rangle_X ,$$
$$\mathcal{E}^{\mathrm{ext}}(F,G) = \int_{\Gamma(\widehat{X})} d\pi(\gamma) \int_{\widehat{X}} dx\, ds\, e^{-s} \left(\frac{\partial}{\partial s}\, \partial_{(x,s)} F(\gamma) \right) \left(\frac{\partial}{\partial s} \partial_{(x,s)} G(\gamma) \right),$$
$$\mathcal{E}^{\mathbb{M}}(F,G) = \mathcal{E}^{\mathrm{int}}(F,G) + \mathcal{E}^{\mathrm{ext}}(F,G).$$

Hence, for any $f, g \in \tilde{\mathcal{P}}$,

$$\tilde{\mathcal{E}}^{\mathrm{int}}(f,g) = \int_{\widehat{X}} d\varkappa(x,s)\, \frac{c(s)}{s} \sum_{i=1}^{d} \left(\frac{\partial}{\partial x^i}\, \partial_{(x,s)} f, \frac{\partial}{\partial x^i}\, \partial_{(x,s)} g \right)_{\mathcal{F}(L^2(\widehat{X},\varkappa))},$$
$$\tilde{\mathcal{E}}^{\mathrm{ext}}(f,g) = \int_{\widehat{X}} d\varkappa(x,s)\, s \left(\frac{\partial}{\partial s}\, \partial_{(x,s)} f, \frac{\partial}{\partial s}\, \partial_{(x,s)} g \right)_{\mathcal{F}(L^2(\widehat{X},\varkappa))},$$
$$\tilde{\mathcal{E}}^{\mathbb{M}}(f,g) = \tilde{\mathcal{E}}^{\mathrm{int}}(f,g) + \tilde{\mathcal{E}}^{\mathrm{ext}}(f,g). \tag{65}$$

Consider the bilinear forms

$$\mathfrak{E}^{\mathrm{int}}(\varphi,\psi) := \int_{\widehat{X}} d\varkappa(x,s)\, \frac{c(s)}{s} \big\langle \nabla_x \varphi(x,s), \nabla_x \psi(x,s) \big\rangle_X,$$
$$\mathfrak{E}^{\mathrm{ext}}(\varphi,\psi) := \int_{\widehat{X}} d\varkappa(x,s)\, s \left(\frac{\partial}{\partial s} \varphi(x,s) \right) \left(\frac{\partial}{\partial s} \psi(x,s) \right),$$
$$\mathfrak{E}^{\mathbb{M}}(\varphi,\psi) := \mathfrak{E}^{\mathrm{int}}(\varphi,\psi) + \mathfrak{E}^{\mathrm{ext}}(\varphi,\psi), \quad \varphi, \psi \in \mathcal{D}(\widehat{X}), \tag{66}$$

on $L^2(\widehat{X}, \varkappa)$. We easily calculate the L^2-generators of these bilinear forms:

$$\mathfrak{E}^{\sharp}(\varphi,\psi) = (-\mathfrak{L}^{\sharp}\varphi, \psi)_{L^2(\widehat{X},\varkappa)}, \quad \varphi, \psi \in \mathcal{D}(\widehat{X}), \tag{67}$$

where for $\varphi \in \mathcal{D}(\widehat{X})$

$$(\mathfrak{L}^{\mathrm{int}}\varphi)(x,s) = \frac{c(s)}{s}\,\Delta_x\varphi(x,s),$$

$$(\mathfrak{L}^{\mathrm{ext}}\varphi)(x,s) = s\left(\frac{\partial^2}{\partial s^2} - \frac{\partial}{\partial s}\right)\varphi(x,s),$$

$$\mathfrak{L}^{\mathbb{M}}\varphi = \mathfrak{L}^{\mathrm{int}}\varphi + \mathfrak{L}^{\mathrm{ext}}\varphi = \frac{c(s)}{s}\,\Delta_x\varphi(x,s) + s\left(\frac{\partial^2}{\partial s^2} - \frac{\partial}{\partial s}\right)\varphi(x,s). \tag{68}$$

Let us now recall the notion of a differential second quantization. Let $(\mathcal{A},\mathcal{D})$ be a densely defined symmetric operator in a real, separable Hilbert space $\mathcal{H}$. We denote by $\mathcal{F}_{\mathrm{alg}}(\mathcal{D})$ the subset of the Fock space $\mathcal{F}(\mathcal{H})$ which is the linear span of the vacuum vector Ψ and vectors of the form $\varphi_1 \odot \varphi_2 \odot \cdots \odot \varphi_n$, where $\varphi_1,\ldots,\varphi_n \in \mathcal{D}$ and $n \in \mathbb{N}$. The differential second quantization $d\,\mathrm{Exp}(\mathcal{A})$ is defined as the symmetric operator in $\mathcal{F}(\mathcal{H})$ with domain $\mathcal{F}_{\mathrm{alg}}(\mathcal{D})$ which acts as follows:

$$d\,\mathrm{Exp}(\mathcal{A})\Psi := 0,$$

$$d\,\mathrm{Exp}(\mathcal{A})\varphi_1 \odot \varphi_2 \odot \cdots \odot \varphi_n := \sum_{i=1}^{n} \varphi_1 \odot \varphi_2 \odot \cdots \odot (\mathcal{A}\varphi_i) \odot \cdots \odot \varphi_n. \tag{69}$$

By e.g. [3, Chap. 6, subsec. 1.1], if the operator $(\mathcal{A},\mathcal{D})$ is essentially self-adjoint on $\mathcal{H}$, then the differential second quantization $(d\,\mathrm{Exp}(\mathcal{A}), \mathcal{F}_{\mathrm{alg}}(\mathcal{D}))$ is essentially self-adjoint on $\mathcal{F}(\mathcal{H})$.

Now, we note that $\tilde{\mathcal{P}} = \mathcal{F}_{\mathrm{alg}}(\mathcal{D}(\widehat{X}))$. By (64), (65), (66), (67), (68), and (69) (see also [3, Chap. 6, Sect. 1]), an easy calculation shows that

$$\tilde{\mathcal{E}}^{\sharp}(f,g) = \left(d\,\mathrm{Exp}(-\mathfrak{L}^{\sharp})f, g\right)_{\mathcal{F}(L^2(\widehat{X},\varkappa))}, \quad f,g \in \tilde{\mathcal{P}},\ \sharp = \mathrm{int},\mathrm{ext},\mathbb{M}.$$

Hence, by (62),

$$\widetilde{H}^{\sharp} f = d\,\mathrm{Exp}(\mathfrak{L}^{\sharp})f, \quad f \in \tilde{\mathcal{P}},\ \sharp = \mathrm{int},\mathrm{ext},\mathbb{M}. \tag{70}$$

Here $\widetilde{H}^{\sharp} := IH^{\sharp}I^{-1}$. To prove the theorem, it suffices to show that the operator $(H^{\sharp},\mathcal{P})$ is essentially self-adjoint on $L^2(\mathbb{K}(X),\mathcal{G})$, or equivalently the operator $(\widetilde{H}^{\sharp},\tilde{\mathcal{P}})$ is essentially self-adjoint on $\mathcal{F}(L^2(\widehat{X},\varkappa))$. By (70), the theorem will follow from the lemma below. □

Lemma 5.2 *Under the assumptions of Theorem 5.1, the operator* $(\mathfrak{L}^{\sharp},\mathcal{D}(\widehat{X}))$ *is essentially self-adjoint on* $L^2(\widehat{X},\varkappa)$, $\sharp = \mathrm{int},\mathrm{ext},\mathbb{M}$.

Proof We will only discuss the hardest case $\sharp = \mathbb{M}$. We denote by $(\mathfrak{L}^{\mathbb{M}}, D(\mathfrak{L}^{\mathbb{M}}))$ the closure of the symmetric operator $(\mathfrak{L}^{\mathbb{M}},\mathcal{D}(\widehat{X}))$ on $L^2(\widehat{X},\varkappa)$. We denote by $\mathcal{S}(X)$

the Schwartz space of real-valued, rapidly decreasing functions on X (see e.g. [23, Sect. V.3]).

Claim. For each $f \in \mathcal{S}(X)$ and $k \in \mathbb{N}$, the function $\varphi(x,s) = f(x)s^k$ belongs to $D(\mathfrak{L}^{\mathbb{M}})$, and $\mathfrak{L}^{\mathbb{M}}\varphi$ is given by the right hand side of (68).

Indeed, for any functions $f \in \mathcal{D}(X)$ and $g \in C_0^\infty(\mathbb{R}_+^*)$, we have $f(x)g(s) \in \mathcal{D}(\widehat{X}) \subset D(\mathfrak{L}^{\mathbb{K}})$. Hence, by approximation, we can easily conclude that, for any functions $f \in \mathcal{S}(X)$ and $g \in C_0^\infty(\mathbb{R}_+^*)$, we have $f(x)g(s) \in D(\mathfrak{L}^{\mathbb{K}})$.

Fix any function $u \in C^\infty(\mathbb{R})$ such that $\chi_{[1,\infty)} \le u \le \chi_{[1/2,\infty)}$. Let

$$C_4 := \max_{t\in[1/2,\,1]} \max\{\,|u'(t)|, |u''(t)|\,\} < \infty.$$

For $n \in \mathbb{N}$, let $u_n(t) := u(nt)$, $t \in \mathbb{R}$. Then

$$\chi_{[1/n,\infty)} \le u_n \le \chi_{[1/(2n),\infty)} \tag{71}$$

and

$$|u_n'(t)| \le C_4\, n \chi_{[1/(2n),\,1/n]}(t), \quad |u_n''(t)| \le C_4\, n^2 \chi_{[1/(2n),\,1/n]}(t), \quad t \in \mathbb{R},\ n \in \mathbb{N}. \tag{72}$$

We also fix any function $v \in C^\infty(\mathbb{R})$ such that $\chi_{(-\infty,\,1]} \le v \le \chi_{(-\infty,\,2]}$. For $n \in \mathbb{N}$, set $v_n(t) := v(t-n)$, $t \in \mathbb{R}$. Hence

$$\chi_{(-\infty,\,n+1]} \le v_n \le \chi_{(-\infty,\,n+2]}, \tag{73}$$

and for some $C_5 > 0$

$$\max\{\,|v_n'(t)|, |v_n''(t)|\,\} \le C_5\, \chi_{[n+1,\,n+2]}, \quad t \in \mathbb{R},\ n \in \mathbb{N}. \tag{74}$$

We fix any $k \in \mathbb{N}$ and set

$$g_n(s) := s^k u_n(s) v_n(s), \quad s \in \mathbb{R}_+^*,\ n \in \mathbb{N}. \tag{75}$$

Clearly, $g_n \in C_0^\infty(\mathbb{R}_+^*)$. We fix $f \in \mathcal{S}(X)$ and set

$$\varphi_n(x,s) := f(x) g_n(s), \quad (x,s) \in \widehat{X},\ n \in \mathbb{N}. \tag{76}$$

Thus, $\varphi_n \in D(\mathfrak{L}^{\mathbb{K}})$. By the dominated convergence theorem,

$$\varphi_n(x,s) \to \varphi(x,s) := f(x)s^k \quad \text{in } L^2(\widehat{X}, \varkappa) \text{ as } n \to \infty. \tag{77}$$

We fix any $\psi \in \mathcal{D}(\widehat{X})$. Then

$$(-\mathfrak{L}^{\mathbb{M}}\varphi_n, \psi)_{L^2(\widehat{X},\varkappa)} = \mathfrak{E}^{\mathbb{M}}(\varphi_n, \psi), \quad n \in \mathbb{N}. \tag{78}$$

It is easy to see that

$$\lim_{n\to\infty} \mathfrak{E}^{\mathbb{M}}(\varphi_n, \psi) = \mathfrak{E}^{\mathbb{M}}(\varphi, \psi). \tag{79}$$

In (78) and (79) , $\mathfrak{E}^{\mathbb{M}}(\cdot,\cdot)$ is given by the formulas in (66). Hence

$$\lim_{n\to\infty} (\mathfrak{L}^{\mathbb{M}}\varphi_n, \psi)_{L^2(\widehat{X},\varkappa)} = (\mathfrak{L}^{\mathbb{M}}\varphi, \psi)_{L^2(\widehat{X},\varkappa)}. \tag{80}$$

We stress that, in (80), the function $\mathfrak{L}^{\mathbb{M}}\varphi \in L^2(\widehat{X}, \varkappa)$ is given by formulas in (68), however we do not yet state that $\varphi \in D(\mathfrak{L}^{\mathbb{M}})$.

By using (71), (72), (73), (74), (75), and (76), it can be easily shown that

$$\sup_{n\in\mathbb{N}} \|\mathfrak{L}^{\mathbb{M}}\varphi_n\|_{L^2(\widehat{X},\varkappa)} < \infty.$$

Hence, by the Banach–Alaoglu and Banach–Saks theorems (see e.g. [18, Appendix, Sect. 2]), there exists a subsequence $(\varphi_{n_j})_{j=1}^{\infty}$ of $(\varphi_n)_{n=1}^{\infty}$ such that the sequence $(\mathfrak{L}^{\mathbb{M}}\xi_i)_{i=1}^{\infty}$ converges in $L^2(\widehat{X}, \varkappa)$. Here

$$\xi_i := \frac{1}{i}\sum_{j=1}^{i} \varphi_{n_j}, \quad i \in \mathbb{N}.$$

We note that, for each $i \in \mathbb{N}$, $\xi_i \in \mathcal{D}(\widehat{X})$, and by (77)

$$\xi_i \to \varphi \quad \text{in } L^2(\widehat{X}, \varkappa) \text{ as } i \to \infty. \tag{81}$$

Furthermore, by (80),

$$\lim_{i\to\infty} (\mathfrak{L}^{\mathbb{M}}\xi_i, \psi)_{L^2(\widehat{X},\varkappa)} = (\mathfrak{L}^{\mathbb{M}}\varphi, \psi)_{L^2(\widehat{X},\varkappa)}, \quad \psi \in \mathcal{D}(\widehat{X}).$$

Hence

$$\mathfrak{L}^{\mathbb{M}}\xi_i \to \mathfrak{L}^{\mathbb{M}}\varphi \quad \text{in } L^2(\widehat{X}, \varkappa) \text{ as } i \to \infty. \tag{82}$$

By (81) and (82), we conclude that $\xi_i \to \varphi$ in the graph norm of the operator $(\mathfrak{L}^{\mathbb{M}}, D(\mathfrak{L}^{\mathbb{M}}))$. Thus, the claim is proven.

We next note that

$$L^2(\widehat{X}, \varkappa) = L^2(X, dx) \otimes L^2(\mathbb{R}^*_+, \lambda) \tag{83}$$

(recall (12)). Evidently, $\mathcal{S}(X)$ is a dense subset of $L^2(X, dx)$. Furthermore, the functions $\{s^k\}_{k=1}^{\infty}$ form a total set in $L^2(\mathbb{R}^*_+, \lambda)$ (i.e., the linear span of this set is

dense in $L^2(\mathbb{R}_+^*, \lambda)$). Indeed, consider the unitary operator

$$L^2(\mathbb{R}_+^*, \lambda) \ni g(s) \mapsto \frac{g(s)}{s} \in L^2(\mathbb{R}_+^*, se^{-s}\, ds).$$

Under this unitary operator, the set $\{s^k\}_{k=1}^{\infty}$ goes over into the set $\{s^k\}_{k=0}^{\infty}$. But the measure $\chi_{\mathbb{R}_+^*}(s)se^{-s}\, ds$ on $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ has Laplace transform which is analytic in a neighborhood of zero, hence the set of polynomials is dense in $L^2(\mathbb{R}_+^*, se^{-s}\, ds)$. Therefore, the set

$$\Upsilon := \text{l. s.}\{f(x)s^k \mid f \in \mathcal{S}(X),\ k \in \mathbb{N}\}$$

is dense in $L^2(\widehat{X}, \varkappa)$. Here l. s. denotes the linear span. By the Claim, the set Υ is a subset of $D(\mathfrak{L}^{\mathbb{M}})$. Note also that the operator $\mathfrak{L}^{\mathbb{M}}$ maps the set Υ into itself.

Since the symmetric operator $(\mathfrak{L}^{\mathbb{M}}, D(\mathfrak{L}^{\mathbb{M}}))$ is an extension of the operator $(\mathfrak{L}^{\mathbb{M}}, \Upsilon)$, to prove that $(\mathfrak{L}^{\mathbb{M}}, D(\mathfrak{L}^{\mathbb{M}}))$ is a self-adjoint operator, it suffices to prove that the operator $(\mathfrak{L}^{\mathbb{M}}, \Upsilon)$ is essentially self-adjoint.

We denote by $L^2_{\mathbb{C}}(\widehat{X}, \varkappa)$ the complex Hilbert space of all complex-valued $\varkappa$-square-integrable functions on $\widehat{X}$. Let $\Upsilon_{\mathbb{C}}$ denote the complexification of Υ, i.e., the set of all functions of the form $\varphi_1 + i\varphi_2$, where $\varphi_1, \varphi_2 \in \Upsilon$. Analogously, we define $L^2_{\mathbb{C}}(X, dx)$ and $\mathcal{S}_{\mathbb{C}}(X)$, the Schwartz space of complex-valued, rapidly decreasing functions on X. We extend the operator $\mathfrak{L}^{\mathbb{M}}$ by linearity to $\Upsilon_{\mathbb{C}}$.

Recall that the Fourier transform determines a unitary operator

$$\mathfrak{F} : L^2_{\mathbb{C}}(X, dx) \to L^2_{\mathbb{C}}(X, dx).$$

This operator leaves the Schwartz space $\mathcal{S}_{\mathbb{C}}(X)$ invariant, and furthermore

$$\mathfrak{F} : \mathcal{S}_{\mathbb{C}}(X) \to \mathcal{S}_{\mathbb{C}}(X)$$

is a bijective mapping. Under $\mathfrak{F}$, the Laplace operator Δ goes over into the operator of multiplication by $-\|x\|_X^2$, see e.g. [24, Sect. IX.1]. Using (83), we obtain the unitary operator

$$\mathfrak{F} \otimes \mathbf{1} : L^2_{\mathbb{C}}(\widehat{X}, \varkappa) \to L^2_{\mathbb{C}}(\widehat{X}, \varkappa).$$

Here $\mathbf{1}$ denotes the identity operator. Clearly $\mathfrak{F} \otimes \mathbf{1} : \Upsilon_{\mathbb{C}} \to \Upsilon_{\mathbb{C}}$ is a bijective mapping. We define an operator $\mathfrak{R}^{\mathbb{M}} : \Upsilon_{\mathbb{C}} \to \Upsilon_{\mathbb{C}}$ by

$$\mathfrak{R}^{\mathbb{M}} := (\mathfrak{F} \otimes \mathbf{1})\mathfrak{L}^{\mathbb{M}}(\mathfrak{F} \otimes \mathbf{1})^{-1}.$$

Explicitly, for each $\varphi \in \Upsilon_{\mathbb{C}}$,

$$(\mathfrak{R}^{\mathbb{M}}\varphi)(x, s) = -\frac{c(s)}{s}\, \|x\|_X^2\, \varphi(x, s) + s\left(\frac{\partial^2}{\partial s^2} - \frac{\partial}{\partial s}\right)\varphi(x, s). \tag{84}$$

It suffices to prove that the operator $(\mathfrak{R}^{\mathbb{M}}, \Upsilon_{\mathbb{C}})$ is essentially self-adjoint on $L^2_{\mathbb{C}}(\widehat{X}, \varkappa)$.

Since the operator $(\mathfrak{R}^{\mathbb{M}}, \Upsilon_{\mathbb{C}})$ is non-positive, by the Nussbaum theorem [21], it suffices to prove that, for each function

$$\varphi(x,s) = f(x)s^k \tag{85}$$

with $f \in \mathcal{D}(X)$ and $k \in \mathbb{N}$,

$$\sum_{n=1}^{\infty} \|(\mathfrak{R}^{\mathbb{M}})^n \varphi\|^{-1/2n}_{L^2_{\mathbb{C}}(\widehat{X},\varkappa)} = \infty. \tag{86}$$

For a function $\varphi(x,s)$ of the form (85), by virtue of (56) and (84), we get

$$\begin{aligned}
&(\mathfrak{R}^{\mathbb{M}}\varphi)(x,s) \\
&\quad = -(a_1 s^k + a_2 s^{k+1} + a_3 s^{k+2})\|x\|_X^2 f(x) + (k(k-1)s^{k-1} - ks^k)f(x) \\
&\quad = (\mathfrak{R}^{\mathbb{M}}_{-1}\varphi)(x,s) + (\mathfrak{R}^{\mathbb{M}}_{0}\varphi)(x,s) + (\mathfrak{R}^{\mathbb{M}}_{1}\varphi)(x,s) + (\mathfrak{R}^{\mathbb{M}}_{2}\varphi)(x,s).
\end{aligned} \tag{87}$$

Here

$$\begin{aligned}
(\mathfrak{R}^{\mathbb{M}}_{-1}\varphi)(x,s) &= k(k-1)s^{k-1}f(x), \\
(\mathfrak{R}^{\mathbb{M}}_{0}\varphi)(x,s) &= (-a_1\|x\|_X^2 - k)s^k f(x), \\
(\mathfrak{R}^{\mathbb{M}}_{1}\varphi)(x,s) &= -a_2\|x\|_X^2 s^{k+1} f(x), \\
(\mathfrak{R}^{\mathbb{M}}_{2}\varphi)(x,s) &= -a_3\|x\|_X^2 s^{k+2} f(x).
\end{aligned} \tag{88}$$

For $l \in \mathbb{N}$, denote

$$m_l := \int_{\mathbb{R}^*_+} s^l \, d\lambda(s) = \int_0^{\infty} s^{l-1} e^{-s} \, ds. \tag{89}$$

Since the Laplace transform of the measure $\chi_{\mathbb{R}^*_+}(s)e^{-s}\,ds$ on $\mathbb{R}$ is analytic in a neighborhood of zero, there exists a constant $C_6 \geq 1$ such that

$$m_l \leq C_6^l \, l!\,, \quad l \in \mathbb{N}. \tag{90}$$

Consider a product $\mathfrak{R}^{\mathbb{M}}_{i_1} \cdots \mathfrak{R}^{\mathbb{M}}_{i_n}\varphi$, where $i_1, \ldots, i_n \in \{-1, 0, 1, 2\}$. Denote by l_j the number of the $\mathfrak{R}^{\mathbb{M}}_j$ operators among the operators $\mathfrak{R}^{\mathbb{M}}_{i_1}, \ldots, \mathfrak{R}^{\mathbb{M}}_{i_n}$. Thus, $l_{-1} + l_0 + l_1 + l_2 = n$. Note that the function $f(x)$ has a compact support in X, hence the function $\|x\|_X^2$ is bounded on $\operatorname{supp}(f)$. Recall also the estimate

$$(2j)! \leq 4^j \, (j!)^2, \quad j \in \mathbb{N}. \tag{91}$$

Hence, by (87), (88), (89), (90), and (91), we get:

$$\|\mathfrak{R}^{\mathbb{M}}_{i_1}\cdots\mathfrak{R}^{\mathbb{M}}_{i_n}\varphi\|_{L^2(\widehat{X},\varkappa)} \le C_7^n(k-l_{-1}+l_1+2l_2)!\,(k-l_{-1}+l_1+2l_2)^{2l_{-1}+l_0} \tag{92}$$

for some constant $C_7 > 0$ which is independent of l_{-1}, l_0, l_1, l_2, n. Since $j! \le j^j$, we get from (92)

$$\begin{aligned}\|\mathfrak{R}^{\mathbb{M}}_{i_1}\cdots\mathfrak{R}^{\mathbb{M}}_{i_n}\varphi\|_{L^2(\widehat{X},\varkappa)} &\le C_7^n(k-l_{-1}+l_1+2l_2)^{k-l_{-1}+l_1+2l_2+2l_{-1}+l_0}\\ &= C_7^n(k-l_{-1}+l_1+2l_2)^{k+l_{-1}+l_0+l_1+2l_2}\\ &\le C_7^n(k+2n)^{k+2n}.\end{aligned}$$

Therefore,

$$\|(\mathfrak{R}^{\mathbb{M}})^n\varphi\|_{L^2_{\mathbb{C}}(\widehat{X},\varkappa)} \le (4C_7)^n(k+2n)^{k+2n}.$$

From here (86) follows. □

Let us recall the notion of a second quantization in a symmetric Fock space. Let $\mathcal{H}$ be a real separable Hilbert space, and let $\mathcal{F}(\mathcal{H})$ be the symmetric Fock space over $\mathcal{H}$. Let B be a bounded linear operator in $\mathcal{H}$, and assume that the operator norm of B is ≤ 1. We define the second quantization of B as a bounded linear operator $\mathrm{Exp}(B)$ in $\mathcal{F}(\mathcal{H})$ which satisfies $\mathrm{Exp}(B)\Psi := \Psi$ (Ψ being the vacuum vector in $\mathcal{F}(\mathcal{H})$) and for each $n \in \mathbb{N}$, the restriction of $\mathrm{Exp}(B)$ to $\mathcal{F}^{(n)}(\mathcal{H})$ coincides with $B^{\otimes n}$.

Let the conditions of Theorem 5.1 be satisfied. For $\sharp = \mathrm{int}, \mathrm{ext}, \mathbb{M}$, recall the non-positive self-adjoint operator $(\mathfrak{L}^\sharp, D(\mathfrak{L}^\sharp))$ in $L^2(\widehat{X}, \varkappa)$. By Lemma 5.2, this operator is essentially self-adjoint on $\mathcal{D}(\widehat{X})$ and, for each $\varphi \in \mathcal{D}(\widehat{X})$, $\mathfrak{L}^\sharp\varphi$ is given by (68). Recall the unitary operator I in formula (63). In view of the bijective mapping $\mathcal{R} : \Gamma_{pf}(\widehat{X}) \to \mathbb{K}(X)$, we can equivalently treat the operator I as a unitary operator

$$I : L^2(\mathbb{K}(X), \mathcal{G}) \to \mathcal{F}(L^2(\widehat{X}, \varkappa)) \tag{93}$$

(recall that the Poisson measure π is concentrated on $\Gamma_{pf}(\widehat{X})$).

Corollary 5.3 *Let the conditions of Theorem 5.1 be satisfied. Then, for* $\sharp = \mathrm{int}, \mathrm{ext}, \mathbb{M}$, *we have*

$$Ie^{tL^\sharp}I^{-1} = \mathrm{Exp}(e^{t\mathfrak{L}^\sharp}), \quad t \ge 0,$$

i.e., under the unitary isomorphism (93), *the semigroup* $(e^{tL^\sharp})_{t\ge 0}$ *with generator* $(L^\sharp, [1]D(L^\sharp))$ *goes over into the semigroup* $(\mathrm{Exp}(e^{t\mathfrak{L}^\sharp}))_{t\ge 0}$—*the second quantization of the semigroup* $(e^{t\mathfrak{L}^\sharp})_{t\ge 0}$ *with generator* $(\mathfrak{L}^\sharp, D(\mathfrak{L}^\sharp))$.

Proof It follows from the proof of Theorem 5.1 that

$$IL^\sharp I^{-1}f = d\,\mathrm{Exp}(\mathfrak{L}^\sharp)f, \quad f \in \mathcal{F}_{\mathrm{alg}}(\mathcal{D}(\widehat{X})),$$

and the operator $d\operatorname{Exp}(\mathfrak{L}^{\sharp})$ is essentially self-adjoint on $\mathcal{F}_{\mathrm{alg}}(\mathcal{D}(\widehat{X}))$. From here the result immediately follows (cf. e.g. [3, Chap. 6, subsec. 1.1]). □

Remark 5.4 Consider the operator $(\mathfrak{L}^{\mathrm{ext}}, D(\mathfrak{L}^{\mathrm{ext}}))$. We define the linear operator

$$\mathfrak{L}^{\mathrm{ext}}_{\mathbb{R}^*_+} u(s) := s\left(\frac{\partial^2}{\partial s^2} - \frac{\partial}{\partial s}\right) u(s), \quad u \in C_0^{\infty}(\mathbb{R}^*_+).$$

It follows from the proof of Lemma 5.2 that this operator is essentially self-adjoint on $L^2(\mathbb{R}^*_+, \lambda)$, and we denote by $(\mathfrak{L}^{\mathrm{ext}}_{\mathbb{R}^*_+}, D(\mathfrak{L}^{\mathrm{ext}}_{\mathbb{R}^*_+}))$ the closure of this operator. Recall that $L^2(\widehat{X}, \varkappa) = L^2(X, dx) \otimes L^2(\mathbb{R}^*_+, \lambda)$. Using (68), it is easy to show that

$$\mathfrak{L}^{\mathrm{ext}} = \mathbf{1} \otimes \mathfrak{L}^{\mathrm{ext}}_{\mathbb{R}^*_+}.$$

Using e.g. [25, Chap. XI], we easily conclude that $(\mathfrak{L}^{\mathrm{ext}}_{\mathbb{R}^*_+}, D(\mathfrak{L}^{\mathrm{ext}}_{\mathbb{R}^*_+}))$ is the generator of the Markov process $Y(t)$ on $\mathbb{R}_+ = [0, \infty)$ given by the following space-time transformation of the square of the 0-dimensional Bessel process $Q(t)$:

$$Y(t) = e^{-2t} Q((e^{2t} - 1)/2).$$

Note that, for each starting point $s > 0$, the process $Y(t)$ is at 0 (so that it has exited $\mathbb{R}^*_+$) with probability $\exp(-s/(1 - e^{-t}))$, and once $Y(t)$ reaches zero it stays there forever (i.e., does not return to $\mathbb{R}^*_+$).

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38 Years with Professor Ludwig Streit

Takeyuki Hida

Abstract This paper focuses on the 38 years of research which Prof. Streit dedicated to the development of the theory of Feynman path integrals, by using the techniques of White Noise Analysis. This paper aims at giving an introductory overview of his achievements.

Keywords white noise • Feynman integral

AMS Subject Classification 60H40 White Noise Theory

1 Introduction

I. A brief interpretation of the theory of the White Noise Analysis.

Let $\dot{B}(t)$ be the white noise which is realized as the time derivative of a Brownian motion $B(t), t \in R^1$. The collection $\{\dot{B}(t), t \in R^1\}$ is a system of idealized elementar random variables, the probability distribution μ of which is a Gaussian measure on the space E^* of generalized functions. To fix the idea the space E^* is taken to be the dual space of a countably-Hilbert nuclear space E dense in $L^2(R^1)$.

The white noise analysis is the calculus of functionals, the domain of which is the measure space (E^*, μ).

The variables of the functional in question are denoted by $\varphi(x), x \in E^*$, where x is viewed as a sample function of the $\dot{B}$.

The variable is a generalized function, even random, and φ is nonlinear in general, so we meet a lot of difficulty. However, the analysis, that is, the white noise analysis, is much interesting and has surprisingly many significant applications.

T. Hida (✉)
Professor Emeritus at Nagoya University, Nagoya, Japan
e-mail: takeyuki@math.nagoya-u.ac.jp

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II. Professor Ludwig Streit and White Noise.
1. I first met Professor Streit in 1975 at Kyoto, where an international conference was held and he was an invited participant.
2. Quantum theory due to Streit in terms of white Noise : We discussed various problems in this direction at ZiF Bielefeld.
3. We also discussed our formulation of the Feynman path integrals at Bielefeld.
4. There have been further developments in the present line. We have had very good collaboration either in Europe or in Nagoya.

2 Some Background

I. What is White Noise Analysis.

At the beginning of white noise theory we used to give a naive interpretation in terms of Gaussian white noise $\dot{B}(t)$, the time derivative of a Brownian motion $B(t)$. At present, having had fruitful results, we can now state the *récit* of the study in the following manner.

We are interested in the study of "random" complex phenomena. Each of them should be represented by a system of random vaiables defined on a certain probability space that we construct. For a mathematical study of those random variables, we propose a approach. First form a system of **indepedent** random variables having the same information as the variables in question. Then, we are given a system of random functions of those independent variables. The functions of independent random variables are much easier to deal with, compared to the functions of dependent random variales. This step is the so-called **reduction**, see [15].

The typical system of independent random variables, actually idealized random variables, is the Gaussian white noise $\{\dot{B}(t), t \in R^1\}$.

II. Notes.

Next, there arises a question: what are the possible, in fact acceptable, cardinal numbers of the system of independent variables. The case of finite or countably infinite number of independent random variables is easy to deal with, but it is not interesting. Whereas the case of continuously many independent random variables is important and much more interesting. There arises, however, a serious problem, that is, a system of continuously many independent *ordinary* random variables has non-separable probability distributions. To avoid this difficulty, we have the idea of taking the time-derivative of an additive process, in particular, a Lévy process, say $\dot{Z}(t)$ where $Z(t)$ is some Lévy process. As for the separability, there is no problem, see [8]. However, we have to pay a price, namely, each $\dot{Z}(t)$ is no longer an ordinary random variable, but an idealized variable.

Professor John R. Klauder has kindly suggested to me to call $\dot{Z}(t)$ an *idealized elementar random variable* (i.e.r.v.). It is often simply called a *noise*.

There is one more remark. A noise is usually parametrized by time or space. For example, $\dot{B}(t)$ or the Poisson noise $\dot{P}(t)$, which is the time derivative of a

Poisson process $P(t)$, depends on time; while another noise $P'(\lambda)$ depends on a space variable λ.

[Remark] Concerning the noise, we often use a phrase, in fact, after Streit, **Raum, Zeit, Rauschen**, cf. H. Weyl, Raum, Zeit, Materie, [24].

3 Quantum Theory in Terms of White Noise

The first joint work with Professor Streit is related to Euclidean fields. The Gaussian case is of particular interest. For example, we see that a multiple Markov Gaussian process has good connection with quantum theory, even in the case where σ-Markov property holds. (See [13].) Further the T-positivity problem can be discussed in this line.

It is to be noted that we have not yet used the space of ordinary white noise functionals.

4 Path Integrals

1. The idea for the path integral.

   The basic idea of our approach to the path integrals in quantum dynamics is to apply the *white noise analysis* to the construction of the *quantum mechanical propagators*.

   In fact, an attempt to give a correct interpretation to the Feynman integral, which had only formal significance before, was one of the motivation of proposing the white noise analysis using **generalized white noise functionals**, or **Hida distributions** named by Streit.

   Actually, there were two problems for us. One is how to realize a "flat" measure on a function space, where the function space itself should be clarified. The other is how to understand the exponential functional of an action.

   The path integral method is, as is well known, viewed as a third method of quantization, which is different from the formulation by W. Heisenberg and another one by E. Schrödinger. Our method of path integral, within the framework of white noise analysis, follows mainly Feynman's method [5] in spirit, see also [11]. However, some other basic quantum mechanical considerations are taken into account.

   While we are working on the problem in question, we have come to realize that we should consider Dirac's ideas, which are mainly found in his textbook [4].

2. We shall quickly explain our approach step by step.

   (i) What does a path mean in quantum dynamics?

   In quantum dynamics, following the Lagrangian dynamics theory, there are many possible paths, that is, trajectories of a particle, where each trajectory may be viewed as a sum of the classical one and fluctuations.

The classical path, denoted by y, is of course uniquely determined by the Lagrangian (with boundary values).

The so-called possible trajectories x in quantum dynamics can be expressed in the form

$$x = y + z,$$

where z is the fluctuation. See [6].

Our first question is to determine the fluctuation z. We propose that z is a Gaussian Markov process, more precisely a Brownian bridge which is a linear function of a Brownian motion $B(t)$. In the next section, we shall explain why a Brownian bridge is fitting for a realization of fluctuation.

(ii) To obtain Feynman's expression of propagator, we first meet the action integral

$$A(t) = \int^t L(x, \dot{x})ds.$$

The integrand involves a term $\dot{B}(s)^2$ to express the kinetic energy. The $\dot{B}(s)^2$ is not an ordinary random function. To come to the propagator we even have to exponentiate the action.

Thus, we shall be concerned with the analysis of generalized functions, actually functionals of $\dot{B}(t)$'s, that is, *white noise functionals*. The book [16] and [12] provides the background for the study of generalized functionals of white noise.

(iii) Integration over the function space $X = \{x\}$, the space of trajectories, can be defined smoothly. To this end, we must specify a measure on X, which is now obvious, since we have taken a white noise, whose probability distribution μ has automatically been introduced.

There is one problem to be reminded. We expect the integration to be done with respect to the uniform measure on X. This problem can be solved in Sect. 6.

(iv) With these background we can come to the actual computation of the propagators. This can be done by using the white noise theory.

(v) We can recognize that our approach can be applied to a pretty large class of Lagrangians.

(vi) Our method of integration on function space can further be applied to other problems in physics as we shall see in the last two sections.

5 Brownian Bridge and a Setup for the Propagator

First we have to explain why the Brownian bridge is involved in the class of quantum mechanical possible trajectories.

In [4] §32, Action principle, there is a statement that $B(t,s) = \int_t^s L(u)du$ satisfies a chain rule, by which we may imagine as the formula for the transition probabilities of a Markov process.

To fix the idea, we consider the case where the time interval is taken to be $[0,T]$. Now the term z that expresses the quantity of fluctuation can be a Markov process $X(t), 0 \le t \le T$. Further assumptions on $X(t)$ can be made as follows.

(1) $X(t)$ is a Gaussian process, since it is a sort of noise.
(2) As a usual requirement, the Gaussian process satisfies $E(X(t)) = 0$ and has the canonical representation by Brownian motion [10], namely

$$X(t) = \int_0^t F(t,u)\dot{B}(u)du.$$

and $X(0) = X(T) = 0$ (bridged).
(3) $X(t)$ is a Gaussian 1-ple Markov process.
(4) The normalized process $Y(t)$ enjoys the projective invariance under time-change.

Theorem 5.1 *The Brownian bridge $X(t)$ over the time interval $[0,T]$ is characterized by the above conditions (1)–(4).*

This theorem have been proved before and the proof is omitted here. We only note that the canonical representation of $X(t)$ is given by

$$X(t) = (T-t)\int_0^t \frac{1}{T-u}\dot{B}(u)du,$$

and the covariance $\Gamma(t,s)$ is

$$\Gamma(t,s) = \sqrt{\frac{s(T-t)}{t(T-s)}}, s \le t.$$

Namely,

$$\Gamma(t,s) = \sqrt{(0,T;s,t)}, s \le t,$$

where $(\cdot,\cdot;\cdot,\cdot)$ is the anharmonic ratio.

Remark In 1981 at the Berlin Conference on Math-Phys, we proposed a white noise approach to path integrals to have quantum mechanical propagators (see [14]; see also [22]). We had, at that time, some idea in mind for the use of a Brownian bridge, and we had many practically good examples of integrand with various kinds of potentials, and satisfactory results have been obtained.

With this background we are ready to propose how to form quantum mechanical propagators.

The possible quantum mechanical trajectories $x(t), t \in [0, T]$ are expressed in the form

$$x(t) = y(t) + \sqrt{\frac{\hbar}{m}} X(t),$$

where $X(t)$ is a Brownian bridge over the time interval $[0, T]$. The fluctuation z in the earlier expression is now taken to be a Brownian bridge.

Recall that the classical trajectory $y(t), t \in [0, T]$, is uniquely determined by the variational principle for the action

$$A[x] = \int_0^T L(x, \dot{x}) dt,$$

where the Lagrangian $L(x, \dot{x})$ in question is assumed to be of the form

$$L(x, \dot{x}) = \frac{1}{2} m(\dot{x})^2 - V(x).$$

The potential $V(x)$ is usually assumed to be regular, but later we can extend the theory to the case where V has certain singularity, even time-dependent (mainly done by the Streit school).

The actual expression and computations of the propagator are given successively as follows:

We follow the Lagrangian dynamics. The possible trajectories are sample paths $y(s), s \in [0, t]$, expressed in the form

$$y(s) = x(s) + \sqrt{\frac{\hbar}{m}} B(s), \tag{1}$$

where the $B(t)$ is an ordinary Brownian motion. Hence the action S is expressed in the form in terms of the quantum trajectory y:

$$A = \int_0^t L(y(s), \dot{y}(s)) ds.$$

Note that the effect of forming a bridge is given by putting the delta-function $\delta_0(y(t) - y_2)$ as a factor of the integrand, where $y_2 = x(t)$.

Now we set

$$S(t_0, t_1) = \int_{t_0}^{t_1} L(t) dt. \tag{2}$$

and set

$$\exp\left[\frac{i}{\hbar}\int_{t_0}^{t_1} L(t)dt\right] = \exp\left[\frac{i}{\hbar}S(t_0,t_1)\right] = B(t_0,t_1).$$

Then, we have , for $0 < t_1 < t_2 < \cdots < t_n < t$,

$$B(0,t) = B(0,t_1)\cdot B(t_1,t_2)\cdots B(t_n,t).$$

Theorem 5.2 *The quantum mechanical propagator $G(0,t;y_1,y_2)$ is given by the following average*

$$G(0,t;y_1,y_2) = \left\langle Ne^{\frac{i}{\hbar}\int_0^t L(y,\dot{y})ds + \frac{1}{2}\int_0^t \dot{B}(s)^2 ds}\delta_o(y(t)-y_2)\right\rangle, \tag{3}$$

where N is the amount of multiplicative renormalization. The average $\langle\ \rangle$ is understood to be the integral with respect to the white noise measure μ.

6 Generalized White Noise Functionals Revisited

It is well-known that there are two classes of generalized white noise functionals; $(L^2)^-$ and $(S)^*$. We use them without discrimination except it is necessary to choose one of them specifically.

It seems better to explain the concept of "renormalization" which makes formal but important basic functionals of the $\dot{B}(t)$'s to be acceptable as generalized white noise functionals. To save time we refer the interpretation to the literature (see [9, 16] and [21]).

We should note that there are generalized white noise functionals involved in the expectation in Theorem 5.2. For instance, the Donsker's delta function $\delta_o(y(t)-y_2)$ is a generalized white noise functional.

There is a Gauss kernel of the form $\exp[c\int_0^t \dot{B}(s)^2 ds]$, where the classical case is $c = -\frac{1}{2}$. In general, we assume $c \neq \frac{1}{2}$, and the Gaussian kernel can be a generalized functional after the multiplication renormalization. Now it seems we have the exceptional case, but it can be treated by combining it with another factor coming from the exponential term. In reality, we combine it with the term that comes from the kinetic energy.

The factor $\exp[\frac{1}{2}\int_0^t \dot{B}(s)^2 ds]$ serves as the *flattening effect* of the white noise measure. One may ask why the functional does so. An intuitive answer to this question is as follows: If we write a Lebesgue measure (exists only virtually) on E^* by dL, the white noise measure μ may be expressed in the form $\exp[-\frac{1}{2}\int_0^t \dot{B}(s)^2 ds]dL$. Hence the factor in question is put to make the measure μ to be a flat measure dL. In fact, this makes sense eventually.

Returning to the average (3) (in Theorem 5.2), which is an integral with respect to the white noise measure μ, it is important to note that the integrand (i.e. the inside of the angular bracket) is "integrable". In other words, the average (3) is a bilinear form of a generalized functional and a test functional.

To be reminded, there are short notes to follow. These are rather crucial. The formula (3) involves a product of functionals of the form like $\varphi(x)\cdot\delta(\langle x,f\rangle - a), f \in L^2(R), a \in \mathbf{C}$. To give a correct interpretation to the expectation of (3) with this choice, it should be checked that it can be regarded as a bilinear form of a pair of a test functional and a generalized functional. The following theorem provides answers to this question.

Theorem 6.1 (Streit et al. [23]) *Let $\varphi(x)$ be a generalized white noise functional. Assume that the $\mathcal{T}$-transform $(\mathcal{T}\varphi)(\xi), \xi \in E$, of φ is extended to a functional of f in $L^2(R)$, in particular a function of $\xi + \lambda f$, and that $(\mathcal{T}\varphi)(\xi - \lambda f)$ is an integrable function of λ for any fixed ξ. If the transform of $(\mathcal{T}\varphi)(\xi - \lambda f)$ is a U-functional, then the pointwise product $\varphi(x)\cdot\delta(\langle x,f\rangle - a)$ is defined and is a generalized white noise functional.*

Proof First a formula for the δ-function is provided.

$$\delta_a(t) = \delta(t-a) = \frac{1}{2\pi}\int e^{ia\lambda}e^{-i\lambda x}d\lambda \text{ (in distribution sense).}$$

Hence, for $\varphi \in (S)^*$ and $f \in L^2(R)$ we have the $\mathcal{T}$-transform

$$\begin{aligned}\mathcal{T}(\varphi(x)\delta(\langle x,f\rangle - a))(\xi) &= \frac{1}{2\pi}\int e^{ia\lambda}e^{-i\lambda\langle x,f\rangle}e^{i\langle x,\xi\rangle}\varphi(x)d\mu(x)d\Lambda \\ &= \frac{1}{2\pi}\int e^{ia\lambda}(\mathcal{T}\varphi)(\xi-\lambda f)d\lambda. \qquad (4)\end{aligned}$$

By assumption this determines a U-functional, which means the product $\varphi(x)\cdot\delta(\langle x,f\rangle - a)$ makes sense and the product is a generalized white noise functional. □

Example 6.2 The above theorem can be applied to a Gauss kernel $\varphi_c(x) = N\exp[c\int x(t)^2dt]$, with $c \neq \frac{1}{2}$. In particular:

(i) The case where c is real and $c < 0$.
We have

$$\begin{aligned}(\mathcal{T}\varphi)(\xi-\lambda f) &= \exp[\frac{c}{1-2c}\int(\xi(t)-\lambda f(t))^2dt] \\ &= \exp[\frac{c}{1-2c}(\|\xi\|^2 - 2\lambda(\xi,f) + \lambda^2\|f\|^2]).\end{aligned}$$

This is an integrable function of real λ. Hence, by the above Theorem 6.1, we have a generalized white noise functional.

(ii) The case where $c = \frac{1}{2} + ia, a \in R - \{0\}$. The same expression as in (i) holds.

Example 6.3 In the following cases, exact values of the propagators can be obtained and, of course, they agree with the known results.

(i) Free particle
(ii) Harmonic oscillator.
(iii) Potentials which are Fourier transforms of measures.

7 Some of Further Developments and Related Topics

[I] In addition to Example 6.3, we have some more interesting potentials, including some which are more singular and time depending. There are satisfactory results in the recent developments.

Example 7.1 Streit et al. [7] have obtained explicit formulae in the following cases:

(1) a time depending Lagrangian of the form

$$L(x(t), \dot{x}(t), t) = \frac{1}{2}m(t)\dot{x}(t)^2 - k(t)^2x(t)^2 - \dot{f}(t)x(t),$$

where $m(t), k(t)$ and $f(t)$ are smooth funtions.

(2) A singular potential $V(x)$ of the form

$$V(x) = \sum_n c^{-n^2}\delta_n(x), \quad c > 0,$$

and others.

[II] The Hopf equation.

There are many approaches to the Navier-Stokes equation.

$$u_{\alpha,t} + u_\beta u_{\alpha,\beta} = -p_\alpha + \mu u_{\alpha,\beta\beta},$$

where $\alpha, \beta = 1, 2, 3$, and where the following notations are used:

$$f_{\alpha,t} = \frac{\partial f_\alpha}{\partial t}$$

$$f_{\alpha,\beta} = \frac{\partial f_\alpha}{\partial x_\beta}$$

and

$$f_{\alpha,\beta\gamma} = \frac{\partial^2 f_\alpha}{\partial x_\beta \partial x_\gamma}.$$

There is an approach to this equation by using the characteristic functional Φ of the measure $P^t(du)$ defined on the phase space $\{u = (u_1, u_2, u_3)\}$:

$$\Phi(\xi, t) = \int e^{i<\xi,u>} P^t(du).$$

E. Hopf shows that the characteristic functional $\Phi(\xi, , t)$ satisfies the following functional differential equation, called **Hopf equation** (see [17]):

$$\frac{\partial \Phi}{\partial t} = \int_R \xi_\alpha(x) \left[i \frac{\partial}{\partial x_\beta} \frac{\partial^2 \Phi}{\partial \xi_\beta(x) dx \partial \xi_\alpha(x) dx} + \mu \Delta_x \frac{\partial \Phi}{\partial \xi_\alpha(x) dx} - \frac{\partial \Pi}{\partial x_\alpha} \right] dx$$

Studying this approach, we may think of two matters. One is a similarity to the Feynman integral in the sense that both cases deal with functional obtained in the form

$$E(\exp[f(u)])$$

where $f(u)$ is a function of a path (trajectory) u. The expectation is taken with respect to the probability measure introduced on the path space.

As the second point, one may think of functionals $\Phi_n, n \geq 0$, that come from the Hopf equation and the Fock space expansion of generalized white noise functionals. In this case we expect that the calculus can be done in a manner similar to the white noise calculus.

We may recall an interesting approach to the Navier-Stokes equation by A. Inoue. See [18].

[III] Towards noncommutative white noise calculus. This comes from many reasons, such as (i) noncommutative geometry, (ii) Hamiltonian dynamics using both variables, p, q. See [3, 19] and [2].

8 Concluding Remarks

(1) There appears a particular quadratic form in the white noise analysis, i.e.

$$\int : \dot{B}(t)^2 : dt.$$

There is a somewhat general quadratic form

$$\int f(t) : \dot{B}(t)^2 : dt + \int \int F(u, v) : \dot{B}(u)\dot{B}(v) : dudv$$

which is called *normal functional*, the first term being the singular part and the second term the regular part. The two terms can be characterized from our viewpoint and play significant roles, respectively. Recall the role of the singular part in the path integral.

(2) Our method of path integrals enables us to deal with the case of very irregular potentials in the propagator (by L. Streit and others).

(3) Some other approaches: A significant result is by C. C. Bernido and M. V. Carpio Bernido [1]. They are using our method of path integral to investigate the entanglement probabilities of two chain like macro-molecules where one polymer lies on a plane and the other perpendicular to it. The entanglement probabilities are calculated and the result shows a characteristic of the polymer.

We also should like to note that Masujima [20] has published a beautiful monograph collecting various approaches to path integrals.

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Quasi-analyticity and Determinacy of the Full Moment Problem from Finite to Infinite Dimensions

Maria Infusino

Abstract This paper is aimed to show the essential role played by the theory of quasi-analytic functions in the study of the determinacy of the moment problem on finite and infinite-dimensional spaces. In particular, the quasi-analytic criterion of self-adjointness of operators and their commutativity are crucial to establish whether or not a measure is uniquely determined by its moments. Our main goal is to point out that this is a common feature of the determinacy question in both the finite and the infinite-dimensional moment problem, by reviewing some of the most known determinacy results from this perspective. We also collect some properties of independent interest concerning the characterization of quasi-analytic classes associated to log-convex sequences.

Keywords Moment problem • Determinacy • Quasi-analytic class • Infinite dimensional moment problem • Realizability • Nuclear space • Convex regularization • Log-convexity

Mathematics Subject Classification (2010) 44A60, 26E10, 47B25, 47A70, 28C05, 28C20

1 Introduction

Among the numerous aspects of the moment problem, the so-called *determinacy question* is certainly one of the most investigated but still far from being completely solved. The moment problem asks whether a given sequence of numbers is the sequence of moments of some non-negative measure with fixed support. If such a measure is unique, then the moment problem is said to be *determinate*. Therefore,

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M. Infusino (✉)
Fachbereich Mathematik und Statistik, Universität Konstanz, Universitätstraße, 10, Konstanz, 78457, Germany
e-mail: infusino.maria@gmail.com

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the determinacy question is to find under which conditions a non-negative measure with given support is completely characterized by its moments.

In this paper we give an overview about how the concept of quasi-analyticity enters in the study of the determinacy question. As spectral theory and moment theory developed in parallel, the determinacy proofs which can be found in literature often seem circular. We review some of them showing the essential role played by quasi-analyticity techniques.

The moment problem was originally posed in a finite-dimensional setting (see e.g. [1, 55]). More precisely, in the *multivariate power moment problem* the starting multisequence $(m_\alpha)_{\alpha\in\mathbb{N}_0^d}$ consists of real numbers and the support of the measure is assumed to be a subset $K \subseteq \mathbb{R}^d$, where $d \in \mathbb{N}$. However, at an early stage, this problem has also been generalized to the case of infinitely many variables (see e.g. [8] for more details on this topic). This abstract formulation of the moment problem is actually very useful in many applications related to the analysis of many-body systems, e.g. in statistical mechanics, spatial ecology, etc. In this setting, each m_n in the starting sequence $(m_n)_{n\in\mathbb{N}_0}$ is an element of the tensor product of n copies of a certain infinite-dimensional space (e.g. for each n, m_n is a generalized function of n variables in $\mathbb{R}^d$) and the support of the measure is assumed to be a non-linear subset of this space (examples of supports are the set of all L^2 functions, the cone of all non-negative generalized functions, the set of all signed measures).

This paper attempts to show that, regardless of the dimension of the setting in which the moment problem is posed, quasi-analyticity theory gives in some sense the best possible general sufficient determinacy conditions. In the literature, there are different approaches to the investigation of the determinacy question for concrete cases in the finite-dimensional context (see [47] for a thorough overview). For instance, the first known determinacy conditions for the one-dimensional moment problem were obtained through techniques involving continued fractions (see e.g. [30, 31, 44, 59]) or using density conditions of polynomials (see e.g. [1, 12, 13, 49, 55, 60]). The determinacy of the higher-dimensional moment problem is still less understood than the one-dimensional case. However, a number of sufficient multivariate determinacy conditions were developed by using polynomial and rational approximation (see e.g. [11, 27, 40, 45, 46]).

The link between quasi-analyticity and determinacy has been known since the early days of the moment theory. In 1926, Carleman first applied quasi-analyticity to the study of the determinacy of the univariate moment problem (see [18]). More precisely, he proved that if the moment sequence $(m_n)_{n\in\mathbb{N}_0}$ of a non-negative measure μ supported on $\mathbb{R}$ fulfills the so-called *Carleman condition*, i.e. $\sum_{n=1}^{\infty} m_{2n}^{-\frac{1}{2n}} = \infty$, then there is no other measure having the same moment sequence as μ. His main idea was to exploit the quasi-analyticity of a certain integral transform, which intrinsically contains the moment data, to get the determinacy of the classical Hamburger moment problem (c.f. Theorem 3.5).

The concept of quasi-analytic function was first introduced by Borel, who observed that there is a larger class of functions, than merely the analytic functions, having the property to be completely determined only by their value and the

values of their derivatives at a single point (see e.g. [17]). Motivated by the theory of partial differential equations, Hadamard proposed the problem to give necessary and sufficient conditions bearing on a sequence $(m_n)_{n\in\mathbb{N}_0}$ such that the class of all infinitely differentiable functions whose $n-$th derivative is bounded by m_n, for each $n \in \mathbb{N}_0$, is quasi-analytic, [29]. Denjoy was the first to provide sufficient conditions [23] and then Carleman, generalizing Denjoy's theorem, gave necessary and sufficient conditions. Carleman's treatise [18] threw a new light on the theory of quasi-analytic functions, revealing its important role in the study of the moment problem. His ideas inspired a large series of subsequent works about quasi-analyticity criteria for functions in one variable (see e.g. [2, 20, 38, 43]) and for multivariate functions (see e.g. [14, 15, 25]).

Both in the higher-dimensional case and in the infinite-dimensional one, the operator theoretical approach is a powerful method to get not only determinacy conditions but also to guarantee the existence of a solution to the moment problem. Actually, there has always been a mutual exchange between spectral theory and moment problem, since the results in moment theory often served as a starting point for new advances in the theory of operators. The quasi-analyticity again enters in a crucial way in the analysis of the moment problem from the operator theoretical point of view.

For the one-dimensional moment problem the basic ideas developed with the traditional methods of continued fractions and orthogonal polynomials can be re-derived by means of the spectral theory of self-adjoint extensions (see e.g. [1, Chapter 4]). In particular, the classical Hamburger and Stieltjes existence theorems and the relative uniqueness results due to Carleman can be obtained using this approach (see [58]). Note that, in the one-dimensional moment problem, the theory of quasi-analytic functions only appears in the uniqueness part via the concept of quasi-analytic vector for an operator.

In contrast to the one-dimensional case, in higher dimensions, one does not know how to prove existence without uniqueness. In fact, in dimension $d \geq 2$, we need to use the spectral theorem for several essential self-adjoint operators and this requires that the involved operators strongly commute (i.e. their resolutions of identity commute). In [42, Theorem 6], Nussbaum proved that the strong commutativity and the essential self-adjointness can actually be derived using again the concept of quasi-analytic vectors. The so-called *multivariate Carleman condition* gives a condition for the existence of a total subset of quasi-analytic vectors for the considered operators directly in terms of the starting multisequence. This yields the existence of a unique measure solving the given moment problem (see [42, Theorem 10]). Other similar but slightly weaker results were proved before Nussbaum's theorem, using the determinacy of certain $1-$sequences derived from the starting positive semidefinite $d-$sequence (see e.g. [24, 26, 55]). For more recent results about partial determinacy see [47, Section 5].

Despite of the fact that it is unknown how to prove the existence of a solution to the moment problem on $\mathbb{R}^d$ with $d \geq 2$ without involving its determinacy, it is instead possible to use partial determinacy to conclude the determinacy of a moment $d-$sequence. Petersen actually proved a general result of this kind, showing

that if all the d marginal measures of a measure μ on $\mathbb{R}^d$ are determinate then μ is determinate, too (see Theorem 3.10). Another determinacy result not involving existence is due to De Jeu, who has recently proved the uniqueness part of the moment problem on $\mathbb{R}^d$ and on the positive octant $\mathbb{R}^d_+$ by following Carleman's path without using spectral theory, [21].

The operator theoretical approach is also applicable to the infinite-dimensional moment problem. In fact, several infinite-dimensional moment problems have been investigated using the theory of generalized eigenfunction expansion for self-adjoint operators (see e.g. [4, 5, 7–9, 35, 57]). This approach is well developed for nuclear spaces in [5, Chapter 8] and [8, Vol. II, Chapter 5], and it is a generalization of the method presented by Krein in [36, 37]. In these works, Krein used the so-called method of directed functionals for self-adjoint operators instead of the spectral projection theorem for an infinite family of strongly commuting self-adjoint operators given in [8, Vol. I, Chapter 3, Section 2]. Further different methods to solve the moment problem on nuclear spaces were introduced in 1975 in [16] and in [19] (see also [32] and [51, Section 12.5]). These approaches are essentially based on Choquet theory and decompositions of positive definite functionals on a commutative nuclear *-algebras into pure states.

We describe in this paper the infinite-dimensional moment problem on the dual Ω' of a nuclear space Ω, showing that the proof scheme used to get the existence of a unique solution to the moment problem on $\mathbb{R}^d$ can be carried over in this case. In fact, thanks to a certain *determining condition*, it is possible to show that the family of operators associated to the starting positive semidefinite sequence has a total subset of quasi-analytic vectors. Hence, they admit unique strongly pairwise commuting self-adjoint extensions by Nussbaum's result. Therefore, by the spectral theorem for infinitely many unbounded self-adjoint operators, there exists a unique measure on $\mathbb{R}^{\mathbb{N}_0}$ representing those operators. It remains to show that this measure is actually concentrated on Ω'. Note that the determining condition is the correspondent of the multivariate Carleman condition in the infinite-dimensional case. However, the infinite-dimensionality involves additional layers such as the uniformity in the index, regularity properties and growth restrictions on the moments as functions.

Let us outline the contents of this paper.
In Sect. 2, we recall the notion of quasi-analytic class of infinitely differentiable functions on $\mathbb{R}$ and we introduce the famous Denjoy-Carleman theorem. We also review some different versions of the Carleman condition known in literature, pointing out the role of the log-convexity in the proof of these results. In particular, we recall the technique of the convex regularization by means of the logarithm, which is important in solving the problem of the equivalence of quasi-analytic classes. In this context, we propose a proof of the Denjoy-Carleman theorem due to Mandelbrojt, which we found interesting since it is based on completely different methods than the classical ones employing holomorphic function theory.

In Sect. 3, we aim to show how quasi-analytic classes enter in the determinacy of the finite-dimensional moment problem. In Sect. 3.2, we give an alternative and

simple proof of the Carleman uniqueness results for the Hamburger and the Stieltjes one-dimensional moment problems, which exploits the quasi-analyticity of a certain Fourier-Stieltjes transform (see proof of Theorem 3.5). Moreover, we recall the importance of the geometry of the support K in the determinacy of the $K-$moment problem. In Sect. 3.3, we focus on the determinacy of the $d-$dimensional moment problem with $d \geq 2$. We first introduce the so-called multivariate Carleman condition (10) and show that it is sufficient for the determinacy of the Hamburger $d-$dimensional moment problem by using a result due to Petersen. Then we sketch the proof of a recent version of the Denjoy-Carleman theorem for quasi-analytic functions in several variables, which can be used to give an alternative proof of the uniqueness result. Finally, we outline the operator theoretical approach to the Hamburger $d-$dimensional moment problem developed by Nussbaum, stressing the points where quasi-analyticity is fundamental to prove not only the uniqueness but also the existence of the solution. We also mention a uniqueness result for the $d-$dimensional version of the Stieltjes moment problem.

In Sect. 4, we present the moment problem on conuclear spaces. We first introduce a sufficient condition for the determinacy of the analogue of the Hamburger moment problem in this infinite-dimensional setting and we prove this uniqueness result without using spectral theoretical tools. Then we review the main results by Berezansky, Kondratiev and Šifrin about the existence and the uniqueness of a solution for the analogues of the Hamburger and the Stieltjes moment problems on conuclear spaces. We point out that, as in the finite-dimensional case, the existence of a solution cannot be proved without using the determinacy of the moment problem and we sketch the steps of this proof where quasi-analyticity enters.

In the appendix, we prove some results about log-convex sequences, which are useful in relation to the quasi-analyticity of the associated classes of functions.

2 Characterization of Quasi-analytic Classes of Functions on $\mathbb{R}$

Let us recall the basic definitions and state some preliminary results concerning the theory of quasi-analytic functions on $\mathbb{R}$. In the following, we denote by $\mathbb{N}_0$ the set of all non-negative integers and by $\mathcal{C}^\infty(X)$ the space of all infinitely differentiable real valued functions on the topological space X.

Definition 2.1 (The class $C\{M_n\}$) Given a sequence of positive real numbers $(M_n)_{n\in\mathbb{N}_0}$, we define the class $C\{M_n\}$ as the set of all functions $f \in \mathcal{C}^\infty(\mathbb{R})$ such that

$$\|D^n f\|_\infty \leq \beta_f B_f^n M_n, \quad \forall\, n \in \mathbb{N}_0$$

where $D^n f$ is the $n-$th derivative of f, $\|D^n f\|_\infty := \sup_{x\in\mathbb{R}} |D^n f(x)|$, and β_f, B_f are positive constants only depending on f.

Definition 2.2 (Quasi-analytic class) The class $C\{M_n\}$ of functions on $\mathbb{R}$ is said to be quasi-analytic if the conditions

$$f \in C\{M_n\},\ (D^n f)(0) = 0, \quad \forall\, n \in \mathbb{N}_0$$

imply that $f(x) = 0$ for all $x \in \mathbb{R}$.

The definition above can be given replacing $(D^n f)(0)$ with $(D^n f)(x_0)$, where x_0 is any other given point in the domain of the function f. Note that the analytic functions on $\mathbb{R}$ correspond to the class $C\{n!\}$. It is obvious from the previous definitions that the following holds.

Proposition 2.3 *Let $(M_n)_{n\in\mathbb{N}_0}$ be a sequence of positive real numbers. $C\{M_n\}$ is quasi-analytic if and only if for any positive constant δ the class $C\{\delta M_n\}$ is quasi-analytic.*

Recall that $C\{M_n\}$ and $C\{M'_n\}$ are said to be *equivalent* if there exist two constants $a, b > 0$ such that $a^n M_n \le M'_n \le b^n M_n$ for any $n \in \mathbb{N}_0$. This means that every function of either of these two classes belongs also to the other. The problem of constructing a sequence $(M'_n)_{n\in\mathbb{N}_0}$ in a simple relationship with a given starting sequence $(M_n)_{n\in\mathbb{N}_0}$ such that the corresponding classes of functions are equivalent has extensively been studied (for more details see [39]). In particular, we introduce here the so-called *convex regularization of by means of the logarithm*.

Definition 2.4 (Log-convexity) A sequence of positive real numbers $(M_n)_{n\in\mathbb{N}_0}$ is said to be log-convex if and only if for all $n \ge 1$ we have that $M_n^2 \le M_{n-1} M_{n+1}$.

Definition 2.5 (Convex regularization by means of the logarithm) Let $(M_n)_{n\in\mathbb{N}}$ be a sequence of positive real numbers with $\liminf_{n\to\infty} M_n^{\frac{1}{n}} = \infty$. Define for any $r \ge 1$ the function $T(r) := \max_{n\in\mathbb{N}} \frac{r^n}{M_n}$. The *convex regularization of* $(M_n)_{n\in\mathbb{N}}$ *by means of the logarithm* is the sequence $(M_n^c)_{n\in\mathbb{N}}$ defined by

$$\ln(M_n^c) := \sup_{t\ge 0} \left(nt - \ln(T(e^t))\right), \tag{1}$$

or equivalently, $M_n^c := \sup_{t\ge 0} \frac{e^{tn}}{T(e^t)} = \sup_{r\ge 1} \frac{r^n}{T(r)}$.

Note that (1) means that for any $t \ge 0$ the line $x \mapsto tx - \ln(T(e^t))$ is not above any of the points $(\ln(M_n^c))_{1\le n<e^t}$. The convex regularized sequence by means of the logarithm is indeed the largest convex minorant (i.e. the convex envelope) of the function $n \mapsto \ln(M_n)$. This means that $(M_n^c)_{n\in\mathbb{N}}$ is a log-convex sequence and that for any $n \in \mathbb{N}$, $M_n^c \le M_n$. Clearly, if $(M_n)_{n\in\mathbb{N}}$ is log-convex then $M_n^c \equiv M_n$ for all $n \in \mathbb{N}$.

This procedure allows to explicitly construct, starting from any sequence $(M_n)_{n\in\mathbb{N}}$ of positive real numbers with $\liminf_{n\to\infty} M_n^{1/n} = \infty$, a log-convex sequence $(M_n^c)_{n\in\mathbb{N}}$ such that the classes $C\{M_n\}$ and $C\{M_n^c\}$ are equivalent (see [39, Theorem 6.5.III]). Therefore, if $\liminf_{n\to\infty} M_n^{1/n} = \infty$, then the class $C\{M_n\}$ is quasi-analytic if and only if $C\{M_n^c\}$ is quasi-analytic.

Remark 2.6 When we deal with quasi-analytic classes the assumption that $\liminf_{n\to\infty} M_n^{\frac{1}{n}} = \infty$ is not restrictive, but actually gives the only interesting case. In fact, if $\liminf_{n\to\infty} M_n^{\frac{1}{n}} = 0$, then $C\{M_n\}$ is equivalent to $C\{0\}$ (which contains only the constants) and if $0 < \liminf_{n\to\infty} M_n^{\frac{1}{n}} < \infty$, then $C\{M_n\}$ is equivalent to $C\{1\}$ (see [39, Theorem 6.5.III]). In both cases, $C\{M_n\}$ is already quasi-analytic.

The problem to give necessary and sufficient conditions bearing on the sequence $(M_n)_{n\in\mathbb{N}_0}$ such that the class $C\{M_n\}$ is quasi-analytic was proposed by Hadamard in [29]. Denjoy was the first to provide sufficient conditions for the quasi-analyticity of a class [23], but the problem was completely solved by Carleman, who generalized Denjoy's theorem and methods giving the first characterization of quasi-analytic classes in [18]. Using the convex regularization by means of the logarithm, other conditions equivalent to Carleman's one were obtained.

Theorem 2.7 (The Denjoy-Carleman Theorem) *Let $(M_n)_{n\in\mathbb{N}_0}$ be a sequence of positive real numbers. Then the following conditions are equivalent*

(a). $C\{M_n\}$ *is quasi-analytic,*

(b). $\sum_{n=1}^{\infty} \frac{1}{\beta_n} = \infty$ *with* $\beta_n := \inf_{k\geq n} \sqrt[k]{M_k}$,

(c). $\sum_{n=1}^{\infty} \frac{1}{\sqrt[n]{M_n^c}} = \infty$,

(d). $\int_1^{\infty} \frac{\ln(T(r))}{r^2} dr = \infty$,

(e). $\sum_{n=1}^{\infty} \frac{M_{n-1}^c}{M_n^c} = \infty$,

where $(M_n^c)_{n\in\mathbb{N}}$ is the convex regularization of $(M_n)_{n\in\mathbb{N}}$ by means of the logarithm and for any $r \geq 1$ the function T is given by $T(r) := \max_{n\in\mathbb{N}} \frac{r^n}{M_n}$.

Condition (b) and (c) are due to Carleman, [18] (see also [20] for a simple but detailed proof). Condition (d) was instead introduced by Ostrowski in [43], who was also the first to provide a new proof of Carleman's theorem. Moreover, Condition (e) was independently given by Mandelbrojt and Bang in [38] and [2], respectively.

A very nice proof of the equivalence of the conditions (b), (c), (d) and (e) is given in [39, Theorem 1.8.VII]. For its simplicity, let us just sketch the proof that (c) and (e) are equivalent. By Proposition 2.3, we can assume w.l.o.g. $M_0 = 1$ and so easily derive from Proposition 1(b) that $M_{n-1}^c \leq (M_n^c)^{1-1/n}$. Hence, (e) implies (c). The converse follows by Carleman's inequality, that is, by using $\sum_{n=1}^{\infty} (a_1 \cdots a_n)^{\frac{1}{n}} \leq e \sum_{n=1}^{\infty} a_n$ for $a_n := M_{n-1}^c / M_n^c$.

To complete this section, we propose the proof of the equivalence of conditions (a), (d) and (e) given by Mandelbrojt in [39] (see in particular Theorem 4.1.III). In contrast to Denjoy, Carleman and Ostrowski, Mandelbrojt's proof is not based on the theory of holomorphic functions but only on some considerations relative to the average values of a real function.

The equivalence of (d) and (e) easily follows by the following

$$\int_1^\infty \frac{\ln(T(r))}{r^2} dr = \ln(T(1)) + 1 + \sum_{n=1}^{\infty} \frac{M_n^c}{M_{n+1}^c}. \tag{2}$$

As mentioned before, a detailed proof of this equality can be found in [39, Theorem 1.8.VII]. We give here just an idea of this proof. For any $t \geq 0$, denote by $N(t)$ the greatest $n \in \mathbb{N}$ such that $tn - \ln(T(e^t)) = \ln M_n$. Then one can easily see that $\ln T(e^t) - \ln T(e^{t'}) = \int_t^{t'} N(s)ds$, for any $t, t' \geq 0$. Since N is a piecewise continuous function and it is monotone increasing, we can denote by t_k the points in which the function N has a jump. Using Definition 2.5, we get that $M_n^c/M_{n+1}^c = t_k$ for any $N(t_k) \leq n \leq N(t_{k+1})$. Combining these two results and making some further calculations, one finally gets (2).

The main ingredient used by Mandelbrojt to prove that (d) and (e) are both necessary and sufficient for quasi-analyticity is the construction of an infinitely differentiable function with compact support which belongs to the class $C\{M_n\}$. Let us preliminarily sketch such a construction.

For a sequence $(\gamma_n)_{n\in\mathbb{N}}$ of positive constants and a function g Lebesgue integrable on $[-\gamma, \gamma]$, we define

$$M(\gamma_1,\dots,\gamma_n; g)(x) := \frac{1}{2^n\gamma_1\cdots\gamma_n} \int_{-\gamma_1}^{\gamma_1} \cdots \int_{-\gamma_n}^{\gamma_n} g(x + t_1 + \cdots + t_n) dt_1 \dots dt_n.$$

Let $(\mu_n)_{n\in\mathbb{N}}$ be a sequence of positive constants with $\sum_{n=1}^{\infty} \mu_n =: \mu < \infty$ and let f be a Lebesgue integrable function supported on $[a, b]$. For any $n \geq 1$, we set

$$M_n(x) := M(\mu_1, \dots, \mu_n; f)(x),$$

which is obviously zero outside the interval $I_n := [a - \sum_{i=1}^n \mu_i, b + \sum_{i=1}^n \mu_i]$ and whose value is independent of the order in which the quantities $\mu_1, \dots, \mu_n$ are taken. This definition is recursive since $M_n(x) = M(\mu_n; M_{n-1})(x)$. For any $n \in \mathbb{N}$, the function $M_n(x)$ is differentiable in I_1 with first derivative equal to

$$(DM_n)(x) = \frac{1}{2\mu_1} M(\mu_2, \dots, \mu_n; f(\cdot + \mu_1) - f(\cdot\mu_1))(x).$$

Thus, $M_n(x)$ has first derivative uniformly bounded in n and so the family $(M_n(x))_{n\in\mathbb{N}}$ is equally graded continuous in $[a - \mu, b + \mu]$. Therefore, it tends

uniformly to a continuous function $\psi(x)$ and so for all $x \in [a-\mu, b+\mu]$

$$\psi(x) = \frac{1}{2\mu_1} \int_{-\mu_1}^{\mu_1} M(\mu_2, \ldots, \mu_n, \ldots; f(\cdot + t))(x)dt.$$

Hence, the function $\psi(x)$ is infinitely differentiable on $[a-\mu, b+\mu]$ and zero outside this interval.

Proof (of (a)⇒(d)) By Remark 2.6, we can directly assume that $\liminf_{n\to\infty} M_n^{\frac{1}{n}} = \infty$. W.l.o.g. we can take $M_0 = 1$, since $C\{M_n\}$ and $C\{\frac{M_n}{M_0}\}$ coincide by Proposition 2.3. Suppose that $\sum_{n=1}^{\infty} M_n^c/M_{n+1}^c < \infty$ and repeat the construction above for $\mu_n := M_{n-1}^c/M_n^c$ and $f := \mathbb{1}_{[-\mu,\mu]}$ with $\mu := \sum_{n=1}^{\infty} \mu_n$. Then we get that the associated limit function ψ is infinitely differentiable on $[-2\mu, 2\mu]$ and zero outside. As a consequence, all the derivatives of the function ψ are zero at $\pm 2\mu$. Furthermore,

$$\psi(0) = \lim_{n\to\infty} \frac{1}{2^n \mu_1 \ldots \mu_n} \int_{-\mu_1}^{\mu_1} \ldots \int_{-\mu_n}^{\mu_n} \mathbb{1}_{[-\mu,\mu]}(t_1 + \ldots t_n)dt_1 \ldots dt_n = 1$$

and it is easy to show that

$$|(D^n\psi)(x)| \leq \frac{1}{\mu_1 \ldots \mu_n} = M_n^c \leq M_n.$$

In conclusion, we constructed $\psi \in C\{M_n\}$ which is not quasi-analytic. □

To prove that (e) implies (a) we need the following lemma.

Lemma 2.8 *Let $(M_n)_{n\in\mathbb{N}_0}$ a sequence of positive real numbers such that $C\{M_n\}$ is not quasi-analytic. Then there exists an infinite differentiable function φ on $[0, 1]$ such that*

1. $(D^n\varphi)(0) = 0$ *and* $(D^n\varphi)(1) = 0$, $\forall n \in \mathbb{N}_0$.
2. $\forall n \in \mathbb{N}$ *and* $\forall x \in [0, 1]$, $|(D^n\varphi)(x)| \leq M_n$.
3. $\varphi \geq 0$ *on* $[0, 1]$.
4. $\varphi(1-x) = \varphi(x)$, $\forall x \in [0, 1]$.

Proof Since a class of functions is invariant under rescaling an translation, we can assume w.l.o.g. that the functions in $C\{M_n\}$ are defined on the interval $[0, 1]$. As $C\{M_n\}$ is not quasi-analytic, there exists a non-zero function $f \in C\{M_n\}$ and a point $a \in [0, 1[$ such that f and all its derivatives vanish at a but for any $\varepsilon > 0$ the function f is not identically zero on $[a, a+\varepsilon]$. For any $0 \leq \alpha < 1-a$, let us define for $x \in [0, 1]$

$$f_1(x) := \int_0^{\alpha x + a} \int_0^t f(\tau)d\tau dt.$$

Then the function f_1 is not identically zero on $[0,1]$ and all its derivatives vanish at 0. Since $f \in C\{M_n\}$, there exists $c > 0$ such that for any $n \in \mathbb{N}_0$ and any $x \in [0,1]$, $|(D^n f)(x)| \leq c^n M_n$. Then $|(D^n f_1)(x)| \leq \alpha^n c^{n-2} M_{n-2}$, that is, $f_1 \in C\{M_{n-2}\}$.

Let $f_2(x) := f_1(x - x^2)$, then $(Df_2)(x) = (1-2x)(Df_1)(x-x^2)$. By induction, it can be easily proved that for any $n \geq 2$ we have

$$|(D^n f_2)(x)| \leq \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{n^{2k}}{k!} \sup_{y\in[0,1]} \left|(D^{n-k} f_1)(y)\right|. \tag{3}$$

Using Taylor formula and the fact that all derivatives of f_1 vanish at zero, we obtain

$$(D^{n-k} f_1)(x) = \frac{1}{(k-1)!} \int_0^x (x-t)^{k-1} (D^n f_1)(t) dt. \tag{4}$$

By (3) and (4), we get

$$\sup_{x\in[0,1]} |(D^n f_2)(x)| \leq \alpha^n c^{n-2} M_{n-2} \sum_{k=0}^{\infty} \frac{n^{2k}}{(k!)^2} \leq e^{2n} \alpha^n c^{n-2} M_{n-2}.$$

Hence, f_2 is in the same class of f_1 and vanishes with all its derivatives at 0 and at 1.

Let us consider the function $f_3(x) := f_2(x)^2$. We can extend f_2 to a periodic even function, using that f_2 and all its derivative coincide at the endpoints. Hence,

$$f_2(x) = \frac{d_0}{2} + \sum_{q=1}^{\infty} (-1)^q d_q \cos(2\pi q x) \quad \text{and} \quad |(D^n f_2)(x)| \leq (2\pi)^n \sum_{q=1}^{\infty} |d_q| q^n,$$

where $d_q := 2(-1)^q \int_0^1 f_2(x) \cos(2\pi q x) dx$. Integrating by parts l times, we get that

$$|d_q| \leq 2(2\pi q)^{-l} e^{2l} \alpha^l c^{l-2} M_{l-2}. \tag{5}$$

Using the binomial formula for the derivative and the Hölder inequality, we obtain that there exists $C > 0$ such that

$$|(D^n f_3)(x)| \leq (4\pi)^n C \sum_{q=1}^{\infty} |d_q| q^n.$$

Furthermore, by (5) for $l = n+2$, we get that

$$|(D^n f_3)(x)| \leq L \left(\sum_{q=1}^{\infty} \frac{1}{q^2} \right) (2c\alpha e^2)^n M_n,$$

where $L := 2C(2\pi)^{-2}(\alpha e^2)^2$. If we choose $\alpha < \frac{1}{2ce^2}$, then the function we are looking for is given by $\varphi(x) := \frac{f_3(x)}{L\left(\sum_{q=1}^{\infty} \frac{1}{q^2}\right)}$. □

Proof (of (e)⇒(a)) Let us show that if $C\{M_n\}$ is not quasi-analytic then $\int_1^{\infty} \frac{\ln(T(r))}{r^2} dr < \infty$. By Remark 2.6, we can again assume that $\liminf_{n\to\infty} M_n^{\frac{1}{n}} = \infty$. Let f be a function on $[0, 1]$ as given by Lemma 2.8 and define

$$F(z) := \int_0^1 e^{-xz} f(x)dx, \quad z \in \mathbb{C},$$

which is an entire function with $F(1) > 0$. Using integration by parts k times and the fact that f vanishes with all its derivatives at 0 and 1, we get that $|F(z)| \leq \frac{M_k}{|z|^k}$. Since this holds for all $k \in \mathbb{N}$ and $\liminf_{n\to\infty} M_n^{1/n} = \infty$, we get

$$|F(z)| \leq \frac{1}{\max\limits_{k\in\mathbb{N}} \frac{|z|^k}{M_k}} = \frac{1}{T(|z|)}. \tag{6}$$

Let $0 < p < 1$ and let us consider the circle C_p given by the equation $\left|\frac{1-z}{z}\right| = p$. Using the Poisson integral formula and the properties of F, it is possible to prove that

$$\frac{1}{2p\pi} \int_{C_p} \frac{\ln|F(z)|}{|z|^2} d|z| \geq \ln|F(1)|.$$

By using (6) in the latter equation, we get that

$$\frac{1}{2p\pi} \int_{C_p} \frac{\ln(T(|z|))}{|z|^2} d|z| \leq -\ln|F(1)|.$$

If we denote by C_p^t the part of C_p between the lines $Im(z) = -t$ and $Im(z) = t$ which contains the point $\frac{1}{p+1}$, then for large values of t we have

$$\frac{1}{2p\pi} \int_{C_p^t} \frac{\ln(T(|z|))}{|z|^2} d|z| \leq -\ln|F(1)|.$$

If $p \to 1$, then C_p^t tends to the segment of the straight line $Re(z) = \frac{1}{2}$ with $-t < Im(z) < t$, which yields

$$\frac{1}{\pi} \int_0^t \frac{\ln(T(r))}{\frac{1}{4} + r^2} dr \leq -\ln(F(1)).$$

As a consequence, the integral $\int_1^{\infty} \frac{\ln(T(r))}{r^2} dr < \infty$. □

3 Uniqueness in the Finite-Dimensional Moment Problem

3.1 The Finite-Dimensional Moment Problem

Let $\mathbb{R}[\mathbf{x}]$ be the algebra of all real polynomials with d real variables and real coefficients. For $\alpha := (\alpha_1, \dots, \alpha_d) \in \mathbb{N}_0^d$ and $\mathbf{x} := (x_1, \dots, x_d) \in \mathbb{R}^d$, we define the following multi-index notation $\mathbf{x}^\alpha := x_1^{\alpha_1} \cdots x_d^{\alpha_d}$ (where $x_j^0 := 1$) and $|\alpha| := \alpha_1 + \cdots + \alpha_d$. Let $\mathcal{M}^*(\mathbb{R}^d)$ be the collection of all non-negative Borel measures on $\mathbb{R}^d$ such that $\mathbf{x}^\alpha \in L^1(\mu)$ for all $\alpha \in \mathbb{N}_0^d$.

Definition 3.1 Let $\mu \in \mathcal{M}^*(\mathbb{R}^d)$ and $\alpha \in \mathbb{N}_0^d$. The $\alpha^{\text{th}}-$*moment* of μ is defined by

$$m_\alpha^\mu := \int_{\mathbb{R}^d} \mathbf{x}^\alpha \, \mu(d\mathbf{x}) = \int_{\mathbb{R}^d} x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_d^{\alpha_d} \mu(dx_1, dx_2, \dots, dx_d).$$

The multisequence $(m_\alpha^\mu)_{\alpha \in \mathbb{N}_0^d}$ is called *moment sequence of* μ.

Note that the set $\mathcal{M}^*(\mathbb{R}^d)$ exactly consists of all the non-negative Borel measures on $\mathbb{R}^d$ with finite moments of all orders. Given a closed subset $K \subseteq \mathbb{R}^d$, we denote by $\mathcal{M}^*(K)$ the set of all measures in $\mathcal{M}^*(\mathbb{R}^d)$ having support contained in K.

The $K-$moment problem asks to determine when a given multisequence is actually the moment sequence of some measure $\mu \in \mathcal{M}^*(K)$.

Problem 3.2 (Full $K-$moment problem) *Let $m = (m_\alpha)_{\alpha \in \mathbb{N}_0^d}$ be a multisequence of real numbers and let $K \subseteq \mathbb{R}^d$ be closed. Find a measure $\mu \in \mathcal{M}^*(K)$ such that $m_\alpha = m_\alpha^\mu$ for all $\alpha \in \mathbb{N}_0^d$.*

If such a measure μ does exists we say that the sequence m is *realized* by μ on K and the measure μ is called *realizing measure* on K. Note that we refer to this moment problem as *finite-dimensional* since the dimension of the supporting set K is finite. Recall that if m is a finite sequence then the $K-$moment problem is called *truncated*.

The statement of Problem 3.2 includes all the classical one-dimensional cases. In fact, if $d = 1$, then we get

- The *Hamburger moment problem* for $K = \mathbb{R}$.
- The *Stieltjes moment problem* for $K = \mathbb{R}_+$.
- The *Hausdorff moment problem* for $K = [0, 1]$.

It is easy to see that the $K-$moment problem can be restated in terms of integral representation of linear functionals by introducing the so-called *Riesz functional*.

Definition 3.3 (Riesz' functional) Given $m = (m_\alpha)_{\alpha \in \mathbb{N}_0^d}$, we define the associated Riesz functional L_m on $\mathbb{R}[\mathbf{x}]$ by $L_m(\mathbf{x}^\alpha) := m_\alpha, \ \alpha \in \mathbb{N}_0^d$.

A necessary condition for a sequence of real numbers to be the moment sequence of some measure in $\mathcal{M}^*(\mathbb{R}^d)$ is the following.

Definition 3.4 (Positive semidefinite sequence) A sequence $m = (m_\alpha)_{\alpha \in \mathbb{N}_0^d}$ of real numbers is said to be *positive semidefinite* if for any $n \in \mathbb{N}$, $\alpha_1, \ldots, \alpha_n \in \mathbb{N}_0^d$ and $\xi_1, \ldots, \xi_n \in \mathbb{R}$,

$$\sum_{j,l=1}^{n} m_{\alpha_j + \alpha_l} \xi_j \xi_l \geq 0,$$

or equivalently, for any $h \in \mathbb{R}[\mathbf{x}]$, $L_m(h^2) \geq 0$.

In the case of the Hamburger moment problem, i.e. when $d = 1$ and $K = \mathbb{R}$, the positive semidefiniteness is also sufficient, but this is not true when $K = \mathbb{R}^d$ with $d \geq 2$.

A measure $\mu \in \mathcal{M}^*(K)$ is called *determinate* if any other measure $\nu \in \mathcal{M}^*(K)$ having the same moment sequence as μ is equal to μ. Equivalently, a sequence of real numbers is called *determining* on K if there exists a unique non-negative measure in $\mathcal{M}^*(K)$ realizing m. In this case, the K-moment problem is also addressed as determinate.

3.2 Determinacy Conditions in the One-Dimensional Case

As far as we know, Carleman was the first to approach the determinacy question with methods involving quasi-analyticity theory. In fact, in his famous work of 1926, he proposed the following result which gives a sufficient condition for the uniqueness of the solution to the Hamburger moment problem (see [18, Chapter VIII]).

Theorem 3.5 *Let $\mu, \nu \in \mathcal{M}^*(\mathbb{R})$ have the same moment sequence $m = (m_n)_{n \in \mathbb{N}_0}$. If m is such that*

$$\sum_{n=1}^{\infty} \frac{1}{\sqrt[2n]{m_{2n}}} = \infty, \tag{7}$$

then $\mu = \nu$.

The original proof by Carleman makes use of the Cauchy transform of the two given measures. Here, we decided to propose a slightly different proof that uses the Fourier-Stieltjes transform but maintains the same spirit of Carleman's proof. In fact, the essential strategy of both proofs is to consider the transform of the difference of the two given measures and show that it belongs to the class $C\{\sqrt{m_{2n}}\}$, which can be proved to be quasi-analytic thanks to (7). This directly leads to the fact that the two original measures coincide and so to the determinacy of the Hamburger moment problem for m. Before giving our proof of Theorem 3.5, let us observe a useful property of the moment sequences.

Remark 3.6 The log-convexity (see Definition 2.4) is a necessary condition for a sequence of positive numbers to be the absolute moment sequence of some non-negative measure defined on $\mathbb{R}$. More precisely, if $\mu \in \mathcal{M}^*(\mathbb{R})$, then the sequence $(M_n)_{n\in\mathbb{N}_0}$ of all its absolute moments, i.e. $M_n = \int_{\mathbb{R}} |x|^n \mu(dx)$, is log-convex. In fact, by Cauchy-Schwarz's inequality, we have that for any $n \in \mathbb{N}$

$$M_n^2 \leq \left(\int_{\mathbb{R}} |x|^{n-1}\mu(dx)\right)\left(\int_{\mathbb{R}} |x|^{n+1}\mu(dx)\right) = M_{n-1}M_{n+1}.$$

It directly follows that the sequence of all even moments of a measure $\mu \in \mathcal{M}^*(\mathbb{R})$, i.e. $m_{2n} = \int_{\mathbb{R}} x^{2n}\mu(dx) = M_{2n}$, is also log-convex.

Proof (of Theorem 3.5) W.l.o.g. assume that all even moments of μ are positive. In fact, if $m_{2n} = 0$ for some $n \geq 1$ then $supp(\mu) \subseteq \{x \in \mathbb{R} : x^{2n} = 0\} = \{0\}$ and thus, the unique realizing measure is $\mu = m_0\delta_0$. By Remark 3.6, the sequence of all even moments $(m_{2n})_{n\in\mathbb{N}_0}$ is log-convex. Hence, the sequence $(\sqrt{m_{2n}})_{n\in\mathbb{N}_0}$ is also log-convex and by assumption it satisfies (7), which can be rewritten as

$$\sum_{n=1}^{\infty} \frac{1}{\sqrt[n]{\sqrt{m_{2n}}}} = \infty.$$

Then, by Denjoy-Carleman's Theorem 2.7, the class $C\{\sqrt{m_{2n}}\}$ is quasi-analytic.

Let us consider the Fourier-Stieltjes transforms of μ and ν, i.e.

$$F_\mu(t) := \int_{\mathbb{R}} e^{-ixt}\mu(dx) \quad \text{and} \quad F_\nu(t) := \int_{\mathbb{R}} e^{-ixt}\nu(dx), \quad t \in \mathbb{R}.$$

The function $(F_\mu - F_\nu) \in \mathcal{C}^\infty(\mathbb{R})$ belongs to $C\{\sqrt{m_{2n}}\}$. In fact, since

$$\frac{d^n}{dt^n}F_\mu(t) = \int_{\mathbb{R}} (-ix)^n e^{-ixt}\mu(dx) \quad \text{and} \quad \frac{d^n}{dt^n}F_\nu(t) = \int_{\mathbb{R}} (-ix)^n e^{-ixt}\nu(dx),$$

we get

$$\left|\frac{d^n}{dt^n}(F_\mu - F_\nu)(t)\right| \leq \int_{\mathbb{R}} |x|^n\mu(dx) + \int_{\mathbb{R}} |x|^n\nu(dx) \leq (c_\mu + c_\nu)\sqrt{m_{2n}},$$

where $c_\mu := \sqrt{\mu(\mathbb{R})}$, $c_\nu := \sqrt{\nu(\mathbb{R})}$. Moreover, since μ and ν have the same moments, we easily get that $\frac{d^n}{dt^n}(F_\mu - F_\nu)(0) = 0$. Then the quasi-analyticity of the class $C\{\sqrt{m_{2n}}\}$ implies that the function $F_\mu - F_\nu$ is identically zero on $\mathbb{R}$. Consequently, by the injectivity of the Fourier-Stieltjes transform, we have that $\mu = \nu$. □

Carleman's condition guarantees that the Hamburger moment problem is determinate unless the even moments tend to infinity quite rapidly. However, this criterion has the disadvantage to only give a sufficient condition for the moment

problem to be determinate on $\mathbb{R}$. Indeed, there exist Hamburger moment sequences $(m_n)_{n\in\mathbb{N}_0}$ such that $\sum_{n=1}^{\infty} \frac{1}{\sqrt[2n]{m_{2n}}} < \infty$ but the correspondent moment problem is determinate (see e.g. [61] for examples).

When we consider a Stieltjes moment sequence, we need to be careful in distinguishing the determinacy in the sense of Stieltjes from the one in the sense of Hamburger. Obviously, an indeterminate Stieltjes moment problem is also an indeterminate Hamburger moment problem. However, there are determinate Stieltjes moment problems which are indeterminate in the sense of Hamburger. Regarding the determinacy of the Stieltjes moment problem, we have the following sufficient criterion (see [18, Chapter VIII]).

Theorem 3.7 *Let $m = (m_n)_{n\in\mathbb{N}_0}$ be the moment sequence of $\mu \in \mathcal{M}^*(\mathbb{R}_+)$. If*

$$\sum_{n=1}^{\infty} \frac{1}{\sqrt[2n]{m_n}} = \infty, \tag{8}$$

then μ is the unique measure in $\mathcal{M}^*(\mathbb{R}_+)$ realizing m.

Condition (8) is well-know as *Stieltjes' condition* since it is sufficient for the determinacy of the Stieltjes moment problem.

Proof Let us consider the measure ν defined on $\mathbb{R}$ as follows

$$d\nu(x) := \frac{1}{2}\left(\mathbb{1}_{[0,+\infty)}(x)d\mu(x^2) + \mathbb{1}_{(-\infty,0]}(x)d\mu(x^2)\right).$$

Then we have that $\nu \in \mathcal{M}^*(\mathbb{R})$ and its moment sequence $q = (q_n)_{n\in\mathbb{N}_0}$ is such that $q_{2n} = m_n$ and $q_{2n+1} = 0$, for all $n \in \mathbb{N}_0$. The conclusion follows by Theorem 3.5 applied to the sequence q. □

This demonstrates that in the general $K-$moment problem, the geometry of K deeply influences its determinateness. Another example is when K is compact. In fact, if two measures $\mu, \nu \in \mathcal{M}^*(\mathbb{R})$ have both compact support K and the same moment sequence m, then by the Stone-Weirstrass theorem we directly get $\mu = \nu$. However, if only one of the two measures has compact support K, then we can still conclude that the correspondent $K-$moment problem for m is determinate, using Carleman's Theorem 3.5 and the following inequality

$$m_{2n} = \int_K x^{2n}\mu(dx) \leq \mu(K)\max_{x\in K} x^{2n}, \quad \forall n \in \mathbb{N}_0.$$

The impact of the geometry of the support on the uniqueness of the realizing measure has been extensively treated in [46], where the authors proved that if K is one-dimensional and virtually compact then every $K-$moment problem is determinate (see [50] and [46, Remark 3.4] for the notion of virtually compact set and recall that such a set is not necessarily compact [46, Example 6.3]). On the other hand, they showed that there exists a large class of non-virtually compact sets

of dimension one which support indeterminate moment sequences. However, as far as we know, it is still open the question if for any K not virtually compact it is possible to construct an indeterminate $K-$moment problem.

The quasi-analyticity plays also a fundamental role in the analysis of the moment problem from an operator theoretical point of view. The uniqueness results given in this section for the one-dimensional moment problem follow indeed from the quasi-analytic vectors theorem. A comprehensive exposition about the classical Hamburger and Stieltjes moment problems via methods from the self-adjoint extension theory of symmetric operators is given by Simon in [58]. In this paper, we will describe the operator theoretical approach only for the higher-dimensional moment problem, because for $d \geq 2$ the quasi-analyticity is already essential to prove the existence of a solution and not only its uniqueness.

3.3 Determinacy Conditions in the Multidimensional Case

The determinacy of the $d-$dimensional moment problem for $d \geq 2$ is a more delicate question, but thanks to quasi-analyticity it is possible to get interesting results also in this case. For a detailed review about this topic, see the comprehensive work of Putinar and Schmüdgen [47]. The quasi-analyticity of functions in several variables has been already treated in [14, 15, 25]. However, we introduce here the analogue of Theorem 2.7 for quasi-analytic classes of functions on $\mathbb{R}^d$, proposing a recent proof due to de Jeu (see [22, Theorem B.1]).

Theorem 3.8 *For $j = 1, \dots, d$, let $(M_j(n))_{n\in\mathbb{N}_0}$ be a sequence of positive real numbers with*

$$\forall\, j \in \{1, \dots, d\}, \quad \sum_{n=1}^{\infty} \frac{1}{\beta_j(n)} = \infty \text{ with } \beta_j(n) := \inf_{k\geq n} \sqrt[k]{M_j(k)}. \tag{9}$$

Let $f \in \mathcal{C}^\infty(\mathbb{R}^d)$ and assume that there exist $A, B \geq 0$ such that for any $\alpha = (\alpha_1, \dots, \alpha_d) \in \mathbb{N}_0^d$

$$\|D^\alpha f\|_\infty \leq AB^{|\alpha|} \prod_{j=1}^{d} M_j(\alpha_j),$$

where $D^\alpha f$ denotes the partial derivative $\frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}} f$, $|\alpha| := \sum_{i=1}^{d} \alpha_i$ and $\|(D^\alpha f)\|_\infty := \sup_{\mathbf{x}\in\mathbb{R}^d} |D^\alpha f(\mathbf{x})|$. If $(D^\alpha f)(0) = 0$, $\forall \alpha \in \mathbb{N}_0^d$, then $f \equiv 0$ on $\mathbb{R}^d$.

Remark 3.9 Note that (9) is equivalent to require that, for each fixed $j \in \{1, \dots, d\}$, any of the conditions (a), (c), (d), (e) in Theorem 2.7 is fulfilled by $(M_j(n))_{n\in\mathbb{N}_0}$.

Proof For $d = 1$, the result reduces to Theorem 2.7. Assume that Theorem 3.8 holds for the dimension $d-1$. For any $\alpha_1, \ldots, \alpha_{d-1} \in \mathbb{N}_0$, let $\phi_{\alpha_1,\ldots,\alpha_{d-1}} : \mathbb{R} \to \mathbb{R}$ be defined by

$$\phi_{\alpha_1,\ldots,\alpha_{d-1}}(b) := \frac{\partial^{\alpha_1+\cdots+\alpha_{d-1}}}{\partial x_1^{\alpha_1}\cdots\partial x_{d-1}^{\alpha_{d-1}}} f(0,\ldots,0,b), \quad \forall b \in \mathbb{R}.$$

Then, all the derivatives of $\phi_{\alpha_1,\ldots,\alpha_{d-1}}$ vanish at $0 \in \mathbb{R}$ by assumption. Moreover, for any $\alpha_d \in \mathbb{N}_0$ and any $b \in \mathbb{R}$,

$$\left| \frac{d^{\alpha_d}}{dx_d^{\alpha_d}} \phi_{\alpha_1,\ldots,\alpha_{d-1}}(b) \right| \leq \left(A\, B^{(\alpha_1+\cdots+\alpha_{d-1})} \prod_{j=1}^{d-1} M_j(\alpha_j) \right) B^{\alpha_d} M_d(\alpha_d).$$

Then by Theorem 2.7, we have that $\phi_{\alpha_1,\ldots,\alpha_{d-1}}$ is identically zero on $\mathbb{R}$, for arbitrary $\alpha_1, \ldots, \alpha_{d-1} \in \mathbb{N}_0$. For each $b \in \mathbb{R}$, define the function $\psi_b : \mathbb{R}^{d-1} \to \mathbb{R}$ as $\psi_b(x_1, \ldots, x_{d-1}) := f(x_1, \ldots, x_{d-1}, b)$, for any $(x_1, \ldots, x_{d-1}) \in \mathbb{R}^{d-1}$. The previous argument shows that ψ_b fulfills all the assumptions of Theorem 3.8 for $d-1$. By inductive assumption, for all $b \in \mathbb{R}$ we have therefore that ψ_b is identically zero on $\mathbb{R}^{d-1}$. Hence, f is identically zero on $\mathbb{R}^d$. □

Let us come back to the determinacy question for the higher-dimensional version of the classical Hamburger moment problem. Namely, we ask whether a measure $\mu \in \mathcal{M}^*(\mathbb{R}^d)$, with $d \geq 2$, is uniquely determined by its moments without any restriction on its support. A fundamental sufficient criterion for uniqueness in this case was obtained by Petersen in [45].

Theorem 3.10 *Let $\mu \in \mathcal{M}^*(\mathbb{R}^d)$ with $d \geq 2$. For $j = 1, \ldots, d$, let $\pi_j : \mathbb{R}^d \to \mathbb{R}$ be given by $\pi_j(x_1, \ldots, x_d) := x_j$ and denote by μ_{π_j} the j–th marginal measure of μ, i.e. the image measure of μ under the mapping π_j. If all the marginal measures $\mu_{\pi_1}, \ldots, \mu_{\pi_d}$ are determinate, then μ is determinate.*

Petersen proved this result by density arguments on polynomials and he also showed that the converse is not true (see [45] for a simple example of determinate measure for which not all marginal measures are determinate). Using Theorems 3.10 and 3.5, we easily get the following.

Theorem 3.11 *Let $\mu, \nu \in \mathcal{M}^*(\mathbb{R}^d)$ have the same moment sequence $m = (m_\alpha)_{\alpha \in \mathbb{N}_0^d}$. If*

$$\sum_{n=1}^{\infty} L_m(x_j^{2n})^{-\frac{1}{2n}} = \infty, \quad \forall\, j = 1, \ldots, d, \tag{10}$$

then $\mu = \nu$.

An alternative proof of Theorem 3.11 has been recently provided by de Jeu in [21, Theorem 2.3], using Theorem 3.8 and the observation that (10) implies (9) for the

sequence $(\sqrt{M_j(2n)})_{n\in\mathbb{N}_0}$ given by $M_j(h) := L_m(x_j^h)$ for any $h \in \mathbb{N}_0$. The proof by de Jeu is very close to the one of Theorem 3.5.

Condition (10) is well-known as *multivariate Carleman's condition* and it is a sharp determinacy condition for the multivariate moment problem in the following sense.

Theorem 3.12 *Let $(M_n)_{n\in\mathbb{N}_0}$ be a log-convex sequence of positive real numbers with $M_0 = 1$. Then the following are equivalent.*

1. *The class $C\{M_n\}$ is quasi-analytic.*
2. *For any $\mu, \nu \in \mathcal{M}^*(\mathbb{R}^d)$ having the same moment multisequence and such that there exists a positive constant c for which*

$$\max\left(\int_{\mathbb{R}^d} \|\mathbf{x}\|^{2n}\,\mu(d\mathbf{x}), \int_{\mathbb{R}^d} \|\mathbf{x}\|^{2n}\,\nu(d\mathbf{x})\right) \leq c\,M_{2n}, \quad \forall\, n \in \mathbb{N},$$

we have that $\mu = \nu$. (Note that $\|\cdot\|$ denotes the Euclidean norm on $\mathbb{R}^d$.)

From Theorems 2.7, 3.11 and Lemma 3, it easily follows that (1) implies (2) in Theorem 3.12. The converse is instead due to Belislé et al. in [3] and we sketch here the main scheme of their proof for $d = 1$.

Proof (of (2)⇒(1) in Theorem 3.12) Suppose that $C\{M_n\}$ is not quasi-analytic and let us take $\varphi \in C\{M_n\}$ as given by Lemma 2.8. W.l.o.g. we can assume that the support of φ is contained in $[a, b]$ with $0 < a < b$. For any $A \subseteq \mathbb{R}$, let us define

$$\omega(A) := \int_A Re(\mathcal{F}(\varphi)^2(x))dx$$

where $\mathcal{F}(\varphi)$ denotes the Fourier transform of φ. Then it is easy to show that for any $n \in \mathbb{N}_0$,

$$\int x^n d\omega(x) = D^n\mathcal{F}\omega(0) = 0 \quad \text{and} \quad \int x^{2n}|\omega|(dx) \leq \|\varphi\|_{L^1} M_{2n}.$$

By taking $\mu := \omega^+$, $\nu := \omega^-$ and $c := \|\varphi\|_{L^1}$, the previous relations respectively give that μ and ν have the same moments and the following holds

$$\max\left(\int_{\mathbb{R}} x^{2n}\,\mu(dx), \int_{\mathbb{R}^d} x^{2n}\,\nu(dx)\right) \leq \int x^{2n} d|\omega|(x) \leq c\,M_{2n}.$$

□

After Petersen, many other sufficient criteria for the multivariate determinacy were developed using polynomial and rational approximation (see e.g. [11, 27, 46, 47]). All these results use that partial determinacy guarantees the uniqueness of the solution of the multidimensional Hamburger moment problem. However, partial

determinacy can be used to prove also the existence part of the moment problem. The first results in this direction were proved by Shohat and Tamarkin in [55], by Devinatz in [24] and by Èskin in [26]. In these works, the authors showed how the determinacy of certain 1-sequences derived from a semidefinite $d-$sequence m ensures both the existence and the uniqueness of a realizing measure for m. Nussbaum in [42] not only reproved these results with different methods, but also gave the following stronger theorem, which we present here in the form given by Berg in [10].

Theorem 3.13 *Let $d \geq 2$ and let $m = (m_\alpha)_{\alpha \in \mathbb{N}_0^d}$ be a positive semidefinite multisequence fulfilling the multivariate Carleman condition* (10)*, then there exists a unique non-negative Borel measure $\mu \in \mathcal{M}^*(\mathbb{R}^d)$ realizing m.*

The proof of this result uses the theory of self-adjointness extensions and makes clear that the multivariate Carleman condition is essential not only for the determinacy but also for the existence of the realizing measure. In fact, as we already mentioned above, the condition of positive semidefiniteness of m solely does not imply the existence of a realizing measure on $\mathbb{R}^d$ when $d \geq 2$ (see Example 6 in [52]). In other words, we will see that we cannot prove an equivalent of Hamburger's existence theorem for higher dimensions without assuming a further condition which guarantees that certain finitely many symmetric self-adjoint operators pairwise strongly commute.

Before proving Theorem 3.13, let us recall some preliminary notions and results from spectral theory. In the following, for an unbounded operator T on a Hilbert space $\mathcal{H}$, we will denote by $\mathcal{D}(T)$ its domain, which we will suppose to be a dense linear subspace of $\mathcal{H}$. For the classical definitions of symmetric, self-adjoint and essentially self-adjoint operators see for example [48, Vol. I, Chapter VIII]. The main tool used by Nussbaum in his proof is the concept of quasi-analytic vector that is intimately related, as we will see, to the multivariate Carleman condition and so to the quasi-analyticity of functions on $\mathbb{R}^d$. From now on we denote by $\mathcal{D}^\infty(T) := \bigcap_{n=1}^{\infty} \mathcal{D}(T^n)$ and by $\mathcal{D}^{qa}(T)$ the set of all quasi-analytic vectors for T, i.e. all vectors $v \in \mathcal{D}^\infty(T)$ such that $\sum_{n=1}^{\infty} ||T^n v||^{-\frac{1}{n}} = \infty$.

The motivation of Nussbaum in [42] was to generalize the classical analytic vectors theorem due to Nelson (see [41]) to the setting of quasi-analytic vectors. Indeed, he managed to prove this result reducing the situation to Theorem 3.5. Let us restate here for convenience Nussbaum's quasi-analytic vectors theorem (see [42, Theorem 2] and [53, Theorem 7.14]).

Theorem 3.14 *Let T be a symmetric operator on a Hilbert space $\mathcal{H}$ and suppose that its domain $\mathcal{D}(T)$ contains a total set $\mathcal{D}$ of quasi-analytic vectors, i.e. $\mathcal{D} \subseteq \mathcal{D}^{qa}(T)$ and $\overline{span(\mathcal{D})} = \mathcal{H}$. Then T is essentially self-adjoint.*

However, to solve the multidimensional moment problem we need more, namely the strong commutativity of a pair of operators (see [42, Theorem 6] and [53, Theorem 7.18]).

Theorem 3.15 *Let A and B be two symmetric operators on a Hilbert space $\mathcal{H}$. Let $\mathcal{D}$ be a set of vectors in $\mathcal{H}$ which are quasi-analytic for both A and B and such that $A\mathcal{D} \subset \mathcal{D}$, $B\mathcal{D} \subset \mathcal{D}$, $AB\phi = BA\phi$, for all $\phi \in \mathcal{D}$. If $\mathcal{D}$ is total in $\mathcal{H}$, then the closures $\overline{A}$ and $\overline{B}$ are strongly commuting self-adjoint operators. Namely, for all $s, t \in \mathbb{R}$, $e^{is\overline{A}}e^{it\overline{B}} = e^{it\overline{A}}e^{is\overline{B}}$.*

Remark 3.16 The hypotheses $A\mathcal{D} \subset \mathcal{D}$ and $B\mathcal{D} \subset \mathcal{D}$ guarantee that $\mathcal{D} \subset \mathcal{D}(A^nB^m)$ for any $n, m \in \mathbb{N}_0$. Then it is easy to see, by induction, that the assumption $AB\phi = BA\phi$ for all $\phi \in \mathcal{D}$ implies

$$A^mB^n\phi = B^nA^m\phi, \quad \forall\, m, n \in \mathbb{N}_0,\ \forall\, \phi \in \mathcal{D}.$$

However, this is not sufficient to conclude the strong commutativity of $\overline{A}$ and $\overline{B}$ (c.f. [48, Section VIII.5, Example 1]).

Proof (of Theorem 3.15) Since $\mathcal{D} \subseteq \mathcal{D}^{\mathrm{qa}}(A)$, $\mathcal{D} \subseteq \mathcal{D}^{\mathrm{qa}}(B)$ and $\mathcal{D}$ is total in $\mathcal{H}$, by Theorem 3.14, the operators A and B are both essentially self-adjoint, i.e. their closures $\overline{A}$ and $\overline{B}$ are self-adjoint. In order to show that these operators also strongly commute, we need to use quasi-analyticity of functions in two variables.
Given $\phi \in \mathcal{D}$, let us consider the functions

$$\begin{aligned} F_1 :\ \mathbb{R}^2 &\to \mathbb{C} \\ (a, b) &\mapsto \langle e^{ib\overline{B}}\phi, e^{-ia\overline{A}}\phi\rangle \end{aligned}$$

and

$$\begin{aligned} F_2 :\ \mathbb{R}^2 &\to \mathbb{C} \\ (a, b) &\mapsto \langle e^{ia\overline{A}}\phi, e^{-ib\overline{B}}\phi\rangle\,. \end{aligned}$$

It is easy to show that $F_1, F_2 \in \mathcal{C}^\infty(\mathbb{R}^2)$. Moreover, for all $\alpha_1, \alpha_2 \in \mathbb{N}_0$

$$\frac{\partial^{\alpha_2}}{\partial b^{\alpha_2}}\frac{\partial^{\alpha_1}}{\partial a^{\alpha_1}}F_1(a, b) = i^{\alpha_2+\alpha_1}\langle \overline{B}^{\alpha_2}e^{ib\overline{B}}\phi, \overline{A}^{\alpha_1}e^{-ia\overline{A}}\phi\rangle$$

and

$$\frac{\partial^{\alpha_2}}{\partial b^{\alpha_2}}\frac{\partial^{\alpha_1}}{\partial a^{\alpha_1}}F_2(a, b) = i^{\alpha_2+\alpha_1}\langle \overline{A}^{\alpha_1}e^{ia\overline{A}}\phi, \overline{B}^{\alpha_2}e^{-ib\overline{B}}\phi\rangle.$$

Hence, by Remark 3.16 we get that

$$\frac{\partial^{\alpha_2}}{\partial b^{\alpha_2}}\frac{\partial^{\alpha_1}}{\partial a^{\alpha_1}}F_1(0, 0) = \frac{\partial^{\alpha_2}}{\partial b^{\alpha_2}}\frac{\partial^{\alpha_1}}{\partial a^{\alpha_1}}F_2(0, 0). \tag{11}$$

For all $\alpha_1, \alpha_2 \in \mathbb{N}_0$, we also have that

$$\left| \frac{\partial^{\alpha_2}}{\partial b^{\alpha_2}} \frac{\partial^{\alpha_1}}{\partial a^{\alpha_1}} (F_1 - F_2)(a, b) \right| \leq 2 M_1(\alpha_1) M_2(\alpha_2), \tag{12}$$

where we set for any $k \in \mathbb{N}_0$

$$M_1(k) := ||\overline{A}^k \phi|| \quad \text{and} \quad M_2(k) := ||\overline{B}^k \phi||.$$

Both $(M_1(k))_{k\in\mathbb{N}_0}$ and $(M_2(k))_{k\in\mathbb{N}_0}$ are log-convex because they are defined by norms. The quasi-analyticity of ϕ for both A and B implies that

$$\sum_{k=1}^{\infty} \frac{1}{\sqrt[k]{M_1(k)}} = \infty \quad \text{and} \quad \sum_{k=1}^{\infty} \frac{1}{\sqrt[k]{M_2(k)}} = \infty. \tag{13}$$

Therefore, by Theorem 3.8, the relations (11), (12) and (13) imply that the function $F_1 - F_2 \equiv 0$ on $\mathbb{R}^2$. Then

$$\langle e^{ib\overline{B}}\phi, e^{-ia\overline{A}}\phi \rangle = \langle e^{ia\overline{A}}\phi, e^{-ib\overline{B}}\phi \rangle, \quad \forall a, b \in \mathbb{R}, \ \forall \phi \in \mathcal{D},$$

which also holds for all $\phi \in \mathcal{H}$, since $\mathcal{D}$ is total in $\mathcal{H}$ and the operators $e^{ia\overline{A}}$ and $e^{ia\overline{B}}$ are continuous. Then the conclusion follows by polarization identity. □

Proof (of Theorem 3.13 for $d = 2$) Let L_m be the Riesz functional on $\mathbb{R}[\mathbf{x}] = \mathbb{R}[x_1, x_2]$ associated to the sequence m (see Definition 3.3). We will apply to this functional the well-known Gelfand-Naimark-Segal (GNS) construction and then we will use the spectral theorem for pairwise strongly commuting self-adjoint extensions of the multiplication operators defined on the Hilbert space given by the GNS-construction.

Since m is a positive semidefinite sequence, the bilinear form given by $\langle f, g \rangle := L_m(fg)$ is a quasi-inner product on $\mathbb{R}[\mathbf{x}]$ and by the Cauchy-Schwarz inequality it follows that the subset $N := \{h \in \mathbb{R}[\mathbf{x}] : L_m(h^2) = 0\}$ is an ideal of the algebra of polynomials $\mathbb{R}[\mathbf{x}]$. Let $\mathcal{H}_m$ be the completion of the pre-Hilbert space $\mathbb{R}[\mathbf{x}]/N$ equipped with the inner product $\langle \cdot, \cdot \rangle$. For $j = 1, 2$, we introduce the operator $X_j : \mathbb{R}[\mathbf{x}]/N \to \mathbb{R}[\mathbf{x}]/N$ defined by

$$X_j\big(h(x_1, x_2)\big) := x_j\, h(x_1, x_2), \quad \text{for any } \ h \in \mathbb{R}[\mathbf{x}]/N.$$

Then X_1, X_2 and $\mathcal{D} := \{x_1^s x_2^n | s, n \in \mathbb{N}_0\}$ fulfill all the assumptions of Theorem 3.15. We only show that $\mathcal{D}$ is a set of quasi-analytic vectors for both X_1 and X_2. Let us fix $s, n \in \mathbb{N}_0$, then by Cauchy-Schwarz's inequality we get that for any $k \in \mathbb{N}$

$$||{X_1}^k x_1^s x_2^n||^2 \leq \big(L_m(x_1^{4k+4s})\big)^{\frac{1}{2}} \big(L_m(x_2^{4n})\big)^{\frac{1}{2}}. \tag{14}$$

Now, let us define the sequence $M_j(k) := L_m(x_j^k)$ for $j = 1, 2$. The log-convexity of the sequence $(M_1(k))_{k\in\mathbb{N}_0}$ easily follows by the Cauchy-Schwarz inequality for the inner product $\langle\cdot,\cdot\rangle$. By Theorem 2.7 and Lemma 3, the multivariate Carleman condition (10) for $j = 1$ guarantees that the class $C\{M_1(k)\}$ is quasi-analytic. By Lemma 5, we get that for the fixed $s \in \mathbb{N}_0$ the class $C\{M_1(k+s)\}$ is also quasi-analytic. Then, by Lemma 3, the class $C\{\sqrt[4]{M_1(4k+4s)}\}$ is quasi-analytic. Since $M_2(4n)$ is constant in k, Proposition 2.3 guarantees that $\sum_{k=1}^{\infty} \frac{1}{\sqrt[4k]{M_1(4k+4s)M_2(4n)}} = \infty$. This together with (14) implies that $\sum_{k=1}^{\infty} ||X_1{}^k x_1^s x_2^n||^{-\frac{1}{k}} = \infty$, i.e. $x_1^s x_2^n$ is a quasi-analytic vector for X_1. The same proof applies to X_2.

Theorem 3.15 guarantees that the closures $\overline{X_1}$ and $\overline{X_2}$ of X_1 and X_2, respectively, are strongly commuting self-adjoint operators. By applying the spectral theorem to $\overline{X_1}$ and $\overline{X_2}$, we get that there exists a unique non-negative measure $\mu \in \mathcal{M}^*(\mathbb{R}^2)$ such that for any $\alpha_1, \alpha_2 \in \mathbb{N}_0$

$$\int_{\mathbb{R}^2} x_1^{\alpha_1} x_2^{\alpha_2} \mu(dx_1, dx_2) = \langle 1, \underbrace{\overline{X_1}\cdots\overline{X_1}}_{\alpha_1 \text{ times}} \underbrace{\overline{X_2}\cdots\overline{X_2}}_{\alpha_2 \text{ times}} \cdot 1\rangle. \tag{15}$$

On the other hand, we have that for any $\alpha_1, \alpha_2 \in \mathbb{N}_0$

$$\langle 1, \underbrace{\overline{X_1}\cdots\overline{X_1}}_{\alpha_1 \text{ times}} \underbrace{\overline{X_2}\cdots\overline{X_2}}_{\alpha_2 \text{ times}} \cdot 1\rangle = \langle 1, (X_1^{\alpha_1} X_2^{\alpha_2})(1)\rangle = L_m(x_1^{\alpha_1} x_2^{\alpha_2}) = m_{(\alpha_1,\alpha_2)}. \tag{16}$$

By (15) and (16), we conclude that $\int_{\mathbb{R}^2} \mathbf{x}^\alpha \mu(d\mathbf{x}) = m_\alpha$ for any $\alpha \in \mathbb{N}_0^2$, i.e. the sequence m is realized on $\mathbb{R}^2$ by the measure μ. Moreover, since m fulfills (10) by assumption, Theorem 3.11 for $n = 2$ guarantees that μ is the unique measure realizing m on $\mathbb{R}^2$. □

Concerning the Stieltjes moment problem in higher dimensions, it is possible to obtain sufficient determinacy conditions using the quasi-analyticity of the Fourier-Laplace transform of a measure supported on $\mathbb{R}^d_+$. This technique is used in [47, Section 2.4], where the authors proved different determinacy conditions corresponding to the different quasi-analyticity criteria given in [15] and [14]. Following the proof in the one-dimensional case (see Theorem 3.7), it is possible to derive from Theorem 3.11 the following sufficient condition for the determinacy of the multidimensional Stieltjes moment problem (see [21] for a detailed proof of this result).

Theorem 3.17 *Let $m = (m_\alpha)_{\alpha\in\mathbb{N}_0^d}$ be the moment sequence of a measure $\mu \in \mathcal{M}^*(\mathbb{R}^d_+)$. If*

$$\sum_{k=1}^{\infty} L_m(x_j^k)^{-\frac{1}{2k}} = \infty, \quad \forall\, j = 1, \ldots, d,$$

then μ is the unique measure realizing m on $\mathbb{R}^d_+$.

As well as in the one-dimensional case, the geometry of the support of a measure on $\mathbb{R}^d$ with $d \geq 2$ can be used to derive other determinacy conditions. First of all, the compactness of $K \subset \mathbb{R}^d$ guarantees the determinacy of the multivariate $K-$moment problem for any $d \in \mathbb{N}$ (the considerations made at the end of Sect. 3.2 can be straightforwardly generalized to higher dimensions). Moreover, in [46, Section 3] the authors showed higher-dimensional determinacy criteria based on the geometry of the support and provided examples of non-compact higher-dimensional sets which support determinate measures (see also [47, Section 9] for a summary of the results in [46]). Another powerful method to study the determinacy of the multidimensional moment problem is to use disintegration techniques. In particular, Putinar and Schmüdgen have recently proved through such techniques a general result which reduces the determinacy question to lower dimensions and it has a very broad class of applications, [47, Section 8].

4 Uniqueness in the Infinite-Dimensional Moment Problem

4.1 The Moment Problem on Conuclear Spaces

In the following we are going to introduce an infinite-dimensional version of the moment problem, in particular we will consider the moment problem on conuclear spaces. For simplicity, from now on, all the spaces are assumed to be separable and real.

Let us consider a family $(H_k)_{k\in K}$ of Hilbert spaces (K is an index set containing 0) which is directed by topological embedding, i.e.

$$\forall\ k_1, k_2 \in K\ \exists k_3\ :\ H_{k_3} \subseteq H_{k_1}\ ,\ H_{k_3} \subseteq H_{k_2}.$$

We assume that each H_k is topologically embedded into H_0. Let Ω be the projective limit of the family $(H_k)_{k\in K}$ endowed with the associated projective limit topology and let us assume that Ω is nuclear, i.e. for each $k_1 \in K$ there exists $k_2 \in K$ such that the embedding $H_{k_2} \subseteq H_{k_1}$ is quasi-nuclear.

Let us denote by Ω' the topological dual space of Ω. We control the classical rigging by identifying H_0 and its dual H_0'. With this identification one can define the duality pairing between elements in H_k and in its dual $H_k' = H_{-k}$ using the inner product in H_0. For this reason, in the following we will denote by $\langle f, \eta\rangle$ the duality pairing between $\eta \in \Omega'$ and $f \in \Omega$ (see [6, 8] for more details).

Consider the $n-$th ($n \in \mathbb{N}_0$) symmetric tensor power $\Omega^{\otimes n}$ of the space Ω which is defined as the projective limit of all $H_k^{\otimes n}$; for $n = 0$, $H_k^{\otimes 0} = \mathbb{R}$. Then its dual space is

$$\left(\Omega^{\otimes n}\right)' = \bigcup_{k\in K} \left(H_k^{\otimes n}\right)' = \bigcup_{k\in K} (H_k')^{\otimes n} = \bigcup_{k\in K} H_{-k}^{\otimes n}, \tag{17}$$

which we can equip with the weak topology.

A generalized process μ is a finite measure defined on the Borel $\sigma-$algebra on Ω'. Moreover, we say that a generalized process μ is *concentrated on* a measurable subset $\mathcal{S} \subseteq \Omega'$ if $\mu(\Omega' \setminus \mathcal{S}) = 0$.

Definition 4.1 (Finite $n-$th local moment) Given $n \in \mathbb{N}$, a generalized process μ on Ω' has *finite $n-$th local moment* (or local moment of order n) if for every $f \in \Omega$ we have

$$\int_{\Omega'} |\langle f, \eta\rangle|^n \mu(d\eta) < \infty.$$

Definition 4.2 ($n-$th generalized moment function) Given $n \in \mathbb{N}$, a generalized process μ on Ω' has $n-$th generalized moment function in the sense of Ω' if μ has finite $n-$th local moment and if the functional $f \mapsto \int_{\Omega'} |\langle f, \eta\rangle|^n \mu(d\eta)$ is continuous on Ω. In fact, by the Kernel Theorem, for such a generalized process μ there exists a symmetric functional $m_\mu^{(n)} \in (\Omega^{\otimes n})'$, which will be called the *$n-$th generalized moment function in the sense of* Ω', such that for any $f^{(n)} \in \Omega^{\otimes n}$ we have

$$\langle f^{(n)}, m_\mu^{(n)}\rangle = \int_{\Omega'} \langle f^{(n)}, \eta^{\otimes n}\rangle \mu(d\eta).$$

By convention, $m_\mu^{(0)} := \mu(\Omega')$.

In analogy to the finite-dimensional case, we will denote by $\mathcal{M}^*(\mathcal{S})$ the collection of all generalized processes concentrated on a measurable subset $\mathcal{S}$ of Ω' with generalized moment functions (in the sense of Ω') of any order. Moreover, let us simply denote by $\mathcal{F}(\Omega')$ the collection of all infinite sequences $(m^{(n)})_{n\in\mathbb{N}_0}$ such that each $m^{(n)} \in \left(\Omega^{\otimes n}\right)'$ is a symmetric functional, namely the tensor product $(\Omega')^{\otimes n}$ is considered to be symmetric.

The full moment problem, which in this infinite-dimensional context is often called the *full realizability problem*, addresses exactly the following question.

Problem 4.3 (Full realizability problem on $\mathcal{S} \subseteq \Omega'$) *Let $\mathcal{S}$ be a measurable subset of Ω' and let $m = (m^{(n)})_{n\in\mathbb{N}_0} \in \mathcal{F}(\Omega')$. Find a generalized process μ with generalized moments (in the sense of Ω') of any order and concentrated on $\mathcal{S}$ such that $m^{(n)} = m_\mu^{(n)}$ for all $n \in \mathbb{N}_0$, i.e. $m^{(n)}$ is the $n-$th generalized moment function of μ for any $n \in \mathbb{N}_0$.*

If such a measure μ does exist we say that m is *realized* by μ on $\mathcal{S}$. Note that the statement of the problem requires that one finds a measure concentrated on $\mathcal{S}$ and not only on Ω'.

An obvious positivity property which is necessary for an element in $\mathcal{F}(\Omega')$ to be the moment sequence of some measure on Ω' is the following.

Definition 4.4 (Positive semidefinite sequence) A sequence $m \in \mathcal{F}(\Omega')$ is said to be *positive semidefinite* if for any $f^{(j)} \in \Omega^{\otimes j}$

$$\sum_{j,l=0}^{\infty} \langle f^{(j)} \otimes f^{(l)}, m^{(j+l)} \rangle \geq 0.$$

This is a straightforward generalization of the classical notion of positive semidefiniteness considered in the finite-dimensional moment problem (see Definition 3.4). Note that, as we work with real spaces, we choose the involution on Ω considered in [8] to be the identity.

A measure $\mu \in \mathcal{M}^*(\mathcal{S})$ is called *determinate* on $\mathcal{S}$ if any other measure $\nu \in \mathcal{M}^*(\mathcal{S})$ having the same generalized moment functions as μ is equal to μ.

4.2 Determinacy Condition for the Realizability Problem on Conuclear Spaces

As well as for the $d-$dimensional moment problem with $d \geq 2$, the role of quasi-analyticity in the infinite-dimensional moment problem is fundamental not only to develop sufficient determinacy conditions but also to obtain the existence of a solution. The following notion is the crucial element to get analogues of Theorems 3.11 and 3.13 for the realizability problem.

Definition 4.5 (Determining sequence) Let $m \in \mathcal{F}(\Omega')$ and let E be a countable total subset of Ω, i.e. the linear span of E is dense in Ω. Let us define the sequence $(m_n)_{n\in\mathbb{N}_0}$ as follows

$$m_0 := \sqrt{|m^{(0)}|} \text{ and } m_n := \sqrt{\sup_{f_1,\dots,f_{2n}\in E} |\langle f_1 \otimes \cdots \otimes f_{2n}, m^{(2n)} \rangle|}, \ \forall\, n \geq 1. \tag{18}$$

The sequence m is said to be *determining* if and only if there exists a countable total subset E of Ω such that for any $n \in \mathbb{N}_0$, $m_n < \infty$ and the class $C\{m_n\}$ is quasi-analytic (see Definition 2.2 and Theorem 2.7).

Note that from (17) it follows that for any sequence $m \in \mathcal{F}(\Omega')$ there exists a sequence $(k^{(n)})_{n\in\mathbb{N}_0} \subset K$ s.t. for any $n \in \mathbb{N}_0$ we have $m^{(n)} \in H^{\otimes n}_{-k^{(n)}}$. If we denote by

$$d(k^{(n)}, E) := \sup_{f\in E} \|f\|_{H_{k^{(n)}}}, \tag{19}$$

then for the m_n's defined in (18) we have

$$m_n \leq (d(k^{(2n)}, E))^n \|m^{(2n)}\|^{\frac{1}{2}}_{H^{\otimes 2n}_{-k^{(2n)}}}.$$

Hence, we can see that a preferable choice for E is the one for which the sequence $\left(d(k^{(2n)}, E)\right)_{n\in\mathbb{N}}$ grows as little as possible. For instance, in [34, Lemma 4.5] we proved that it is possible to explicitly construct such a set E in the case when Ω is the space of all infinitely differentiable functions with compact support in $\mathbb{R}^d$. This explicit construction is based on quasi-analyticity theory and uses a technique similar to the one of [28, Chapter 4, Section 9].

Let us prove now the correspondent of Theorem 3.11 for Problem 4.3 in the case $\mathcal{S} = \Omega'$ (c.f. [8, Vol. II, Theorem 2.1] and [9]). Before stating the theorem, we need some preliminary considerations.

Let $m \in \mathcal{F}(\Omega')$ be the moment sequence of a measure μ on Ω'. For any $\varphi \in \Omega$ and any $n \in \mathbb{N}_0$, we define

$$m_{\varphi,n} := \langle \varphi^{\otimes n}, m^{(n)} \rangle.$$

Therefore, we have

$$m_{\varphi,n} = \int_{\Omega'} \langle \varphi, \eta \rangle^n \mu(d\eta) = \int_{\mathbb{R}} t^n \mu_{\pi_\varphi}(dt),$$

where $\pi_\varphi(\eta) := \langle \varphi, \eta \rangle$ for all $\eta \in \Omega'$ and μ_{π_φ} is the image measure of μ under π_φ. Note that the sequence $(m_{\varphi,n})_{n\in\mathbb{N}_0}$ is a log-convex sequence of real numbers and if μ is a probability then $m_{\varphi,0} = 1$.

Theorem 4.6 *Let Ω' be a Suslin space and let $\mu, \nu \in \mathcal{M}^*(\Omega')$ have the same generalized moment sequence $m = (m^{(n)})_{n\in\mathbb{N}_0}$. If there exists a countable total subset E of Ω such that for all $\varphi \in E$ the class $C\{m_{\varphi,n}\}$ is quasi-analytic, then $\mu = \nu$. In particular, if m is determining, then the conclusion holds.*

Proof Since for any $\varphi \in E$ the class $C\{m_{\varphi,n}\}$ is quasi-analytic and the sequence $(m_{\varphi,n})_{n\in\mathbb{N}_0}$ is log-convex, by Lemma 3 and Theorem 3.5, it follows that $\mu_{\pi_\varphi} = \nu_{\pi_\varphi}$ on $\mathbb{R}$. To show that $\mu = \nu$ on Ω', it is enough to prove that μ and ν coincide on all the cylindrical sets

$$C(f_1, \ldots, f_n; B) := \{\eta \in \Omega' : (\langle f_1, \eta \rangle, \ldots, \langle f_n, \eta \rangle) \in B\},$$

with $n \in \mathbb{N}, f_1, \ldots, f_n \in E$ and B in the Borel $\sigma-$algebra $\mathcal{B}(\mathbb{R}^n)$ on $\mathbb{R}^n$. In fact, since E is total in Ω and Ω' is Suslin, a theorem due to Fernique (see [54, Lemma 18]) guarantees that the Borel $\sigma-$algebra on Ω' is generated by all the cylinders above.

Since for any $n \in \mathbb{N}$ and for any $f_1, \ldots, f_n \in E$, we have already proved that $\mu_{\pi_{f_j}} = \nu_{\pi_{f_j}}$ on $\mathbb{R}$ for all $j \in \{1, \ldots, n\}$, Petersen's Theorem 3.10 implies that $\mu(C(f_1, \ldots, f_n; B)) = \nu(C(f_1, \ldots, f_n; B))$ for any $B \in \mathcal{B}(\mathbb{R}^n)$.

In particular, if m is determining then there exists a countable total subset E of Ω such that $C\{m_n\}$ is quasi-analytic, where m_n is defined as in (18). Then for any $\varphi \in E$ and $n \in \mathbb{N}_0$ we get $\sqrt{m_{\varphi,2n}} \leq m_n$, which implies that $C\{\sqrt{m_{\varphi,2n}}\}$ is quasi-analytic. Hence, by Lemma 3, $C\{m_{\varphi,n}\}$ is quasi-analytic. Then the conclusion follows by the first part of this proof. □

Let us state now the analogue of Theorem 3.13 for Problem 4.3 in the case $\mathcal{S} = \Omega'$ (see [8, Vol. II, Theorem 2.1] and [9]).

Theorem 4.7 *Let Ω' be a Suslin space. If $m \in \mathcal{F}(\Omega')$ is a positive semidefinite sequence which is also determining, then there exists a unique non-negative generalized process $\mu \in \mathcal{M}^*(\Omega')$ such that for any $n \in \mathbb{N}_0$ and for any $f^{(n)} \in \Omega^{\otimes n}$*

$$\left\langle f^{(n)}, m^{(n)} \right\rangle = \int_{\Omega'} \left\langle f^{(n)}, \eta^{\otimes n} \right\rangle \mu(d\eta).$$

The original proof of Theorem 4.7 in [8] uses a slightly less general definition of determining sequence. Indeed, the authors require that the class

$$C\left\{ d(k^{(2n)}, E)^n \left\| m^{(2n)} \right\|^{1/2}_{H^{\otimes 2n}_{-k^{(2n)}}} \right\}$$

is quasi-analytic, which in turn implies that $C\{m_n\}$ is also quasi-analytic. Nevertheless, their proof also works using just the bound given by Definition 4.5. The latter has actually the advantage to guarantee that, whenever m is realizable on Ω, the sequence $(m_n)_{n\in\mathbb{N}_0}$ is log-convex. This is an essential property to obtain necessary and sufficient conditions for the realizability problem on semi-algebraic sets (see [34] for more details on this topic).

Proof (Sketch) The general scheme of the proof of Theorem 4.7 is very similar to the one of Theorem 3.13. As in the finite-dimensional case, the GNS construction is used to define a Hilbert space $\mathcal{H}_m$ associated to the starting positive semidefinite sequence $m \in \mathcal{F}(\Omega')$, which is now a sequence of functionals and no more of real numbers. Consider the set $\mathscr{P}_\Omega(\Omega')$ of all polynomials on Ω' of the form

$$P(\eta) := \sum_{j=0}^{N} \langle f^{(j)}, \eta^{\otimes j} \rangle, \tag{20}$$

where $f^{(0)} \in \mathbb{R}$ and $f^{(j)} \in \Omega^{\otimes j}$, $j = 1, \ldots, N$ with $N \in \mathbb{N}$. Let us define the Riesz functional L_m associated to $m \in \mathcal{F}(\Omega')$ as

$$\begin{aligned} L_m : \quad & \mathscr{P}_\Omega(\Omega') \quad \to \mathbb{R} \\ & P(\eta) = \sum_{n=0}^{N} \langle p^{(n)}, \eta^{\otimes n} \rangle \mapsto L_m(P) := \sum_{n=0}^{N} \langle p^{(n)}, m^{(n)} \rangle. \end{aligned}$$

Since m is positive semidefinite, the bilinear form given by $\langle P, Q \rangle := L_m(PQ)$ is a quasi-inner product on $\mathscr{P}_\Omega(\Omega')$. After the factorization of $\mathscr{P}_\Omega(\Omega')$ with respect to $N := \{P \in \mathscr{P}_\Omega(\Omega') : L_m(P^2) = 0\}$ and the subsequent completion of this quotient space, we obtain a Hilbert space $\mathcal{H}_m$.

For any $e \in E$, let us introduce the multiplication operator A_e on $\mathcal{H}_m$ defined by

$$A_e P := \sum_{j=0}^{N} \langle e \otimes f^{(j)}, \eta^{\otimes(j+1)} \rangle, \quad \text{for any } P \in \mathscr{P}_\Omega\left(\Omega'\right) \text{ as in (20).}$$

Thanks to the determining condition, it is possible to show that the domain of each of these operators contains a countable total subset of quasi-analytic vectors, namely, the set all the polynomials $P_k(\eta) := \langle f_1 \otimes \cdots \otimes f_k, \eta^{\otimes k} \rangle$ with $k \in \mathbb{N}$ and $f_1, \ldots, f_k \in E$. Indeed, for any $e \in E$ and any $k \in \mathbb{N}$ we have that $P_k \in \cap_{n=1}^{\infty} \mathcal{D}(A_e^n)$. Moreover, for any $n \in \mathbb{N}$ we get

$$\begin{aligned} \|A_e^n P_k\| &= \langle A_e^n P_k, A_e^n P_k \rangle^{\frac{1}{2}} = L_m(\langle f_1 \otimes \cdots \otimes f_k \otimes \underbrace{e \otimes \cdots \otimes e}_{n \text{ times}}, \eta^{\otimes(k+n)} \rangle^2)^{\frac{1}{2}} \\ &= \langle f_1^{\otimes 2} \otimes \cdots \otimes f_k^{\otimes 2} \otimes \underbrace{e \otimes \cdots \otimes e}_{2n \text{ times}}, m^{(2(k+n))} \rangle^{\frac{1}{2}} \leq m_{k+n}. \end{aligned}$$

By Definition 4.5, the class $C\{m_n\}$ is quasi-analytic and the sequence $(m_n)_{n\in\mathbb{N}}$ is log-convex. Then, by Lemma 5, the class $C\{m_{k+n}\}$ is also quasi-analytic. Hence, the previous estimate shows that each P_k is a quasi-analytic vector for A_e. As in the finite-dimensional case, it is possible to show that these operators admit unique self-adjoint extensions, which are pairwise strongly commuting. Therefore, by the spectral theorem for infinitely countable many unbounded self-adjoint operators (see [8, Vol. I, Section 2]), there exists a unique measure representing those operators. Hence, this spectral measure μ realizes m on $\mathbb{R}^E$.

The final part of the proof consists in showing that the spectral measure is actually supported on Ω'. Moreover, since m is determining by assumption, Theorem 4.6 also guarantees that the measure μ is the unique measure realizing m on Ω'. □

Remark 4.8 The $d-$dimensional moment problem on $\mathbb{R}^d$ is a special case of Problem 4.3 for $\Omega = H_0 = \mathbb{R}^d$. Hence, an analogue of Theorem 4.7 can be proved also in the finite-dimensional case, where the condition $m := (m^{(n)})_{n\in\mathbb{N}_0} \in \mathcal{F}\left(\mathbb{R}^d\right)$ holds for any multisequence of real numbers. In fact, if $\{e_1, \ldots, e_d\}$ denotes the canonical basis of $\mathbb{R}^d$ then we have that for each $n \in \mathbb{N}_0$,

$$m^{(n)} := \sum_{\substack{n_1,\ldots,n_d \in \mathbb{N}_0 \\ n_1+\cdots+n_d=n}} m^{(n)}_{(n_1,\ldots,n_d)} \underbrace{e_1 \otimes \cdots \otimes e_1}_{n_1 \text{ times}} \otimes \cdots \otimes \underbrace{e_d \otimes \cdots \otimes e_d}_{n_d \text{ times}} \in \mathbb{R}^{dn}.$$

The determining condition on m reduces to the requirement that the class

$$C\left\{\sqrt{\max_{\substack{n_1,\ldots,n_d \in \mathbb{N}_0 \\ n_1+\cdots+n_d=2n}} |m^{(2n)}_{n_1,\ldots,n_d}|}\right\} \tag{21}$$

is quasi-analytic. This follows by taking $E := \{e_1, \ldots, e_d\}$ in Definition 4.5. Note that the quasi-analyticity of the class (21) implies the multivariate Carleman condition. Hence, Theorem 4.7 gives here a slightly weaker version than Theorem 3.13, but it is now clear that it is the quasi-analyticity the key stone on which both results are based. Let us also underline that, whenever the starting sequence m is realizable on $\mathbb{R}^d$, the sequence in (21) is log-convex.

The infinite-dimensional analogue of the Stieltjes moment problem was considered by Šifrin in [56], where he develops the analysis of the infinite-dimensional moment problem on dual cones in conuclear spaces. In particular, applying Šifrin's result to a generating cone $\mathcal{K}$ of a nuclear space Ω as before, it is possible to obtain a version of Theorem 4.7 for the realizability problem on the dual cone of such a $\mathcal{K}$, but with the difference that the determining condition is replaced by the requirement that the class $C\{\sqrt{m_n}\}$ is quasi-analytic where the m_n's are defined as in Definition 4.5. This condition is slightly more general than the one given by Šifrin in [56], which can be rewritten as

$$\sum_{n=1}^{\infty} \frac{1}{\sqrt[4n]{d(k^{(2n)}, E)^{2n} \left\| m^{(2n)} \right\|_{H^{\otimes 2n}_{-k^{(2n)}}}}} = \infty, \tag{22}$$

where $d(k^{(2n)}, E)$ is defined as in (19) and E is total in Ω. Condition (22) is called *generalized Stieltjes' condition*. In fact, it is easy to see that the difference between (22) and the original determining condition given by Berezansky and Kondratiev, i.e.

$$\sum_{n=1}^{\infty} \frac{1}{\sqrt[2n]{d(k^{(2n)}, E)^{2n} \left\| m^{(2n)} \right\|_{H^{\otimes 2n}_{-k^{(2n)}}}}} = \infty,$$

is the same as the difference between Stieltjes' condition (8) and Carleman's condition (7) in the one-dimensional case.

As in the finite-dimensional case, the geometry of the support $\mathcal{S}$ again allows to get easier conditions for realizability (see [33] for some examples).

Appendix: Log-Convexity and Quasi-analyticity

We conclude this paper with some properties of log-convex sequences which are useful in relation to the quasi-analyticity of the associated classes of functions.

Proposition 1 *For a sequence of positive real numbers $(M_n)_{n\in\mathbb{N}_0}$ the following are equivalent*

(a). $(M_n)_{n\in\mathbb{N}_0}$ *is log-convex.*
(b). $\left(\frac{M_n}{M_{n-1}}\right)_{n\in\mathbb{N}}$ *is monotone increasing.*
(c). $(\ln(M_n))_{n\in\mathbb{N}}$ *is convex.*

Proof The conditions (a) and (b) are obviously equivalent. If (c) holds, then

$$2\ln M_n \leq \ln M_{n+1} + \ln M_{n-1},$$

which implies (a). Let us assume (b), then for any $n, m, k \in \mathbb{N}$ such that $n \leq k \leq m$ we have

$$\frac{1}{k-n}\sum_{j=n+1}^{k} \ln\left(\frac{M_j}{M_{j-1}}\right) \leq \frac{1}{m-k}\sum_{j=k+1}^{m} \ln\left(\frac{M_j}{M_{j-1}}\right), \tag{23}$$

where we used the fact that the denominators of the pre-factors are equal to the number of summands in both sums. The inequality (23) is equivalent to

$$(m-n)\ln M_k \leq (k-n)\ln M_m + (m-k)\ln M_n,$$

which gives the convexity of the sequence $(\ln(M_n))_{n\in\mathbb{N}}$ and so (c). □

Corollary 2 *If a sequence of positive real numbers $(M_n)_{n\in\mathbb{N}_0}$ is log-convex with $M_0 = 1$, then $(\sqrt[n]{M_n})_{n\in\mathbb{N}}$ is monotone increasing.*

Proof From (b) in Proposition 1, it follows that for any $n \in \mathbb{N}$

$$M_n = \frac{M_n}{M_0} = \prod_{j=1}^{n} \frac{M_j}{M_{j-1}} \leq \left(\frac{M_n}{M_{n-1}}\right)^n,$$

which gives $M_{n-1}^n \leq M_n^{n-1}$, or equivalently, $M_{n-1}^{1/n-1} \leq M_n^{1/n}$. □

Lemma 3 *Assume that $(M_n)_{n\in\mathbb{N}_0}$ is a log-convex sequence of positive real numbers. $C\{M_n\}$ is quasi-analytic if and only if for some (and hence for any) $j \in \mathbb{N}$ the class $C\{\sqrt[j]{M_{jn}}\}$ is quasi-analytic.*

Proof W.l.o.g. we can assume that $M_0 = 1$. (In fact, if $M_0 \neq 1$ then one can always apply the following proof to the sequence $(\frac{M_n}{M_0})_{n\in\mathbb{N}_0}$ by Proposition 2.3.)

Let us first note that, by Theorem 2.7, it is enough to prove $\sum_{n=1}^{\infty} \frac{1}{\sqrt[n]{M_n}} = \infty$ if and only if for some $j \in \mathbb{N}$, $\sum_{n=1}^{\infty} \frac{1}{\sqrt[jn]{M_{jn}}} = \infty$. By Corollary 2, we have

$$\sum_{n=1}^{\infty} \frac{1}{\sqrt[n]{M_n}} = \sum_{n=1}^{\infty} \left(\frac{1}{\sqrt[jn]{M_{jn}}} + \cdots + \frac{1}{\sqrt[jn+(j-1)]{M_{jn+j-1}}} \right) + \sum_{n=1}^{j-1} \frac{1}{\sqrt[n]{M_n}}$$
$$\leq j \sum_{n=1}^{\infty} \frac{1}{\sqrt[jn]{M_{jn}}} + \sum_{n=1}^{j-1} \frac{1}{\sqrt[n]{M_n}},$$

which gives the necessity part. On the other hand, if $\sum_{n=1}^{\infty} \frac{1}{\sqrt[jn]{M_{jn}}}$ diverges for some $j \in \mathbb{N}$, then also $\sum_{n=1}^{\infty} \frac{1}{\sqrt[n]{M_n}}$ diverges since it contains more summands than the former series. □

Lemma 4 *Let $(M_n)_{n\in\mathbb{N}_0}$ be a sequence of positive real numbers. Then, for any $k \in \mathbb{N}_0$, $\sum_{n=1}^{\infty} \frac{M_{n+k-1}}{M_{n+k}} = \infty$ if and only if $\sum_{n=1}^{\infty} \frac{M_{n-1}}{M_n} = \infty$.*

Proof These two series differ only by a finite number of positive summands. □

Lemma 5 *Let $(M_n)_{n\in\mathbb{N}_0}$ be a log-convex sequence of positive real numbers. $C\{M_n\}$ is quasi-analytic if and only if for some (and hence for any) $k \in \mathbb{N}_0$ the class $C\{M_{n+k}\}$ is quasi-analytic.*

Proof By Theorem 2.7 and Lemma 4, $C\{M_n\}$ is quasi-analytic if and only if

$$\sum_{n=1}^{\infty} \frac{M_{n+k-1}}{M_{n+k}} = \infty. \tag{24}$$

Note that the sequence $(M_{n+k})_{n\in\mathbb{N}_0}$ is also log-convex. Hence, by Theorem 2.7, (24) is equivalent to the quasi-analyticity of the class $C\{M_{n+k}\}$. □

Theorem 6 *Let $(M_n)_{n\in\mathbb{N}_0}$ be a log-convex sequence of positive real numbers. If we have $\sum_{n=1}^{\infty} \frac{1}{\sqrt[2n]{M_{2n}}} = \infty$, then $\sum_{n=1}^{\infty} \frac{1}{\sqrt[2n]{M_{2n+h}}} = \infty$ for any $h \in \mathbb{N}_0$.*

Proof By Proposition 2.3, we can assume w.l.o.g. that $M_0 = 1$. Let us consider separately the cases when h is even or odd.
If h is even, then the conclusion directly follows by applying Lemma 5.
If h is odd, then we need some more considerations. Let us first note that for bounded $(M_n)_{n\in\mathbb{N}_0}$, the result is obvious. Suppose $(M_n)_{n\in\mathbb{N}_0}$ diverges, then there exists $N \in \mathbb{N}$

such that for any $n \geq N$ we have that $M_n \geq 1$. Hence, for any $n \geq N$, we get that

$$\frac{1}{\sqrt[2n-1]{M_{2n-1}}} \leq \frac{1}{\sqrt[2n]{M_{2n-1}}}. \tag{25}$$

Moreover, by Corollary 2, we have that $\frac{1}{\sqrt[2n]{M_{2n}}} \leq \frac{1}{\sqrt[2n-1]{M_{2n-1}}}$, for any $n \in \mathbb{N}$. Hence, since $\sum_{n=1}^{\infty} \frac{1}{\sqrt[2n]{M_{2n}}} = \infty$, also $\sum_{n=1}^{\infty} \frac{1}{\sqrt[2n-1]{M_{2n-1}}} = \infty$. This together with (25) gives that

$$\sum_{n=1}^{\infty} \frac{1}{\sqrt[2n]{M_{2n-1}}} = \infty. \tag{26}$$

Let us consider the sequence $B_n := \sqrt{M_{2n-1}}$ for $n \geq 1$. The log-convexity of $(M_n)_{n\in\mathbb{N}_0}$ implies that $(B_n)_{n\in\mathbb{N}}$ is also log-convex. Then (26) is equivalent to the quasi-analyticity of the class $C\{B_n\}$ by Theorem 2.7. Let $k \in \mathbb{N}$ be such that $h = 2k-1$, then by applying Lemma 5 to the sequence $(B_n)_{n\in\mathbb{N}}$, we get that $C\{B_{n+k}\}$ is quasi-analytic which proves our conclusion. □

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Elements for the Retrieval of the Solar Spectrum on the Surface of Mars from an Array of Photodiodes

Salvador Jiménez and Luis Vázquez

To Prof. Ludwig Streit in his 75th birthday

Abstract We present some elements concerning the retrieval of the Solar irradiance spectrum on the surface of Mars, from data collected by arrays of photodiodes, such as those aboard the "Curiosity" MSL-rover and other missions currently under design.

Keywords Solar irradiance spectrum • Retrieval • Planet mars

Mathematics Subject Classification (2010) Primary 65D05; Secondary 65R32

1 Introduction: Solar Irradiance Sensors

Several probes that have been sent to Mars or are under consideration to be sent in the future to study the atmosphere and the general conditions on the surface of the planet, carry a Solar irradiance sensor (SIS) composed of several photodiodes that measure radiation intensity in different bands.

Measuring the Solar irradiance on the surface of a celestial body is an important step in order to determine the feasibility of human habitability. Also, it is important in order to determine whether Earth-like life could be found.

S. Jiménez (✉)
Dept. Matemática Aplicada, E.T.S.I. Telecomunicación, Universidad Politécnica de Madrid, Avenida Complutense 30, 28040-Madrid, Spain
e-mail: s.jimenez@upm.es

L. Vázquez
Dept. Matemática Aplicada, Facultad de Informática, Universidad Complutense de Madrid, Calle Profesor José García Santesmases, s/n, 28040-Madrid, Spain
e-mail: lvazquez@fdi.ucm.es

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The Solar spectrum can be measured on Earth with different instruments. Typically, this is achieved using a spectrometer: a device that measures intensity for a specific wavelength, that can be then tuned to sample the whole range under consideration in a detailed way and establish the experimental dependence of the intensity versus the wavelength.

Unfortunately, the restrictions of present spatial probes on size and weight of the payload they can carry as well as on the needs of power supply do not allow such instruments to qualify for a mission. Instead, instruments with arrays of photodiodes are preferred due to their robustness as well as their size, weight and power requirements. Contrarily to a spectrometer, that can measure intensity corresponding to a single wavelength (up to some precision), photodiodes measure over extended intervals of wavelength values. In that sense, their measure can be considered as an integrated value.

The corresponding ranges can be either narrow, around a specific wave length, or extended over a wider span. For instance, REMS-MSL[1–3] carries 6 photodiodes that cover different ranges over the ultra-violet (UV) region of the spectrum, with photodiodes devoted to each of three bands, UV-A, UV-B and UV-C:

No.	Range
1	Global UV: 200–370 nm
2	UV-A: 320–370 nm
3	UV-B: 280–320 nm
4	UV-C: 220–280 nm
5	Ozone absorption: 230–290 nm
6	Complementary range: 300–350 nm

Note that photodiodes 2–6 have intersecting ranges and fill-in in a complementary way the spectral range covered by photodiode 1.

METSIS[4, 5] has an array of eleven different photodiodes, some are duplicated on the different faces of the instrument. They cover not only the UV region but also the near infra-red (IR), the visible spectrum (VIS), some specific bands related to the expected dust absorption wavelengths, the water absorption wavelength (H_2O), as well as some other bands related to the Ozone. Some of the ranges are limited on purpose around specific values (those related to the dust can be considered as having only an 8 nm span) but other cover practically the whole region under observation:

No.	Range
1	Total luminosity reference: 230–1200 nm
2	UV-A: 315–400 nm
3	UV-B: 280–315 nm
4	Hartley Band: 200–310 nm
5	Huggins Band: 300–345 nm
6	Dust Optical Depth: 440 nm
7	Dust Optical Depth: 600 nm
8	IR: 700–1100 nm
9	VIS: 400–700 nm
10	UV MRO: 245–290 nm
11	H_2O: 930–950 nm

SISDREAMS[6], due to some limitations in the design, will carry three different photodiodes, one on the top face, the other two being duplicated on the three lateral faces of the instrument.

No.	Range
1	UV-A: 315–400 nm
2	IR: 700–1100 nm
3	Total luminosity reference: 220–1100 nm

2 Mathematical Models

The challenge associated to the use of photodiodes is to reconstruct the dependence of the intensity versus the wavelength from the measures of the intensity accumulated over the different ranges.

In this sense, we can ideally consider that we have for a given photodiode measuring all wavelength contributions from $\lambda_{\min}$ to $\lambda_{\max}$ a value M_{ideal} given by:

$$M_{\text{ideal}} = \int_{\lambda_{\min}}^{\lambda_{\max}} I(\lambda)\, d\lambda\,, \tag{1}$$

where $I(\lambda)$ is the intensity corresponding to wavelength λ. Our goal is to estimate a suitable function $I(\lambda)$. We call this an "ideal" measure since we will see later how to take into account more realistic situations.

To achieve our goal, we suppose that we have the measures from n ideal photodiodes M_j, with $j = 1, \ldots, n$, each covering a wave range given by $[\alpha_j, \beta_j]$:

$$M_j = \int_{\alpha_j}^{\beta_j} I(\lambda)\, d\lambda\,, \quad j = 1, \ldots, n\,. \tag{2}$$

These ranges are not necessarily disjoint and some overlapping may occur among them.

We suppose $I(\lambda)$ exists and is integrable over the different ranges and call $F(\lambda)$ a primitive. We have then

$$M_j = F(\beta_j) - F(\alpha_j)\,, \quad j = 1, \ldots, n\,. \tag{3}$$

We suppose, furthermore, that we may approximate $F(\lambda)$ in some vector space, in principle with infinite dimension, with orthonormal base functions $\phi_k(\lambda)$, $k = 1, \ldots, \infty$, such that the orthogonal projection of F on that space is a Fourier series of the form:

$$\sum_{k=1}^{\infty} a_k \phi_k(\lambda)\,. \tag{4}$$

We suppose that this series converges uniformly to F and that a good approximation is obtained when we truncate the series keeping only the first n terms.

Of these last two hypothesis, the first one is reasonable but the second one is not necessarily guaranteed if n is small.

Assuming all of the above, we can reconstruct approximatively F as

$$F(\lambda) \approx \sum_{k=1}^{n} a_k \phi_k(\lambda)\,, \tag{5}$$

while I is then approximated by

$$I(\lambda) \approx \sum_{k=1}^{n} a_k \phi_k'(\lambda)\,, \tag{6}$$

where $\phi_k'(\lambda)$ are the derivatives of the base functions. The coefficients a_k are determined solving (3) which corresponds to the linear system:

$$\forall j = 1, \ldots, n,\ M_j = \sum_{k=1}^{n} a_k \big[\phi_k(\alpha_j) - \phi_k(\beta_j)\big]. \tag{7}$$

This is the approach used in [7]. Due to the fact that for all three configurations (MSL, METSIS and SISDREAMS) there is a global sensor with a range that overlaps all other ranges, the linear system (7) can present equations that are close to linear combinations of some of the others and we may expect to have a large condition number.

Conversely to the previous process, one may start approximating I in the base of orthonormal functions and consider

$$I(\lambda) \approx \sum_{k=1}^{n} c_k \phi_k(\lambda) \tag{8}$$

instead of (6), and determine the coefficients solving now:

$$\forall j = 1, \ldots, n,\ M_j = \sum_{k=1}^{n} c_k \big[\Phi_k(\alpha_j) - \Phi_k(\beta_j)\big], \tag{9}$$

where, for each k, $\Phi_k(\lambda)$ is a primitive of $\phi_k(\lambda)$.

A way to discriminate both possibilities is to construct matrices A and C, associated respectively to (7) and (9), given by:

$$A_{jk} = \phi_k(\alpha_j) - \phi_k(\beta_j), \qquad C_{jk} = \Phi_k(\alpha_j) - \Phi_k(\beta_j), \tag{10}$$

compute their condition number, and choose the method that gives a smaller value, since that approach would be less sensitive to errors.

As an illustration we present some results in the cases of METSIS and SISDREAMS. We reconstruct the irradiance spectrum of the black body radiation, considering what would be the ideal values measured by the corresponding array of photodiodes. We have used as base functions Chebyshev polynomials, with a change of variables to adjust the whole range to the usual interval for those polynomials. We represent the results for METSIS in Fig. 1. We have also computed the irradiance spectrum allowing a 1 % error in all data, which should be within the characteristics of the actual sensors, with no significant variation of the results. A more thorough analysis, using the stochastic ideas in [8] is under consideration.

The case for SISDREAMS is different since from the three values we can only fit a parabola, which is poorly adapted to represent the general shape of the black body radiation. To overcome this limitation, we include an extra measure, that of a "virtual sensor", with an arbitrary value that we adjust in order to minimize the integral of the resulting third degree polynomial. We represent the results in Fig. 2.

3 Responsivities

A real photodiode does not provide the same response to all wavelengths inside the nominal range it covers. Some responsivity function r that depends on λ has to be taken into account. We may understand that a more realistic measure can be represented, instead of by (1), by:

$$M = \int_{\lambda_{\min}}^{\lambda_{\max}} I(\lambda)\, r(\lambda)\, d\lambda\,. \tag{11}$$

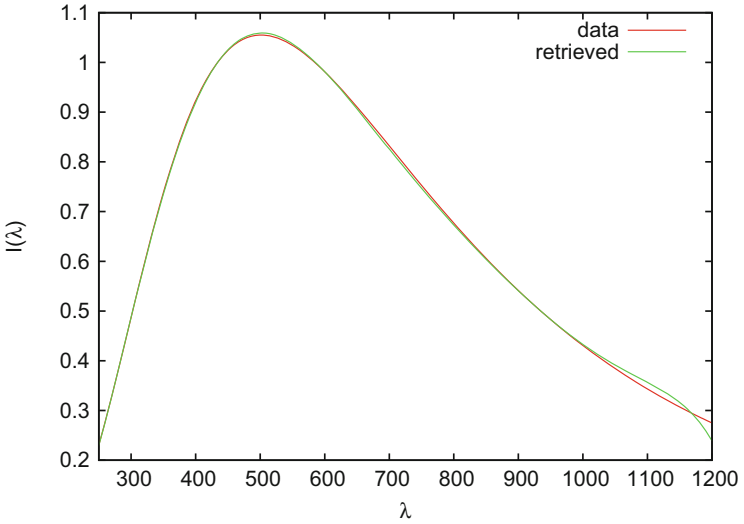

Fig. 1 Approximation of the spectrum of the black body using METSIS photodiodes

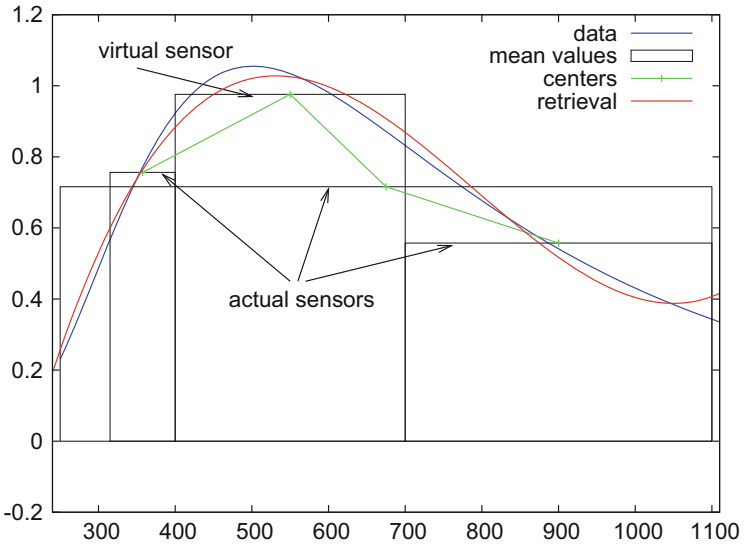

Fig. 2 Approximation of the spectrum of the black body using SISDREAMS photodiodes and a virtual one

The values of the responsivity function $r(\lambda)$ for a specific photodiode can be tabulated by experimental measures on the laboratory with sufficient precision. In this sense the presence of r would not suppose a significant difference in the approach, but some other factors have to be considered: from missions to Mars [9],

it is known that dust will deposit erratically on all exposed surfaces, including those of the photodiodes, reducing in this case their sensibility. But it is also known [9] that winds that can remove a large part of the dust and cleanse the devices, allowing them to recover part of their lost sensitivity. Also, the response of the photodiodes can be degraded due to exposition to the radiation itself, especially to the most energetic one as well as to high energy protons from the Solar wind.

We may use the tabulated values of r as a primer but we devise an iterative process to approximate the actual values.

For each photodiode j, we start considering a first approximation to the mean value of the responsivity in the corresponding range defined as:

$$\bar{r}_j^0 = \frac{1}{\beta_j - \alpha_j} \int_{\alpha_j}^{\beta_j} r_j(\lambda)\, d\lambda\,, \quad j = 1, \ldots, n\,. \tag{12}$$

We consider that the measures M_j given by the photodiodes correspond to

$$M_j = \int_{\alpha_j}^{\beta_j} I(\lambda)\, r_j(\lambda)\, d\lambda\,, \quad j = 1, \ldots, n\,. \tag{13}$$

In order to approximate $I(\lambda)$, we define $I^0(\lambda)$ such that

$$\int_{\alpha_j}^{\beta_j} I^0(\lambda)\, d\lambda = \frac{M_j}{\bar{r}_j^0}\,, \quad j = 1, \ldots, n\,, \tag{14}$$

and construct it through the interpolation process as in the previous section. Once we have it, we estimate a new set of average values

$$\bar{r}_j^1 = \frac{\int_{\alpha_j}^{\beta_j} I^0(\lambda)\, r_j(\lambda)\, d\lambda}{\int_{\alpha_j}^{\beta_j} I^0(\lambda)\, d\lambda} = \frac{\bar{r}_j^0}{M_j} \int_{\alpha_j}^{\beta_j} I^0(\lambda)\, r_j(\lambda)\, d\lambda\,, \quad j = 1, \ldots, n\,. \tag{15}$$

From here, we define $I^1(\lambda)$ such that

$$\int_{\alpha_j}^{\beta_j} I^1(\lambda)\, d\lambda = \frac{M_j}{\bar{r}_j^1}\,, \quad j = 1, \ldots, n\,, \tag{16}$$

and construct it. We then iterate this process, defining further approximations $\bar{r}_j^p$ and $I^p(\lambda)$, $p = 2, \ldots$, until achieving convergence [10].

In this way we can take into account deviations of the responsivity from the nominal values.

As an illustration, we present in Figs. 3 and 4 the retrieved irradiance for a Hamamatsu deuterium (D_2) lamp both in vacuum and with some ozone, with the photodiodes corresponding to the REMS settings with filters that modify the responsivity. The algorithm converges in five iterations to values with an error less

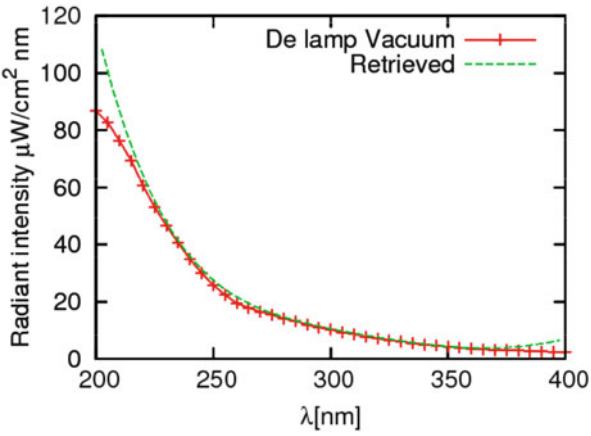

Fig. 3 Approximation of the spectrum of the D_2 lamp in vacuum using REMS photodiodes with filters

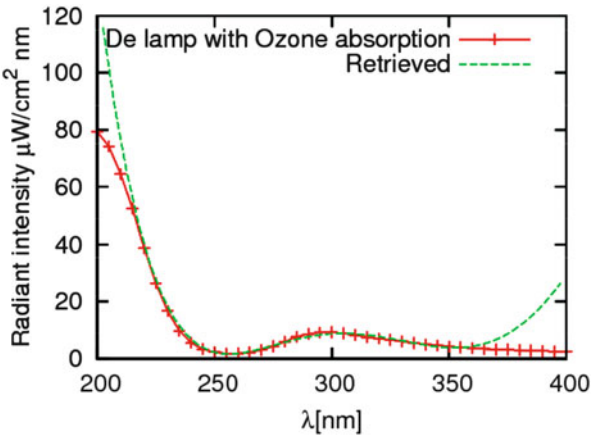

Fig. 4 Approximation of the spectrum of the D_2 lamp with a weak ozone absorption band using REMS photodiodes with filters

than 0.6 % [10]. As we see, we can discriminate accurately both cases: with and without the presence of ozone.

A more realistic approach should take into account that the photodiodes response depend on the angle θ of the light coming directly from the Sun with the normal to their surface:

$$M = \int_{\lambda_{\min}}^{\lambda_{\max}} I(\lambda)\, r(\lambda, \theta)\, d\lambda\,, \tag{17}$$

where the responsivity function depends now both on λ and on θ. An iterative method similar to the previous one can be used, starting with the values of r tabulated for different angles from calibrations in the laboratory.

4 Radiative Transfer

The real emission from the Sun is not that of black body but has some irregularities. Furthermore, the presence of dust, concentration of water vapour and ozone etc., on the atmosphere alter in a characteristic way the radiation that reaches the surface of the planet. From Radiative Transfer techniques it is possible to have information on these different possible scenarios. Also, other instruments on board the same probe can give an idea of the atmosphere situation at the precise time of the measurements. This is useful to adapt the interpolation techniques to try and match the measures of some of these cases, in order to identify more precisely the actual irradiance.

For instance, in [7] we used a combination of approximation by rational functions and polynomials to reproduce the expected curve in the UV region, from 220 to 400 nm. We used a linear combination of the polynomial $Q(\lambda)$ given by the right handside of (6) with Gauss-Legendre polynomials as base functions and the rational function approximation $R(\lambda)$, choosing the coefficients in a way to minimize the total integral.

As another option, we have used natural cubic spline intepolation plus conditions on the spectrum provided by the Radiative Transfer models to retrieve the spectrum in a scenario of a Martian atmosphere with high dust concentration. The result can be seen in Fig. 5. The retrieval is qualitatively correct and a good quantitatively approximation.

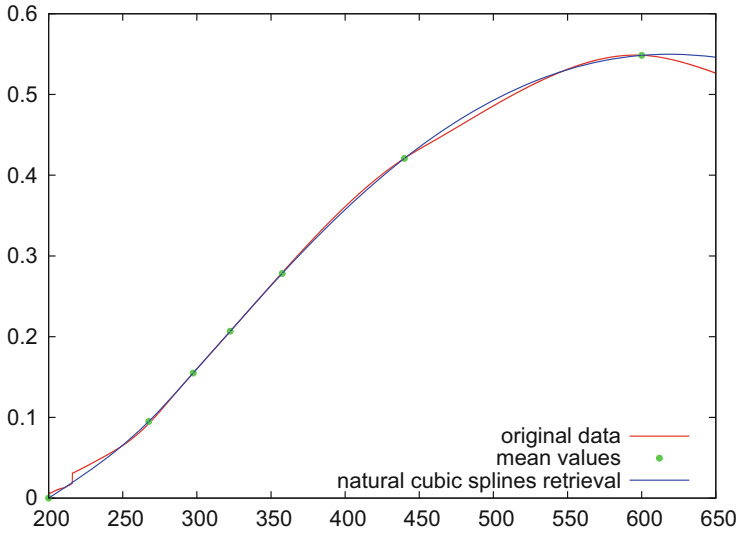

Fig. 5 Approximation in the lower part of the spectrum by natural splines with additional conditions determined by Radiative Transfer

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Stochastic Processes on Ends of Tree and Dirichlet Forms

Witold Karwowski

Abstract We present main ideas and compare two constructions of stochastic processes on the ends (leaves) of the trees with varying numbers of edges at the nods. In one of them the trees are represented by spaces of numerical sequences and the processes are obtained by solving a class of Chapman-Kolmogorov Equations. In the other the trees are described by the set of nodes and edges. To each node there is naturally associated a finite dimensional function space and the Dirichlet form on it. Having a class of Dirichlet forms at the nodes one can under certain conditions build a Dirichlet form on L^2 space of funcions on the ends of the trees. We show that the state spaces of two approaches are homeomorphic but the second yields larger class of processes.

Keywords p-adics • Trees • Stochastic processes • Jump processes • Ultrametric spaces

Mathematics Subject Classification (2010) Primary 60J75; Secondary 05C05, 31C25

1 Introduction

The physicists became interested in ultrametric spaces in mainly two contexts. In 1980s of the last century it had been conjectured that at high energy collisions when dynamics at Planck distances had to be taken into account the structure of space-time was no longer that of a real linear space but might have a non-Archimedean metric. The p-adic numbers [20] turned out to be natural object to be implemented in the theory. The expected physical applications prompted research leading to formulation and studies of p-adic analogs of Quantum Mechanics and Quantum Field Theory [4–6, 19, 23]. Another contact point of Physics and ultrametric spaces was the theory of spin glasses. It has been observed that relaxation in a large system

W. Karwowski (✉)
Institute of Pysics, Opole University, Opole, Poland
e-mail: witoldkarwowski@o2.pl

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of interacting spins is (below certain temperature) not exponential but proportional to $t^{-\alpha}$, $\alpha, t > 0$. It has been explained roughly speaking by assuming hierarchical structure of dynamics and modelled by random processes on hierarchical spaces. Again p-adics were the natural mathematical objects for constructing the physical models [22]. Independently the studies of random processes on p-adics appeared in mathematical literature. Aldous and Evans [8, 10] constructed and discussed spherically symmetric processes in terms of Lèvy–Khinchin formula. Albeverio and Karwowski [1] constructed the same class [7] of processes on p-adics by solving Chapman-Kolmogorov equations and computing transition functions of the processes. They found explicit formulas for the Dirichlet forms and generators. They also gave complete spectral description of the generators. Yasuda [24] extended their method to local fields.

The method of constructing stochastic processes by solving Chapman-Kolmogorov equations was independent of algebraic structure but relied on non-Archimedean metric space properties of p-adics. Exploiting this property Karwowski and Vilela Mendes [16] constructed a class of processes without spherical and translation symmetry. Such processes were required for some physical applications [21]. Further studies of [16] processes were carried out in [3] and [7]. Next generalizations of [1] processes went beyond the state space of p-adics. While p-adic numbers considered as a metric space can be identified with leaves of a tree having $p + 1$ edges at every node Albeverio and Karwowski [2] constructed a class of processes on leaves of the trees with varying number of edges attached to a node. Similarly as in [1] they provided formulas for transition function, the Dirichlet form and the generator of the process.

Due to well known correspondence between regular Dirichlet forms and Markov processes [11, 12] one may first define a Dirichlet form and then obtain the process. Such approach has been successfully used in study of random processes on hierarchical spaces. Before listing some examples we remark that the Dirichlet forms for the processes discussed in [16] and [3] could have been obtained by multiplicative functional transformation of the spherically symmetric Dirichlet forms introduced in [1]. Kaneko [13] constructed a class of regular Dirichlet forms yielding spatially inhomogeneous processes. In this class there were forms which could not have been obtained by multiplicative functional transformation of the spherically symmetric forms.

Using the method of Dirichlet forms Karwowski and Yasuda [15, 17] studied processes of diffusion in $\mathbb{R}$ and $\mathbb{R}^2$ consisting of diffusion and jumps on some fractal subsets. They characterized class of admissible jump parts in terms of Haussdorff dimension of the fractal.

Recently Kaneko [14] introduced a new class of processes on leaves of multi-branching trees. Let $\mathbb{S}_B$ stands for the non-Arhimedean space of the leaves and μ for the ambient measure on $\mathbb{S}_B$. Given a Dirichlet form on $L^2(\mathbb{S}_B, \mu)$ put H for the generator of the corresponding transition semigroup. Then according to property of the balls for any node V of the tree there corresponds a finite dimensional eigenspace $\mathcal{H}_V$ of H and $\bigoplus_V \mathcal{H}_V = L^2(\mathbb{S}_B, \mu)$. Let H_V be a positive Hermitean matrix in $\mathcal{H}_V$. Then there is a positive self-adjoint operator $\tilde{H}$ with $D(\tilde{H})$ dense in $L^2(\mathbb{S}_B, \mu)$ such

that $\tilde{H} \restriction \mathcal{H}_V = H_V$. The question arises. What are the conditions for a given family of operators H_V so that $\tilde{H}$ is the generator of a Hunt process in $\mathbb{S}_B$? Kaneko has formulated the problem in terms of Dirichlet forms and found sufficient conditions. He provided examples which went beyond the scope of Ref. [2].
In this note we present and compare the classes of Markov processes discussed in references [2] and [14].

We prove that although the state spaces are defined in different manners they are essentially identical. More precisely they are homeomorphic under a map preserving their tree structures. We also show that for any Radon measure μ on the state space $\mathbb{S}_B$ with $\operatorname{supp}\mu = \mathbb{S}_B$ there is an orthogonal system $e^k_{\alpha,M}$ assigned to any node $\{\alpha\}_{-(M+1)}$, $\alpha \in \mathbb{S}_B, M \in \mathbb{Z}, k = 1, 2, \ldots, s_{\alpha,M}$. The total system of the vectors corresponding to all nodes in $\mathbb{S}_B$ is complete in $L^2(\mathbb{S}_B, \mu)$ if $\mu(\mathbb{S}_B) = \infty$. If $\mu(\mathbb{S}_B) = 1$ then this system and a non-zero constant function form an orthogonal basis in $L^2(\mathbb{S}_B, \mu)$. It will also be evident that the class of processes discussed in [14] is wider than that of [2]. In Sect. 2 we introduce the state spaces $\mathbb{S}_B$ of Ref.[2] and Σ^+ of Ref. [14] and show their equivalence. We continue the presentation using $\mathbb{S}_B$ as the state space. In Sect. 3 we briefly present the main facts about the constructions of the processes according to [2] (Sect. 3.1) and [14] (Sect. 3.3). In Sect. 3.2 we provide main information on the Dirichlet form and the transition semigroup generators for the processes obtained in Sect. 3.1.

2 The State Space

Let as usual $\mathbb{Z}$, $\mathbb{N}$ and $\mathbb{N}_0$ stand for the sets of integers, positive integers and non-negative integers respectively. For any $k \in \mathbb{Z}$ let S_k be the family of all sequences $\{\alpha_i\}_{i\le k}$ such that $\alpha_i \in \mathbb{N}_0$ and $\alpha_i = 0$ for all $i \le N$ for some $N \le k$, $N \in \mathbb{Z}$. Put

$$S = \bigcup_{k\in\mathbb{Z}} S_k.$$

To simplify notations we put

$$\{\alpha\}_k := \{\alpha_i\}_{i\le k}.$$

If $\alpha_i = 0$ for all $i \le k$ then we write $\{\alpha\}_k = \{0\}_k$.

Definition 2.1 Let B_{α_k} be a function defined on S with values in $\mathbb{N} \setminus \{1\}$. We say that $\{\alpha\}_k \in S_B \subset S$ iff $0 \le \alpha_{i+1} \le B_{\alpha_k} - 1$ for every $i < k$. □

Clearly $\{0\}_k \in S_B$ for any $k \in \mathbb{Z}$.

Definition 2.2 We say that a sequence $\{\alpha_i\}_{i\in\mathbb{Z}}$ belongs to the set $\mathbb{S}_B$ iff $\{\alpha\}_k \in S_B$ for all $k \in \mathbb{Z}$. □

To simplify notations we write

$$\alpha := \{\alpha_i\}_{i\in\mathbb{Z}}. \tag{1}$$

Let q be a real number, $q > 1$. For any pair $\alpha, \beta \in \mathbb{S}_B$ we define

$$\begin{aligned} \rho_q(\alpha,\alpha) &= 0 \\ \rho_q(\alpha,\beta) &= q^{-i_0}, \end{aligned} \tag{2}$$

where i_0 is such that $\alpha_{i_0} \neq \beta_{i_0}$ and $\alpha_i = \beta_i$ if $i < i_0$.

Proposition 2.3 *ρ_q is a metric on $\mathbb{S}_B$ satisfying the non-Archimedean triangle inequality*

$$\rho_q(\alpha,\beta) \leq \max\{\rho_q(\alpha,\gamma), \rho_q(\gamma,\beta)\}. \tag{3}$$

□

It is clear that for any $q, q' > 1$ the metrics ρ_q and $\rho_{q'}$ are equivalent. Thus we fix a real number $q > 1$ throughout the paper and drop the subscript q. Set

$$\mathbb{S}_B^k := \{\alpha \in \mathbb{S}_B; \alpha_i = 0 \, for \, i \geq k\}, \tag{4}$$

and

$$\mathbb{S}_{B,0} := \bigcup_{k\in\mathbb{Z}} \mathbb{S}_B^k. \tag{5}$$

Proposition 2.4 *[2] $\mathbb{S}_B$ equipped with the metric ρ is a complete metric space and $\mathbb{S}_{B,0}$ is a dense subset of it.* □

Given $\alpha \in \mathbb{S}_B$ and $N \in \mathbb{Z}$ the set

$$K(\alpha, q^N) = \{\beta \in \mathbb{S}_B; \rho(\alpha,\beta) \leq q^N\} \tag{6}$$

will be called a ball of radius q^N centered at α. The following facts are the consequences of (3):

1. If $\beta \in K(\alpha, q^N)$ then $K(\beta, q^N) = K(\alpha, q^N)$.
2. If $\alpha, \beta \in \mathbb{S}_B$ then the balls $K(\alpha, q^N), K(\beta, q^N)$ are either disjoint or identical.
3. If $\alpha \in \mathbb{S}_B$ and $\alpha_i = 0$ for $i < -N$, then $K(\alpha, q^N) = K(0, q^N)$.

It follows from (6) that $K(\alpha, q^N)$ is uniquely defined by $\{\alpha\}_{-(N+1)}$ and thus we can identify

$$\{\alpha\}_{-(N+1)} = K(\alpha, q^N). \tag{7}$$

It will be convenient to introduce following notation:

Definition 2.5

1. We say that $\{\alpha\}_{k+1}$ is the B-product of $\{\alpha\}_k$ and $\{\alpha_{k+1}\}$ iff

$$\{\alpha\}_{k+1} = \{\alpha\}_k \times \{\alpha_{k+1}\} \tag{8}$$

and

$$0 \leq \alpha_{k+1} \leq B_{\{\alpha\}_k} - 1. \tag{9}$$

2. We say that $\{\alpha\}_{k+l}$, $l \in \mathbb{N}$ is the B-product of $\{\alpha\}_k$ and the ordered l-tuple $\{\alpha_{k+1}, \ldots, \alpha_{k+l}\}$

$$\{\alpha\}_{k+l} = \{\alpha\}_k \times \{\alpha_{k+1}, \ldots, \alpha_{k+l}\}$$

iff

$$\{\alpha\}_{k+l} = (\ldots((\{\alpha\}_k \times \{\alpha_{k+1}\}) \times \{\alpha_{k+2}\}) \times \cdots \times \{\alpha_{k+l}\}), \tag{10}$$

where all products are B-products in the sense of 1. We then write

$$\{\alpha\}_{k+l} = \{\alpha\}_k \times \{\alpha_{k+1}\} \times \cdots \times \{\alpha_{k+l}\}. \tag{11}$$

□

Remark 2.6 Whenever we write a formula like the right side of (11) we always mean the B-product. □

With this notation one easily sees that

$$K(\alpha, q^{N+1}) = \{\alpha\}_{-(N+2)} = \bigcup_{\gamma} \{\alpha\}_{-(N+2)} \times \{\gamma\}, \tag{12}$$

where the union is taken over the values of γ satisfying:
$0 \leq \gamma \leq B_{\{\alpha\}_{-(N+2)}} - 1$. Thus the ball $K(\alpha, q^{(N+1)})$ is the union of $B_{\{\alpha\}_{-(N+2)}}$ disjoint balls of radius q^N. Take $N, M \in \mathbb{Z}, N > M$. Iterating formula (12) we find a family of disjoint balls of radius q^M such that $K(\alpha, q^N)$ can be expressed as their union. Once the function $B_{\{\alpha\}_k}$ is defined, this family depends on $\alpha \in \mathbb{S}_B$ and the numbers N, M. We denote this family by $\mathcal{K}(\alpha, N, M)$ and by $n(\alpha, N, M)$ the number of balls in it. Note that $\mathcal{K}(\alpha, N, M) \subsetneq \mathcal{K}(\alpha, N+1, M)$. Consequently $n(\alpha, N, M)$ increases to infinity as N varies from $M+1$ to $+\infty$. Let $M \in \mathbb{Z}$ be given. Then according to property 3 of the balls for any $\beta \in \mathbb{S}_B$ there is $N > M$ such that $\beta \in K(0, q^N)$. Thus

$$\mathbb{S}_B = \bigcup_{N>M} K(0, q^N). \tag{13}$$

On the other hand $\beta \in K(0, q^N)$ implies that β belongs to one of the balls in the family $\mathcal{K}(0, N, M)$. Set

$$\mathcal{K}(M) := \bigcup_{N>M} \mathcal{K}(0, N, M). \tag{14}$$

Then $\mathcal{K}(M)$ is a countable family of disjoint balls of radius q^M

$$\mathcal{K}(M) = \{K_i^M\}_{i\in\mathbb{N}}, \tag{15}$$

where K_i^M is a ball of radius q^M and $K_i^M \cap K_j^M = \emptyset$ iff $i \neq j$. As a consequence of (12), (13) we have

$$\mathbb{S}_B = \bigcup_{i\in\mathbb{N}} K_i^M. \tag{16}$$

Let p be a prime number. Put $B_{\{\alpha\}_k} = p$ for all $\{\alpha\}_k \in S$. Then $\mathbb{S}_B$ can be identified with the set of p-adic numbers $\mathbb{Q}_p$. If in addition $q = p$, then the $\mathbb{S}_B$ metric coincides with that of $\mathbb{Q}_p$. We also have

Proposition 2.7 *[2] A ball in $\mathbb{S}_B$ is both open and compact.* □

In contrast with the above description of the trees and their leaves Kaneko [14] following Kigami [18] used different formulation. We shall briefly describe his approach and show that two formulations are equivalent.

Let a countably infinite set T and a map $\mathcal{A} : T \times T \to \{0, 1\}$ be given. In what follows we always assume $\mathcal{A}(x, x) = 0$ and $\mathcal{A}(x, y) = \mathcal{A}(y, x)$. The elements of T are called nodes and the pairs $x, y \in T$ with $\mathcal{A}(x, y) = 1$ are called wedges. A sequence $a_i \in T,\ i = 0, 1, \ldots, n$ is called a path if $\mathcal{A}(a_i, a_{i+1}) = 1,\ i = 0, 1, \ldots, n-1$. If $i \neq j \Rightarrow a_i \neq a_j$ the path is called simple. If $(a_0, \ldots, a_n)$ is a simple path then n is called the length of the path. If for any pair $x, y \in T$ there is a path $a_i \in T,\ i = 0, 1, \ldots, n$ with $a_0 = x,\ a_n = y$ then $(T, \mathcal{A})$ is called a non-directed tree. Put $V(x) = \{y; \mathcal{A}(x, y) = 1\}$. The class of non-directed trees admitted in [14] is limited by following requirements

(i) for any $x \in T$ the set $V(x)$ is finite and $\sharp V(x) \geq 3$,
(ii) $(T, \mathcal{A})$ does not admit any path $(a_0, a_1, \ldots, a_{n-1}, a_n)$ with $a_0 = a_n$ and distinct edges $(a_0, a_1), (a_1, a_2), \ldots, (a_{n-1}, a_n)$.

Lemma 2.8 (Kaneko,private comm) *The condition (ii) is equivalent to the following; If $(a_0, a_1, \ldots, a_n)$ and $(a_{n-1}, a_n, \ldots, a_{n+m})$ are simple paths then $(a_0, \ldots, a_{n+m})$ is a simple path.* □

The condition (ii) eliminates trees with cycles from the consideration. An infinite sequence $a_i \in T,\ i \in \mathbb{N}_0$ is called a geodesic ray if for any $n \in \mathbb{N}$ the sequence

$a_i,\ i = 0, \ldots, n$ is a simple path. Put $\mathcal{R}$ for the set of all geodesic rays in the tree $\{T, \mathcal{A}\}$ and define an equivalence relation "$\sim$" on $\mathcal{R}$ by

Definition 2.9 $(a_0, a_1, \ldots) \sim (b_0, b_1, \ldots)$ if there is $k \in \mathbb{Z}$ such that $a_{k+m} = b_m$ for any $m \in \mathbb{N}_0$. □

We denote the quotient space $\mathcal{R}/\sim$ by Σ and call its elements the ends of the tree. Let $\Delta \in \Sigma$ be fixed and denote $\Sigma^+ = \Sigma \setminus \Delta$. Let $(\delta_0, \delta_1, \ldots)$ be a representative sequence for Δ then to any $x \notin (\delta_0, \delta_1, \ldots)$ and $i \in \mathbb{N}_0$ there is a simple path $(a_0, \ldots, a_n)$ with $a_0 = x$ and $a_n = \delta_i$. In particular there is $i_x \in \mathbb{N}_0$ such that the length of $(a_0, \ldots, a_n)$ is minimal. We denote the minimal length by $\ell(x)$ and define the map $\pi : T \to T$ by

$$\pi(x) = \begin{cases} a_1 \text{ if } x \notin \{\delta_0, \delta_1 \ldots\}, \\ \delta_{i+1} \text{ if } x = \delta_i \text{ for some } i \geq 0. \end{cases} \tag{17}$$

Put $T_m = \{x \in T | \ell(x) - i_x = m\}$ for $m \in \mathbb{Z}$. Then $m \neq m' \Rightarrow T_m \cap T_{m'} = \emptyset$ and $T = \bigcup_{m \in \mathbb{Z}} T_m$.

Now we are going to demonstrate that the above description of trees is equivalent to that in terms of numerical sequences as formulated in [2] . Let $\mathbb{S}_B$ be given. Take S_B for the set T of nodes. Define the function $\mathcal{A}$ as follows:
If $\{\alpha\}_k \in S_B$ and $0 \leq \gamma \leq B_{\{\alpha\}_k} - 1$ then

$$\begin{cases} \mathcal{A}(\{\alpha\}_{k-1}, \{\alpha\}_k) = \mathcal{A}(\{\alpha\}_k, \{\alpha\}_k \times \gamma) = 1, \\ \mathcal{A}(\{\alpha\}_k, \cdot) = 0 \text{ otherwise}. \end{cases} \tag{18}$$

Hence

$$V(\{\alpha\}_k) = \{\{\alpha\}_{k-1}, \{\alpha\}_{k+\gamma}\}, \tag{19}$$

where $0 \leq \gamma \leq B_{\{\alpha\}_k} - 1$ and

$$\sharp V(\{\alpha\}_k) = B_{\{\alpha\}_k} + 1 \geq 3. \tag{20}$$

Let $\{\alpha\}_k, \{\beta\}_l \in S_B$ and $\{\alpha\}_k \neq \{\beta\}_l$. Then there is $N \leq \min\{l, k\}$, such that $\{\alpha\}_N = \{\beta\}_N$. Take the maximal N with this property and define the sequence of nods

$$a_i = \{\alpha\}_{k-i},\ 0 \leq i \leq k - N$$

and

$$a_i = \{\beta\}_{2N-k+i},\ k - N + 1 \leq i \leq n = k + l - 2N.$$

Then $(a_0, \ldots, a_n)$ is a simple path and $a_0 = \{\alpha\}_k,\ a_n = \{\beta\}_l$. Hence $(T, \mathcal{A})$ is a non-directed tree. By Definition 2.1 the condition (i) is satisfied. Conditions (ii) is also easily verified.

By definition of $\mathbb{S}_B$ the sequences $a_{\pm i} \in S_B,\ i \in \mathbb{N}_0$ are the geodesic rays iff there is $\alpha \in \mathbb{S}_B$ and $n \in \mathbb{Z}$ such that $a_{\pm i} = \{\alpha\}_{n\pm i}$. Following Definition 2.9. we introduce the equivalence relation $\sim$, in the set $\mathcal{R}$ of geodesic rays and find that to any $\alpha \in \mathbb{S}_B$ there is the equivalence class α consisting of geodesic rays

$$A_{\alpha,n} = \{\{\alpha\}_{n+k}\ k \in \mathbb{N},\ n \in \mathbb{Z}\}. \tag{21}$$

Moreover there is the equivalence class Δ consisting of the geodesic rays $O_{\alpha,n} = \{\{\alpha\}_{n-k},\ k \in \mathbb{N}\},\ n \in \mathbb{Z},\ \alpha \in \mathbb{S}_B\}$. We denote the set of all equivalence classes $\{\alpha \in \mathbb{S}_B, \Delta\}$ by Σ and put $\Sigma^+ = \Sigma \setminus \Delta$. Thus $\mathbb{S}_B$ can be identified with Σ^+.
We summarise our discussion in following theorem.

Theorem 2.10 *Given S_B and the map $\mathcal{A} : S_B \times S_B \to \{0, 1\}$ defined by (18). Then $(\mathbb{S}_B, \mathcal{A})$ is a non-directed tree satisfying conditions (i), (ii). Put $\Delta = \{O_{\alpha,n}\}_{\alpha\in\mathbb{S}_B, n\in\mathbb{Z}}$. Then (21) defines a one to one correspondence between $\mathbb{S}_B$ and Σ^+.* □

Let now a tree $(T, \mathcal{A})$ satisfying the conditions (i), (ii) be given. Choose $\Delta \in \Sigma$. We shall define a function $G : T \to S$ in an infinite sequence of steps.

Step 0. Let $(\delta_0, \delta_1, \ldots)$ be a representative sequence for Δ. For every $i \in \mathbb{N}_0$ define $G\delta_i = \{0\}_i$.
We apply following inductive procedure. In step $n,\ n \in \mathbb{N}$ we first specify a set $T^{(n)} \subset T$ by the property that for any $y \in T^{(n)}$ the map $G\pi(y)$ has already been defined. Put $T^{(n)}_x = \{y \in T^{(n)}; \pi(y) = x\}$. We have $Gx = \{\alpha\}_k$ for some $\{\alpha\}_k \in S_k$. Then for $y \in T^{(n)}$ we define $Gy = \{\alpha\}_k \times \gamma$, so that $0 \le \gamma \le \sharp V(x) - 2$ and the G is one to one.

Step 1. Set $T^{(1)} = V(\delta_0) \setminus \{\delta_1\}$ and define Gy for $y \in T^{(1)}$.

Step 2. Set

$$T^{(2)} = [V(\delta_1) \setminus \{\delta_2, \delta_0\}\}] \cup \{y \in T; \pi(y) \in T^{(1)}],$$

and define Gy for $y \in T^{(2)}$.

Step n. Set

$$T^{(n)} = [V(\delta_{n-1}) \setminus \{\delta_n, \delta_{n-2}\}] \cup \{y \in T; \pi(y) \in T^{(n-1)}\}$$

and define Gy for $y \in T^{(n)}$.

If $y = \delta_i,\ i \in \mathbb{N}_0$ then Gy is defined in step 0. If $y \notin \{\delta_0, \delta_1, \ldots\}$ then there is i_y and $l(y)$ so that $\pi^{l(y)}(y) = \delta_{i_y}$. If i_y is the minimal number with this property then $y \in T^{(n)}$ where $n = l(y) + i_y$. Observing that $\sharp T^{(n)} < \infty$ we conclude that for every $y \in T$ the element Gy is defined in finite number of steps.

Let $Gy = \{\alpha\}_k$. Denote $B_{\{\alpha\}_k} = V(y) - 1$. Then we have

$$GT = S_B. \tag{22}$$

Let the sequence $(a_{-i}, a_{-i+1}, \ldots)$, where $a_{-i} = \delta_i,\ i \leq 0$ be a geodesic ray. Define $b_k = a_k$ if $k \geq -i$ and $b_k = \delta_{-k}$ if $k < i$. Then

$$\{(b_k, b_{k+1}, \ldots),\ k \in \mathbb{Z}\} \tag{23}$$

is a class of equivalence of geodesic rays. The class (23) defines the sequence $\beta = \{\beta_i\}_{i\in\mathbb{Z}}$ such that $\{\beta\}_k = Gb_k$ and $\{\beta\}_k \in S_k$. Hence $\beta \in \mathbb{S}_B$. Thus we have proved

Theorem 2.11 *Let $(T, \mathcal{A})$ be a non-directed tree satisfying conditions (i), (ii). Then there is a space S_B, the corresponding space $\mathbb{S}_B$ and a one to one map G of T onto S_B such that if $(\delta_0, \delta_1, \ldots)$ is a given representative sequence of Δ then $G\delta_i = \{0\}_i,\ i \in \mathbb{N}_0$, and for any $\alpha \in \mathbb{S}_B,\ k \in \mathbb{Z}$ there is $B_{\{\alpha\}_k} = V(y) - 1$, where $\{\alpha\}_k = Gy$. The map G determines a one to one correspondence between Σ^+ and $\mathbb{S}_B$.* □

For any $x \in T$ define $S_x = \{y \in T | \pi^k(y) = x$ for some non-negative integer $k\}$ and $\Sigma_x = \{\xi \in \Sigma^+ | \xi$ admits a geodesic ray $(a_0, a_1, \ldots),\ a_0, a_1, \ldots \in S_x$ as a representative sequence of $\xi\}$. Taking the family $\Sigma_S^+ = \bigcup_{x\in S\subset T} \Sigma_x^+$ for the family of open sets defines a topology in Σ^+. However if $x \in T_{-(M+1)}$ then $x \leftrightarrows \{\alpha\}_{-(M+1)} \in S_B$ for some $\alpha \in \mathbb{S}_B$ and $\Sigma_x^+ \leftrightarrows K(\alpha, q^M)$. Thus Σ^+ and $\mathbb{S}_B$ are homeomorphic.

3 Stochastic Processes on $\mathbb{S}_B$

3.1 Chapman-Kolmogorov Equation Method

In this section we present main ideas of the construction of stochastic processes on $\mathbb{S}_B$ developed in Ref. [2]. We begin by constructing Markov processes on $\mathcal{K}(M)$. Let $\alpha^i \in K_i^M$, $i \in \mathbb{N}$. Then according to (7)

$$K_i^M = K(\alpha^i, q^M) = \{\alpha^i\}_{-(M+1)}. \tag{24}$$

Put $P_{\{\alpha^i\}_{-(M+1)}\{\alpha^j\}_{-(M+1)}}(t), t \in \mathbb{R}_+$ for the transition probability from K_i^M to K_j^M in time t. We shall temporally use the simplified notation

$$P_{ij} := P_{\{\alpha^i\}_{-(M+1)}\{\alpha^j\}_{-(M+1)}}(t). \tag{25}$$

Thus the forward and backward Chapman-Kolmogorov equations read:

$$\dot{P}_{ij}(t) = -\tilde{a}_j P_{ij}(t) + \sum_{\substack{l=1 \\ l\neq j}}^{\infty} \tilde{u}_{lj} P_{il}, \tag{26a}$$

$$\dot{P}_{ij}(t) = -\tilde{a}_j P_{ij}(t) + \sum_{\substack{l=1 \\ l\neq j}}^{\infty} \tilde{u}_{il} P_{lj}, \tag{26b}$$

$i, j \in \mathbb{N}$. We impose the initial condition

$$P_{ij}(0) = \delta_{ij}. \tag{27}$$

The coefficients $\tilde{a}_j$ and $\tilde{u}_{lj}$ will be defined according to the following intuitive requirements. If at time t the process is in the ball $K(\alpha, q^N)$, then the probability that at time $t + \Delta t > t$ the process is outside of $K(\alpha, q^N)$ is set equal to $a(\alpha, N)\Delta t$. We call $a(\alpha, N)$ the intensity of the state $K(\alpha, q^N)$ and assume

(i) The intensity of the state $K(\alpha, q^N)$ depends only on the radius of the ball, i.e. on N, and is independent of α. Hence

$$P\left(X_{t+\Delta t} \in (\mathbb{S}_B - K(\alpha, q^N))|X_t \in K(\alpha, q^N)\right) = a(N)\Delta t.$$

(ii) The Probability that during a short time Δt the process jumps over a distance q^N and reaches a state in $K(\alpha, q^{N'})$ is the same as the probability to reach a state in $K(\beta, q^{N'})$ where $M \leq N' < N$ and $\rho(\alpha, \beta) = q^{N'+1}$.

(iii) The coefficients $\tilde{a}_j$ satisfy the following relation:

$$\tilde{a}_j = \sum_{\substack{l=1 \\ l\neq j}}^{\infty} \tilde{u}_{jl}. \tag{28}$$

To meet requirement (i) we proceed as follows. We define a sequence $a(N)$, $N \in \mathbb{Z}$ such that

$$a(N) \geq a(N+1) \tag{29a}$$

and

$$\lim_{N\to\infty} a(N) = 0, \quad \lim_{N\to-\infty} a(N) = W, \tag{29b}$$

where W is either a positive real number or $+\infty$. Put

$$U(N+1) = a(N) - a(N+1). \tag{30}$$

We interpret $U(N+1)\Delta t$ as the probability that the process leaves a ball $K(\alpha, q^N)$ but stays in the ball $K(\alpha, q^{N+1})$ i.e. it jumps to one of the balls

$$\{\alpha\}_{-(N+2)} \times \{\gamma\},\ \gamma = 0, \ldots, B_{\{\alpha\}_{-(N+2)}} - 1,\ \gamma \neq \alpha_{-(N+1)}. \tag{31}$$

Let $\rho(\alpha^l, \alpha^j) = q^{N+m}$, $m \in \mathbb{N}$. Define

$$B(\alpha^j, m, M) = (B_{\{\alpha^j\}_{-(M+m+1)}} - 1)B_{\{\alpha^j\}_{-(M+m)}} \cdots B_{\{\alpha^j\}_{-(M+2)}} \tag{32}$$

Set

$$u(\alpha^j, m, M) := B^{-1}(\alpha^j, m, M)U(M+m). \tag{33}$$

It follows from (i), (ii) that $u(\alpha^j, m, M)\Delta t$ is the probability that the process jumps from $\{\alpha^l\}_{-(M+1)}$ to $\{\alpha^j\}_{-(M+1)}$ during the time Δt. Thus we define

$$\tilde{u}_{lj} = u(\alpha^j, m, M). \tag{34}$$

To underline the fact that the elementary balls have radius q^M we write

$$\tilde{a}_j = \tilde{a}_j(M). \tag{35}$$

Lemma 3.1

$$\tilde{a}_j(M) = a(M). \tag{36}$$

□

Specifying the coefficients in equations (26a) as defined by (34) and (35) the solution satisfying initial conditions (27) is found to be given by

$$P_{ii} = \sum_{n=0}^{\infty} \left(B_{\{\alpha^i\}_{-(M+n+2)}} \cdots B_{\{\alpha^i\}_{-(M+2)}}\right)^{-1} \left(B_{\{\alpha^i\}_{-(M+n+2)}} - 1\right) \exp\left\{-\left(a(M+n) + u(\alpha^i, 1, M+n)\right)t\right\}. \tag{37}$$

If $\rho(\alpha^i, \alpha^j) = q^{M+k}$, $k \in \mathbb{N}$ then

$$P_{ij}(t) = B^{-1}(\alpha^j, k, M)\left(Pij^{M,M+k} - P_{ij}^{M,M+k-1}\right) = B^{-1}(\alpha^j, k, M)B^{-1}_{\{\alpha^i\}_{-(M+k+1)}}\left(B_{\{\alpha^i\}_{-(M+k+1)}} - 1\right)$$

$$[\sum_{n=0}^{\infty}\left(B_{\{\alpha^i\}_{-(M+k+n+2)}}\cdots B_{\{\alpha^i\}_{-(M+k+2)}}\right)^{-1}\left(B_{\{\alpha^i\}_{-(M+k+n+2)}}-1\right)$$
$$\exp\left\{-\left(a(M+k+n)+u(\alpha^i,1,M+k+n)\right)t\right\}$$
$$-\exp\left\{-\left(a(M+k-1)+u(\alpha^i,1,M+k-1)\right)t\right\}]. \tag{38}$$

Formulas (37), (38) give the explicit form of the transition functions for a class of processes on $\mathcal{K}(M)$. The next step of our discussion is to construct the transition functions on $\mathbb{S}_B$.

Let $\alpha,\beta\in\mathbb{S}_B$. Then $\{\alpha\}_{-(M+1)}=\{\alpha^i\}_{-(M+1)}$ and $\{\beta\}_{-(M+1)}=\{\alpha^j\}_{-(M+1)}$ for some $i,j\in\mathbb{N}$. Recall that in the extended notation we had $P_{\{\alpha\}_{-(M+1)}\{\beta\}_{-(M+1)}}(t)=P_{ij}(t)$. Thus

$$P_{\{\alpha\}_{-(M+1)}\{\alpha\}_{-(M+1)}}(t)$$
$$=\sum_{n=0}^{\infty}\left(B_{\{\alpha\}_{-(M+n+2)}}\cdots B_{\{\alpha\}_{-(M+2)}}\right)^{-1}\left(B_{\{\alpha\}_{-(M+n+2)}}-1\right)$$
$$\times\exp\left\{-\left(a(M+n)+u(\alpha,1,M+n)\right)t\right\} \tag{39}$$

and

$$P_{\{\alpha\}_{-(M+1)}\{\beta\}_{-(M+1)}}(t)=B^{-1}(\beta,k,M)B^{-1}_{\{\alpha\}_{-(M+k+1)}}\left(B_{\{\alpha\}_{-(M+k+1)}}-1\right)$$
$$[\sum_{n=0}^{\infty}\left(B_{\{\alpha\}_{-(M+k+n+2)}}\cdots B_{\{\alpha\}_{-(m+k+2)}}\right)^{-1}\left(B_{\{\alpha\}_{-(M+k+n+2)}}-1\right)$$
$$\times\exp\left\{-\left(a(M+k+n)+u(\alpha,1,m+k+n)\right)t\right\}$$
$$-\exp\left\{-\left(a(M+k-1)+u(\alpha,1,M+k-1)\right)t\right\}], \tag{40}$$

when $\rho(\alpha,\beta)=q^{M+k}$.
Let $M,N\in\mathbb{Z}$ and $M\le N$. Then $\{\beta\}_{-(N+1)}$ is an union of the balls of radius q^M i.e.

$$\{\beta\}_{-(N+1)}=\bigcup_{\gamma}\{\beta\}_{-(N+1)}\times\{\gamma_{-N}\}\times\cdots\{\gamma_{-(M+1)}\}, \tag{41}$$

where the union runs over all B-products of $\{\beta\}_{-(N+1)}$ and the $(N-M)$-tuples γ. Then we define

$$P_{\{\alpha\}_{-(M+1)}\{\beta\}_{-(N+1)}}(t)=\sum_{\gamma}P_{\{\alpha\}_{-(M+1)}\{\beta\}_{-(N+1)}\times\{\gamma_{-N}\}\times\cdots\times\{\gamma_{-(M+1)}\}}(t). \tag{42}$$

It can be shown that the function (42) does not depend on M provided $M \leq N$. Since $\alpha = \bigcap_{M \leq N} \{\alpha\}_{-(M+1)}$ we set

$$P(\alpha, \{\beta\}_{-(N+1)}, t) = P_{\{\alpha\}_{-(M+1)}\{\beta\}_{-(N+1)}}(t) \tag{43}$$

We shall show in the next subsection that (43) defines the transition function for a stochastic process on $\mathbb{S}_B$.

3.2 Markovian Semigroup and Its Generator

We begin by defining a Borel measure on $\mathbb{S}_B$. Recall that $\mathcal{K}(M)$ defined by (14) is the family of all disjoint balls of radius q^M. Then

$$\mathcal{K} := \bigcup_{M \in \mathbb{Z}} \mathcal{K}(M)$$

is the family of all balls in $\mathbb{S}_B$. Set

$$\mu(\{0\}_{-1}) = 1, \tag{44}$$

and

$$\mu(\{\alpha\}_{-(M+1)}) = B_{\{\alpha\}_{-(M+1)}} \mu(\{\alpha\}_{-M}) \tag{45}$$

for all $\alpha \in \mathbb{S}_B$ and $M \in \mathbb{Z}$.
Equation (44) and multiple application of (45) define a set function on $\mathcal{K}$. Note that by (45) the numbers $\mu(\{\alpha\}_{-(M+1)\times\{\gamma\}})$, $0 \leq \gamma \leq B_{\{\alpha\}_{-(M+1)}} - 1$ are equal. By standard arguments [9] μ can be extended to a Borel measure on $\mathbb{S}_B$. Similarly for any $\alpha \in \mathbb{S}_B$ and $t > 0$, $P(\alpha, \{\beta\}_{-(k+1)}, t)$ defines a set function on $\mathcal{K}$ and can be extended to a Borel measure on $\mathbb{S}_B$. Given a ball $\{\beta\}_{-(k+1)}$ and $t > 0$, then $P(\alpha, \{\beta\}_{-(k+1)}, t)$ is a function of $\alpha \in \mathbb{S}_B$ and by (43) it is constant on every ball $\{\alpha\}_{-(k+1)}$. It follows that for any Borel set $A \subset \mathbb{S}_B$, $P(\alpha, A, t)$ is a μ-measurable function. Thus $P(\alpha, A, t)$ is a family of positive integral kernels. For a real valued Borel function u on $\mathbb{S}_B$ put $p_t u(\eta) = \int_{\mathbb{S}_B} P(\eta, d\xi, t) u(\xi)$ whenever the integral makes sense. It is shown in reference [2] that p_t defines a strongly continuous self-adjoint Markovian semigroup T_t, $t > 0$ in $L^2(\mathbb{S}_B, \mu)$.

Hence it has the representation

$$T_t = e^{-Ht}, t \geq 0$$

where H is a non-negative self-adjoint operator acting in $L^2(\mathbb{S}_B, \mu)$. Let $f \in L^2(\mathbb{S}_B, \mu)$. Then by definition

$$(Hf)(\eta) = \lim_{t \downarrow 0} t^{-1} \left[f(\eta) - (T_t f)(\eta) \right] = \lim_{t \downarrow 0} t^{-1} \left[f(\eta) - \int_{\mathbb{S}_B} f(\xi) P(\eta, d\xi, t) \right]$$

whenever the strong limit exists. By direct computation one checks that the characteristic function of any ball in $\mathbb{S}_B$ belongs to the domain $D(H)$ of H. For any $\alpha \in \mathbb{S}_B$ and $M \in \mathbb{Z}$ we have

$$H\chi_{\{\alpha\}_{-(M+1)}}(\eta) = \begin{cases} a(M) \text{ if } \eta \in \{\alpha\}_{-(M+1)}, \\ -B^{-1}(\alpha, k, M)\left(a(M+k-1) - a(M+k)\right) \\ \text{if } \rho(\eta, \alpha) = q^{M+k}. \end{cases} \tag{46}$$

The spectral properties of H are described by

Theorem 3.2 *Let $-H$ denote the generator of the strongly continuous semigroup T_t with the kernel defined by (43).*
Then

(a). To any $M \in \mathbb{Z}$ such that $a(M) > 0$ and $\alpha \in \mathbb{S}_B$ there corresponds an eigenvalue $h_{M,\alpha}$ of H given by

$$h_{M,\alpha} = \left(B_{\{\alpha\}_{-(M+2)}} - 1 \right)^{-1} \left(B_{\{\alpha\}_{-(M+2)}} a(M) - a(M+1) \right) \tag{47}$$

and a $B_{\{\alpha\}_{-(M+2)}} - 1$ dimensional eigenspace spanned by vectors of the form

$$e_{M,\alpha} = \sum_{\gamma=0}^{s} b_\gamma \chi_{\{\alpha\}_{-(M+2)} \times \{\gamma\}}, \tag{48}$$

where

$$\sum_{\gamma=0}^{s} b_\gamma = 0 \text{ and } s = B_{\{\alpha\}_{-(M+2)}} - 1. \tag{49}$$

If $a(M) = 0$ then $\chi_{\{\alpha\}_{-(M+1)}}$ is an eigenvector of H to the eigenvalue 0.

(b). The linear hull spanned by the vectors $e_{M,\alpha}$, $M \in \mathbb{Z}$, $\alpha \in \mathbb{S}_B$ is dense in $L^2(\mathbb{S}_B, \mu)$.

□

Put D_0 for the linear hull spanned by all functions $\chi_{\{\alpha\}_{-(M+1)}}$, $\alpha \in \mathbb{S}_B$ and $M \in \mathbf{Z}$. Since $\chi_{\{\alpha\}_{-(M+1)}} \in D(H)$ we have $D_0 \subset D(H)$.

By Theorem 3.2 (a), the eigenfunctions $e^k_{M,\alpha} \left\| e^k_{M,\alpha} \right\|^{-1}$ of H are defined as linear combinations of the characteristic functions for the balls and thus belong to D_0.

Hence by Theorem 3.2 (b) D_0 is dense in $D(H)$ in the graph norm. As the result we have

Corollary 3.3 *D_0 is an operator core for H in $L^2(\mathbb{S}_B, \mu)$.*

Since $-H$ is the generator of the strongly continuous Markov semigroup $T_t,\ t > 0$ constructed above, the quadratic form

$$\mathcal{E}(f, g) = \left(H^{\frac{1}{2}} f, H^{\frac{1}{2}} g\right)$$

defined for all $f, g \in D[\mathcal{E}] = D(H^{\frac{1}{2}})$ is according to [11, 12] a closed, symmetric Markovian quadratic form i.e. a Dirichlet form in $L^2(\mathbb{S}_B, \mu)$.
Since D_0 is a core for H it is also a core for $H^{\frac{1}{2}}$ i.e.

(a). D_0 is dense in $D[\mathcal{E}]$ in the norm $(\mathcal{E}_1(\cdot,\cdot))^{\frac{1}{2}} = [\mathcal{E}(\cdot,\cdot) + (\cdot,\cdot)]^{\frac{1}{2}}$.
Put $C_0(\mathbb{S}_B)$ for the space of real valued continuous functions of compact support on $\mathbb{S}_B$. Then by the Weierstrass-Stone theorem
(b). D_0 is dense in $C_0(\mathbb{S}_B)$ in the uniform norm topology.

In the Fukushima terminology a set $D_0 \subset D[\mathcal{E}] \cap C_0(\mathbb{S}_B)$ satisfying (a) and (b) is called a core for $\mathcal{E}$ and a Dirichlet form which has a core is called regular. The regular Dirichlet forms can be expressed uniquely in terms of the Beurling-Deny representation which in our case reads

$$\mathcal{E}(u, v) = \int\int_{\mathbb{S}_B \times \mathbb{S}_B \setminus d} (u(\eta) - u(\xi))(v(\eta) - v(\xi)) J(d\eta, d\xi) \tag{50}$$

for $u, v \in D[\mathcal{E}] \cap C_0(\mathbb{S}_B)$.
Here $J(d\eta, d\xi)$ is a symmetric positive Borel measure on $\mathbb{S}_B \times \mathbb{S}_B$ off the diagonal d. Let $\rho(\alpha, \beta) = q^{M+k},\ M \in \mathbb{Z},\ k \in \mathbb{N}$. By direct computations one gets

$$\begin{aligned} J\left(\{\alpha\}_{-(M+1)}, \{\beta\}_{-(M+1)}\right) &= \tfrac{1}{2}\mu\left(\{\alpha\}_{-(M+1)}\right) \\ &\quad \times B^{-1}(\beta, k, M)\left(a(M+k+1) - a(M+k)\right) \end{aligned} \tag{51}$$

which determines the measure J uniquely.

Remark The formula (51) seems to contradict the symmetry of J. However a direct computation shows that

$$\mu\left(\{\alpha\}_{-(M+1)}\right) B^{-1}(\beta, k, M) = \mu\left(\{\beta\}_{-(M+1)}\right) B^{-1}(\alpha, k, M)$$

so that after all J is symmetric. □

3.3 The Dirichlet Forms Method

Let μ be a Radon measure on $\mathbb{S}_B$ with $\text{supp}\mu = \mathbb{S}_B$. Recall that for any $\alpha \in \mathbb{S}_B$ and $M \in \mathbb{Z}$ the sequence $\{\alpha\}_{-(M+1)}$ determines the ball $K(\alpha, q^M)$. If $s = B_{\{\alpha\}_{-(M+1)}} - 1$ then

$$\{\alpha\}_{-(M+1)} = \bigcup_{\gamma=0}^{s} \{\alpha\}_{-(M+1)} \times \gamma.$$

Denote the characteristic function of the ball $\{\alpha\}_{-(M+1)} \times \gamma$ by $\chi_{\alpha,M,\gamma}$. The linear hull spanned by $\chi_{\alpha,M,\gamma}$, $\alpha \in \mathbb{S}_B$, $M \in \mathbb{Z}$, $0 \le \gamma \le B_{\{\alpha\}_{-(M+1)}} - 1 \equiv s_{\alpha,M}$ is identical with D_0 and so it is dense in $L^2(\mathbb{S}_B, \mu)$. Put $\mathcal{H}_{\alpha,M}$ for the subspace of $L^2(\mathbb{S}_B, \mu)$ spanned by the functions $\chi_{\alpha,M,\gamma}$, $0 \le \gamma \le s_{\alpha,M}$. Let $\mathcal{H}^{\perp}_{\alpha,M}$ be the orthogonal complement of $\chi_{\{\alpha\}_{-(M+1)}}$ in $\mathcal{H}_{\alpha,M}$. Then the functions

$$e^k_{\alpha,M} = \sum_{\gamma=0}^{s_{\alpha,M}} b^k_\gamma \chi_{\alpha,M,\gamma}$$

form an orthogonal basis in $\mathcal{H}^{\perp}_{\alpha,M}$ iff the coefficients b^k_γ satisfy

$$\sum_{\gamma=0}^{s_{\alpha,M}} b^k_\gamma \mu(\{\alpha\}_{-(M+1)} \times \gamma) = 0$$

and

$$\sum_{\gamma=0}^{s_{\alpha,M}} b^k_\gamma b^{k'}_\gamma \mu(\{\alpha\}_{-(M+1)} \times \gamma) = \delta_{kk'}.$$

Note that $e^k_{\alpha,M}$, $e^{k'}_{\alpha',M'}$ are orthogonal unless $M = M'$, $\{\alpha\}_{-(M+1)} = \{\alpha'\}_{-(M+1)}$, $k = k'$. Hence

$$E = \{e^k_{\alpha,M} |\ \alpha \in \mathbb{S}_B,\ M \in \mathbb{Z},\ 1 \le k \le s_{\alpha,M}\} \tag{52}$$

is an orthonormal system in $L^2(\mathbb{S}_B, \mu)$. Note that $E \subset D_0$. Next theorem is a generalization of Theorem 3.1 in [3].

Theorem 3.4

(a) If $\mu(\mathbb{S}_B) = \infty$ then the orthonormal system (52) is a basis in $L^2(\mathbb{S}_B, \mu)$.
(b) If $\mu(\mathbb{S}_B) = 1$ then the orthonormal system (52) and the identity function form a basis in $L^2(\mathbb{S}_B, \mu)$.

Proof Let $f \in L^2(\mathbb{S}_B, \mu)$ be orthogonal to the system (52). In particular $f \perp \mathcal{H}^{\perp}_{\beta,N}, \{\beta\}_{-(N+1)} \subset \{\alpha\}_{-(M+1)}$ implies $f(x) \equiv C \in \mathbb{R}$ for $x \in \{\alpha\}_{-(M+1)}$ i.e. $\int_{\{\alpha\}_{-(M+1)}} f(x)\mu(dx) = C\mu(\{\alpha\}_{-(M+1)})$. Similarly, if $f \perp \mathcal{H}^{\perp}_{\beta,N}, \{\beta\}_{-(N+1)} \subset \{\alpha\}_{-(M+2)}$ then $f(x) = C'$ and $\int_{\{\alpha\}_{-(M+2)}} f(x)\mu(dx) = C'\mu(\{\alpha\}_{-(M+2)})$. Since $\{\alpha\}_{-(M+1)} \subset \{\alpha\}_{-(M+2)}$ we have $C = C'$. Taking $M \to \infty$ we obtain $f(x) \equiv C$ for $x \in \mathbb{S}_B$. If $\mu(\mathbb{S}_B) = \infty$ then $f \in L^2(\mathbb{S}_B, \mu)$ implies $C = 0$. If $\mu(\mathbb{S}_B) = 1$ then $f(x) \equiv 1$ completes the system (52) to orthonormal basis for $L^2(\mathbb{S}_B, \mu)$. □

The situation described in Theorem 3.4 has already occured, when we discussed spectral property of the generator H. The eigenspaces of H were the examples of the spaces $\mathcal{H}^{\perp}_{\alpha,M}$.

Let U be a finite set of disjoint balls $K_i,\ i = 1, 2, \ldots, n$ in $\mathbb{S}_B$ and $\mathcal{E}$ a symmetric bilinear form on the real linear space C spanned by the functions $\chi_{K_i}, i = 1, 2, \ldots, n$. Thus $C \ni u = \sum_i u_i \chi_{K_i}$. The pair $(\mathcal{E}, C)$ is called a Dirichlet space if

(i) $\mathcal{E}(u, u) \geq 0$ for any $u \in C$,
(ii) $\mathcal{E}(\chi_{K_i}, \chi_{K_j}) \leq 0$ if $i \neq j$,
(iii) If $v = 1$ on every $K_i\ i = 1, 2, \ldots, n$ then $\mathcal{E}(u, v) = 0$ for every $u \in C$.

If $(\mathcal{E}, C)$ is a Dirichlet space then there is a matrics $A_{ij},\ i, j = 1, 2, \ldots, n$ such that $\mathcal{E}(u, v) = \Sigma_{i,j} A_{ij} u_i v_j$. Then $A_{ij} = A_{ji}$ and $\Sigma_j A_{ij} = 0$. Alternatively we have the representation $\mathcal{E}(u, v) = \frac{1}{2}\Sigma_{i,j} A_{ij}(u_i - u_j)(v_i - v_j)$. A symmetric bilinear form $\mathcal{E}$ on C satisfying (i) is called non-negative.
In particular we can take $C = \mathcal{H}_{\alpha,M}$.

Presently we address the following problem elaborated by Kaneko [14]. Given a Dirichlet form $\mathcal{E}$ in $L^2(\mathbb{S}_B, \mu)$. When does it induce "local" Dirichlet forms on the $\mathcal{H}_{\alpha,M}$ spaces. Conversely, given a family of Dirichlet forms on the $\mathcal{H}_{\alpha,M}$ spaces, when does it determine a Dirichlet form on $L^2(\mathbb{S}_B, \mu)$.

Let a Dirichlet space $(\mathcal{E}, \mathcal{F})$ in $L^2(\mathbb{S}_B, \mu)$ be such that $D_0 \in \mathcal{F}$. Define

$$\mathcal{E}_{\alpha,M}(u, v) = \mathcal{E}(u, v) - (u)_{\alpha,M}(v)_{\alpha,M}\mathcal{E}(\chi_{\{\alpha\}_{-(M+1)}}, \chi_{\{\alpha\}_{-(M+1)}}) \tag{53}$$

where $(u)_{\alpha,M} = \mu(\{\alpha\}_{-(M+1)})^{-1} \int_{\{\alpha\}_{-(M+1)}} u(\eta)\mu(d\eta)$ and put $P_{\alpha,M}$ for the orthogonal projection onto $\mathcal{H}_{\alpha,M}$.

Proposition 3.5 *If $\mathcal{E}(P_{\alpha,M}u, \chi_{\{\alpha\}_{-(M+1)}}) = 0$ for any $u \in L^2(\mathbb{S}_B, \mu),\ \alpha \in \mathbb{S}_B$ and $M \in \mathbb{Z}$, then $(\mathcal{E}_{\alpha,M}, \mathcal{H}_{\alpha,M})$ is a Dirichlet space.* □

Remark 3.6 Let $-H$ be the generator of a strongly continuous Markovian semigroup $T_t,\ t > 0$ constructed in Sects. 3.1, 3.2 and

$$\mathcal{E}(f, g) = (H^{1/2}f, H^{1/2}g),\ f, g \in D(H^{1/2})$$

the corresponding Dirichlet form. It can be shown that then

$$\mathcal{E}(P_{\alpha,M}u, \chi_{\{\alpha\}_{-(M+l)}}) = 0 \tag{54}$$

for any $u \in L^2(\mathbb{S}_B, \mu)$, $\alpha \in \mathbb{S}_B$, $M \in \mathbb{Z}$ and $l \geq 1$. Hence in particular the assumptions of Proposition 3.5 are satisfied and $(\mathcal{E}_{\alpha,M}, \mathcal{H}_{\alpha,M})$ is a Dirichlet space.

Remark 3.7 If $\mathcal{E}$ is a regular Dirichlet form on $L^2(\mathbb{S}_B, \mu)$ with vanishing killing measure, then its Beurling-Deny representation reads

$$\mathcal{E}(u,v) = \frac{1}{2}\int_{\mathbb{S}_B\times\mathbb{S}_B\setminus d}(u(\xi)-u(\eta))(v(\xi)-v(\eta))J(d\xi,d\eta)$$

$u, v \in \mathcal{F}$.

Theorem 3.8 *Given a regular Dirichlet space $(\mathcal{E},\mathcal{F})$ such that $\mathcal{E}(P_{\alpha,M}u, \xi_{\{\alpha\}_{(M+l)}}) = 0$, $l \geq 0$. The following conditions are equivalent:*

(1) If $u \in \mathcal{H}_{\alpha,M}$, $v \in \mathcal{H}_{\alpha',M'}$ and $\mathcal{H}_{\alpha,M} \neq \mathcal{H}_{\alpha',M'}$ then $\mathcal{E}(u,v) = 0$.
(2) The measure $J(d\xi,d\eta)$ is absolutely continuous with respect to the product measure $\mu(d\xi)\mu(d\eta)$ and the density function is constant at every direct product of the balls $\{\ldots,\alpha_{M+2},\alpha_{M+1},\gamma\}\times\{\ldots,\alpha_{M+2},\alpha_{M+1},\gamma'\}$, $\gamma \neq \gamma'$.

□

Given a sequence $\{(\mathcal{E}_k,\mathcal{F}_k)\}_{k=0}^{\infty}$ of Dirichlet spaces on $L^2(\mathbb{S}_B,\mu)$. If $\mathcal{H}_{\alpha,M} \in \mathcal{F}_k$ then we put

$$\mathcal{E}_{k,\alpha,M} = \mathcal{E}_k(P_{\alpha,M}u, P_{\alpha,M}v),\ u,v \in \mathcal{F}_k.$$

Definition 3.9 If a sequence $\{(\mathcal{E}_k,\mathcal{F}_k)\}_{k=0}^{\infty}$ of Dirichlet spaces on $L^2(\mathbb{S}_B,\mu)$ is such that $\mathcal{F}_k \subset \mathcal{F}_{k+1}$ for any $k \in \mathbb{N}_0$, and for any $\alpha \in \mathbb{S}_B$, $M \in \mathbb{Z}$ and $u, v \in \mathcal{H}_{\alpha,M}$ the condition $\mathcal{H}_{\alpha,M} \in \mathcal{F}_k$ implies $\mathcal{E}_{k,\alpha,M}(u,v) = \mathcal{E}_{k+1,\alpha,M}(u,v)$ then the sequence $\{(\mathcal{E}_k,\mathcal{F}_k)\}_{k=0}^{\infty}$ is called nodewise consistent.

Put $\mathcal{H}^k_{\alpha,M}$ for the linear space spanned by $\bigcup_{l=0}^{k}\mathcal{H}_{\alpha,M+l}$. From now on we shall make following

Assumption 3.10 *For any $\alpha \in \mathbb{S}_B$ and $M \in \mathbb{Z}$ the inequality*

$$\sup\{\lambda|\mathcal{E}(u,u) = \lambda(u,u); u \in \mathcal{H}_{\alpha,M+k}\setminus\{0\},\ k \in \mathbb{N}_0\} < \infty.$$

Proposition 3.11 *If $(\mathcal{E},\mathcal{F})$ is a regular Dirichlet space and condition (1) of theorem (3.8) holds, then for any pair (α,M) the symmetric bilinear form*

$$\mathcal{E}^k_{\alpha,M}(u,v) := \mathcal{E}_{\alpha,M}(u,v) + \mathcal{E}_{\alpha,M+1}(u,v) + \ldots + \mathcal{E}_{\alpha,M+k}(u,v)$$

with domain $\mathcal{H}^k_{\alpha,M}$ is a Dirichlet space and the sequence $\{(\mathcal{E}^k_{\alpha,M},\mathcal{H}^k_{\alpha,M})\}_{k=0}^{\infty}$ of the Dirichlet spaces is nodewise consistent. □

According to the last proposition any Dirichlet space $(\mathcal{E},\mathcal{F})$ satisfying Assumption 3.10 defines for any pair (α,M) a sequence of nodewise consistent Dirichlet spaces. We shall now proceed in opposite direction. In our discussion the crucial

role will be played by the concept of admissible family of the Dirichlet spaces. Let

$$\{(\mathcal{E}_{\alpha,M}, \mathcal{H}_{\alpha,M}),\ \alpha \in \mathbb{S}_B,\ M \in \mathbb{Z}\} \tag{55}$$

be a family of Dirichlet spaces in $L^2(\mathbb{S}_B, \mu)$ with vanishing killing measure and such that $u \perp \mathcal{H}^{\perp}_{\alpha,M},\ v \in \mathcal{H}^{\perp}_{\alpha,M}$ implies $\mathcal{E}_{\alpha,M}(u, v) = 0$.

The family (55) is called admissible if the symmetric bilinear form

$$\mathcal{E}^k_{\alpha,M}(u, v) := \mathcal{E}_{\alpha,M}(u, v) + \mathcal{E}_{\alpha,M+1}(u, v) + \ldots + \mathcal{E}_{\alpha,M+k}(u, v)$$

with domain $\mathcal{H}^k_{\alpha,M}$ satisfies $\mathcal{E}^k_{\alpha,M}(\chi_{\{\alpha\}_{-(M+1)}\times\gamma}, \chi_{\{\alpha\}_{-(M+1)}\times\gamma'}) \le 0$ for any $\gamma \ne \gamma'$.

Lemma 3.12 *If the family (55) is admissible then*

(i) $(\mathcal{E}^k_{\alpha,M}, \mathcal{H}^k_{\alpha,M})$ *is a Dirichlet space for any* (α, M) *and* $k \in \mathbb{N}_0$,
(ii) the sequence $\{(\mathcal{E}^k_{\alpha,M}, \mathcal{H}^k_{\alpha,M})\}_{k=0}^{\infty}$ *of Dirichlet spaces is nodewise consistent.*

Chose $m \ge -(M+1)$. Put Γ_k for the set of all B-products $\{\{\alpha\}_{-(M+1)} \times \gamma_1 \times \gamma_2 \times \ldots \times \gamma_{m+M+k+1}\},\ k \in \mathbb{N}_0$ and define

$$\mathcal{E}^{(m)}_{\alpha,M} := \sum\nolimits_{g\in\Gamma_i(k)} \mathcal{E}_g \tag{56}$$

and

$$\mathcal{H}^{(m)}_{\alpha,M} := \bigoplus\nolimits_{g\in\Gamma_i(k)} \mathcal{H}_g, \tag{57}$$

where $i(k) = m+M+k+1$. Define the map $\Pi : \mathbb{S}_B \times \mathbb{S}_B \setminus \{diagonal\} \to S_B \times S_B$ as follows: If $\xi, \eta \in \mathbb{S}_B,\ \xi \ne \eta$ then $\Pi(\xi, \eta) = (\{\xi\}_{-(N+1)}, \{\eta\}_{-(N+1)})$, where $N \in \mathbb{Z}$ is such that $\{\xi\}_{-(N+2)} = \{\eta\}_{-(N+2)}$. and $\{\xi\}_{-(N+1)} \ne \{\eta\}_{-(N+1)}$. Finally we put $I_{\alpha,M+k} = \{\alpha\}_{-(M+k+1)} \times \{\alpha\}_{-(M+k+1)} \setminus \bigcup_{g\in\Gamma_{i(k)}} g \times g$. Note that $(\xi, \eta) \in I_{\alpha,M+k}$ iff $\{\xi\}_{-(M+k+1)} = \{\eta\}_{-(M+k+1)} = \{\alpha\}_{-(M+k+1)}$ and $-(m+1) < N \le M+k$.

With this notation we have

Proposition 3.13 *If a family (55) is admissible then the sequence*

$$\{\mathcal{E}^{(m)}_{\alpha,M+k}, \mathcal{H}^{(m)}_{\alpha,M+k}\}_{k\in\mathbb{N}_0}$$

is nodewise consistent and for any $k \in \mathbb{N}_0$ *and* $u, v \in \mathcal{H}^{(m)}_{\alpha,M+k}$ *the quadratic form* $\mathcal{E}^{(m)}_{\alpha,M+k}(u, v)$ *admits representation*

$$\mathcal{E}^{(m)}_{\alpha,M+k}(u, v) = \frac{1}{2}\int\int_{I_{\alpha,M+k}} (u(\xi) - u(\eta))(v(\xi) - v(\eta))K_{\{\alpha\}_{-(M+k+1)}} \times(\Pi(\xi, \eta))\mu(d\xi)\mu(d\eta). \tag{58}$$

where $K_{\{\alpha\}_{(M+k+1)}}(\{\xi\}_{-(N+1)}, \{\eta\}_{-(N+1)}) = (\mu(\{\xi\}_{-(N+1)})\mu(\{\eta\}_{-(N+1)}))^{-1}$ $\mathcal{E}^{M+k-N-1}_{\alpha,M+k}(\chi_{\{\xi\}_{-(N+1)}}, \chi_{\{\eta\}_{-(N+1)}})$.

Put

$$\mathcal{H}^{(m)}_* = \{u \in \bigcup_{k=0}^{\infty} \mathcal{H}^{(m)}_{\alpha,M+k} | \lim_{k\to\infty} \mathcal{E}^{(m)}_{\alpha,M+k}(u,u) < \infty\} \tag{59}$$

and

$$\mathcal{E}^{(m)}_* = \lim_{k\to\infty} \mathcal{E}^{(m)}_{\alpha,M+k}. \tag{60}$$

Then we have

Proposition 3.14 *If a family (55) of Dirichlet spaces is admissible then the family* $\{\mathcal{E}^{(m)}_*, \mathcal{H}^{(m)}_*\}$ *of the symmetric bilinear forms satisfies*

$$\mathcal{E}^{(m+1)}_*(u,v) = \mathcal{E}^{(m)}_*(u,v)$$

for any $u, v \in \mathcal{H}^{(m)}_*$ *and* $m \geq -(M+1)$.

Note that $\mathcal{H}^{(m)}_*$, $\mathcal{E}^{(m)}_*$ and $\bigcup_{m=-(M+1)}^{\infty} \mathcal{H}^{(m)}_*$ are independent of α and M. Put

$$\mathcal{H}_* = \bigcup_{m=-(M+1)}^{\infty} \mathcal{H}^{(m)}_*.$$

In virtue of Proposition 3.14 we can define following quadratic form with domain $\mathcal{H}_*$

$$\mathcal{E}_*(u,v) = \mathcal{E}^{(m)}_*(u,v),\ u, v \in \mathcal{H}_* \tag{61}$$

where m is such that $u, v \in \mathcal{H}^{(m)}_*$. The form (61) with domain $\mathcal{H}_*$ is not closed but is closable. Its closure is characterise by following theorem

Theorem 3.15 *If a family (55) of the Dirichlet forms is admissible and* $\lim_{k\to\infty} \mathcal{E}^k_{\alpha,M}(\chi_{\{\alpha\}_{-(M+1)}}, \chi_{\{\alpha\}_{-(M+1)}}) < \infty$ *for any* $\alpha \in \mathbb{S}_B$, $M \in \mathbb{Z}$, *then there exists a regular Dirichlet space* $(\mathcal{E}, \mathcal{F})$ *on* $L^2(\mathbb{S}_B, \mu)$ *such that* $\mathcal{E}_{\alpha,M}(u,v) = \mathcal{E}(u,v) - (u)_{\alpha,M}(v)_{\alpha,M}\mathcal{E}(\chi_{\{\alpha\}_{-(M+1)}}, \chi_{\{\alpha\}_{-(M+1)}})$ *for any* $u, v \in \mathcal{H}_{\alpha,M}$. □

When discussing special cases of the Dirichlet forms $(\mathcal{E}_{\alpha,M}, \mathcal{H}_{\alpha,M})$ it is convenient to have a sufficient conditions for the assumptions of Theorem 3.15 to hold which can be directly verified. We shall formulate below a result in this direction. If $(\mathcal{E}_{\alpha,M}, \mathcal{H}_{\alpha,M})$ is a Dirichlet space then the corresponding matrix denoted $H^{\alpha,M}_{i,j}$ is real symmetric and non-positive defined. Hence there is $s_{\alpha,M}+1$ dimensional orthogonal basis of its eigenfunctions in $\mathcal{H}_{\alpha,M}$ and the condition $\mathcal{E}_{\alpha,M}(\chi_{\{\alpha\}_{-(M+1)}}, u) = 0$ for

any $u \in \mathcal{H}_{\alpha,M}$ implies that $\chi_{\{\alpha\}_{-(M+1)}}$ is an eigenfunction to the eigenvalue 0. We chose the system (52) so that $e^k_{\alpha,M}$ are eigenfunctions for $H^{\alpha,M}_{i,j}$ and put $\lambda^k_{\alpha,M}$ for the corresponding eigenvalues. We also set $\lambda_{\alpha,M} = \max_k \lambda^k_{\alpha,M}$. The sufficient condition we mentioned is given in terms of a sequence $\{I^M\}_{M\in\mathbb{Z}}$ of the functions defined by

$$I^M(\xi,\xi') = \frac{1}{2}(H^{\alpha,M-1}_{\gamma,\gamma'} - \sum_{i=1}^{i=\infty} \lambda_{\alpha,M+i}(\frac{1}{\mu(\{\alpha\}_{-(M+i)})} - \frac{1}{\mu(\{\alpha\}_{-(M+i+1)})}))$$

if $\xi^{(')} = \{\alpha\}_{-(M+1)} \times \gamma^{(')}$ for some $\alpha \in \mathbb{S}_B$ and $\gamma \neq \gamma'$.

$$I^M(\xi,\xi') = \frac{1}{2}(\frac{\lambda_{\alpha,M-l}}{\mu(\{\alpha\}_{-(M-l)})} - \sum_{i=1}^{i=\infty} \lambda_{\alpha,M-l+i}(\frac{1}{\mu(\{\alpha\}_{-(M-l+i-1)})} - \frac{1}{\mu(\{\alpha\}_{-(M-l+i)})}))$$

if $\xi^{(')} = \{\alpha\}_{-(M+-l)} \times \gamma^{(')}$ for some $\alpha \in \mathbb{S}_B$, $l \leq 0$ and $\gamma \neq \gamma'$. Otherwise $I^M(\xi,\xi') = 0$. Then we have

Theorem 3.16 *If every function in $\{I^M\}_{M\in\mathbb{Z}}$ is real and non-negative, then there exists a regular Dirichlet space $(\mathcal{E},\mathcal{F})$ on $L^2(\mathbb{S}_B,\mu)$ such that*

$$\mathcal{E}_{\alpha,M}(u,v) = \mathcal{E}(u,v) - (u)_{\alpha,M}(v)_{\alpha,M}\mathcal{E}(\chi_{\{\alpha\}_{-(M+1)}}, \chi_{\{\alpha\}_{-(M+1)}})$$

for any $u, v \in \mathcal{H}_{\alpha,M}$ and any $\alpha \in \mathbb{S}_B$, $M \in \mathbb{Z}$. □

To summarise the discussion presented in this note we compare classes of the processes obtained in references [2] and [14]. Although the methods are different the results are finally formulated in terms of Dirichlet forms and the semigroup generators. In [2] the measure μ is determined by the structure of $\mathbb{S}_B$. The process obtained is determined by the sequence $\{a_M\}_{M\in\mathbb{Z}}$. Any $\mathcal{H}^{\perp}_{\alpha,M}$ is an eigenspace of the generator corresponding to one eigenvalue $\lambda_{\alpha,M}$. The formulation of [14] is more general. Given $\mathbb{S}_B$ the measure μ is merely assumed to be Radon. The sequence $\{a_M\}_{M\in\mathbb{Z}}$ is not explicite introduced. Any $\mathcal{H}^{\perp}_{\alpha,M}$ is spanned by eigenfunctions of the generator but the eigenvalues do not have to be equal.

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Completing Canonical Quantization, and Its Role in Nontrivial Scalar Field Quantization

John R. Klauder

Abstract The process of canonical quantization is redefined so that the classical and quantum theories coexist when $\hbar > 0$, just as they do in the real world. This analysis not only supports conventional procedures, it also reveals new quantization procedures that, among several examples, permit nontrivial quantization of scalar field models such as ϕ_n^4 for every spacetime dimension $n \geq 2$.

Keywords Enhanced quantization procedures • Model problem solutions

1 Conventional & Enhanced Quantization

1.1 Conventional Canonical Quantization

The standard recipe for canonical quantization is simply stated. For a single degree of freedom, one version reads:

Classical Theory: Choose canonically conjugate, classical phase space coordinates p and q, along with a classical Hamiltonian $H_c(p, q)$, and adopt dynamical equations, i.e., Hamilton's equations of motion, that follow from the stationary variation of a classical (C) action functional given by

$$A_C \equiv \int_0^T [p(t)\dot{q}(t) - H_c(p(t), q(t))]\, dt\ . \tag{1}$$

Quantum Theory: Promote the phase space coordinates to Hermitian operators, $p \to P$ and $q \to Q$, that satisfy Heisenberg's commutation relation $[Q, P] = i\hbar\mathbb{1}$. Choose a Hermitian Hamiltonian operator $\mathcal{H}(P, Q)$, with dynamical equations, i.e., Schrödinger's equation and its adjoint, that follow from the stationary variation of a

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J.R. Klauder
Department of Physics and Department of Mathematics, University of Florida, Gainesville, FL 32611-8440, USA
e-mail: klauder@phys.ufl.edu

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quantum (Q) action functional given by

$$A_Q \equiv \int_0^T \langle \psi(t)|\,[i\hbar\,(\partial/\partial t) - \mathcal{H}(P,Q)]\,|\psi(t)\rangle\,dt\ , \tag{2}$$

where $|\psi\rangle$—and its adjoint $\langle\psi|$—denote vectors in a complex Hilbert space.

Comments: Clearly, the classical and quantum theories have several fundamental differences: For a single degree of freedom, classical phase space is two dimensional, while in quantum theory the Hilbert space is infinite dimensional. In the classical theory, one chooses $\hbar = 0$, while in the quantum theory $\hbar \simeq 10^{-27}$erg·s as determined by experimental measurement. To relate the classical and quantum models, it is traditional to choose $\mathcal{H}(P,Q) = H_c(P,Q)$, modulo possible $\mathcal{O}(\hbar)$ corrections. While covariance under canonical coordinate transformations leads to many possible choices of coordinates, quantization results are generally better [1] if the original coordinates p and q are chosen as "Cartesian coordinates"—despite the fact that classical phase space is *not* endowed with a metric structure that would permit the identification of such coordinates.

Although canonical quantization as sketched above is highly successful, there are certain cases where the so-defined quantum theory is less than satisfactory. We claim that the triviality of ϕ^4 scalar field models in high enough spacetime dimensions are such cases. We aim to overcome that triviality.

1.2 Enhanced Canonical Quantization

In the real world $\hbar > 0$, and so there must be a formulation of the classical theory that accepts that fact [2]. The action functional for the quantum theory assumes that general variations of the Hilbert space vectors are possible. But suppose that is not the case, and we are able to vary only certain Hilbert space vectors that can be varied *without* disturbing the system. One such variation involves translating the system to a new position, but according to Galilean covariance we can move the observer a corresponding amount instead of moving the system. Likewise we can imagine putting the system into uniform motion with a constant velocity, but again Galilean covariance asserts we can get the same result by putting the observer into uniform motion instead of the system. Thus if we assume that some normalized reference state $|\eta\rangle$ is relevant for our problem, e.g., under appropriate conditions, the ground state for our system, then we can imagine that we can vary the set of states denoted by

$$|p,q\rangle \equiv e^{-iqP/\hbar}\,e^{ipQ/\hbar}\,|\eta\rangle\ , \tag{3}$$

a set of states recognized as *canonical coherent states* [3], which offer translation of $|\eta\rangle$ to a new position by q as well as to a new velocity as represented by a new momentum p. Here the operators P and Q, which (for the present) we assume to be

irreducible, obey the usual commutation relation $[Q, P] = i\hbar\mathbb{1}$, and, moreover, are chosen as *self adjoint*—a stronger condition than simply being Hermitian—which is necessary to generate unitary transformations that preserve the normalization of $|\eta\rangle$. It is convenient to choose $|\eta\rangle$ such that $\langle\eta|P|\eta\rangle = \langle\eta|Q|\eta\rangle = 0$, called "physical centering", in which case $\langle p, q|P|p, q\rangle = p$ and $\langle p, q|Q|p, q\rangle = q$, two equations that determine the physical meaning of p and q. Armed with this set of states, we declare as a classical observer that we can only vary p and q in the limited set of states $\{|p, q\rangle\}$, and thus we are led to a restricted (R) quantum action functional given by

$$\begin{aligned} A_{Q(R)} &\equiv \int_0^T \langle p(t), q(t)|\,[\,i\hbar\,(\partial/\partial t) - \mathcal{H}(P, Q)\,]\,|p(t), q(t)\rangle\, dt \\ &= \int_0^T [p(t)\,\dot{q}(t) - H(p(t), q(t))]\, dt\ , \end{aligned} \tag{4}$$

where $\langle p, q|\,i\hbar\,(\partial/\partial t)\,|p, q\rangle = \langle\eta|\,[(P + p\,\mathbb{1})\,\dot{q} - Q\dot{p}\,]\,|\eta\rangle = p\,\dot{q}$. Here we have introduced the important relation that

$$\begin{aligned} H(p, q) &\equiv \langle p, q|\,\mathcal{H}(P, Q)\,|p, q\rangle \\ &= \langle\eta|\,\mathcal{H}(P + p\mathbb{1}, Q + q\mathbb{1})\,|\eta\rangle \\ &= \mathcal{H}(p, q) + \mathcal{O}(\hbar; p, q)\ . \end{aligned} \tag{5}$$

Observe that the restricted quantum action functional $A_{Q(R)}$ resembles the classical action functional and differs from it only by the fact that $\hbar > 0$. The conventional classical Hamiltonian may be obtained as

$$H_c(p, q) \equiv \lim_{\hbar\to 0} H(p, q)\ , \tag{6}$$

but that limit may change the character of $H(p, q)$ in unphysical ways. The additional term $\mathcal{O}(\hbar; p, q)$ in (5) depends on the choice of $|\eta\rangle$, and generally would change if $|\eta\rangle$ is changed. This is to be expected since our limited set of states $\{|p, q\rangle\}$ involves *projections* in Hilbert space, and different choices of $|\eta\rangle$ lead to different projections.

Classical mechanics also involves canonical coordinate transformations which relate new canonical coordinates $(\tilde{p}, \tilde{q})$ to our present coordinates (p, q) by means of the one form

$$p\,dq = \tilde{p}\,d\tilde{q} + d\widetilde{G}(\tilde{p}, \tilde{q})\ . \tag{7}$$

We define the coherent states to transform as scalars under such coordinate transformations such that $|p, q\rangle = |p(\tilde{p}, \tilde{q}), q(\tilde{p}, \tilde{q})\rangle \equiv |\,\tilde{p}, \tilde{q}\rangle$, so that the restricted

quantum action functional becomes

$$\begin{aligned} I_{Q(R)} &= \int_0^T \langle\, \tilde{p}(t), \tilde{q}(t) | \, [\, i\hbar\, (\partial/\partial t) - \mathcal{H}(P,Q)\,] \, | \tilde{p}(t), \tilde{q}(t) \rangle \, dt \\ &= \int_0^T [\, \tilde{p}(t)\, \dot{\tilde{q}}(t) + \dot{\widetilde{G}}(\tilde{p}(t), \tilde{q}(t)) - \widetilde{H}(\tilde{p}(t), \tilde{q}(t))\,] \, dt \, , \end{aligned} \tag{8}$$

where $\widetilde{H}(\tilde{p}, \tilde{q}) \equiv H(p,q)$, and which leads to the proper enhanced classical equations of motion without changing the quantum operators in any way.

Next, let us return to the original coordinates (p,q) and observe that in these canonical coordinates the relation (5) has *exactly* the feature characterized by the choice of p and q as "Cartesian coordinates". And indeed, we can now show that these are Cartesian coordinates after all. The Hilbert space norm generates a metric for vectors determined by $d(|\psi\rangle, |\phi\rangle)^2 = \| \, |\psi\rangle - |\phi\rangle \, \|^2$. However, in quantum theory the overall phase of a vector carries no physics and we can instead consider the ray (R) metric determined by $d_R(|\psi\rangle, |\phi\rangle)^2 = \min_\alpha \| \, |\psi\rangle - e^{i\alpha} \, |\phi\rangle \, \|^2$. If we evaluate a rescaled version of the ray metric for two coherent states that are infinitesimally close to each other, we obtain (a.k.a., the Fubini-Study metric)

$$\begin{aligned} d\sigma_R(p,q)^2 &\equiv (2\hbar) \, [\, \| \, d|p,q\rangle \, \|^2 - |\, \langle\, p,q | d | p,q \rangle \, |^2] \\ &= (2/\hbar) \, [\, \langle Q^2 \rangle \, dp^2 + \langle PQ + QP \rangle dp \, dq + \langle P^2 \rangle \, dq^2 \,] \, , \end{aligned} \tag{9}$$

where here $\langle (\cdot) \rangle \equiv \langle \eta | (\cdot) | \eta \rangle$. For a general choice of $|\eta\rangle$, the two-dimensional space $\{p,q\}$ is always flat, and up to a linear coordinate transformation, this metric involves Cartesian coordinates. Specifically, for the common choice where $(\omega\, Q + iP) \, |\eta\rangle = 0$, i.e., an oscillator ground state, then

$$d\sigma_R(p,q)^2 = \omega^{-1} \, dp^2 + \omega \, dq^2 \, , \tag{10}$$

and p and q are indeed Cartesian coordinates according to the Hilbert space metric. Of course, we can now assign that metric to the classical phase space if so desired. It is in this sense that the coordinates p and q are Cartesian.

Conventional canonical quantization is confirmed! *It is important to appreciate that what has been shown so far is equivalent to the standard canonical quantization procedure!* Specifically, we have identified phase-space coordinates p and q that are indeed Cartesian coordinates and the quantum Hamiltonian operator is indeed the same function of the variables as is the classical Hamiltonian, modulo terms of order $\hbar$.

However, there is more to the story.

Reducible Canonical Operators

Let us consider the example with a classical Hamiltonian given by

$$H_c(\vec{p}\,, \vec{q}\,) = \tfrac{1}{2} \, (\vec{p}^{\,2} + m_0^2 \vec{q}^{\,2}) + \lambda \, (\vec{q}^{\,2})^2 \, , \tag{11}$$

where $\overrightarrow{p} = \{p_1, p_2, \ldots, p_N\}$, and $\overrightarrow{q} = \{q_1, q_2, \ldots, q_N\}$, with $N \leq \infty$. Here, $\overrightarrow{p}^2 \equiv \Sigma_{n=1}^N p_n^2$, $\overrightarrow{q}^2 \equiv \Sigma_{n=1}^N q_n^2$, and for $N = \infty$ we require that $\overrightarrow{p}^2 + \overrightarrow{q}^2 < \infty$. It is clear that this model is invariant under orthogonal rotations $\overrightarrow{p} \to O\overrightarrow{p}$, $\overrightarrow{q} \to O\overrightarrow{q}$, where $O \in \mathbf{O}(N, \mathbb{R})$, and such models are called *Rotationally Symmetric* models [4]. As a consequence of rotational invariance, every solution is equivalent to a solution for $N = 1$ if $\overrightarrow{p} \parallel \overrightarrow{q}$ at time $t = 0$, or to a solution for $N = 2$ if $\overrightarrow{p} \nparallel \overrightarrow{q}$ at time $t = 0$. Moreover, solutions for $N = \infty$ may be derived from those for $N < \infty$ by the limit $N \to \infty$, provided we maintain $\overrightarrow{p}^2 + \overrightarrow{q}^2 < \infty$.

A conventional canonical quantization begins with $\overrightarrow{p} \to \overrightarrow{P}$, $\overrightarrow{q} \to \overrightarrow{Q}$, which are irreducible operators that obey $[Q_l, P_n] = i\hbar\delta_{l,n}\mathbb{1}$ as the only non-vanishing commutation relation. For a free model, with mass m and $\lambda = 0$, the quantum Hamiltonian $\mathcal{H}_0 = \frac{1}{2} : (\overrightarrow{P}^2 + m^2\overrightarrow{Q}^2) :$, where $: (\cdot) :$ denotes normal ordering, has the feature that the Hamiltonian operator for $N = \infty$ is obtained as the limit of those for which $N < \infty$. Moreover, with the ground state $|0\rangle$ of the Hamiltonian operator chosen as the fiducial vector for canonical coherent states, namely,

$$|\overrightarrow{p}, \overrightarrow{q}\rangle = \exp[-i\overrightarrow{q} \cdot \overrightarrow{P}/\hbar] \exp[i\overrightarrow{p} \cdot \overrightarrow{Q}/\hbar]|0\rangle \ , \tag{12}$$

it follows that

$$\langle \overrightarrow{p}, \overrightarrow{q}\,| \tfrac{1}{2} : (\overrightarrow{P}^2 + m^2\overrightarrow{Q}^2) : |\overrightarrow{p}, \overrightarrow{q}\rangle = \tfrac{1}{2}(\overrightarrow{p}^2 + m^2\overrightarrow{q}^2) = H(\overrightarrow{p}, \overrightarrow{q}) \tag{13}$$

as desired, for all $N \leq \infty$.

However, canonical quantization of the interacting models with $\lambda > 0$ leads to trivial results for $N = \infty$. To show this we assume that the Schrödinger representation of the ground state of an interacting model is real, unique, and rotationally invariant. As a consequence, the characteristic function (i.e., the Fourier transform) of the ground-state distribution has the form (note: $|f|^2 \equiv \Sigma_{n=1}^N f_n^2$ and $r^2 \equiv \Sigma_{n=1}^N x_n^2$)

$$\begin{aligned} C_N(\overrightarrow{f}) &= \int e^{i\Sigma_{n=1}^N f_n x_n/\hbar}\, \Psi_0(r)^2\, \Pi_{n=1}^N dx_n \\ &= \int e^{i|f|r\cos(\theta)/\hbar}\, \Psi_0(r)^2\, r^{N-1}\, dr\, \sin(\theta)^{N-2}\, d\theta\, d\Omega_{N-3} \\ &\simeq M' \int e^{-|f|^2 r^2/2(N-2)\hbar^2}\, \Psi_0(r)^2\, r^{N-1}\, dr d\Omega_{N-3} \\ &\to \int_0^\infty e^{-b|f|^2/\hbar}\, w(b)\, db \end{aligned} \tag{14}$$

assuming convergence, where a steepest descent integral has been performed for θ, and in the last line we have taken the limit $N \to \infty$. Additionally, $w(b) \geq 0$, and $\int_0^\infty w(b)db = 1$. This is the result based on symmetry. Uniqueness of the ground state then ensures that $w(b) = \delta(b - 1/4\tilde{m})$, for some $\tilde{m} > 0$, implying

that the quantum theory is that of a free theory, i.e., *the quantum theory is trivial! In addition, the classical limit of the resultant quantum theory is a free theory, which differs from the original, nonlinear classical theory.*

The way around this unsatisfactory result is to let the representations of $\overrightarrow{P}$ and $\overrightarrow{Q}$ be *reducible*. The weak correspondence principle, namely $H(\overrightarrow{p}, \overrightarrow{q}) \equiv \langle \overrightarrow{p}, \overrightarrow{q} | \mathcal{H} | \overrightarrow{p}, \overrightarrow{q} \rangle$, ensures that the enhanced classical Hamiltonian depends only on the proper variables. A detailed study [4] of the proper reducible representation, still in accord with the argument above that limits the ground-state functional form to a Gaussian, leads to the following formulation. Let $\overrightarrow{R}$ and $\overrightarrow{S}$ represent a new set of operators, independent of the former operators, and which obey the commutation relation $[S_l, R_n] = \imath\hbar\delta_{l,n}\mathbb{1}$. We introduce two Hamiltonian operators:

$$\begin{aligned} \mathcal{H}_{0\,PQ} &\equiv \tfrac{1}{2} : (\overrightarrow{P}^2 + m^2(\overrightarrow{Q} + \zeta \overrightarrow{S})^2) : , \\ \mathcal{H}_{0\,RS} &\equiv \tfrac{1}{2} : (\overrightarrow{R}^2 + m^2(\overrightarrow{S} + \zeta \overrightarrow{Q})^2) : , \end{aligned} \tag{15}$$

where $0 < \zeta < 1$. These two operators have a common, unique, Gaussian ground state $|0, 0; \zeta\rangle$. Let new coherent states, which span the Hilbert space of interest, be defined with this ground state as the fiducial vector, as given by

$$|\overrightarrow{p}, \overrightarrow{q}\,\rangle \equiv \exp[-i\overrightarrow{q} \cdot \overrightarrow{P}/\hbar] \exp[i\overrightarrow{p} \cdot \overrightarrow{Q}/\hbar] |0, 0; \zeta\rangle \ , \tag{16}$$

and it follows that

$$\begin{aligned} &\langle \overrightarrow{p}, \overrightarrow{q} | \mathcal{H}_{0\,PQ} + \mathcal{H}_{0\,RS} + 4v : \mathcal{H}_{0\,RS}^2 : | \overrightarrow{p}, \overrightarrow{q}\,\rangle \\ &\quad = \tfrac{1}{2}[\overrightarrow{p}^2 + m^2(1 + \zeta^2)\overrightarrow{q}^2] + v\zeta^4 m^4 (\overrightarrow{q}^2)^2 \\ &\quad \equiv \tfrac{1}{2}(\overrightarrow{p}^2 + m_0^2 \overrightarrow{q}^2) + \lambda (\overrightarrow{q}^2)^2 \end{aligned} \tag{17}$$

as required. This example shows that enhanced quantization techniques that make use of reducible kinematical operator representations can lead to a nontrivial and fully satisfactory solution to certain problems.

The next section illustrates yet another procedure that serves to generalize canonical quantization.

1.3 Enhanced Affine Quantization

Affine Variables and Their Algebra

We return to the study of a single degree of freedom. Importantly, the canonical operators P and Q, which have the whole real line for their spectrum and satisfy the Heisenberg commutation rule $[Q, P] = i\hbar\mathbb{1}$, imply a second commutation relation

as well. If we multiply the Heisenberg commutator by Q, we find $i\hbar Q = [Q,P]Q = [Q,PQ]$, and finally the Lie algebra

$$[Q,D] = i\hbar Q\,, \qquad D \equiv \tfrac{1}{2}(PQ+QP)\,. \tag{18}$$

The variables D and Q are called *affine coordinates* and the commutation relation (18) is called an *affine commutation relation*. Clearly D has the dimensions of $\hbar$, and we will find it convenient to choose Q as dimensionless (or consider Q/q_0 and choose units so that $q_0 = 1$). If the representation for P and Q is *irreducible*, then the representation for D and Q is *reducible*. The irreducible sub-representations of D and Q are one where $Q > 0$ and a similar, second one where $Q < 0$; a third representation with $Q = 0$ is less important. Initially, let us consider the irreducible representation where $Q > 0$.

If $Q > 0$ is a self-adjoint operator, then it follows that P, although Hermitian, can never be self adjoint. Thus, P can not serve as the generator of unitary transformations, so canonical coherent states do not exist in this case. However, although P can not be self adjoint, the operator D can be self adjoint; hence we choose a different algebra made from the affine variables. We choose a new normalized fiducial vector $|\eta\rangle$ and introduce a set of *affine coherent states* [3], which are defined by

$$|p,q\rangle \equiv e^{ipQ/\hbar}\, e^{-i\ln(q)D/\hbar}\,|\eta\rangle\,, \tag{19}$$

for all $(p,q) \in \mathbb{R}\times\mathbb{R}^+$, i.e., $q > 0$. While a self-adjoint P serves to *translate* Q, e.g., $e^{iqP/\hbar}\,Q\,e^{-iqP/\hbar} = Q + q\mathbb{1}$, it follows that a self-adjoint D serves to *dilate* Q, e.g., $e^{i\ln(q)D/\hbar}\,Q\,e^{-i\ln(q)D/\hbar} = qQ$; as already partially noted, it is useful to treat q and Q as dimensionless. If we choose $|\eta\rangle$ so that $[\tilde{\beta}\,(Q-1)+iD]\,|\eta\rangle = 0$—a rough analog of $(\omega Q + iP)\,|\eta\rangle = 0$ for the Heisenberg algebra—it follows that $\langle\eta|Q|\eta\rangle = 1$ and $\langle\eta|D|\eta\rangle = 0$. Moreover, $\langle p,q|Q|p,q\rangle = q$ as well as $\langle p,q|D|p,q\rangle = p\,q$.

It is also important to consider reducible affine operator representations as well. In this case, we introduce a fiducial vector $|\eta\rangle = |\eta_+\rangle \oplus |\eta_-\rangle$ and $Q = Q_+ \oplus Q_-$,where $\langle\eta_\pm|Q_\pm|\eta_\pm\rangle = \pm 1$. We introduce reducible affine coherent states given by

$$|p,q\pm\rangle \equiv |p,q_+\rangle \oplus |p,q_-\rangle\,, \tag{20}$$

where $p \in \mathbb{R}$, $\pm\, q_\pm > 0$, $\pm\, Q_\pm > 0$, and

$$|p,q_\pm\rangle \equiv e^{ipQ_\pm/\hbar}\, e^{-i\ln(|q|)D/\hbar}\,|\eta_\pm\rangle\,. \tag{21}$$

In particular, with the indicated choice of the fiducial vector, the coherent state overlap function is given, for separate $\pm$ in each vector, by

$$\begin{aligned}&\langle p', q' \pm |p, q \pm\rangle \\ &\quad = \theta(q'q)\,[\tfrac{1}{2}(\sqrt{q'/q} + \sqrt{q/q'}) + i\,\tfrac{1}{2}\sqrt{q'q}\,(p'-p)/\tilde{\beta}]^{-2\tilde{\beta}/\hbar}\ , \end{aligned} \tag{22}$$

where $\theta(y) \equiv 1$ if $y > 0$ and $\theta(y) \equiv 0$ if $y < 0$.

Affine Quantization as Canonical Quantization

Given a quantum action functional, once again we assume that we can only vary a subset of Hilbert space vectors, in particular, either the irreducible affine coherent states $\{|p, q\rangle\}$ or the reducible affine coherent states $\{|p, q \pm\rangle\}$. This leads to two versions of the restricted quantum action functional:

$$\begin{aligned} A_{Q(R)} &= \textstyle\int_0^T \langle\, p(t), q(t)|\,[i\hbar(\partial/\partial t) - \mathcal{H}'(D, Q)]\,|p(t), q(t)\rangle\, dt \\ &= \textstyle\int_o^T [-q(t)\dot{p}(t) - H(p(t), q(t))]\, dt\ , \end{aligned} \tag{23}$$

in which $q(t) > 0$, as well as, for identical $\pm$ in both vectors,

$$\begin{aligned} A_{Q(R\pm)} &= \textstyle\int_0^T \langle\, p(t), q(t) \pm |\,[i\hbar(\partial/\partial t) - \mathcal{H}'(D, Q)]\,|p(t), q(t) \pm\rangle\, dt \\ &= \textstyle\int_0^T [-q(t)\dot{p}(t) - H(p(t), q(t))]\, dt\ , \end{aligned} \tag{24}$$

where now $|q(t)| > 0$. Note that this latter case is especially useful if the Hamiltonian has a singularity at $q = 0$. *However, the important point is:* **The restricted quantum action functional, based on affine coherent states, is again identical to the form of a canonical classical system, enhanced, because in these equations, $\hbar > 0$! Stated otherwise, enhanced affine quantization effectively serves as enhanced canonical quantization.**

To complete the story we observe that

$$\begin{aligned} H(p, q) &\equiv \langle p, q \pm |\mathcal{H}'(D, Q)|p, q \pm\rangle \\ &= \langle \mathcal{H}'(D + p|q|\,Q, |q|\,Q)\rangle = \mathcal{H}'(pq, q) + \mathcal{O}(\hbar; p, q)\ , \end{aligned} \tag{25}$$

as well as

$$\begin{aligned} H(p, q) &\equiv \langle p, q \pm |\mathcal{H}(P, Q)|p, q \pm\rangle \\ &= \langle \mathcal{H}(P/|q| + p, |q|\,Q)\rangle = \mathcal{H}(p, q) + \mathcal{O}(\hbar; p, q)\ . \end{aligned} \tag{26}$$

It is important to appreciate that the coordinates (p, q) used in the affine coherent states can be changed to a new set of coordinates $(\tilde{p}, \tilde{q})$ in the very same manner as was the case for the coordinates used in the canonical coherent states. While the phase-space geometry induced by the canonical coherent states (9) led to a flat space, the Fubini-Study metric for the affine coherent states, given by

$$d\sigma_R(p,q)^2 = \tilde{\beta}^{-1} q^2 dp^2 + \tilde{\beta}\, q^{-2} dq^2 \,, \tag{27}$$

corresponds to a different phase-space geometry, namely, a space of constant negative curvature, $-2/\tilde{\beta}$. However, this difference in induced phase-space geometry does not affect the suitability of enhanced affine quantization to serve as enhanced canonical quantization.

A Simple Example

A simple example serves to illustrate the power of enhanced affine quantization. As the classical Hamiltonian, we choose $H_c(p,q) = p^2/2m - e^2/|q|$, which we call a one-dimensional 'hydrogen atom' problem. Classical solutions fall into the singularity in a finite time. For the Hamiltonian operator we choose $\mathcal{H} = P^2/2m - e^2/|Q|$, and thus the enhanced affine classical Hamiltonian is given by

$$H(p,q) = p^2/2m - C/|q| + C'/q^2 \,, \tag{28}$$

where $C \equiv e^2\langle |Q|^{-1}\rangle \propto e^2$ and $C' \equiv \langle P^2\rangle/2m \propto \hbar^2/m$. Observe that $C' \simeq \hbar^2/(me^2)\,C$, *a ratio that is seen to be the Bohr radius!*. Thus we see that the enhanced affine classical Hamiltonian prevents all singularities and has a stable minimum at a distance from the singularity of approximately the Bohr radius. Since $\hbar > 0$ in the real world, we are led to claim that the enhanced classical Hamiltonian is 'more physical' than the conventional classical Hamiltonian with which we started, for which $\hbar = 0$. It would be hard to achieve the same features from an enhanced canonical quantization.

It is important to emphasize that for enhanced affine quantization of Hamiltonians of the general form $P^2 + V(Q)$, the enhanced classical Hamiltonian always contains a term of the form q^{-2} with a coefficient proportional to $\hbar^2$. This fact anticipates the naturalness of an actual term proportional to $\hbar^2$ and involving inverse squared operators in the quantum Hamiltonian of other models, suggesting that it may not be out of place.

These musings provide an important clue for the next topic of discussion.

2 Scalar Field Quantization Without Divergences

We next consider a special class of infinitely-many degrees-of-freedom problems associated with a covariant scalar field. For ϕ_n^4 models, standard canonical quantization procedures have obtained self-consistent solutions for spacetime dimensions $n = 2, 3$, e.g., [5], but those same methods have failed to provide suitable results for $n \geq 4$, leading instead to trivial quantum solutions equivalent to (generalized) free theories. It is our believe that for higher spacetime dimensions ($n \geq 4$), we can find nontrivial solutions by choosing affine quantization procedures, and that this technique also leads to new solutions for $n = 2, 3$ as well, which exhibit compatibility for 'mixed models' in ways we will describe. The reason behind this believe is based on the form of the ground-state distribution we are led to, which has integrable singularities when certain field values are zero. As we shall see, this particular form of the ground-state distribution has the decided advantage that a perturbation series for the interaction does *not* exhibit divergences! Our ground-state wave function with square-integrable singularities when certain fields vanish leads to terms in the quantum Hamiltonian proportional to $\hbar^2$, and in our case involve inverse squared field operators. Although an affine quantization is in order, the insight outlined above for these models means that we can proceed to develop the theory in a more direct manner [6].

2.1 Free vs. Pseudofree Models

It is self evident that $\lim_{g\to 0}(A_0 + gA_I) = A_0$, except when it is false. Consider the action functional for an anharmonic oscillator given by

$$A_g = \int_0^T \{\tfrac{1}{2}[\dot{y}(t)^2 - y(t)^2] - g\, y(t)^w\}\, dt\,, \tag{29}$$

and the domain of functions allowed by this expression. If the exponent $w = +4$, then the limit as $g \to 0$ leads to the free action $A_0 = \int_0^T \frac{1}{2}[\dot{y}(t)^2 - y(t)^2]dt$, but if $w = -4$ that is *not* the case. Instead, when $w = -4$, the limit as $g \to 0$ is $A_0' \equiv \int_0^T \frac{1}{2}[\dot{y}(t)^2 - y(t)^2]dt$ *supplemented with the requirement that* $\int_0^T y(t)^{-4}\, dt < \infty$, which is a fundamentally different domain from that of the free action functional. We refer to the theory described by A_0' as a *pseudofree theory*. A pseudofree theory is the one that is continuously connected to the interacting theories. The pseudofree theory may coincide with the usual free theory, as is the case when $w = +4$, but when $w = -4$, the pseudofree and the free theories are different. This distinction applies to the quantum theories as well. In particular, the free and pseudofree quantum theories are identical for $w = +4$ and distinct for $w = -4$. If one considered making a perturbation analysis of the interacting theory, one would have to start with the pseudofree theory and *not* with the free theory when these two theories differ.

A rather similar situation applies to scalar fields. Consider the classical action given by

$$A_{g_0} = \int (\tfrac{1}{2}\{[\partial_\mu \phi(t,x)]^2 - m_0^2 \phi(t,x)^2\} - g_0 \phi(t,x)^4)\, dt\, d^s x\ , \tag{30}$$

where $x \in \mathbb{R}^s$, $s \geq 1$. Provided $m_0 > 0$ and $g_0 > 0$, a multiplicative inequality [7, 8] implies, for $n = s + 1$, and now where $x \in \mathbb{R}^n$, that

$$\{g_0 \int \phi(x)^4\, d^n x\}^{1/2} \leq C'' \int \{[\nabla \phi(x)^2] + m_0^2 \phi(x)^2\}\, d^n x\ , \tag{31}$$

where $C'' = (4/3)[g_0^{1/2}\, m_0^{(n-4)/2}]$ if $n \leq 4$, while $C'' = \infty$ if $n \geq 5$, which in the latter case means that there are fields for which the left side of (31) diverges, but the right side is finite. [Remark: The divergent cases are *exactly* the *non*-renormalizable models when quantized—and that fact holds true for all the non-renormalizable models of the form ϕ_n^p as well [8]!] Thus, when $n \geq 5$, (31) ensures that the classical pseudofree model is different from the classical free model; and thus we expect that the quantum pseudofree and quantum free models are also different. We will be guided in choosing the pseudofree model by the requirement that it connects smoothly with the interacting models.

2.2 Choosing the Pseudofree Model

Formally, the action functional determines the quantum Hamiltonian, which, in turn, determines the ground-state wave function. The reverse of this ordering is also formally true, so let us start with a study of the lattice regularized form of the presumptive ground-state wave function, $\tilde{\Psi}_0(\phi) \equiv \exp[-U(\phi)/2]$, where, as usual, $U(\phi)$ is determined by the 'large-field' behavior of the potential, and thus $U(\phi)$ is well behaved when ϕ is 'small'. On the lattice, $\{\phi(x)\}$, at $t = 0$, is replaced by $\{\phi_k\}$, where $k \in \mathbb{Z}^s$ labels the site on a (spatial) hypercubic, periodic, lattice with lattice spacing $a > 0$ and a total number of (spatial) sites $L^s \equiv N' < \infty$. The continuum limit arises when $a \to 0$, $L \to \infty$, but $(La)^s = N' a^s$ is fixed and finite, at least initially. Many moments of the ground-state distribution diverge in the continuum limit, such as

$$\int [\Sigma_k' \phi_k^2]^p\, e^{-U(\phi)}\, \Pi_k' d\phi_k = \mathcal{O}(N'^p)\ , \tag{32}$$

where the estimated value arises because there are N'^p terms each of $\mathcal{O}(1)$, and as $N' \to \infty$, divergences arise, for all $p \geq 1$. [Remark: In (32) Σ_k' and Π_k' denote a sum and product over all sites in a single spatial slice.] These divergences seem to arise from the fact that the continuum limit involves an infinite number of integration variables, but the continuum limit need not lead to divergences. To understand this remark, let us first change the integration variables from "Cartesian coordinates" to

"hyperspherical coordinates" by the transformation $\phi_k \equiv \kappa\,\eta_k$, where $\kappa^2 \equiv \Sigma'_k \phi_k^2$, $1 \equiv \Sigma'_k \eta_k^2$, $0 \le \kappa < \infty$, and $-1 \le \eta_k \le 1$, for all k. In the new variables, (32) becomes

$$\int [\kappa^2]^p \, e^{-U(\kappa\,\eta)} \, \kappa^{N'-1} \, d\kappa \, 2\delta(1 - \Sigma'_k \eta_k^2) \, \Pi'_k d\eta_k \, . \tag{33}$$

No longer do we have N'^p terms of order $\mathcal{O}(1)$, but it is the power $N' - 1$ of the hyperspherical radius κ that leads to divergences as $N' \to \infty$. Moreover, a steepest descent analysis as $N' \to \infty$—which makes the support of the measure in (33) *disjoint*, at least partially, for a change of parameters in U—leads to divergences in any perturbation analysis. However, if the ground-state distribution contained an additional factor, namely, $\kappa^{-(N'-R)}$, where $R > 0$ is fixed and finite, it would effectively change the κ-factor from $\kappa^{N'-1}$ to κ^{R-1}—a procedure we call *measure mashing*—and, as a result, the divergences would disappear as $N' \to \infty$! Stated otherwise, measure mashing would nullify the steepest descent argument, and thus a perturbation analysis would not involve divergences. In summary, the "trick" in securing a finite version of scalar field quantization—one that also smoothly passes to its own pseudofree theory—is a direct result of mashing the measure.

To achieve measure mashing, we now assume the ground-state distribution has the form

$$\Psi_0(\phi)^2 \equiv \{\Pi'_k [\Sigma'_l J_{k,l} \, \phi_l^2]^{-(1-2ba^s)/2}\} \, e^{-U'(\phi)} \, , \tag{34}$$

where $J_{k,l} \equiv 1/(2s+1)$ for $l = k$ and for l equal to each site of the $2s$ spatially nearest neighbors of k; $J_{k,l} \equiv 0$ otherwise. Specifically, $R \equiv 2ba^s N'$, where $b > 0$ has the dimensions of $(\text{length})^{-s}$ to make R dimensionless. In turn, the functional form of the lattice ground state determines the functional form of the lattice-regularized Hamiltonian operator. Roughly speaking, the denominator term fixes the small-field dependence of the potential, while $U'(\phi)$ leads to the large-field behavior of the potential. However, to fix the Hamiltonian, we let the chosen denominator (involving $J_{k,l}$) of the ground-state wave function determine the small-field potential, but for the large-field behavior, we specify the form of the Hamiltonian itself. This leads us to the lattice regularized form of the quantum Hamiltonian operator given by

$$\begin{aligned} \mathcal{H} = &-\tfrac{1}{2} a^{-2s} \hbar^2 \textstyle\sum'_k \dfrac{\partial^2}{\partial \phi_k^2} \, a^s + \tfrac{1}{2} \textstyle\sum'_{k,k*} (\phi_{k*} - \phi_k)^2 \, a^{s-2} + \tfrac{1}{2} m_0^2 \textstyle\sum'_k \phi_k^2 \, a^s \\ &+ g_0 \textstyle\sum'_k \phi_k^4 \, a^s + \tfrac{1}{2} \hbar^2 \textstyle\sum'_k \mathcal{F}_k(\phi) \, a^s - E_0 \, , \end{aligned} \tag{35}$$

where k^* denotes each of the s nearest neighbors to k in the positive sense, and the all-important counterterm $\mathcal{F}_k(\phi)$ is given by

$$\begin{aligned}\mathcal{F}_k(\phi) \;&= \tfrac{1}{4}(1-2ba^s)^2 a^{-2s}\left(\sum_t' \frac{J_{t,k}\phi_k}{[\Sigma_m' J_{t,m}\phi_m^2]}\right)^2 \\ &\quad -\tfrac{1}{2}(1-2ba^s)a^{-2s}\sum_t' \frac{J_{t,k}}{[\Sigma_m' J_{t,m}\phi_m^2]} \\ &\quad +(1-2ba^s)a^{-2s}\sum_t' \frac{J_{t,k}^2\phi_k^2}{[\Sigma_m' J_{t,m}\phi_m^2]^2}\;. \end{aligned} \tag{36}$$

Although $\mathcal{F}_k(\phi)$ does not depend only on ϕ_k, it nevertheless becomes a local potential in the formal continuum limit. The constant E_0 is chosen to ensure that $\mathcal{H}\Psi_0(\phi) = 0$. Note that local field powers do not involve normal ordering, but instead, they are defined by an operator product expansion, realized effectively by a multiplicative renormalization of the parameters [6].

At this point, the reader may be wondering what is the relation of enhanced quantization, the topic in the first part of this article, and the approach taken to describe scalar field quantization in the second part of this article. In the first part we introduced coherent states, both canonical and affine. Coherent states of any kind are normally based on a fiducial vector, i.e., our $|\eta\rangle$, and for a field theory with an infinite number of degrees of freedom, the usual fiducial vectors (e.g., Gaussian functions) are generally inappropriate. A safe fiducial vector to use is the ground state of the associated Hamiltonian, and for the scalar field case under discussion, the ground-state wave function, as given by the square root of (34), leads to affine coherent states being appropriate [9], and thus our scalar field analysis is a form of affine quantization.

From the Hamiltonian operator we can determine the form of the (Euclidean) lattice action functional as given by

$$I = \tfrac{1}{2}\Sigma_{k,k^*}(\phi_{k^*}-\phi_k)^2 a^{n-2} + \tfrac{1}{2}m_0^2\Sigma_k\phi_k^2 a^n + g_0\,\Sigma_k\phi_k^4 a^n + \tfrac{1}{2}\hbar^2\,\Sigma_k\mathcal{F}_k(\phi)\,a^n\;, \tag{37}$$

where $n = s+1$, Σ_k signifies a sum over the entire, finite, n-dimensional spacetime lattice, and now k^* runs over all n nearest neighbors to k in the positive sense. The Euclidean-spacetime generating functional is given, in turn, by

$$S(h) = M\int e^{Z^{-1/2}\Sigma_k h_k\phi_k a^n/\hbar - I/\hbar}\;\Pi_k d\phi_k\;, \tag{38}$$

where Z denotes the field-strength renormalization constant, Π_k is a product over all sites in the (finite) spacetime lattice, and M is chosen so that $S(0) = 1$. Based on the distribution underlying this integral, preliminary Monte Carlo studies (J. Stankowicz, private communication) show a positive, non-vanishing

renormalized coupling constant vs. the bare coupling constant for ϕ_4^4. This result compares with an apparently vanishing renormalized coupling constant vs. the bare coupling constant that follows from a Monte Carlo study of conventional canonical quantization procedures [10].

2.3 Discussion of Scalar Field Quantization

The counterterm $\mathcal{F}_k(\phi)$ does not depend on g_0 and thus it remains as $g_0 \to 0$. The result of that limit is the pseudofree model, and it differs from the usual free model. This kind of interacting theory provides a valid quantization of the non-renormalizable models such as ϕ_n^4, $n \geq 5$. However, we can also extend the use of the new Hamiltonian operator to lower dimensions as well, even though, for the classical theory, the free and pseudofree models are the same. The purpose of extending the new form of the Hamiltonian is to ensure the uniqueness of 'mixed models'. For example, consider the case of ϕ_3^4, which is a super-renormalizable model that has been studied perturbatively and non-perturbatively with the same self-consistent results; e.g., see [5]. But, suppose we studied the mixed model given by $g_0\phi_3^4 + g_0'\phi_3^8$, which is a sum of a super-renormalizable and a non-renormalizable model, or the mixed model $g_0''\phi_5^4 + g_0'''\phi_5^8$, which is the sum of two different non-renormalizable models, etc. Conventional canonical quantization procedures would not be able to make any sense of such mixed models, but the new version, which treats each ingredient of such models in the same manner, would make perfectly good sense as the coupling constants are turned on, then off, then on again, etc., in any order. In this regard we are also proposing new and different quantization procedures for models like ϕ_2^4 and ϕ_3^4, and other super-renormalizable models. [Remark: Of course, the original solutions for super-renormalizable models have their own role to play for different physical situations.] On these grounds, we advocate accepting the lattice Hamiltonian (35) and the lattice action (37) for all $n \geq 2$.

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Stochastic Solutions of Nonlinear PDE's and an Extension of Superprocesses

Rui Vilela Mendes

Abstract Stochastic solutions provide new rigorous results for nonlinear PDE's and, through its local non-grid nature, are a natural tool for parallel computation. There are two different approaches for the construction of stochastic solutions: MacKean's and superprocesses. Here one shows how to extend the McKean construction to equations with derivatives and non-polynomial interactions. On the other hand, when restricted to measures, superprocesses can only be used to generate solutions for a limited class of nonlinear PDE's. A new class of superprocesses, namely superprocesses on signed measures and on ultradistributions, is proposed to extend the stochastic solution approach to a wider class of PDE's.

Keywords Stochastic solutions • Superprocesses

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1 Introduction: Stochastic Solutions and Measure-Valued Processes

A *stochastic solution* of a linear or nonlinear partial differential equation is a stochastic process which, starting from a point x in the domain generates after time t a boundary measure that, sampling the initial condition at $t = 0$, provides the solution at the point x and time t. For illustration consider the McKean [1] construction of a stochastic solution for the KPP equation

$$\frac{\partial v}{\partial t} = \frac{1}{2}\frac{\partial^2 v}{\partial x^2} + v^2 - v \qquad\qquad v(0,x) = g(x) \tag{1}$$

R.V. Mendes (✉)
Faculdade de Ciências C6, CMAF – University of Lisbon, Campo Grande, 1749-016 Lisboa, Portugal
e-mail: rvmendes@fc.ul.pt; rvilela.mendes@gmail.com

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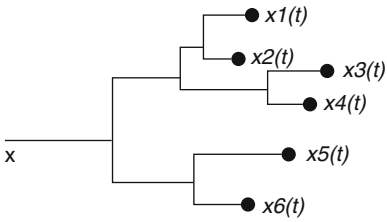

Fig. 1 The McKean process

Let $G(t,x)$ be Green's operator for the heat equation $\partial_t v(t,x) = \frac{1}{2}\frac{\partial^2}{\partial x^2} v(t,x)$

$$G(t,x) = e^{\frac{1}{2}t\frac{\partial^2}{\partial x^2}}$$

and write the KPP equation in integral form

$$v(t,x) = e^{-t} G(t,x)\, g(x) + \int_0^t e^{-(t-s)} G(t-s,x)\, v^2(s,x)\, ds \tag{2}$$

Denoting by (ξ_t, Π_x) a Brownian motion starting from time zero and coordinate x, Eq. (2) may be rewritten as

$$\begin{aligned} v(t,x) &= \Pi_x \left\{ e^{-t} g(\xi_t) + \int_0^t e^{-(t-s)} v^2(s, \xi_{t-s})\, ds \right\} \\ &= \Pi_x \left\{ e^{-t} g(\xi_t) + \int_0^t e^{-s} v^2(t-s, \xi_s)\, ds \right\} \end{aligned} \tag{3}$$

The *stochastic solution process* is a composite process: a Brownian motion plus a branching process with exponential holding time T, $P(T > t) = e^{-t}$ (Fig. 1). At each branching point the particle splits into two, the new particles going along independent Brownian paths. At time $t > 0$, if there are n particles located at $x_1(t), x_2(t), \cdots x_n(t)$, the solution of (1) is obtained by

$$v(t,x) = \mathbb{E}_x \{ g(x_1(t))\, g(x_2(t)) \cdots g(x_n(t)) \} \tag{4}$$

An equivalent interpretation, that corresponds to the second equality in (3), is of a process starting from time t at x and propagating backwards-in-time to time zero. When it reaches $t = 0$ the process samples the initial condition, that is, it generates a measure μ at the $t = 0$ boundary which yields the solution by (4).

The construction of solutions for nonlinear equations, through the stochastic interpretation of the integral equations, has become an active field in recent years, applied for example to Navier-Stokes [2–6], to Vlasov-Poisson [7–9], to Euler [10] to magnetohydrodynamics [11] and to a fractional version of the KPP equation [12]. In addition to providing new exact results for nonlinear PDE's, the stochastic solutions are also a promising tool for numerical implementation, in particular for

parallel computation using for example the recently develop probabilistic domain decomposition method [13–15]. This method decomposes the integration domain into subdomains, uses in each one a deterministic algorithm with Dirichlet boundary conditions, the values at the boundaries being obtained by a stochastic algorithm. This minimizes the time-consuming communication problem between subdomains and allows for extraordinary improvements in computer time.

There are basically two methods to construct stochastic solutions. The first method, which will be called the McKean method, as illustrated above, is essentially a probabilistic interpretation of the Picard series. The differential equations are written as integral equations which are rearranged in a such a way that the coefficients of the successive terms in the Picard iteration obey a normalization condition. The Picard iteration is then interpreted as an evolution and branching process, the stochastic solution being equivalent to importance sampling of the normalized Picard series. The second method [16, 17] constructs the boundary measures of a measure-valued stochastic process (a superprocess) and obtains the solution of the differential equation by a scaling procedure. For a detailed comparison of the two methods refer to [18].

As developed in the past, both methods lead to boundary measure-valued processes which are used to integrate a boundary function. As representations of solutions of the nonlinear equations of physical interest both methods have serious limitations. For the McKean method it is not clear how to handle nonpolynomial interaction terms and terms with derivatives. For the measure-valued superprocesses, in addition to these problems, they can only be applied to a limited class of nonlinear partial differential equations. In this paper both problems will be addressed, namely how to handle derivatives and nonpolynomial interactions in the McKean construction and how to extend superprocesses from measure-valued to ultradistribution-valued processes.

2 Stochastic Solutions with Derivatives and Non-polynomial Terms

To extend the construction of stochastic solutions to cases more general than those dealt with in the past, techniques must be developed to handle derivatives and nonpolynomial interactions. Sometimes the direct handling of derivatives may be avoided if the derivative of the propagation kernel is smooth. This is the case in the configuration space Navier-Stokes equation [5], where by an integration by parts the derivative of the heat kernel is controlled by a majorizing kernel and absorbed in the probability measure. However, in general this is not possible.

Sometimes the nonpolynomial interaction case may be reduced to the polynomial case by expanding the interaction term in a Taylor series and normalizing the coefficients to obtain a probabilistic interpretation. Again, this is not always possible.

Here the solution of both problems (derivatives and non-polynomials) is illustrated in the example of the SOLEDGE2D equations [19] which describe plasma dynamics in the scrape-off layer. Other examples and details may be found in [20]. One deals with the Cauchy problem, namely the equations are defined in the full space with initial conditions at $t = 0$. This is the most natural setting when the McKean approach is used. Spatial boundary conditions are easier to implement through the superprocess formulation, with or without a scaling limit (see [18]). Here the nonpolynomial and derivative terms will be treated as operator labels at the branching points of the process.

The SOLEDGE2D equations are [19]

$$\begin{aligned} \partial_t N + \frac{1}{q}\partial_\theta \Gamma + \frac{\chi}{\eta} N &= D\partial_r^2 N \\ \partial_t \Gamma + \frac{1}{q}(1-\chi)\,\partial_\theta\left(\frac{\Gamma^2}{N} + N\right) + \frac{\chi}{\eta}(\Gamma - \Gamma_0) &= \nu\partial_r^2 \Gamma \end{aligned} \tag{5}$$

where Γ and N are the dimensionless parallel momentum and density, (r, θ) are the radial and poloidal coordinates and the mask function χ equals one in a region where an obstacle is located and zero elsewhere.

To construct a stochastic representation for the solution one needs to identify a stochastic process associated to the linear component (to the full linear component or part of it) and then, through an integral equation, construct the branching mechanism representing the nonlinear part.

2.1 The $\chi = 1$ Case

In the $\chi = 1$ case the system (5) is linear

$$\begin{aligned} \partial_t N + \frac{1}{q}\partial_\theta \Gamma + \frac{1}{\eta} N &= D\partial_r^2 N \\ \partial_t \Gamma + \frac{1}{\eta}(\Gamma - \Gamma_0) &= \nu\partial_r^2 \Gamma \end{aligned} \tag{6}$$

the solution being

$$\begin{aligned} \begin{pmatrix} N(t) \\ \Gamma(t) \end{pmatrix} = e^{t\left(-\frac{1}{q}C\partial_\theta + B\partial_r^2 - \frac{1}{\eta}\right)} \left\{ \begin{pmatrix} N(0) \\ \Gamma(0) \end{pmatrix} \right. \\ \left. + \int_0^t d\tau e^{-\tau\left(-\frac{1}{q}C\partial_\theta + B\partial_r^2 - \frac{1}{\eta}\right)} \begin{pmatrix} 0 \\ \frac{\Gamma_0}{\eta} \end{pmatrix} \right\} \end{aligned} \tag{7}$$

with B and C the matrices

$$B = \begin{pmatrix} D & 0 \\ 0 & \nu \end{pmatrix}; \qquad C = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

2.2 The $\chi = 0$ Case

The linear part of the system for $\chi = 0$ is:

$$\begin{aligned} \partial_t N + \frac{1}{q}\partial_\theta \Gamma &= D\partial_r^2 N \\ \partial_t \Gamma + \frac{1}{q}\partial_\theta N &= \nu \partial_r^2 \Gamma \end{aligned} \tag{8}$$

Given the initial conditions at time zero $\begin{pmatrix} N(0,r,\theta) \\ \Gamma(0,r,\theta) \end{pmatrix}$ the solution of this system is

$$\begin{pmatrix} N(t,r,\theta) \\ \Gamma(t,r,\theta) \end{pmatrix} = \exp t \left\{ -\frac{1}{q} A\partial_\theta + B\partial_r^2 \right\} \begin{pmatrix} N(0,r,\theta) \\ \Gamma(0,r,\theta) \end{pmatrix} \tag{9}$$

A being the matrix

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

However, for the construction of a stochastic solution to the nonlinear equation, through a probabilistic interpretation of the integral equation, it is convenient to have a stochastic process that operates in a simple way on the arguments of the functions. Therefore, instead of the full linear part, only the diffusion associated to the first term in (8) will be used. It also provides an easier handling of the ∂_θ derivative.

For the nonlinear equations one writes

$$\begin{aligned} N(t,r,\theta) &= e^{tD\partial_r^2} N(0,r,\theta) - \frac{1}{q}\int_0^t d\tau e^{\tau D\partial_r^2} \partial_\theta \Gamma(t-\tau,r,\theta) \\ \Gamma(t,r,\theta) &= e^{t\nu\partial_r^2} \Gamma(0,r,\theta) - \frac{1}{q}\int_0^t d\tau e^{\tau\nu\partial_r^2} \partial_\theta \left\{ \frac{\Gamma^2}{N} + N \right\} (t-\tau,r,\theta) \end{aligned} \tag{10}$$

Denote by $\xi_s^{(N)}$ and $\xi_s^{(\Gamma)}$ two Brownian motions in the $r-$coordinate with diffusion coefficients $\sqrt{2D}$ and $\sqrt{2\nu}$. Then the Eq. (10) may be reinterpreted as defining a

probabilistic processes for which the expectation values are the functions $N(t,r,\theta)$ and $\Gamma(t,r,\theta)$, that is

$$\begin{aligned} N(t,r,\theta) &= \mathbb{E}_{(t,r,\theta)}\left[p\frac{1}{p}N\left(0,\xi_t^{(N)},\theta\right)\right. \\ &\quad \left. -\frac{t}{q(1-p)}\int_0^t \frac{1-p}{t}d\tau\,\partial_\theta\Gamma\left(t-\tau,\xi_\tau^{(N)},\theta\right)\right] \\ \Gamma(t,r,\theta) &= \mathbb{E}_{(t,r,\theta)}\left[p\frac{1}{p}\Gamma\left(0,\xi_t^{(\Gamma)},\theta\right)\right. \\ &\quad \left. -\frac{2t}{q(1-p)}\int_0^t \frac{1-p}{t}d\tau\,\partial_\theta\left\{\frac{1}{2}\frac{\Gamma^2}{N}+\frac{1}{2}N\right\}\left(t-\tau,\xi_\tau^{(\Gamma)},\theta\right)\right] \end{aligned} \tag{11}$$

$\mathbb{E}_{(t,r,\theta)}$ denotes the expectation value of a backwards-in-time stochastic process started from (t,r,θ). The processes that construct the solution at the point (t,r,θ) are backwards-in-time processes that start from time t and propagate to time zero. With probability p the process reach time zero and the contribution to the expectation value is $\frac{1}{p}N\left(0,\xi_t^{(N)},\theta\right)$ (or $\frac{1}{p}\Gamma\left(0,\xi_t^{(\Gamma)},\theta\right)$). With probability $(1-p)$ the process is interrupted at a time τ chosen with uniform probability in the interval $(t,0)$. For the process associated to N, the process changes its nature, becomes a Γ process and picks up a factor $-\frac{t}{q(1-p)}$. For the case of the process Γ, with probability $\frac{1}{2}$, this process either changes to a N process or branches into a N and a Γ process. In both cases it picks up a factor $-\frac{2t}{q(1-p)}$.

Notice that the propagation process acts only on the $r-$coordinate. Therefore the derivative ∂_θ, the square in Γ^2 and the quotient in $\frac{\Gamma^2}{N}$ may all be treated as operators which are kept as labels at each branching point. When all the lines of the process reach time zero, the initial condition is sampled at the arrival r_0-coordinate. This initial condition is not simply a number but a function of θ ($\Gamma(0,r_0,\theta)$ or $N(0,r_0,\theta)$). It implies that both the initial condition and all its derivatives at the argument θ must be provided. This initial functions are then backtracked throughout the sample lines, the multiplicative factors are picked up at each τ interrupt and the operators applied whenever a labelled branching point is reached. This provides the contribution of each sample path to the expectation value. Figure 2 displays an example of a sample path, where the operators picked up along the way are denoted by flags.

Notice the order of the operators at each branching point. For example, at the leftmost $\delta-$labelled point the operation is

$$\partial_\theta\left\{\frac{\Gamma^2\left(0,r_0^{(1)},\theta\right)}{N\left(0,r_0^{(2)},\theta\right)}\right\}$$

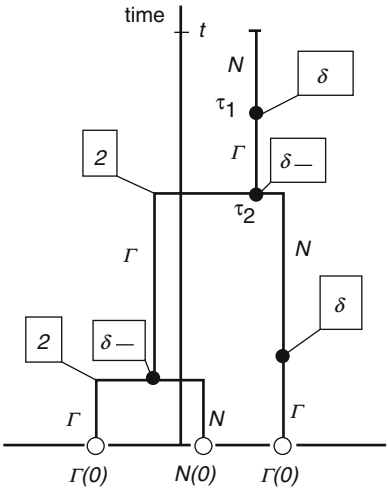

Fig. 2 A sample path of the $N-\Gamma$ stochastic process

and the whole contribution of this sample path to the $N-$expectation value is

$$\partial_\theta^2 \left\{ \left(\partial_\theta \left\{ \frac{\Gamma^2\left(0, r_0^{(1)}, \theta\right)}{N\left(0, r_0^{(2)}, \theta\right)} \right\} \right)^2 \left\{ \partial_\theta \Gamma\left(0, r_0^{(3)}, \theta\right) \right\}^{-1} \right\}$$

times the factor $\left(\frac{1}{p}\right)^3 \frac{4t\tau_1\tau_2^2}{q^4(1-p)^4}$.

The branching, being identical to a Galton-Watson process, has a finite number of branches almost surely. Therefore, with a uniform unit bound on the quantities at each branching vertex, one obtains almost sure convergence of the expectation value. In conclusion:

Proposition 2.1 *If the initial conditions* $\left|\frac{\Gamma^2}{N}, N, \Gamma\right|$ *and all its derivatives are bound by a constant M, the above described process provides a solution to the SOLEDGE2D equations up to time* $t \leq \frac{q}{M}$ *a.s.*

This bound, which is obtained by a worst case analysis, is in practice too severe because the probability of the generated trees is a fast decreasing function of the number of branches.

3 Superprocesses

A superprocess describes the evolution of a population, without a fixed number of units, that evolves according to the laws of chance. Given a countable dense subset Q of $[0, \infty)$ and a countable dense subset F of a separable metric space E, the

countable set

$$M_1 = \left\{ \sum_{i=1}^{n} \alpha_i \delta_{x_i} : x_1 \cdots x_n \in F; \alpha_1 \cdots \alpha_n \in Q; n \geq 1 \right\} \tag{12}$$

is dense on the space $M(E)$ of finite Borel measures on E (theorem 1.8 in [21]). This is at the basis of the interpretation of the limits of evolving particle systems as measure-valued superprocesses. On the other hand the representation of an evolving measure as a collection of measures with point support is also useful for the construction of solutions of nonlinear partial differential equations as scaling limits of measure-valued superprocesses.

However, as far as representations of solutions of nonlinear PDE's, superprocesses constructed in the space $M(E)$ of finite measures have serious limitations. The set of interaction terms that can be handled is limited (essentially to $u^{\alpha}(x)$ with $\alpha \leq 2$) and derivative interactions cannot be included as well. The first obvious generalization would be to construct superprocesses on distributions of point support, because any such distribution is a finite sum of deltas and their derivatives [22]. However, because in a general branching process the number of branches is not bounded, one really needs a framework that can handle arbitrary sums of deltas and their derivatives. This requirement leads naturally to the space of ultradistributions of compact support.

Ultradistributions may be characterized as Fourier transforms of distributions of exponential type [23]. However, the representation of ultradistributions by analytical functions is actually simpler and also more convenient for practical calculations. Let $\mathcal{S}$ be the Schwartz space of functions of rapid decrease and $\mathcal{U} \subset \mathcal{S}$ those functions in $\mathcal{S}$ that may be extended into the complex plane as entire functions of rapid decrease on strips. $\mathcal{U}'$, the dual of $\mathcal{U}$, is Silva's space of tempered ultradistributions [24, 25].

Let first $E = \mathbb{R}$. Define B_η as the complement in $\mathbb{C}$ of the strip $Im(z) \leq \eta$

$$B_\eta = \{z : Im(z) > \eta\} \tag{13}$$

and H_η the set of functions which are holomorphic and of polynomial growth in B_η

$$\varphi(z) \in H_\eta \Longrightarrow \exists M, \alpha : |\varphi(z)| < M|z|^{\alpha}, \forall z \in B_\eta \tag{14}$$

Let H_ω be the union of all such spaces

$$H_\omega = \underset{\eta \geq 0}{\cup} H_\eta \tag{15}$$

and in H_ω define the equivalence relation Π by

$$\varphi \overset{\Pi}{\simeq} \psi \text{ if } \varphi - \psi \text{ is a polynomial}$$

Then, the space of tempered ultradistribution is

$$\mathcal{U}' = H_\omega / \Pi \tag{16}$$

The relation to ultradistributions as entities $f(x)$ in $\mathbb{R}$ is obtained by the generalized Stieltjes transform

$$\varphi(z) = \frac{p(z)}{2\pi i} \int \frac{f(x)}{p(x)(x-z)} dx + P(z) \tag{17}$$

$p(z)$ being a polynomial such that $f/p \sim O\left(t^{-1}\right)$ and $P(z)$ an arbitrary polynomial. In this sense one may say that $[\varphi] \in H_\omega / \Pi$ is the Stieltjes image of the ultradistribution f. Operations with $f(x)$ are performed using their analytical images. For example f is integrable in $\mathbb{R}$ if there is an y_0 and a $\varphi(z)$ in the Stieltjes image such that $\varphi(x + iy_0) - \varphi(x - iy_0)$ is integrable in $\mathbb{R}$ in the sense of distributions.

An ultradistribution vanishes in an open set $A \in \mathbb{R}$ if $\varphi(x + iy) - \varphi(x - iy) \to 0$ for $x \in A$ when $y \to 0$ or, equivalently, if there an analytical extension of φ to the vertical strip $Rez \in A$. The support of f is the complement in $\mathbb{R}$ of the largest open set where f vanishes.

All these notions are easily generalized to $\mathbb{R}^n$ [25] by considering products of semiplanes as in (13) and the corresponding polynomial bounds. For the equivalence relation Π one uses pseudopolynomials, that is, functions of the form

$$\sum_{j,k} \rho\left(z_1, \cdots, \hat{z_j}, \cdots, z_n\right) z_j^k$$

$\hat{z_j}$ meaning that this variable is absent from the arguments of ρ.

An ultradistribution f in $\mathbb{R}^n$ has compact support if there is a disk D such that any φ in the Stieltjes image has an analytic extension to $(\mathbb{C}/D)^n$.

For our purposes, the most important property of ultradistributions of compact support is the fact that any such ultradistribution has a representation as a series of multipoles

$$f(x) = \sum_{r_1=0}^{\infty} \cdots \sum_{r_n=0}^{\infty} p_{r_1,\cdots,r_n} \delta^{(r_1,\cdots,r_n)}(x-a)$$

a being a point in the support of f. This result follows from the fact that for compact support one may apply to the Stieltjes image the Cauchy theorem over a closed contour. The space of tempered ultradistributions of compact support will be denoted as $\mathcal{U}_0'$.

Let the underlying space E be $\mathbb{R}^n$. Denote by $(X_t, P_{0,\nu})$ a branching stochastic process with values in $\mathcal{U}_0'$ and transition probability $P_{0,\nu}$ starting from time 0 and $\nu \in \mathcal{U}_0'$. The process is assumed to satisfy the *branching property,* that is, given $\nu = \nu_1 + \nu_2$

$$P_{0,\nu} = P_{0,\nu_1} * P_{0,\nu_2} \tag{18}$$

After the branching $\left(X_t^1, P_{0,\nu_1}\right)$ and $\left(X_t^2, P_{0,\nu_2}\right)$ are independent and $X_t^1 + X_t^2$ has the same law as $(X_t, P_{0,\nu})$. In terms of the *transition operator* V_t operating on functions on $\mathcal{U}$ this would be

$$\langle V_t f, \nu_1 + \nu_2 \rangle = \langle V_t f, \nu_1 \rangle + \langle V_t f, \nu_2 \rangle \tag{19}$$

with V_t defined by $e^{-\langle V_t f, \nu \rangle} \triangleq P_{0,\nu} e^{-\langle f, X_t \rangle}$ or

$$\langle V_t f, \nu \rangle = -\log P_{0,\nu} e^{-\langle f, X_t \rangle} \tag{20}$$

$f \in \mathcal{U}, \nu \in \mathcal{U}_0'$.

Underlying the usual construction of superprocesses, in the form that is useful for the representation of solutions of PDE's, there is a stochastic process with paths that start from a particular point in E, then propagate and branch, but the paths preserve the same nature after the branching. In terms of measures it means that one starts from an initial δ_x which at the branching point originates other $\delta' s$ with at most some scaling factors. It is to preserve this pointwise interpretation that, in this larger setting, one considers ultradistributions in $\mathcal{U}_0'$, because, as seen above, any ultradistribution in $\mathcal{U}_0'$ may be represented as a multipole expansion at any point of its support. Therefore an arbitrary transition in the process X_t in $\mathcal{U}_0'$ may be associated to a branching of paths in E and along these new paths new distributions with point support will propagate. As a result the construction now proceeds as in the measure-valued case.

In $M = [0, \infty) \times E$ consider a set $Q \subset M$ and the associated exit process $\xi = (\xi_t, \Pi_{0,x})$ with parameter k defining the lifetime. The process starts from $x \in E$ carrying along an ultradistribution in $\mathcal{U}_0'$ with support on the path. At each branching point of the ξ_t-process there is a transition ruled by the P probability in $\mathcal{U}_0'$ leading to one or more elements in $\mathcal{U}_0'$. These $\mathcal{U}_0'$ elements are then carried along by the new paths of the ξ_t-process. The whole process stops at the boundary ∂Q, finally defining an exit process $\left(X_Q, P_{0,\nu}\right)$ on $\mathcal{U}_0'$. If the initial ν is δ_x one writes

$$u(x) = \langle V_Q f, \nu \rangle = -\log P_{0,x} e^{-\langle f, X_Q \rangle} \tag{21}$$

$\langle f, X_Q \rangle$ being computed on the (space-time) boundary with the exit ultradistribution generated by the process.

The connection with nonlinear PDE's is established by defining the whole process to be a $(\xi, \psi)-$*superprocess* if $u(x)$ satisfies the equation

$$u + G_Q \psi(u) = K_Q f \tag{22}$$

where G_Q is the Green operator,

$$G_Q f(r, x) = \Pi_{0,x} \int_0^\tau f(s, \xi_s)\, ds \tag{23}$$

and K_Q the Poisson operator

$$K_Q f(x) = \Pi_{0,x} 1_{\tau<\infty} f(\xi_\tau) \tag{24}$$

$\psi(u)$ means $\psi(0,x;u(0,x))$ and τ is the first exit time from Q.

The superprocess is constructed as follows: Let $\varphi(s,x;z)$ be the branching function at time s and point x. Then for $e^{-w(0,x)} \triangleq P_{0,x} e^{-\langle f, X_Q\rangle}$ one has

$$P_{0,x} e^{-\langle f, X_Q\rangle} \triangleq e^{-w(0,x)} = \Pi_{0,x}\left[e^{-k\tau} e^{-f(\tau,\xi_\tau)} + \int_0^\tau dske^{-ks}\varphi\left(s,\xi_s; e^{-w(\tau-s,\xi_s)}\right)\right] \tag{25}$$

τ is the first exit time from Q and $f(\tau,\xi_\tau) = \langle f, X_Q\rangle$ is computed with the exit boundary ultradistribution. For measure-valued superprocesses the branching function would be

$$\varphi(s,y;z) = c\sum_0^\infty p_n(s,y) z^n \tag{26}$$

with $\sum_n p_n = 1$ and c the branching intensity, but now it may be a more general function.

For the interpretation of the superprocesses as generating solutions of PDE's, an essential role is played by a transformation of Eq. (25) that uses $\int_0^\tau ke^{-ks}ds = 1 - e^{-k\tau}$ and the Markov property $\Pi_{0,x} 1_{s<\tau} \Pi_{s,\xi_s} = \Pi_{0,x} 1_{s<\tau}$. This is lemma 1.2 in ch. 4 of Ref. [16]. Because it only depends on the Markov properties of the $(\xi_t, \Pi_{0,x})$ process it also holds in this more general context. A proof is included in the Appendix with the notations used in this paper.

Using the lemma, Eq. (25) for $e^{-w(0,x)}$ is converted into

$$e^{-w(0,x)} = \Pi_{0,x}\left[e^{-f(\tau,\xi_\tau)} + k\int_0^\tau ds\left[\varphi\left(s,\xi_s; e^{-w(\tau-s,\xi_s)}\right) - e^{-w(\tau-s,\xi_s)}\right]\right] \tag{27}$$

Eq. (22) is now obtained by a limiting process. Let in (27) replace $w(0,x)$ by $\beta w_\beta(0,x)$ and f by βf. β is interpreted as the mass of the particles and when the $\mathcal{U}_0'$-valued process $X_Q \to \beta X_Q$ then $P_\mu \to P_{\frac{\mu}{\beta}}$.

$$e^{-\beta w(0,x)} = \Pi_{0,x}\left[e^{-\beta f(\tau,\xi_\tau)} + k_\beta \int_0^\tau ds\left[\varphi_\beta\left(s,\xi_s; e^{-\beta w(\tau-s,\xi_s)}\right) - e^{-\beta w(\tau-s,\xi_s)}\right]\right] \tag{28}$$

Two scaling limits will be used in this paper. The first one, which is the one used in the past for superprocesses on measures, defines

$$u_\beta^{(1)} = \left(1 - e^{-\beta w_\beta}\right)/\beta \quad ; \quad f_\beta^{(1)} = \left(1 - e^{-\beta f}\right)/\beta \tag{29}$$

and

$$\psi_\beta^{(1)}\left(0, x; u_\beta^{(1)}\right) = \frac{k_\beta}{\beta}\left(\varphi\left(0, x; 1 - \beta u_\beta^{(1)}\right) - 1 + \beta u_\beta^{(1)}\right) \tag{30}$$

one obtains from (28)

$$u_\beta^{(1)}(0, x) + \Pi_{0,x}\int_0^\tau ds \psi_\beta^{(1)}\left(s, \xi_s; u_\beta^{(1)}\right) = \Pi_{0,x} f_\beta^{(1)}(\tau, \xi_\tau) \tag{31}$$

that is

$$u_\beta^{(1)} + G_Q \psi_\beta^{(1)}\left(u_\beta^{(1)}\right) = K_Q f_\beta^{(1)} \tag{32}$$

When $\beta \to 0, f_\beta^{(1)} \to f$ and if ψ_β goes to a well defined limit ψ then u_β tends to a limit u solution of (22) associated to a superprocess. Also one sees from (29) that in the $\beta \to 0$ limit

$$u_\beta^{(1)} \to w_\beta = -\log P_{0,x} e^{-\langle f, X_Q\rangle} \tag{33}$$

as in Eq. (21). The superprocess corresponds to a cloud of ultradistribution "particles" for which both the mass and the lifetime tend to zero.

3.1 Measure-Valued Superprocesses and Nonlinear PDE's

Here one restricts oneself to measure-valued superprocesses, that is, in terms of paths, to $\delta' s$ propagating along the paths of the $(\xi_t, \Pi_{0,x})$ process and simply branching to new δ measures at each branching point. Let us construct a superprocess providing a solution to the equation

$$\frac{\partial u}{\partial t} = \frac{1}{2}\frac{\partial^2 u}{\partial x^2} - u^\alpha \tag{34}$$

for $1 < \alpha \leq 2$. Comparing with (22) one should have

$$\psi(0, x; u) = u^\alpha$$

Then from (30) and (26), with $z = 1 - \beta u_\beta^{(1)}$ one has

$$\begin{aligned}\varphi(0,x;z) &= \sum_n p_n z^n = z + \frac{\beta}{k_\beta} u_\beta^{(1)\alpha} = z + \frac{\beta}{k_\beta}\frac{(1-z)^\alpha}{\beta^\alpha} \\ &= z + \frac{1}{k_\beta \beta^{\alpha-1}}\left(1 - \alpha z + \frac{\alpha(\alpha-1)}{2} z^2\right. \\ &\quad \left. - \frac{\alpha(\alpha-1)(\alpha-2)}{3!} z^3 + \cdots\right)\end{aligned} \tag{35}$$

Choosing $k_\beta = \frac{\alpha}{\beta^{\alpha-1}}$ the terms in z cancel and for $1 < \alpha \leq 2$ the coefficients of all the remaining z powers are positive and may be interpreted as branching probabilities. It would not be so for $\alpha > 2$. Then

$$p_0 = \frac{1}{\alpha}; \quad p_1 = 0; \quad \cdots \quad p_n = \frac{(-1)^n}{\alpha}\binom{\alpha}{n} \quad n \geq 2 \tag{36}$$

with $\sum_n p_n = 1$. With this choice of probabilities p_n for branching into new δ measures and with $k_\beta = \frac{\alpha}{\beta^{\alpha-1}}$ and $\beta \to 0$ one obtains a superprocess which, through (21), provides a solution to the Eq. (34). $\alpha = 2$ is an upper bound for this representation, because for $\alpha > 2$ some of the $p_n's$ would be negative and would not be interpretable as branching probabilities.

For the particular case

$$\frac{\partial u}{\partial t} = \frac{1}{2}\frac{\partial^2 u}{\partial x^2} - u^2 \tag{37}$$

$$p_1 = 0; \quad p_0 = p_2 = \frac{1}{2}; \quad k_\beta = \frac{2}{\beta} \tag{38}$$

When $\beta \to 0$, the solutions are given by (21) and the superprocesses correspond to the scaling limit of processes where both the mass and the lifetime of the particles tend to zero and at each bifurcation point one has probability p_0 of dying without offspring or creating n new δ measures with probabilities p_n.

Superprocesses are usually associated with nonlinear PDE's in the scaling limit $\beta \to 0$ of (30) and (31). However other limits may also be useful. For example with $p_n = \delta_{n,2}$, $\beta = 1$ and $k_\beta = 1$ one obtains

$$\begin{aligned}\psi_\beta^{(1)}\left(0,x;u_\beta^{(1)}\right) &= \frac{k_\beta}{\beta}\left(\varphi\left(0,x;1-\beta u_\beta^{(1)}\right) - 1 + \beta u_\beta^{(1)}\right) \\ &= \frac{k_\beta}{\beta}\left(\sum p_n\left(1-\beta u_\beta^{(1)}\right)^n - 1 + \beta u_\beta^{(1)}\right)\end{aligned}$$

$$= \frac{k_\beta}{\beta}\left(\beta^2 u_\beta^{(1)2} - \beta u_\beta^{(1)}\right)$$
$$\to u^2 - u \tag{39}$$

Therefore, in this case, one is led to the KPP equation

$$\frac{\partial u}{\partial t} = \frac{1}{2}\frac{\partial^2 u}{\partial x^2} - u^2 + u \tag{40}$$

However in this case, because $\beta = 1$ instead of $\beta \to 0$, the solution is given by $(1 - e^{-w})$ instead of (21). Because of the natural stochastic clock provided by the linear u term, a stochastic solution for the Cauchy problem of the KPP equation may be constructed by the McKean method [1], as seen before. However, the interpretation as an exit measure, allows for the construction of solutions with arbitrary boundary conditions.

3.2 Superprocesses on Signed Measures and Ultradistributions

When superprocesses are generalized from measures to ultradistributions of compact support, a general aim would be, of course, to characterize all the admissible transition kernels and branching mechanisms compatible with the new formulation. I will leave this for future work and just present a few examples of transitions and branchings which provide stochastic representations for a wider class of nonlinear PDE's.

Although the scaling limit $\beta \to 0$ of measure-valued superprocesses allows the construction of solutions for equations which do not possess a natural Poisson clock, it has the severe limitation of requiring a polynomial branching function $\varphi(s, x; z)$. This automatically restricts the nonlinear terms in the PDE's to be powers of u. In addition, these terms must be such that all coefficients in the z^n expansion in Eq. (26) are positive to be interpretable as branching probabilities. As seen before, it was this requirement that led to the restriction $1 < \alpha \leq 2$ in (34).

The variable z that appears in $\varphi_\beta(s, x; z)$ is in fact $z = e^{-\beta w(\tau - s, \xi_s)} = P_{0,x} e^{-\langle \beta f, X\rangle}$. When restricting the superprocess to measures, the delta measure, at each branching point, may at most branch into other deltas (with positive coefficients) and therefore $\varphi(s, x; z)$ must be a sum of monomials in z. When one generalizes to $\mathcal{U}_0'$ ultradistributions of compact support, changes of sign and transitions from deltas to their derivatives are allowed. In the end, the exponential $e^{-\langle \beta f, X\rangle}$ will be computed by evaluation of the function on the ultradistribution that reaches the boundary. To find out the equation that is represented by the process one needs to compute the $\psi_\beta\left(0, x; u_\beta\right)$ of Eq. (30) for the corresponding $\varphi(s, x; z)$ in the $\beta \to 0$ limit. Recalling that $\varphi(s, x; z) = \varphi_\beta\left(s, \xi_s; e^{-\beta w(\tau - s, \xi_s)}\right)$ and $z = e^{-\beta w_\beta}$, one concludes that

there are basically two new transitions at the branching points:

(1) A change of sign in the point support ultradistribution

$$e^{\langle \beta f, \delta_x \rangle} = e^{\beta f(x)} \to e^{\langle \beta f, -\delta_x \rangle} = e^{-\beta f(x)} \tag{41}$$

which corresponds to

$$z \to \frac{1}{z} \tag{42}$$

and

(2) A change from $\delta^{(n)}$ to $\pm\delta^{(n+1)}$, for example

$$e^{\langle \beta f, \delta_x \rangle} = e^{\beta f(x)} \to e^{\langle \beta f, \pm \delta'_x \rangle} = e^{\mp \beta f'(x)} \tag{43}$$

which corresponds to

$$z \to e^{\mp \partial_x \log z} \tag{44}$$

Case (1) corresponds to an extension of superprocesses on measures to superprocesses on signed measures and the second to superprocesses in $\mathcal{U}'_0$.

How these transformations provide stochastic representations of solutions for other classes of PDE's, will be illustrated by two examples:

First, let

$$\varphi^{(1)}(0, x; z) = p_1 e^{\partial_x \log z} + p_2 e^{-\partial_x \log z} + p_3 z^2 \tag{45}$$

This branching function means that at the branching point, with probability p_1 a derivative is added to the propagating ultradistribution, with probability p_2 a derivative is added plus a change of sign and with probability p_3 the ultradistribution branches into two identical ones. Using the transformation and scaling limit (29) one has, for small β

$$\begin{aligned} z \to e^{\mp \partial_x \log z} &= e^{\mp \partial_x \log\left(1 - \beta u_\beta^{(1)}\right)} \\ &= 1 \pm \beta \partial_x u_\beta^{(1)} + \frac{\beta^2}{2} \left\{ \left(\partial_x u_\beta^{(1)} \right)^2 \pm \partial_x u_\beta^{(1)2} \right\} + O\left(\beta^3\right) \end{aligned} \tag{46}$$

$$z \to z^2 = \left(1 - \beta u_\beta^{(1)}\right)^2 = 1 - 2\beta u_\beta^{(1)} + \beta^2 u_\beta^{(1)2} \tag{47}$$

Then, computing $\psi_\beta\left(0,x;u_\beta^{(1)}\right)$ with $p_1=p_2=\frac{1}{4}$ and $p_3=\frac{1}{2}$ one obtains

$$\begin{aligned}\psi_\beta^{(1)}\left(0,x;u_\beta^{(1)}\right) &= \frac{k_\beta}{\beta}\left(\varphi^{(1)}(0,x;z)-z\right)\\ &= \frac{k_\beta}{\beta}\left(\varphi^{(1)}\left(0,x;1-\beta u_\beta^{(1)}\right)-1+\beta u_\beta^{(1)}\right)\\ &= \frac{k_\beta}{\beta}\left(\frac{1}{8}\beta^2\left(\partial_x u_\beta^{(1)}\right)^2+\frac{1}{2}\beta^2 u_\beta^{(1)2}+O\left(\beta^3\right)\right)\end{aligned} \tag{48}$$

meaning that, with $k_\beta=\frac{4}{\beta}$, the superprocess provides, in the $\beta\to 0$ limit, a solution to the equation

$$\frac{\partial u}{\partial t}=\frac{1}{2}\frac{\partial^2 u}{\partial x^2}-2u^2-\frac{1}{2}\left(\partial_x u\right)^2 \tag{49}$$

For the second example a different scaling limit will be used, namely

$$u_\beta^{(2)}=\frac{1}{2\beta}\left(e^{\beta w_\beta}-e^{-\beta w_\beta}\right)\quad;\quad f_\beta^{(2)}=\frac{1}{2\beta}\left(e^{\beta f}-e^{-\beta f}\right) \tag{50}$$

Notice that, as before, $u_\beta^{(2)}\to w_\beta$ and $f_\beta^{(2)}\to f$ when $\beta\to 0$. In this case with $z=e^{\beta w_\beta}$ one has

$$\begin{aligned}z &= -2\beta u_\beta^{(2)}+2\sqrt{\beta^2 u_\beta^{(2)2}+1}\\ &= 2-2\beta u_\beta^{(2)}+\beta^2 u_\beta^{(2)2}+O\left(\beta^4\right)\end{aligned} \tag{51}$$

and

$$\begin{aligned}\frac{1}{z} &= 2\beta u_\beta^{(2)}+2\sqrt{\beta^2 u_\beta^{(2)2}+1}\\ &= 2+2\beta u_\beta^{(2)}+\beta^2 u_\beta^{(2)2}+O\left(\beta^4\right)\end{aligned} \tag{52}$$

For the integral equation, instead of (31), one has

$$u_\beta^{(2)}(0,x)+\Pi_{0,x}\int_0^\tau ds\psi_\beta^{(2)}\left(s,\xi_s;u_\beta^{(2)}\right)=\Pi_{0,x}f_\beta^{(2)}(\tau,\xi_\tau) \tag{53}$$

with

$$\psi_\beta^{(2)}\left(0,x;u_\beta^{(2)}\right)=k_\beta\left(\frac{1}{2\beta}\left(\varphi(0,x;z)-\varphi\left(0,x;\frac{1}{z}\right)\right)-u_\beta^{(2)}\right) \tag{54}$$

Let now

$$\varphi^{(2)}(0,x;z) = p_1 z^2 + p_2 \frac{1}{z} \tag{55}$$

This branching function means that with probability p_1 the ultradistribution branches into two identical ones and with probability p_2 it changes its sign. Therefore, in this case, one is simply extending the superprocess construction to signed measures. Using (51) and (52) one computes $\psi_\beta^{(2)}\left(0,x;u_\beta^{(2)}\right)$ obtaining

$$\psi_\beta^{(2)}\left(0,x;u_\beta^{(2)}\right) = k_\beta\left\{-p_1 8u_\beta^{(2)}\left(1+\frac{1}{2}\beta^2 u_\beta^{(2)2}\right) + p_2 u_\beta^{(2)} - u_\beta^{(2)} + O\left(\beta^4\right)\right\} \tag{56}$$

and with $p_1 = \frac{1}{10}; p_2 = \frac{9}{10}$ and $k_\beta = \frac{5}{2\beta^2}$ one obtains in the in the $\beta \to 0$ limit

$$\psi_\beta^{(2)}\left(0,x;u_\beta^{(2)}\right) \to -u_\beta^{(2)3} \tag{57}$$

meaning that this superprocess provides a solution to the equation

$$\frac{\partial u}{\partial t} = \frac{1}{2}\frac{\partial^2 u}{\partial x^2} + u^3 \tag{58}$$

In conclusion: Extending the superprocess construction to signed measures and ultradistributions, stochastic solutions are obtained for a much larger class of partial differential equations.

4 Final Remarks

Stochastic solutions are powerful tools both to construct new exact solutions of nonlinear PDE's and to develop faster numerical algorithms for parallel computing. Two related methods are used to construct the stochastic solutions. Both use limiting processes, as in branching particle systems, to generate boundary measures which sample the initial (boundary) conditions. The limitations in the classical constructions, are the handling of derivatives, nonpolynomial terms and negative branching coefficients which cannot be interpreted as probabilities. To overcome these limitations one used either operator labels at the branching vertices or an extension of superprocesses from measures to ultradistributions. In reality these methods are closely related. In the first one keeps the propagating entities as delta measures but then has to backtrack the initial conditions from the final boundary time to apply the operators at each vertex. In the second the propagating entities are modified at each vertex, the final generated entity being directly applied to the initial conditions without any backtracking.

Notice however that there are cases where backtracking of the initial conditions through the tree is needed even in case without derivatives or nonpolynomial terms. This is, for example, the case of Navier-Stokes or magnetohydrodynamics [11], because of the Leray product at each vertex.

The simple superprocess examples treated here deal with the kind of terms that will appear in PDE's with local interactions. More general nonlocal interactions or integral equations would require a more general treatment of the ultradistribution superprocesses, where the allowed transitions are not simply changes of sign and derivatives.

Appendix: Proof of a Lemma

Let

$$u(x,t) = \Pi_{0,x}\left\{e^{-kt}u(\xi_t,0) + \int_0^t ke^{-ks}\Phi(\xi_s,t-s)\,ds\right\} \tag{59}$$

Then

$$\Pi_{0,x}\int_0^t ku(\xi_s,t-s)\,ds = \Pi_{0,x}\left\{\int_0^t ke^{-k(t-s)}u(\xi_{s+t-s},0)\,ds + \int_0^t kds\int_0^{t-s} kds'e^{-ks'}\Phi\left(\xi_{s+s'},t-s-s'\right)\right\} \tag{60}$$

Summing (59) and (60)

$$\begin{aligned} &u(x,t) + \Pi_{0,x}\int_0^t ku(\xi_s,t-s)\,ds \\ &= \Pi_{0,x}\left\{\left(e^{-kt} + \int_0^t ke^{-k(t-s)}ds\right)u(\xi_t,0)\right. \\ &\quad +k\int_0^t e^{-ks}\Phi(\xi_s,t-s)\,ds \\ &\quad \left.+k\int_0^t ds\int_0^{t-s} kds'e^{-ks'}\Phi\left(\xi_{s+s'},t-s-s'\right)ds'\right\} \end{aligned} \tag{61}$$

Changing variables in the last integral in (61) from (s, s') to $(s, \sigma = s + s')$ one obtains for the last term

$$k \int_0^t d\sigma \int_0^\sigma k ds e^{-k(\sigma - s)} \Phi(\xi_\sigma, t - \sigma)\, ds$$

and finally

$$\begin{aligned} & u(x,t) + \Pi_{0,x} k \int_0^t u(\xi_s, t-s)\, ds \\ &= \Pi_{0,x} \left\{ u(\xi_t, 0) + k \int_0^t \Phi(\xi_s, t-s)\, ds \right\} \end{aligned} \tag{62}$$

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Maximum Likelihood Drift Estimation for the Mixing of Two Fractional Brownian Motions

Yuliya Mishura

Abstract We construct the maximum likelihood estimator (MLE) of the unknown drift parameter $\theta \in \mathbb{R}$ in the linear model

$$X_t = \theta t + \sigma_1 B^{H_1}(t) + \sigma_2 B^{H_2}(t),\ t \in [0, T],$$

where B^{H_1} and B^{H_2} are two independent fractional Brownian motions with Hurst indices $\frac{1}{2} \le H_1 < H_2 < 1$. The formula for MLE is based on the solution of the integral equation with weak polar kernel.

Keywords Independent fractional Brownian motions • Linear model • Unknown drift parameter • Maximum likelihood estimator

1 Introduction: The Elements of Stochastic Calculus for fBm

Consider the continuous-time linear model

$$X(t) = \theta t + \sigma_1 B^{H_1}(t) + \sigma_2 B^{H_2}(t),\ t \in [0, T],$$

where B^{H_1} and B^{H_2} are two independent fractional Brownian motions with Hurst indices $\frac{1}{2} \le H_1 < H_2 < 1$, $\sigma_1, \sigma_2 > 0$.

An adapted stochastic process $\{B^H(t), t \ge 0\}$ is the fractional Brownian motion with Hurst parameter $H \in (1/2, 1)$, if it is a centered Gaussian process with the covariance function

$$\mathsf{E}\left[B^H(t)B^H(s)\right] = \frac{1}{2}\left(t^{2H} + s^{2H} - |t-s|^{2H}\right).$$

Y. Mishura (✉)
Taras Shevchenko National University of Kyiv, Volodymyrska 64, 01601, Kyiv, Ukraine
e-mail: yumishura@gmail.com

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Denote by $L_H^2[0,T]$ the completion of the space of simple functions $f\colon [0,T]\to\mathbb{R}$ with respect to the scalar product

$$\langle f,g\rangle_H^2 := \alpha_H \int_0^T \int_0^T f(t)g(s)\,|t-s|^{2H-2}\,dsdt,$$

where $\alpha_H = H(2H-1)$. For a step function of the form

$$f(t) = \sum_{k=0}^{n-1} a_k \mathbf{1}_{[t_k,t_{k+1})},$$

where $\{t_0 < t_1 < \cdots < t_n\}$ is a partition of $[0,T]$, the integral $I^H(f)$ of f with respect to B^H is defined by

$$I^H(f) = \int_0^T f(t)dB^H(t) = \sum_{k=0}^{n-1} a_k \left(B^H(t_{k+1}) - B^H(t_k)\right).$$

I^H maps isomorphically the space of step functions on $[0,T]$ with the scalar product $\langle\cdot,\cdot\rangle_H$ into $L^2(\Omega)$, therefore, I^H can be extended to $L_H^2[0,T]$.

Define a square integrable kernel

$$K_H(t,s) = \begin{cases} \beta_H s^{1/2-H}\int_s^t (u-s)^{H-3/2}u^{H-1/2}du, & \text{if } t>s \\ 0, & \text{otherwise,}\end{cases}$$

where $\beta_H = \left(\frac{\alpha_H}{\mathrm{B}(H-1/2,2-2H)}\right)^{\frac{1}{2}}$.

The map

$$(K_H^* f)(s) = \int_s^T f(t)\partial_t K(t,s)dt = \beta_H s^{1/2-H}\int_s^T f(t)t^{H-1/2}(t-s)^{H-3/2}dt$$

is an isometry between the space of step functions and can be extended to a Hilbert space isomorphism between $L_H^2[0,T]$ and $L^2[0,T]$. This implies that the process

$$W(t) = I^H\left((K_H^*)^{-1}\mathbf{1}_{[0,t]}\right)$$

is a standard Wiener process on $[0,T]$, moreover, for any $f\in L_H^2[0,T]$,

$$I^H(f) = \int_0^T (K_H^* f)(s)dW(s). \tag{1}$$

In particular, putting in the last formula $f = \mathbf{1}_{[0,t]}$, one gets the following well-known representation of B^H:

$$B^H(t) = \int_0^t K_H(t,s)dW(s).$$

For these transformations, see [7].

Finally, we define the so-called fundamental martingale, or Molchan martingale M^H, for B^H. Let

$$l_H(t,s) = c_H s^{1/2-H}(t-s)^{1/2-H}\mathbf{1}_{(0,t)}(s),$$

where

$$c_H = \Big(\frac{\Gamma(3-2H)}{2H\Gamma(\frac{3}{2}-H)^3\Gamma(H+\frac{1}{2})}\Big)^{\frac{1}{2}}.$$

Consider square-integrable Gaussian martingale

$$M^H(t) = \int_0^t l_H(t,s)dB^H(s) = (2-2H)^{\frac{1}{2}}\int_0^t s^{1/2-H}dW(s).$$

The paper is organized as follows. In Sect. 2 we reduce the main problem to the solution of the integral equation with the weak polar kernel and establish the existence-uniqueness result for this equation. Appendix contains an auxiliary result concerning the existence and uniqueness of the solution of the corresponding integral equation of the 1st kind. We prove this fact directly, by constructing the unique solution.

Note that the elements of stochastic analysis of fBm are contained in [2, 5, 10], and the problems of statistical drift parameter estimation are treated, among others, in [1, 3, 4, 6, 11].

2 Main Problem

Now, let $\frac{1}{2} \le H_1 < H_2 < 1$, $\{\widetilde{B}^{H_1}(t), B^{H_2}(t),\ t \ge 0\}$, $i = 1,2$, be two processes defined on the space $(\Omega, \mathfrak{F}, (\mathfrak{F})_t)$ and P_θ be a probability measure under which $\widetilde{B}^{H_1}$ and B^{H_2} are independent, B^{H_2} is a fractional Brownian motion with Hurst parameter H_2, and $\widetilde{B}^{H_1}$ is a fractional Brownian motion with Hurst parameter H_1 and with drift $\frac{\theta}{\sigma_1}$, i.e.,

$$\sigma_1\widetilde{B}^{H_1}(t) = \theta t + \sigma_1 B^{H_1}(t).$$

The probability measure P_0 corresponds to the case when $\theta = 0$. Our main problem is the construction of maximum likelihood estimator for $\theta \in \mathbb{R}$ by the observations of the process $Z(t) = \theta t + \sigma_1 B^{H_1}(t) + \sigma_2 B^{H_2}(t),\ t \in [0,T]$. However, the form of the process Z (two fBm's with different Hurst indices) does not allow to construct the estimator immediately. To simplify the construction, we apply to Z

the linear transformation of the following form:

$$Y(t) = \int_0^t l_{H_1}(t,s)dZ(s) = \theta \int_0^t l_{H_1}(t,s)ds + \sigma_1 M^{H_1}(t) + \sigma_2 \int_0^t l_{H_1}(t,s)dB^{H_2}(s)$$
$$= \theta c_{H_1} B\Big(\frac{3}{2} - H_1, \frac{3}{2} - H_1\Big)t^{2-2H_1} + \sigma_1 M^{H_1}(t) + \sigma_2 \int_0^t l_{H_1}(t,s)dB^{H_2}(s). \tag{2}$$

This process is preferable since it involves Gaussian martingale M^H.

Lemma 2.1 *The linear transformation* (2) *is correctly defined.*

Proof It is sufficient to establish the existence of the integral $\int_0^t l_{H_1}(t,s)dB^{H_2}(s)$ for any $t \in [0,T]$. But we have that for any $u, s \in [0,t]$

$$|u-s|^{2H_2-2} \le t^{2H_2-2H_1}|u-s|^{2H_1-2},$$

therefore

$$||l_{H_1}(t,\cdot)||^2_{H_2} := \alpha_{H_2} \int_0^t \int_0^t l_{H_1}(t,s)l_{H_1}(t,u)\,|u-s|^{2H_2-2}\,dsdu$$
$$\le \alpha_{H_2} t^{2H_2-2H_1} \int_0^t \int_0^t l_{H_1}(t,s)l_{H_1}(t,u)\,|u-s|^{2H_1-2}\,dsdu$$
$$= \alpha_{H_2} t^{2H_2-2H_1} ||l_{H_1}(t,\cdot)||^2_{H_1} = \alpha_{H_2} t^{2H_2-2H_1} E|M^{H_1}(t)|^2$$
$$= \frac{\alpha_{H_2}\gamma^2_{H_1}}{2-2H_1} t^{2H_2-4H_1+2} < \infty,$$

whence the proof follows. □

As it was mentioned, process Y is more convenient to deal with since it involves martingale with a drift. Furthermore, it follows from the next result that processes Z and Y are observed simultaneously, so, we can reduce the original problem to the equivalent problem of the construction of maximum likelihood estimator of $\theta \in \mathbb{R}$ basing on the linear transformation Y.

Lemma 2.2 *Processes Z and Y are observed simultaneously.*

Proof Taking into account (2), it is enough to present Z via Y. But it follows from (2), from Fubini theorem for integrals w.r.t fBm (Theorem 2.6.5 [8]), and from elementary integral transformations, that for any $t \in [0,T]$

$$\int_0^t (t-s)^{H_1-\frac{3}{2}} \int_0^s l_{H_1}(s,u)dZ(u)ds = \int_0^t u^{\frac{1}{2}-H_1} \int_u^t (t-s)^{H_1-\frac{3}{2}}(s-u)^{\frac{1}{2}-H_1}dsdZ(u)$$
$$= B\Big(H_1 - \frac{1}{2}, \frac{3}{2} - H_1\Big) \int_0^t u^{\frac{1}{2}-H_1}dZ(u) = \int_0^t (t-s)^{H_1-\frac{3}{2}}Y(s)ds$$
$$= \Big(H_1 - \frac{1}{2}\Big)^{-1} \int_0^t (t-s)^{H_1-\frac{1}{2}}dY(s),$$

whence

$$Z(t) = B\Big(H_1 - \frac{1}{2}, \frac{3}{2} - H_1\Big)^{-1} \int_0^t \int_s^t (u-s)^{H_1-3/2} u^{H_1-1/2} du dY(s),$$

and the proof follows. □

Denote $\gamma_{H_1} = c_{H_1} B\Big(\frac{3}{2} - H_1, \frac{3}{2} - H_1\Big)$. Now the main problem can be formulated as follows. Let $\frac{1}{2} \le H_1 < H_2 < 1$, $\{\widetilde{X}_1(t) = \widetilde{M}^{H_1}(t), X_2(t) := \int_0^t l_{H_1}(t,s) dB^{H_2}(s),\ t \ge 0\}$, be two processes defined on the space $(\Omega, \mathfrak{F})$ and P_θ be a probability measure under which $\widetilde{X}_1$ and X_2 are independent, B^{H_2} is a fractional Brownian motion with Hurst parameter H_2, and $\widetilde{X}_1$ is a martingale with square characteristics

$$\langle \widetilde{X}_1 \rangle(t) = t^{2-2H_1}$$

and with drift $\frac{\theta \gamma_{H_1}}{\sigma_1} t^{2-2H_1}$, i.e.,

$$\widetilde{X}_1(t) = \widetilde{M}^{H_1}(t) = \frac{\theta \gamma_{H_1}}{\sigma_1} t^{2-2H_1} + M^{H_1}(t).$$

Also, denote $X_1(t) = M^{H_1}(t)$. Our main problem is the construction of maximum likelihood estimator for $\theta \in \mathbb{R}$ by the observations of the process

$$Y(t) = \theta \gamma_{H_1} t^{2-2H_1} + \sigma_1 X_1(t) + \sigma_2 X_2(t).$$

Consider the martingale $\widetilde{M}^{H_1}$ with a drift:

$$\begin{aligned} \widetilde{M}^{H_1}(t) &= \frac{\theta \gamma_{H_1}}{\sigma_1} t^{2-2H_1} + (2-2H_1)^{\frac{1}{2}} \int_0^t s^{1/2-H_1} dW(s) \\ &= \frac{\theta \gamma_{H_1}}{\sigma_1} (2-2H_1)^{\frac{1}{2}} (2-2H_1)^{\frac{1}{2}} \int_0^t s^{\frac{1}{2}-H_1} s^{\frac{1}{2}-H_1} ds + (2-2H_1)^{\frac{1}{2}} \int_0^t s^{1/2-H_1} dW(s) \\ &= (2-2H_1)^{\frac{1}{2}} \int_0^t s^{\frac{1}{2}-H_1} d\widetilde{W}(s), \end{aligned} \tag{3}$$

where $\widetilde{W}(t)$ is a Wiener process with a drift defined under the measure P_θ by the equation:

$$d\widetilde{W}(t) := dW(t) + \theta \frac{\gamma_{H_1} (2-2H_1)^{\frac{1}{2}}}{\sigma_1} t^{\frac{1}{2}-H_1} dt.$$

By Girsanov theorem and independence of X_1 and X_2,

$$\frac{dP_\theta}{dP_0} = \exp\Big\{\theta \cdot \frac{\gamma_{H_1}}{\sigma_1}(2-2H_1)^{\frac{1}{2}} \int_0^T s^{\frac{1}{2}-H_1} d\widetilde{W}(s) - \frac{1}{2}\theta^2 \cdot \frac{\gamma_{H_1}^2}{\sigma_1^2} T^{2-2H_1}\Big\}$$

$$= \exp\Big\{\theta \cdot \frac{\gamma_{H_1}}{\sigma_1}\widetilde{X}_1(T) - \frac{1}{2}\theta^2 \cdot \frac{\gamma_{H_1}^2}{\sigma_1^2} T^{2-2H_1}\Big\}.$$

The derivative above is not the likelihood function of a parameter θ since it is not measurable with respect to the observed σ-algebra

$$\mathfrak{F}_T^Y := \sigma\{Y(t), t \in [0,T]\} = \mathfrak{F}_T^X := \sigma\{X(t), t \in [0,T]\},$$

where $X(t) = X_1(t) + X_2(t)$.

We shall proceed as in [4]: let μ_θ be the probability measure induced by Y on the space of continuous functions with the supremum topology under probability P_θ. Then for any measurable set A:

$$\mu_\theta(A) = \int_A \Phi(x)\mu_0 dx,$$

where $\Phi(x)$ is such measurable functional that $\Phi(X) = E_0\Big(\frac{dP_\theta}{dP_0}\Big|\mathfrak{F}_T^X\Big)$. The latter means that $\mu_\theta \ll \mu_0$ for any $\theta \in \mathbb{R}$. Taking into account that $\widetilde{X}_1 = X_1$ under P_0 and the fact that the vector process (X_1, X) is Gaussian, we get that the corresponding likelihood function is given by

$$L_T(X,\theta) = E_0\Big(\frac{dP_\theta}{dP_0}\Big|\mathfrak{F}_T^X\Big) = E_0\Big(\exp\Big\{\theta \cdot \frac{\gamma_{H_1}}{\sigma_1}X_1(T) - \frac{1}{2}\theta^2 \cdot \frac{\gamma_{H_1}^2}{\sigma_1^2}T^{2-2H_1}\Big\}|\mathfrak{F}_T^X\Big)$$

$$= \exp\Big\{\theta \cdot \frac{\gamma_{H_1}}{\sigma_1}E_0(X_1(T)|\mathfrak{F}_T^X) + \frac{1}{2}\theta^2 \cdot \frac{\gamma_{H_1}^2}{\sigma_1^2}\Big(V(T) - T^{2-2H_1}\Big)\Big\}, \qquad (4)$$

where $V(t) = E_0\Big(\big(X_1(t) - E_0(X_1(t)|\mathfrak{F}_t^X)\big)^2|\mathfrak{F}_t^X\Big),\ t \in [0,T]$.

For that follows let the coefficients σ_1 and σ_2 be equal to one.

Thus, we arrive at the following problem: to find the projection $P_X X_1(T)$ of $X_1(T)$ onto $\{X(t) = X_1(t) + X_2(t), t \in [0,T]\}$. We recall from Sect. 1 that

$$W_i(t) = \int_0^t \big((K_{H_i}^*)^{-1}\mathbf{1}_{[0,t]}\big)\, dB^{H_i}(s),\ i = 1,2,$$

are standard Wiener processes, which are obviously independent. Also from Sect. 1 we have

$$X_1(t) = (2-2H_1)^{\frac{1}{2}} \int_0^t s^{1/2-H_1} dW_1(s),\ B^{H_2}(t) = \int_0^t K_{H_2}(t,s) dW_2(s). \tag{5}$$

Then, using (1), we can write

$$X_2(t) = \int_0^t K_{H_1,H_2}(t,s) dW_2(s),$$

where

$$K_{H_1,H_2}(t,s) = \beta_{H_2} c_{H_1} s^{1/2-H_2} \int_s^t (t-u)^{1/2-H_1} u^{H_2-H_1} (u-s)^{H_2-3/2} du. \tag{6}$$

Similarly to (1), we have for $f \in L^2_{H_2}[0,T]$

$$\int_0^T f(s) dX_2(s) = \int_0^T (K^*_{H_1,H_2} f)(s) dW_2(s), \tag{7}$$

where

$$(K^*_{H_1,H_2} f)(s) = \int_s^T f(t) \partial_t K_{H_1,H_2}(t,s) dt.$$

The projection of $X_1(T)$ onto $\{X(t), t \in [0,T]\}$ is a centered X-measurable Gaussian random variable, therefore, it has a form

$$P_X X_1(T) = \int_0^T h_T(t) dX(t)$$

with $h_T \in L^2_{H_1}[0,T]$. Note that h_T still can be a distribution.

This projection for all $u \in [0,T]$ must satisfy

$$E_0\Big(X(u) P_X X_1(T)\Big) = E_0\Big(X(u) X_1(T)\Big). \tag{8}$$

Using (8) together with independency of X_1 and X_2, we arrive at

$$E_0\Big(X_1(u) \int_0^T h_T(t) dX_1(t) + X_2(u) \int_0^T h_T(t) dX_2(t)\Big) = E_0\Big(X(u) X_1(T)\Big) = u^{2-2H_1}. \tag{9}$$

From (5), (6), (7), (8) and (9) we get

$$(2-2H_1) \int_0^u h_T(s) s^{1-2H_1} ds + \int_0^T h_T(s) r_{H_1,H_2}(s,u) ds = u^{2-2H_1} \tag{10}$$

where

$$r_{H_1,H_2}(s,u) = \int_0^{s\wedge u} \partial_s K_{H_1,H_2}(s,v) K_{H_1,H_2}(u,v) dv.$$

This kernel can be written alternatively as $r_{H_1,H_2}(t,s) = \partial_t R_{H_1,H_2}(t,s)$, where

$$R_{H_1,H_2}(t,s) = \int_0^{t\wedge s} K_{H_1,H_2}(t,u) K_{H_1,H_2}(s,u) du = \mathsf{E}\,[X_2(t)X_2(s)]$$

$$= \alpha_{H_2} \int_0^t \int_0^s (t-u)^{1/2-H_1} u^{1/2-H_1} (s-v)^{1/2-H_1} v^{1/2-H_1} |u-v|^{2H_2-2} dv\, du.$$

Differentiating (10) with respect to u, we arrive to

$$(2-2H_1) h_T(u) u^{1-2H_1} + \int_0^T h_T(s) k(s,u) ds = (2-2H_1) u^{1-2H_1}, \tag{11}$$

where

$$k(s,u) = \partial_u r_{H_1,H_2}(s,u) = \int_0^{s\wedge u} \partial_s K_{H_1,H_2}(s,v) \partial_u K_{H_1,H_2}(u,v) dv. \tag{12}$$

Theorem 2.3 *Let $H_2 - H_1 > \frac{1}{4}$. Then there exists a sequence $T_n \to \infty$ such that integral equation (11) has unique solution h_{T_n} on any interval $[0, T_n]$ and $h_{T_n}(\cdot)\cdot^{\frac{1}{2}-H_1} \in L_2[0, T_n]$.*

Proof We denote C_{H_1,H_2} constants which values are not so important; their values can change from line to line. At first, we can apply the changing of variables $u = s + (t-s)z$ to (6) and transform the kernel $K_{H_1,H_2}(t,s)$ from (6) to the following form:

$$K_{H_1,H_2}(t,s) = \beta_{H_2} c_{H_1} s^{\frac{1}{2}-H_2} (t-s)^{H_2-H_1} \int_0^1 (1-z)^{\frac{1}{2}-H_1} (s+(t-s)z)^{H_2-H_1} z^{H_2-\frac{3}{2}} dz. \tag{13}$$

Then we can differentiate (13) and after inverse changing of variables we get that

$$\partial_t K_{H_1,H_2}(t,s) = (H_2-H_1)\Bigg(\frac{K_{H_1,H_2}(t,s)}{t-s} + \beta_{H_2} c_{H_1} s^{\frac{1}{2}-H_2} \frac{1}{t-s} \int_s^t (t-r)^{\frac{1}{2}-H_1} r^{H_2-H_1-1} (r-s)^{H_2-\frac{1}{2}} dr \Bigg). \tag{14}$$

Further, we have the following bound for kernel $K_{H_1,H_2}(t,s)$ on the interval $[0,T]$:

$$0 \le K_{H_1,H_2}(t,s) \le \beta_{H_2} c_{H_1} B\Big(\frac{3}{2} - H_1, H_2 - \frac{1}{2}\Big) t^{H_2-H_1} s^{\frac{1}{2}-H_2} (t-s)^{H_2-H_1}, \tag{15}$$

and it follows from (14) and (15) that

$$0 \le \partial_t K_{H_1,H_2}(t,s) \le \beta_{H_2} c_{H_1} s^{\frac{1}{2}-H_2}\Big(B\Big(\frac{3}{2}-H_1, H_2-\frac{1}{2}\Big)t^{H_2-H_1}(t-s)^{H_2-H_1-1}$$
$$+B\Big(\frac{3}{2}-H_1, H_2+\frac{1}{2}\Big)t^{H_2-H_1-1}(t-s)^{H_2-H_1}\Big) \le C_{H_1,H_2} s^{\frac{1}{2}-H_2} t^{H_2-H_1}(t-s)^{H_2-H_1-1}. \tag{16}$$

Now we can substitute the bound from (16) into (12) and get that

$$0 \le k(s,u) \le C_{H_1,H_2} u^{H_2-H_1} s^{H_2-H_1} \int_0^{s\wedge u} v^{1-2H_2}(u-v)^{H_2-H_1-1}(s-v)^{H_2-H_1-1}dv. \tag{17}$$

Let, for example, $s < u$. Note that

$$(u-v)^{H_2-H_1-1} = (u-v)^{H_2+H_1-2}(u-v)^{1-2H_1} \le (u-v)^{H_2+H_1-2}(u-s)^{1-2H_1}.$$

Then it follows from (17) that

$$0 \le k(s,u) \le C_{H_1,H_2} u^{H_2-H_1} s^{H_2-H_1}(u-s)^{1-2H_1}$$
$$\times \int_0^s v^{1-2H_2}(u-v)^{H_2+H_1-2}(s-v)^{H_2-H_1-1}dv. \tag{18}$$

In order to bound the integral in the right-hand side of (18), we apply the first statement from lemma 2.2 [9], according to which for $\mu, \nu > 0$, $c > 1$

$$\int_0^1 t^{\mu-1}(1-t)^{\nu-1}(c-t)^{-\mu-\nu}dt = B(\mu,\nu)c^{-\nu}(c-1)^{-\mu}.$$

Therefore, with $\mu = 2-2H_2$, $\nu = H_2-H_1$ and $c = \frac{u}{s}$

$$\begin{aligned}
&\int_0^s v^{1-2H_2}(u-v)^{H_2+H_1-2}(s-v)^{H_2-H_1-1}dv \\
&= s^{-1}\int_0^1 v^{1-2H_2}\Big(\frac{u}{s}-v\Big)^{H_2+H_1-2}(1-v)^{H_2-H_1-1}dv \\
&= B(2-2H_2, H_2-H_1)s^{-1}\Big(\frac{u}{s}\Big)^{H_1-H_2}\Big(\frac{u}{s}-1\Big)^{2H_2-2} \\
&= C_{H_1,H_2} s^{1-H_2-H_1} u^{H_1-H_2}(u-s)^{2H_2-2},
\end{aligned} \tag{19}$$

and it follows from (18) and (19) that for $s < u$

$$0 \le k(s,u) \le C_{H_1,H_2} s^{1-2H_1}(u-s)^{2H_2-2H_1-1}. \tag{20}$$

Evidently, for $u < s$

$$0 \le k(s,u) \le C_{H_1,H_2} u^{1-2H_1}(s-u)^{2H_2-2H_1-1}. \tag{21}$$

Now we rewrite equation (11) in the equivalent form

$$\gamma_{H_1}^2 u^{\frac{1}{2}-H_1} = \gamma_{H_1}^2 h(u) u^{\frac{1}{2}-H_1} + \int_0^T h(s) s^{\frac{1}{2}-H_1} s^{H_1-\frac{1}{2}} u^{H_1-\frac{1}{2}} k(s,u) ds, \tag{22}$$

or

$$\gamma_{H_1}^2 u^{\frac{1}{2}-H_1} = \gamma_{H_1}^2 \tilde{h}_T(u) + \int_0^T \tilde{h}_T(s) k_1(s,u) ds, \tag{23}$$

where $k_1(s,u) = s^{H_1-\frac{1}{2}} u^{H_1-\frac{1}{2}} k(s,u)$, $\tilde{h}_T(u) = h(u) u^{\frac{1}{2}-H_1}$ and it follows from (20) and (21) that for $s < u$

$$k_1(s,u) \le C_{H_1,H_2} u^{H_1-\frac{1}{2}} s^{\frac{1}{2}-H_1} (u-s)^{2H_2-2H_1-1}$$

and for $u < s$

$$k_1(s,u) \le C_{H_1,H_2} s^{H_1-\frac{1}{2}} u^{\frac{1}{2}-H_1} (s-u)^{2H_2-2H_1-1}.$$

Therefore, taking into account that for $H_2 - H_1 > \frac{1}{4}$ we have that $4H_2 - 4H_1 - 2 > -1$, it is possible to bound $L_2[0,T]^2$ – norm of the kernel:

$$\begin{aligned}
\|k_1\|_{L_2[0,T]^2} &= \int_0^T \int_0^T k_1^2(s,u) ds du = \int_0^T \int_0^u k_1^2(s,u) ds du + \int_0^T \int_u^T k_1^2(s,u) ds du \\
&\le C_{H_1,H_2} \Big(\int_0^T \int_0^u u^{2H_1-1} s^{1-2H_1} (u-s)^{4H_2-4H_1-2} ds du \\
&\quad + \int_0^T \int_u^T s^{2H_1-1} u^{1-2H_1} (s-u)^{4H_2-4H_1-2} ds du \Big) \\
&\le C_{H_1,H_2} \Big(\int_0^T u^{4H_2-4H_1-1} du + T^{2H_1-1} \int_0^T u^{1-2H_1} (T-u)^{4H_2-4H_1-1} du \Big) \\
&\le C_{H_1,H_2} T^{4H_2-4H_1} < \infty.
\end{aligned} \tag{24}$$

It means that the integral operator $K_T f(u) = \int_0^T k_1(s,u) f(u) du$ is compact linear self-adjoint operator from $L_2[0,T]$ into $L_2[0,T]$ and Fredholm alternative can be applied to equation (23). To avoid the question concerning eigenvalues and eigenfunctions, we produce the following trick.

It is very easy to see that for any $a > 0$

$$K(ta, sa) = K(t, s)a^{\frac{1}{2}+H_2-2H_1},\ \partial_t K_{H_1,H_2}(ta, sa) = \partial_t K(t, s)a^{-\frac{1}{2}+H_2-2H_1},$$
$$k(ta, sa) = a^{2H_2-4H_1}k(t, s), \tag{25}$$

whence

$$k_1(ta, sa) = k_1(t, s)a^{2H_2-2H_1-1}.$$

Therefore we can put in equation (23) $s = s'T, u = u'T$ and $\hat{h}_T(z) = \tilde{h}_T(Tz)$, and equation (23) will be reduced to the equivalent form (we omit superscripts)

$$(uT)^{\frac{1}{2}-H_1} = \hat{h}_T(u) + T^{2H_2-2H_1}\gamma_{H_1}^{-2}\int_0^1 \hat{h}_T(s)k_1(s, u)ds = \hat{h}_T(u)$$
$$+\lambda\int_0^1 \hat{h}_T(s)k_1(s, u)ds, \tag{26}$$

with $\lambda = T^{2H_2-2H_1}\gamma_{H_1}^{-2}$. Since operator K_1 is compact linear self-adjoint operator from $L_2[0, T]$ into $L_2[0, T]$, as it was mentioned above, it has no more than countable number of eigenvalues any of them are real numbers, and with only one possible condensation point 0. Taking the sequence $T_n \to \infty$ in such a way that

$$\lambda_n = T_n^{2H_1-2H_2}\gamma_{H_1}^2$$

will be not an eigenvalue, we get that equation (26) with T_n as upper bound of integration has unique solution whence the proof follows. □

Now we establish the form of maximum likelihood estimate.

Theorem 2.4 *Let $H_2 - H_1 > \frac{1}{4}$. Then the likelihood function has a form*

$$L_T(X, \theta) = \exp\{\theta\gamma_{H_1}N(T) - \frac{1}{2}\theta^2\gamma_{H_1}^2\langle N\rangle(T)\}, \tag{27}$$

and maximum likelihood estimate has a form

$$\hat{\theta}(T) = \frac{N(T)}{\gamma_{H_1}\langle N\rangle(T)}, \tag{28}$$

where $N(t) = E_0(X_1(t)|\mathfrak{F}_t^X)$ is a square integrable Gaussian $\mathfrak{F}_t^X$-martingale, $N(T) = \int_0^T h_T(t)dX(t)$ with $h_T(t)t^{\frac{1}{2}-H_1} \in L_2[0, T]$, $h_T(t)$ be a unique solution to (11) and $\langle N\rangle(T) = (2 - 2H_1)\int_0^T h_T(t)t^{1-2H_1}dt$.

Proof We start with (4). Consider Gaussian process $N(t) = E_0(X_1(t)|\mathfrak{F}_t^X)$. Since $X_1(t)$ is $\mathfrak{F}_t$-martingale and $\mathfrak{F}_t^X \subset \mathfrak{F}_t$, the process N is a $\mathfrak{F}_t^X$-martingale with respect

to probability measure P_0. Furthermore, we can present $V(t)$ as

$$V(t) = E_0(X_1^2(t)|\mathfrak{F}_t^X) - N^2(t).$$

Note that $X_1^2(t) - t^{2-2H}$ is $\mathfrak{F}_t$-martingale. Therefore,

$$E_0\left(N^2(t) - \left(t^{2-2H} - V(t)\right)|\mathfrak{F}_s^X\right) = E_0\left(E_0(X_1^2(t)|\mathfrak{F}_t^X) - t^{2-2H}|\mathfrak{F}_s^X\right)$$
$$= E_0\left(X_1^2(t) - t^{2-2H}|\mathfrak{F}_s^X\right) = E_0(X_1^2(s)|\mathfrak{F}_s^X) - s^{2-2H} = N^2(s) - \left(s^{2-2H} - V(s)\right), \tag{29}$$

therefore the quadratic variation of the martingale N equals $\langle N\rangle(t) = t^{2-2H} - V(t)$, and the likelihood ratio is reduced to

$$L_T(X,\theta) = \exp\left\{\theta\gamma_{H_1}N(T) - \frac{1}{2}\theta^2\gamma_{H_1}^2\langle N\rangle(T)\right\}, \tag{30}$$

so, we get (27) and (28). Now, taking (11) into account, we get that

$$\langle N\rangle(T) = E_0(N^2(T)) = E_0\Big(\int_0^T h_T(u)dX(u)\Big)^2$$
$$= E_0\Big(\int_0^T h_T(u)d(X_1(u) + X_2(u)\Big)^2$$
$$= E_0\Big(\int_0^T h_T(u)dX_1(u)\Big)^2 + E_0\Big(\int_0^T h_T(u)dX_2(u)\Big)^2$$
$$= (2-2H_1)\int_0^T h_T^2(u)u^{1-2H_1}du$$
$$+ \int_0^T\int_t^T h_T(u)\partial_u K_{H_1,H_2}(u,t)du\int_t^T h_T(s)\partial_s K_{H_1,H_2}(s,t)dsdt$$
$$= (2-2H_1)\int_0^T h_T^2(u)u^{1-2H_1}du$$
$$+ \int_0^T h_T(u)\int_0^T h_T(s)\int_0^{s\wedge u}\partial_s K_{H_1,H_2}(s,t)\partial_u K_{H_1,H_2}(u,t)dtdsdu$$
$$= \int_0^T h_T(u)\Big((2-2H_1)h_T(u)u^{1-2H_1} + \int_0^T h_T(s)k(s,u)ds\Big)du$$
$$= (2-2H_1)\int_0^T h_T(u)u^{1-2H_1}du,$$

whence the proof follows. □

In what follows, saying "$T \to \infty$" we have in mind that the corresponding property holds for any sequence $T_n \to \infty$ that has only finite common points with the sequence of eigenvalues of operator K_1. Proof of the following result repeats the proof of the corresponding statements from [4] so is omitted.

Theorem 2.5 *The estimator $\hat{\theta}_T$ is unbiased and the corresponding estimation error is normal*

$$\hat{\theta}_T - \theta \sim N\Big(0, \frac{1}{\int_0^T h_T(s) s^{1-2H_1} ds}\Big).$$

Now we establish the asymptotic behavior of the estimator.

Theorem 2.6 *Let $H_2 - H_1 > \frac{1}{4}$. Estimator $\hat{\theta}_T$ is strongly consistent and*

$$\lim_{T\to\infty} T^{2-2H_2} E_\theta(\hat{\theta}_T - \theta)^2 = \frac{1}{\int_0^1 h_0(u) u^{\frac{1}{2}-H_1} du}.$$

Proof At first we rewrite equation (23) in the equivalent form, changing $u = u'T, s = s'T$ and omitting superscripts:

$$\gamma_{H_1}^2 u^{\frac{1}{2}-H_1} T^{\frac{1}{2}-H_1} = \gamma_{H_1}^2 \tilde{h}_T(uT) + T^{2H_2-2H_1} \int_0^1 \tilde{h}_T(sT) k_1(s,u) ds, \tag{31}$$

or

$$\gamma_{H_1}^2 u^{\frac{1}{2}-H_1} = \gamma_{H_1}^2 \tilde{h}_T(uT) T^{H_1-\frac{1}{2}} + T^{2H_2-2H_1} \int_0^1 \tilde{h}_T(sT) T^{H_1-\frac{1}{2}} k_1(s,u) ds, \tag{32}$$

Denote $\mu = T^{2H_2-2H_1}$. Let $h_\mu(u) = \mu \tilde{h}_T(uT) T^{H_1-\frac{1}{2}}$. Then, taking into account (25), equation (31) can be rewritten as

$$\gamma_{H_1}^2 u^{\frac{1}{2}-H_1} = \frac{1}{\mu} \gamma_{H_1}^2 h_\mu(u) + \int_0^1 h_\mu(s) k_1(s,u) ds. \tag{33}$$

Note that

$$\langle N \rangle(T) = \int_0^T h_T(s) s^{1-2H_1} ds = \int_0^T \tilde{h}_T(s) s^{\frac{1}{2}-H_1} ds = T^{2-2H_2} \int_0^1 h_\mu(u) u^{\frac{1}{2}-H_1} du.$$

Define the operator K

$$(Kf)(u) = \int_0^1 f(s) k_1(s,u) ds$$

and the scalar product $\langle f,g\rangle = \int_0^1 f(s)g(s)ds, f,g \in L_2[0,1]$. Then equation (33) can be rewritten as

$$\gamma_{H_1}^2 u^{\frac{1}{2}-H_1} = \frac{1}{\mu}\gamma_{H_1}^2 h_\mu(u) + Kh_\mu(u). \tag{34}$$

Note that

$$\begin{aligned}\langle Kf,f\rangle &= \int_0^1 (Kf)(t)f(t)dt = \int_0^1 (\int_0^1 f(s)k_1(t,s)ds)f(t)dt\\ &= \int_0^1\int_0^1 f(t)t^{H_1-1/2}f(s)s^{H_1-1/2}\int_0^{s\wedge t}\partial_s K_{H_1,H_2}(s,v)\partial_t K_{H_1,H_2}(t,v)dvdsdt\\ &= \int_0^1 dv\int_v^1 \partial_s K_{H_1,H_2}(s,v)f(s)s^{H_1-1/2}ds\int_v^1 \partial_t K_{H_1,H_2}(t,v)f(t)t^{H_1-1/2}dt \geq 0.\end{aligned} \tag{35}$$

Introduce corresponding the first type auxiliary integral equation

$$\gamma_{H_1}^2 u^{\frac{1}{2}-H_1} = (Kh)(u). \tag{36}$$

It follows from Lemma 1 that (36) has the unique solution, say, h_0, obviously, not depending on μ. The function $\delta_\mu = h_\mu - h_0$ satisfies two equations $K\delta_\mu + \frac{1}{\mu}\gamma_{H_1}^2 h_\mu = 0$ and $K\delta_\mu + \frac{1}{\mu}\gamma_{H_1}^2\delta_\mu = -\frac{h_0}{\mu}$. Multiplying the 2nd equation by δ_μ and integrating, we get

$$\langle K\delta_\mu,\delta_\mu\rangle + \frac{1}{\mu}\gamma_{H_1}^2\|\delta_\mu\|^2 = \frac{1}{\mu}|\langle h_0,\delta_\mu\rangle|, \tag{37}$$

and it follows from (37) and (35) that $\gamma_{H_1}^2\|\delta_\mu\|^2 \leq |\langle h_0,\delta_\mu\rangle| \leq \|h_0\|\|\delta_\mu\|$, which implies that $\|\delta_\mu\| \leq \|h_0\|$. Multiplying the 1st equation by h_0 and integrating we get

$$\langle K\delta_\mu,h_0\rangle + \frac{1}{\mu}\gamma_{H_1}^2\langle h_\mu,h_0\rangle = 0.$$

Note that inequality $\|\delta_\mu\| \leq \|h_0\|$ implies that

$$|\langle h_\mu,h_0\rangle| \leq |\langle\delta_\mu,h_0\rangle| + \|h_0\|^2 \leq 2\|h_0\|^2 < \infty,$$

and hence

$$\gamma_{H_1}^2|\langle\delta_\mu,u^{\frac{1}{2}-H_1}\rangle| = |\langle\delta_\mu,Kh_0\rangle| = |\langle K\delta_\mu,h_0\rangle| = \frac{1}{\mu}\gamma_{H_1}^2|\langle h_\mu,h_0\rangle| \to 0 \tag{38}$$

as $T \to \infty$. It means that $\lim_{T\to\infty} \int_0^1 h_\mu(u) u^{\frac{1}{2}-H_1} du = \int_0^1 h_0(u) u^{\frac{1}{2}-H_1} du$. Therefore

$$T^{2-2H_2} E_\theta(\hat{\theta}_T - \theta)^2 = \frac{1}{\int_0^1 h_\mu(u) u^{\frac{1}{2}-H_1} du} \to \frac{1}{\int_0^1 h_0(u) u^{\frac{1}{2}-H_1} du},$$

whence the proof follows. □

Remark 2.7 In outline, our method of proof follows the method of the corresponding result from [4], however Lemma 1 is specific to our case.

Appendix

We recall some notions from fractional calculus. For the details see [12]. Fractional integrals are defined as

$$(I^\alpha_{a+} f)(x) = \frac{1}{\Gamma(\alpha)} \int_a^x f(t)(x-t)^{\alpha-1} dt$$

and

$$(I^\alpha_{b-} f)(x) = \frac{1}{\Gamma(\alpha)} \int_x^b f(t)(t-x)^{\alpha-1} dt,$$

while fractional derivatives are defined as

$$(\mathcal{D}^\alpha_{a+} f)(x) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_a^x f(t)(x-t)^{-\alpha} dt$$

and

$$(\mathcal{D}^\alpha_{b-} f)(x) = -\frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_x^b f(t)(t-x)^{-\alpha} dt.$$

Fractional differentiation and integration are inverse operators on the appropriate functional classes. Also, we shall use the following integration by parts formula for fractional derivatives,

$$\int_a^b (\mathcal{D}^\alpha_{a+} f)(x) g(x) dx = \int_a^b f(x) (\mathcal{D}^\alpha_{b-} g)(x) dx.$$

Lemma 1 *For any constant $C > 0$ integral equation*

$$u^{1/2-H_1} = C(Kh)(u), \ u \in (0, 1] \tag{39}$$

of the 1st kind has the unique solution.

Proof We can present equation (39) in equivalent form

$$u^{1/2-H_1} = C\int_0^1 h(s)k_1(s,u)ds,\ u \in (0,1],$$

or

$$u^{1-2H_1} = C\int_0^1 \breve{h}(s)\int_0^{s\wedge u} \partial_s K_{H_1,H_2}(s,v)\partial_u K_{H_1,H_2}(u,v)dvds,\ u \in (0,1],$$

where $\breve{h}(s) = h(s)s^{1/2-H_1}$, or, at last,

$$u^{1-2H_1} = C\int_0^u \left(\int_v^1 \breve{h}(s)\partial_s K_{H_1,H_2}(s,v)ds\right)\partial_u K_{H_1,H_2}(u,v)dv. \tag{40}$$

Now, taking into account the transition from equation (10) to (11) with the help of differentiation, we can perform the inverse operation and get from (40) the following equivalent equation

$$u^{2-2H_1} = C(2-2H_1)\int_0^u K_{H_1,H_2}(u,v)\left(\int_v^1 \breve{h}(s)\partial_s K_{H_1,H_2}(s,v)ds\right)dv, u \in [0,1]. \tag{41}$$

The right-hand side of equation (41) can be rewritten as

$$C(2-2H_1)\int_0^u K_{H_1,H_2}(u,v)q(v)dv,$$

where $q(v) = \int_v^1 \breve{h}(s)\partial_s K_{H_1,H_2}(s,v)ds$. At first, solve the equation

$$u^{2-2H_1} = C_1\int_0^u K_{H_1,H_2}(u,v)q(v)dv,$$

with $C_1 = C(2-2H_1)$. Taking into account (6), the latter equation can be rewritten in equivalent form

$$u^{2-2H_1} = C_1\beta_{H_2}\int_0^u v^{1/2-H_2}\int_v^u (u-z)^{1/2-H_1}z^{H_2-H_1}(z-v)^{H_2-3/2}dzq(v)dv,$$

or

$$u^{2-2H_1} = C_1\beta_{H_2}\int_0^u z^{H_2-H_1}(u-z)^{1/2-H_1}\int_0^z v^{1/2-H_2}(z-v)^{H_2-3/2}q(v)dvdz,$$

or, at last,

$$u^{2-2H_1} = C_2(I_{0+}^{3/2-H_1}p)(u),$$

where $C_2 = C_1\beta_{H_2}\Gamma(3/2-H_2)$ and

$$p(z) = z^{H_2-H_1}\int_0^z v^{1/2-H_2}(z-v)^{H_2-3/2}q(v)dv. \tag{42}$$

It means that

$$\begin{aligned} p(u) &= C_2^{-1}(\mathcal{D}_{0+}^{3/2-H_1}(\cdot^{2-2H_1}))(u) \\ &= (C_2\Gamma(H_1-1/2))^{-1}\Big(\int_0^u (u-t)^{H_1-3/2}t^{2-2H_1}dt\Big)'_u = C_3u^{1/2-H_1}, \end{aligned} \tag{43}$$

where $C_3 = \frac{(3/2-H_1)B(H_1-1/2,3-2H_1)}{C_2\Gamma(H_1-1/2)}$. Furthermore, comparing (42) and (43), we get that

$$C_3z^{1/2-H_2} = \int_0^z v^{1/2-H_2}(z-v)^{H_2-3/2}q(v)dv = \Gamma(H_2-1/2)(I_{0+}^{H_2-1/2}(\cdot^{1/2-H_2}q))(z),$$

whence

$$\begin{aligned} v^{1/2-H_2}q(v) &= C_3(\Gamma(H_2-1/2))^{-1}(\mathcal{D}_{0+}^{H_2-1/2}\cdot^{1/2-H_2})(v) \\ &= C_3(\Gamma(H_2-1/2)\Gamma(3/2-H_2))^{-1}\Big(\int_0^v (v-t)^{1/2-H_2}t^{1/2-H_2}dt\Big)'_v \\ &= C_4v^{1-2H_2}, \end{aligned}$$

where $C_4 = C_3(2-2H_2)(\Gamma(H_2-1/2)\Gamma(3/2-H_2))^{-1}$. Obviously, $q(v) = C_4v^{1/2-H_2}$, and we arrive at the equation

$$C_4v^{1/2-H_2} = \int_v^1 \check{h}(s)\partial_sK_{H_1,H_2}(s,v)ds. \tag{44}$$

Note that

$$\partial_sK_{H_1,H_2}(s,v) = \beta_{H_2}\Gamma(3/2-H_1)v^{1/2-H_2}\Big(\mathcal{D}_{v+}^{H_1-1/2}\Big(\cdot^{H_2-H_1}(\cdot-v)^{H_2-3/2}\Big)\Big)(s),$$

so, with the help of integration by parts formula, equation (44) can be rewritten as

$$\begin{aligned} C_5 &= \int_v^1 \check{h}(s)\Big(\mathcal{D}_{v+}^{H_1-1/2}\Big(\cdot^{H_2-H_1}(\cdot-v)^{H_2-3/2}\Big)\Big)(s)ds \\ &= \int_v^1 (\mathcal{D}_{1-}^{H_1-1/2}\check{h})(s)s^{H_2-H_1}(s-v)^{H_2-3/2}ds \\ &= (\Gamma(H_2-1/2))^{-1}(I_{1-}^{H_2-1/2}(\mathcal{D}_{1-}^{H_1-1/2}\check{h})\cdot^{H_2-H_1})(v), \end{aligned} \tag{45}$$

where $C_5 = C_4(\beta_{H_2}\Gamma(3/2-H_1))^{-1}$. The latter equation means that

$$(\mathcal{D}_{1-}^{H_1-1/2}\check{h})(v)v^{H_2-H_1} = C_6(1-v)^{1/2-H_1},$$

$C_6 = \frac{C_5\Gamma(H_1-1/2)}{\Gamma(3/2-H_1)}$. At last, we get that

$$h(v) = v^{H_1-1/2}\check{h}(v) = C_6 v^{H_1-1/2}(I_{1-}^{H_1-1/2}(\cdot^{H_1-H_2}(1-\cdot)^{1/2-H_1}))(v),$$

and this solution of equation (39) is unique. □

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Existence of Density for Solutions of Mixed Stochastic Equations

Taras Shalaiko and Georgiy Shevchenko

Abstract We consider a mixed stochastic differential equation $\mathrm{d}X_t = a(t, X_t)\mathrm{d}t + b(t, X_t)\mathrm{d}W_t + c(t, X_t)\mathrm{d}B_t^H$ driven by independent multidimensional Wiener process and fractional Brownian motion. Under Hörmander type conditions we show that the distribution of X_t possesses a density with respect to the Lebesgue measure.

Keywords Mixed stochastic differential equations • Existence of denisty • Hörmander condition • Malliavin differentiability

Mathematics Subject Classification (2010) 60H10, 60H07, 60G22

1 Introduction

In this paper we study a so-called mixed stochastic differential equation (SDE) in $\mathbb{R}^d$

$$X_t = X_0 + \int_0^t a(s, X_s)\mathrm{d}s + \int_0^t b(s, X_s)\mathrm{d}W_s + \int_0^t c(s, X_s)\mathrm{d}B_s^H \tag{1}$$

driven by a multidimensional standard Wiener process and a multidimensional fractional Brownian motion (fBm) with Hurst parameter $H \in (1/2, 1)$ (see next section for precise definitions). Recently such equations gained a lot of attention thanks to their modeling features. There is already a large literature devoted to

T. Shalaiko (✉)
Department of Probability Theory, Statistics and Actuarial Mathematics, Taras Shevchenko National University of Kyiv, Volodymyrska 64, Kyiv 01601, Ukraine

Department of Mathematical Economics II,
Mathematical Institute of the Manhheim University, A5, 6, D-68131 Mannheim, Germany
e-mail: tshalaik@mail.uni-mannheim.de

G. Shevchenko
Department of Probability Theory, Statistics and Actuarial Mathematics, Taras Shevchenko National University of Kyiv, Volodymyrska 64, Kyiv 01601, Ukraine
e-mail: zhora@univ.kiev.ua; zhoraster@gmail.com

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them; the few papers we cite here give an extensive overview of existing results. The unique solvability result in the form suitable for our needs is obtained in the paper [12]; although the result is formulated there for equations with delay, it is a fortiori valid for usual equations. The paper [11] contains useful estimates of the solution and results on its integrability. Finally, we mention the paper [13], where the Malliavin differentiability of the solution is obtained.

The main aim of this article is to provide conditions under which the solution to (1) has a density with respect to the Lebesgue measure. For Itô SDEs, such issues were addressed by many authors, see [8] and references therein. Existence and regularity of density for SDEs driven by fBm we proved in [1, 9, 10] and in [6] (in case of $H \in [1/3, 1/2]$) under Hörmander type conditions.

Equation (1) can be treated in the rough path sense by passing from an Itô integral to a Stratonovich integral and adding the correspondent correction term to a drift. Malliavin regularity and existence of a density of solutions to rough differential equations is currently an active research topic. Among the others we mention the following works: in [3] the existence of density was established for the differential equations driven by Gaussian signals with "not too rough" sample paths (such as fBm with Hurst index $H > 1/3$) under simplified Hörmander condition, under Hörmander condition and "non-degeneracy" of a driving Gaussian signal (this case covers the fBm with a Hurst index $H > 1/4$) the existence (but not a smoothness) of the density was proven in [4]; the existence and smoothness of the density were finally obtained in [7] for a general class of rough Gaussian signals, including fBm with Hurst index $H > 1/4$. The recent paper [2] contains a generalization of these results to equations driven by Gaussian rough paths. However, in all cited papers the authors assume that a driving signal consists of independent *identically distributed* rough paths, thus, those results can not be applied to our mixed SDE (1).

The paper is organised as follows. In Sect. 2 we introduce our notation, describe the main object and briefly discuss Malliavin calculus of variations for fractional Brownian motion. In Sect. 3, we prove that the distribution of the solution $X_t, t > 0$ possesses density w.r.t. Lebesgue measure under a simplified version of the Hörmander condition. Section 4 contains the result on existence and smoothness of the density under a strong version of the Hörmander condition. The Appendix contains some technical lemmas and the Norris lemma for a mixed SDE.

2 Preliminaries

2.1 Definitions and Notation

Throughout the paper, $|\cdot|$ will denote the absolute value of a number, the Euclidean norm of a vector, and the operator norm of a matrix. $\langle \cdot, \cdot \rangle$ stays for the usual scalar product in the Euclidean space. We will use the symbol C to denote a generic constant, whose value is not important and may change from one line to another.

We will write a subscript if a constant is relevant or if its value depends on some parameters.

For a matrix $A = (a_{i,j})$ of arbitrary size, we denote by a_i its i-th row and by $a_{\cdot,j}$ its j-th column.

The classes of continuous and θ-Hölder continuous functions on $[a, b]$ will be denoted respectively by $C[a, b]$ and $C^\theta[a, b]$. For a function $f\colon [a, b] \to \mathbb{R}$ denote by $\|f\|_{\infty,[a,b]}$ its supremum norm and by

$$\|f\|_{\theta,[a,b]} = \sup_{a\le s<t\le b} \frac{|f(t) - f(s)|}{|t - s|^\theta}$$

its θ-Hölder seminorm. If there is no ambiguity, we will use the notation $\|f\|_\infty$ and $\|f\|_\theta$.

Finally, for a function $h \in C^2(\mathbb{R}^d)$ denote by $\partial_x h = (\frac{\partial}{\partial x_1}h, \dots, \frac{\partial}{\partial x_d}h)$ its gradient and by $\partial^2_{xx} h = (\frac{\partial^2}{\partial x_i \partial x_j}h)_{i,j=1,\dots,d}$ its second derivative matrix.

2.2 Main Equation and Assumptions

For a fixed time horizon $T > 0$, let $\{\Omega, \mathscr{F}, \mathbf{F} = (\mathscr{F}_t)_{t\in[0,T]}, \mathsf{P}\}$ be a standard stochastic basis. Equation (1) is driven by two independent sources of randomness: an m-dimensional $\mathbf{F}$-Wiener process $\{W_t = (W^1_t, \dots, W^m_t), t \in [0, T]\}$ and an l-dimensional fBm $\{B^H_t = (B^{H,1}_t, \dots, B^{H,l}_t), t \ge [0, T]\}$ with Hurst index $H \in (1/2, 1)$, i.e. a centered Gaussian process having the covariance

$$\mathsf{E}\left[B^{H,i}_t B^{H,j}_s\right] = \frac{\delta_{i,j}}{2}(t^{2H} + s^{2H} - |t - s|^{2H}).$$

It is well known that the fBm B^H has a modification with γ-Hölder continuous path for any $\gamma < H$, in the following we will assume that the process itself is Hölder continuous.

Equation (1) is understood as a system of SDEs on $[0, T]$

$$X^i_t = X^i_0 + \int_0^t a_i(s, X_s)\mathrm{d}s + \sum_{j=1}^m \int_0^t b_{i,j}(s, X_s)\mathrm{d}W^j_s + \sum_{k=1}^l \int_0^t c_{i,k}(s, X_s)\mathrm{d}B^{H,k}_s,$$

$i = 1, \dots, d$, with a non-random initial condition $X_0 \in \mathbb{R}^d$. In this equation, the integral w.r.t. W is understood in a usual Itô sense, the one w.r.t. B^H is understood in a pathwise sense, as Young integral. More information on its definition and properties can be found in [5].

The coefficients $a_i, b_{i,j}, c_{i,k}\colon [0,T]\times\mathbb{R}^d \to \mathbb{R}^d$, $i = 1,\dots,d, j = 1,\dots,m, k = 1,\dots,l$ are assumed to satisfy the following conditions.

A1 for all $t \in [0,T]$ $a(t,\cdot), b(t,\cdot) \in C^1(\mathbb{R}^d)$, $c(t,\cdot) \in C^2(\mathbb{R}^d)$;
A2 for all $t \in [0,T]$, $x \in \mathbb{R}^d$

$$|a(t,x)| + |b(t,x)| + |c(t,x)| \le C(1+|x|);$$

A3 for all $t \in [0,T]$, $x \in \mathbb{R}^d$ $|\partial_x c(t,x)| \le C$;
A4 there exists $\beta > 0$ such that for all $t,s \in [0,T]$, $x \in \mathbb{R}^d$

$$|c(t,x) - c(s,x)| \le C|t-s|^\beta(1+|x|), \quad |\partial_x c(t,x) - \partial_x c(s,x)| \le C|t-s|^\beta.$$

The continuous differentiability implies that $a, b, \partial_x c$ are locally Lipschitz continuous. Therefore, by [12, Theorem 4.1], equation (1) has a unique solution which is Hölder continuous of any order $\theta \in (0, 1/2)$.

2.3 Ad Hoc Malliavin Calculus

Here we summarize some facts from the Malliavin calculus of variations, see [8] for a deeper exposition. Denote by $S[0,T]$ the set the of step functions of the form $f(t) = \sum_{k=1}^n c_k \mathbf{1}_{[a_k,b_k)}(t)$ defined on $[0,T]$. Let $L_H^2[0,T]$ denote the separable Hilbert space obtained by completing $S[0,T]$ w.r.t. the scalar product

$$\langle f,g\rangle_{L_H^2[0,T]} = \int_0^T\int_0^T f(t)g(s)\phi(t,s)\mathrm{d}t\mathrm{d}s,$$

where $\phi(t,s) = H(2H-1)|t-s|^{2H-2}$.

Consider the product space

$$\mathfrak{H} = \left(L_H^2[0,T]\right)^l \times \left(L^2[0,T]\right)^m.$$

It is also a separable Hilbert space with a scalar product

$$\langle f,g\rangle_{\mathfrak{H}} = \sum_{i=1}^{l}\langle f_i,g_i\rangle_{L_H^2[0,T]} + \sum_{i=l+1}^{l+m}\langle f_i,g_i\rangle_{L^2[0,T]}.$$

The map

$$\mathscr{I}\colon (\mathbf{1}_{[0,t_1)},\dots,\mathbf{1}_{[0,t_l)},\mathbf{1}_{[0,s_1)},\dots,\mathbf{1}_{[0,s_m)}) \mapsto (B_{t_1}^{H,1},\dots,B_{t_l}^{H,l},W_{s_1}^1,\dots,W_{s_m}^m)$$

can be extended by linearity to $S[0,T]^{l+m}$. It appears that for $f, g \in S[0,T]^{l+m}$

$$\mathsf{E}\left[\langle \mathscr{I}(f), \mathscr{I}(g)\rangle\right] = \langle f, g\rangle_{\mathfrak{H}},$$

so $\mathscr{I}$ can be extended to an isometry between $\mathfrak{H}$ and a subspace of $L^2(\Omega;\mathbb{R}^{m+l})$.

For $\xi = F(\mathscr{I}(f_1),\ldots,\mathscr{I}(f_n))$, where $f_1,\ldots,f_n \in \mathfrak{H}$ and $f_i = (f_{i,1},\ldots,f_{i,m+l})$, $i = 1,\ldots,n$, $F\colon \mathbb{R}^{n(m+l)} \to \mathbb{R}$ is a continuously differentiable finitely supported function, define the Malliavin derivative $\mathsf{D}\xi$ as an element of $\mathfrak{H}$, whose j-th coordinate equal to

$$\sum_{i=1}^{n} \partial_{(i-1)(l+m)+j} F(\mathscr{I}(f_1),\ldots,\mathscr{I}(f_n)) f_{i,j}, j = 1,\ldots,l+m.$$

Denote for $p \geq 1$ by $\mathbb{D}^{1,p}$ the closure of the space of smooth cylindrical random variables with respect to the norm

$$\|\xi\|^p_{\mathbb{D}^{1,p}} = \mathsf{E}\left[\,|\xi|^p + \|\mathsf{D}\xi\|^p_{\mathfrak{H}}\,\right]^{1/p}.$$

D is closable in this space and its closure will be denoted likewise. Finally, the Malliavin derivative is a (possibly, generalized) function from $[0,T]$ to $\mathbb{R}^{l+m}$, so we can introduce the notation

$$\mathsf{D}\xi = \left\{\mathsf{D}_t\xi = \left(\mathsf{D}^{H,1}_t\xi,\ldots,\mathsf{D}^{H,l}_t\xi,\mathsf{D}^{W,1}_t\xi,\ldots,\mathsf{D}^{W,m}_t\xi\right),\ t\in[0,T]\right\}.$$

We say that $\xi \in \mathbb{D}^{1,p}_{loc}$ if exists a sequence $\{\xi_n(\omega),\Omega_n\}_{n\geq 1}$ such that $\Omega_n \subset \Omega_{n+1}$ for $n \geq 1$, $P\left(\Omega \setminus \left(\bigcup_{n\geq 1}\Omega_n\right)\right) = 0$; $\xi_n \in \mathbb{D}^{1,p}$ and $\xi|_{\Omega_n} = \xi_n|_{\Omega_n}$ for all $n \geq 1$.

For the reader convenience we state here the theorem concerning the Mallivian differentiability of the solution to (1) in the case of SDE with non-homogeneous coefficients. The proof is similar to that of [13, Theorem 2]

Theorem 2.1 *Suppose that coefficients a, b, c of (1) satisfy the assumptions*

B1 *for all $t \in [0,T]$ $a(t,\cdot), b(t,\cdot) \in C^1(\mathbb{R}^d)$, $c(t,\cdot) \in C^2(\mathbb{R}^d)$;*
B2 *$a, b, \partial_x a, \partial_x b, \partial_x c, \partial^2_{xx} c$ are bounded;*
B3 *there exists $\beta > 0$ such that for all $t, s \in [0,T]$, $x \in \mathbb{R}^d$*

$$|c(t,x) - c(s,x)| \leq C|t-s|^\beta(1+|x|), \quad |\partial_x c(t,x) - \partial_x c(s,x)| \leq C|t-s|^\beta.$$

Then $X_t \in \bigcap_{p\geq 1}\mathbb{D}^{1,p}$.

3 Existence of Density Under Simplified Hörmander Condition

In this section we prove that a solution to (1) possesses density of a distribution under a quite strong condition, which we call a simplified Hörmander condition. More precisely, we will assume in this section that the coefficients of (1) satisfy

$$\mathsf{span}\{c_{\cdot,k}(0,X_0), b_{\cdot,j}(0,X_0) \mid 1 \le k \le l, 1 \le j \le m\} = \mathbb{R}^d. \tag{2}$$

The first step to establish the existence of density is to show the (local) Malliavin differentiability of the solution to (1).

Theorem 3.1 *If the coefficients of* (1) *satisfy the assumptions* A1–A4*, then* $X_t \in \bigcap_{p\ge 1} \mathbb{D}^{1,p}_{loc}$.

Proof Define $\Omega_n = \{\omega : \|X_\cdot(\omega)\|_{\infty,[0,t]} < n\}$, $n \ge 1$. Obviously, $\Omega_n \subset \Omega_{n+1}, n \ge 1$ and, since $\|X_\cdot(\omega)\|_{\infty,[0,t]} < \infty$ a.s., $\bigcup_{n\ge 1} \Omega_n = \Omega$. Consider a smooth function $\psi = \psi(x)$, $x \in \mathbb{R}$ such that

- for all $x \in \mathbb{R}$ $0 \le \psi(x) \le 1$;
- $\psi(x) = 1, x \in [-1, 1]$;
- $\psi(x) = 0$, $x \notin [-2, 2]$.

For $n \ge 1$, put $\Psi_n = \Psi_n(x_1, \dots, x_d) = (\int_0^{x_1} \psi(y/n)\mathrm{d}y, \dots, \int_0^{x_d} \psi(y/n)\mathrm{d}y)$, define $d^{(n)}(s,x) = d(t, \Psi_n(x))$, $d \in \{a, b, c\}$, and let $X^{(n)}$ solve

$$X^{(n)}_t = X_0 + \int_0^t a^{(n)}(s, X^{(n)}_s)\mathrm{d}s + \int_0^t b^{(n)}(s, X^{(n)}_s)\mathrm{d}W_s + \int_0^t c^{(n)}(s, X^{(n)}_s)\mathrm{d}B^H_s.$$

Since the functions a_n, b_n, c_n satisfy assumptions B1–B3, in view of Theorem 2.1, $X^{(n)}_t \in \bigcap_{p\ge 1} \mathbb{D}^{1,p}$. It is not hard to see that $X^{(n)}_t(\omega) = X_t(\omega)$ for $\omega \in \Omega_n$, which concludes the proof. □

Now we are to prove the main result of this section.

Theorem 3.2 *Suppose that the coefficients of* (1) *satisfy assumptions* A1–A4 *and the simplified Hörmander condition* (2)*. Then for all* $t > 0$ *the law of* X_t *is absolutely continuous with respect to the Lebesgue measure in* $\mathbb{R}^d$.

Proof By the classical condition for existence of density (see e.g. [8, Theorem 2.1.2]) and thanks to the previous theorem, it is enough to verify the non-degeneracy of the Mallivain covariation matrix $M(t) = (M_{i,j}(t))_{i,j=1,\dots,d}$ with $M_{i,j}(t) = \langle \mathsf{D}X^i_t, \mathsf{D}X^i_t\rangle_{\mathscr{H}}$. Define the matrix-valued process $J_{t,0} = (J_{t,0}(i,j))_{i,j=1,\dots,d}$

as the solution to

$$J_{t,0}(i,j) = \delta_{i,j} + \sum_{r=1}^{d}\Bigg[\int_0^t \frac{\partial a_i}{\partial x_r}(s,X_s)J_{s,0}(r,j)\mathrm{d}s + \sum_{k=1}^{m}\int_0^t \frac{\partial b_{i,k}}{\partial x_r}(s,X_s)J_{s,0}(r,j)\mathrm{d}W_s^k + \sum_{q=1}^{l}\int_0^t \frac{\partial c_{i,q}}{\partial x_r}(s,X_s)J_{s,0}(r,j)\mathrm{d}B_s^{H,q}\Bigg]. \tag{3}$$

where $\delta_{i,j} = \mathbf{1}_{i=j}$ is the Kronecker delta. The system above is linear, hence, possesses a unique solution. In view of Lemma 1, $J_{t,0}$ is non-degenerate; denoting $J_{t,s} = J_{t,0}J_{s,0}^{-1}$ and applying Lemma 2 one can write

$$M(t) = \sum_{k=1}^{m}\int_0^t (J_{t,s}b_{\cdot,k}(s,X_s))(J_{t,s}b_{\cdot,k}(s,X_s))'\mathrm{d}s + \sum_{q=1}^{l}\int_0^t\int_0^t \varphi_H(s,u)(J_{t,s}c_{\cdot,q}(s,X_s))(J_{t,u}c_{\cdot,q}(u,X_u))'\mathrm{d}s\mathrm{d}u = J_{t,0}C_tJ_{t,0}',$$

where

$$C_t = \sum_{k=1}^{m}\int_0^t (J_{s,0}^{-1}b_{\cdot,k}(s,X_s))(J_{s,0}^{-1}b_{\cdot,k}(s,X_s))'\mathrm{d}s + \sum_{q=1}^{l}\int_0^t\int_0^t \varphi_H(s,u)(J_{s,0}^{-1}c_{\cdot,q}(s,X_s))(J_{u,0}^{-1}c_{\cdot,q}(u,X_u))'\mathrm{d}s\mathrm{d}u.$$

Again, due to the invertibility of $J_{t,0}$, M_t is invertible if and only if so is C_t. Assuming the contrary, there exists a non-zero vector $v \in \mathbb{R}^d$ such that $v'C_tv = 0$. Write

$$v'C_tv = \sum_{k=1}^{m}\|\langle J_{\cdot,0}b_{\cdot,k}(\cdot,X_\cdot), v\rangle\|_{L^2[0,t]}^2 + \sum_{q=1}^{l}\left\|\langle J_{\cdot,0}c_{\cdot,q}(\cdot,X_\cdot), v\rangle\right\|_{L_H^2[0,t]}^2.$$

Since the functions

$$s \mapsto \langle J_{s,0}^{-1}b_{\cdot,k}(s,X_s), v\rangle,\ k = 1,\dots,m,$$
$$s \mapsto \langle J_{s,0}^{-1}c_{\cdot,q}(s,X_s), v\rangle,\ q = 1,\dots,l$$

are continuous, they must be equal zero for all $s \in [0, t]$. For $s = 0$ we get

$$\sum_{i=1}^{d} b_{i,k}(0, X_0)v_i = 0, k = 1, \ldots, m;$$

$$\sum_{i=1}^{d} c_{i,q}(0, X_0)v_i = 0, q = 1, \ldots, l.$$

This, however, contradicts the assumption (2). Consequently, M_t is invertible, as required. □

4 Existence of Density Under Strong Hörmander Condition

In this section we consider a homogeneous version of (1):

$$X_t = X_0 + \int_0^t a(X_s)\mathrm{d}s + \int_0^t b(X_s)\mathrm{d}W_s + \int_0^t c(X_s)\mathrm{d}B_s^H. \tag{4}$$

In this section we assume that Hurst index $H \in (1/2, 2/3)$, and some $\theta \in ((H - 1/2)/(3 - 4H), 1/2)$ is fixed. The role of the restriction $\theta > (H - 1/2)/(3 - 4H)$ will become clear in the proof of the Norris lemma for (4) (Lemma 5). Now we just remark that the expression $(H - 1/2)/(3 - 4H)$ is increasing for $H \in (1/2, 3/4)$ and is equal to $1/2$ for $H = 2/3$, so the upper bound $H < 2/3$ arises naturally.

We impose the following condition on the coefficients of (4):

C1 $a, b, c \in C_b^\infty(\mathbb{R}^d)$ with all derivatives bounded.

Under this assumption the solution is infinitely differentiable in the Malliavin sense: $X_t \in \bigcap_{k,p=1}^{\infty} \mathbb{D}^{k,p} = \mathbb{D}^\infty$, which can be shown similarly to its differentiability under B1–B3.

The aim of this section is to investigate the existence of a density and properties of this density of a distribution of X_t under the strong Hörmander condition, which reads as follows.

Set $V_0 = a$, $V_j(\cdot) = b_{\cdot,j}(\cdot)$ for $j = 1, \ldots, m$ and $V_{j+m}(\cdot) = c_{\cdot,j}(\cdot)$ for $j = 1, \ldots, l$. Using the Lie bracket $[\cdot, \cdot]$, define the set

$$\Upsilon_k = \{[V_{i_1}, \ldots, [V_{i_{k-1}}, V_{i_k}] \ldots], (i_1, \ldots, i_k) \in \{1, \ldots, d\}^k\}.$$

It is said that the vector field $\Upsilon_0 = \{V_j\}_{j=1,\ldots,m+l}$ satisfies the Hörmander condition at the point X_0, if for some positive integer n_0 one has

$$\mathsf{span}\left\{V(X_0), V \in \bigcup_{k=1}^{n_0} \Upsilon_k\right\} = \mathbb{R}^d. \tag{5}$$

The main result of this section is the following theorem.

Theorem 4.1 *Assume that coefficients of (4) satisfy assumption* C1 *and the Hörmander condition (5). Then the law of X_t for all $t > 0$ possesses a smooth density with respect to the Lebesgue measure in $\mathbb{R}^d$.*

Proof Using the usual condition for existence of a smooth density (see e.g. [8, Theorem 2.1.4]) and taking into account that all moments of the Jacobian $J_{t,s}$ are finite, it is enough to show that the matrix inverse to the reduced Malliavin covariance matrix of X_t possesses all moments.

Recall from Theorem 3.2 that the reduced Malliavin covariance matrix of the solution to (4) can be written as

$$C(t) = \sum_{k=1}^{m} \int_0^t (J_{s,0}^{-1} b_{\cdot,k}(X_s))(J_{s,0}^{-1} b_{\cdot,k}(X_s))' \mathrm{d}s$$

$$+ \sum_{q=1}^{l} \int_0^t \int_0^t \varphi_H(s,u)(J_{s,0}^{-1} c_{\cdot,q}(X_s))(J_{u,0}^{-1} c_{\cdot,q}(X_u))' \mathrm{d}s\mathrm{d}u.$$

To simplify the notation, we assume from now that $t = 1$. We are to prove that $\mathsf{E}[\,|\det C_t|^{-p}\,] < \infty$ for all $p \geq 1$. Due to [8, Lemma 2.3.1] it suffices to prove that the entries of C_t possess all moments and for any $p \geq 2$ there exists C_p such that for all $\varepsilon > 0$ it holds

$$\sup_{\|v\|=1} \mathsf{P}\{\langle v, C_1 v\rangle \leq \varepsilon\} \leq C_p \varepsilon^p.$$

Write

$$\langle v, C_1 v\rangle = \sum_{k=1}^{m} \left\| \langle J_{\cdot,0}^{-1} b_{\cdot,k}(X_\cdot), v\rangle \right\|_{L^2[0,1]}^2 + \sum_{q=1}^{l} \left\| \langle J_{\cdot,0}^{-1} c_{\cdot,q}(X_\cdot), v\rangle \right\|_{L_H^2[0,1]}.$$

It is well known that $\|f\|_{L_H^2[0,1]} \leq \|f\|_{L^2[0,1]}$. Therefore,

$$\langle v, C_1 v\rangle \geq C \sum_{k=1}^{m+l} \|G_k\|_{L_H^2[0,1]}, \text{ where } G_k = \langle J_{\cdot,0}^{-1} V_k(X_\cdot), v\rangle.$$

Applying [1, Lemma 4.4] we get that

$$\langle v, C_1 v\rangle \geq C \sum_{k=1}^{m+l} \frac{\|G_k\|_\infty^{2(3+1/\theta)}}{\|G_k\|_\theta^{2(2+1/\theta)}}$$

for $\theta > H - 1/2$. Thus,

$$\mathsf{P}\left\{\langle v, C_1 v\rangle \le \varepsilon\right\} \le \mathsf{P}\left\{C\sum_{k=1}^{m+l}\frac{\|G_k\|_\infty^{2(3+1/\theta)}}{\|G_k\|_\theta^{2(2+1/\theta)}} \le \varepsilon\right\}.$$

From [1, Lemma 4.5] and Theorem 5 we obtain the following estimate

$$\mathsf{P}\left\{C\sum_{k=1}^{m+l}\frac{\|G_k\|_\infty^{2(3+1/\theta)}}{\|G_k\|_\theta^{2(2+1/\theta)}} \le \varepsilon\right\} \le C\varepsilon^p + \min_{k=1,\dots,m+l}\mathsf{P}\left\{\|\langle v, J_{\cdot,0}V_k(X_\cdot)\rangle\|_\infty \le \varepsilon^\alpha\right\}.$$

Now let V be a bounded vector field with bounded derivatives of all order. The chain rule implies

$$J_{t,0}^{-1}V(X_t) = V(X_0) + \int_0^t J_{s,0}^{-1}([V_0, V] + \frac{1}{2}\sum_{k=1}^{m+l}[V_k,[V_k,V]])(X_s)\mathrm{d}s$$
$$+\sum_{k=1}^{m}\int_0^t J_{s,0}^{-1}[V_k,V](X_s)\mathrm{d}W_s + \sum_{k=m+1}^{l+m}\int_0^t J_{s,0}^{-1}[V_k,V](X_s)\mathrm{d}B_s^H.$$

Thus, applying Theorem 5 once more, we obtain

$$\mathsf{P}\left\{\|\langle v, J_{\cdot,0}V(X_\cdot)\rangle\|_\infty < \varepsilon\right\} \le C\varepsilon^p + \min_{k=1,\dots,m+l}\mathsf{P}\left\{\left\|\langle v, J_{\cdot,0}^{-1}[V_k,V](X_\cdot)\rangle\right\|_\infty \le \varepsilon^\alpha\right\}.$$

Let n_0 be the integer from the Hörmander condition. Iterating our consideration above, we obtain

$$\mathsf{P}\left\{\langle v, C_1 v\rangle \le \varepsilon\right\} \le C\varepsilon^p + \min_{V\in\bigcup_{k=1}^{n_0}\Upsilon_k}\mathsf{P}\left\{\left\|\langle v, J_{\cdot,0}^{-1}V(X_\cdot)\rangle\right\|_\infty \le \varepsilon^\alpha\right\}$$

for all ε small enough. Since $\{V(x_0), V \in \bigcup_{k=1}^{n_0}\Upsilon_k\}$ spans $\mathbb{R}^d$, there exists v such that $\langle v, V(x_0)\rangle \ne 0$. Hence, there exists $\varepsilon_0(p)$ such that for all $\varepsilon < \varepsilon_0(p)$ the second term vanishes. As a result,

$$\mathsf{P}\left\{\langle v, C_1 v\rangle \le \varepsilon\right\} \le C_p\varepsilon^p$$

for all $\varepsilon \le \varepsilon_0(p)$, as required. □

Appendix: Technical Lemmas

The following two lemmas concern the Jacobian of the flow generated by the solution X to equation (1). These are quite standard facts, so we just sketch the proofs.

Lemma 1 *Under assumptions* A1–A4 *the matrix valued process* $J_{t,0} = (J_{t,0}(i,j))_{i,j=1,\dots,d}$ *given by* (3) *has an inverse* $Z_{t,0} = (Z_{t,0}(i,j))_{i,j=1,\dots,d}$ *for all* $t > 0$. *Moreover,* $\{Z_{t,0}, t \geq 0\}$ *satisfies the following system of equations*

$$\begin{aligned} Z_{t,0}(i,j) = \delta(i,j) - \sum_{r=1}^{d} \Bigg[\int_0^t \frac{\partial a_r}{\partial x_j}(s, X_s) Z_{s,0}(i,r) \mathrm{d}s \\ + \sum_{k=1}^{m} \int_0^t \frac{\partial b_{r,k}}{\partial x_j}(s, X_s) Z_{s,0}(i,r) \mathrm{d}W_s^k + \sum_{q=1}^{l} \int_0^t \frac{\partial c_{r,q}}{\partial x_j}(s, X_s) Z_{s,0}(i,r) \mathrm{d}B_s^{H,q} \\ - \sum_{u=1}^{d} \sum_{v=1}^{d} \int_0^t \frac{\partial b_{r,v}}{\partial x_u}(s, X_s) \frac{\partial b_{u,v}}{\partial x_j}(s, X_s) Z_{s,0}(i,r) \mathrm{d}s \Bigg]. \end{aligned} \tag{6}$$

Proof The equation (6) is linear, thus possesses a unique solution $Z_{t,0}$. So we need to verify that $Z_{t,0}J_{t,0} = J_{t,0}Z_{t,0} = I_d$, the identity matrix. The equality clearly holds for $t = 0$. To show it for $t > 0$, it is enough to show that the differentials of $Z_{t,0}J_{t,0}$ and of $J_{t,0}Z_{t,0}$ vanish. But this can be routinely checked using the Itô formula. □

Denote for $t \geq s$ $J_{t,s} = J_{t,0}J_{s,0}^{-1}$.

Lemma 2 *Under assumptions* A1–A4*, the Malliavin derivatives of the solution to* (1) *are given by*

$$\mathsf{D}_s^{W,k} X_t = J_{t,s} b_{\cdot,k}(s, X_s) \mathbf{1}_{s \leq t},\ k = 1, \dots, m, \tag{7}$$

$$\mathsf{D}_s^{H,q} X_t = J_{t,s} c_{\cdot,q}(s, X_s) \mathbf{1}_{s \leq t},\ q = 1, \dots, l. \tag{8}$$

Proof The argument is exactly the same for both equations, so we prove only (7). Evidently, $\mathsf{D}_s^{W,k} X_t = 0$ for $s > t$, so suppose that $s \leq t$. Due to the closedness of the derivative, we can freely differentiate (1) as if the integrals were finite sums, in particular, using the chain rule, we can write for $i = 1, \dots, d$

$$\mathsf{D}_s^{W,k} \int_0^t a_i(u, X_u) \mathrm{d}u = \int_0^t \mathsf{D}_s^{W,k} a_i(u, X_u) \mathrm{d}u = \sum_{r=1}^{d} \int_s^t \frac{\partial}{\partial x_r} a_i(u, X_u) \mathsf{D}_s^{W,k} X_u^r \mathrm{d}u$$

and similarly

$$\mathsf{D}_s^{W,k}\int_0^t c_{i,q}(u,X_u)\mathrm{d}B_u^{H,q}=\sum_{r=1}^d\int_s^t\frac{\partial}{\partial x_r}c_{i,q}(u,X_u)\mathsf{D}_s^{W,k}X_u^r\mathrm{d}B_s^{H,q},q=1,\dots,l,$$

$$\mathsf{D}_s^{W,k}\int_0^t b_{i,j}(u,X_u)\mathrm{d}W_u^j=\sum_{r=1}^d\int_s^t\frac{\partial}{\partial x_r}b_{i,j}(u,X_u)\mathsf{D}_s^{W,k}X_u^r\mathrm{d}W_s^j,j=1,\dots,m,j\neq k.$$

To differentiate the integral w.r.t. W^k, approximate it by an integral sum and note that we will have an extra term corresponding to the derivative of the increment of W^k on the interval containing s. Passing to the limit, we get

$$\mathsf{D}_s^{W,k}\int_0^t b_{i,k}(u,X_u)\mathrm{d}W_u^k=b_{i,k}(s,X_s)+\sum_{r=1}^d\int_s^t\frac{\partial}{\partial x_r}b_{i,k}(u,X_u)\mathsf{D}_s^{W,k}X_u^r\mathrm{d}W_s^k.$$

Therefore, we have for $s\le t$ the following linear equation on $\mathsf{D}_s^{W,k}X_u$:

$$\mathsf{D}_s^{W,k}X_t=b_{\cdot,k}(s,X_s)+\sum_{r=1}^d\Bigg[\int_s^t\frac{\partial}{\partial x_r}a(u,X_u)\mathsf{D}_s^{W,k}X_u^r\mathrm{d}u$$

$$+\sum_{q=1}^l\int_s^t\frac{\partial}{\partial x_r}c_{\cdot,q}(u,X_u)\mathsf{D}_s^{W,k}X_u^r\mathrm{d}B_s^{H,q}+\sum_{j=1}^m\int_s^t\frac{\partial}{\partial x_r}b_{\cdot,j}(u,X_u)\mathsf{D}_s^{W,k}X_u^r\mathrm{d}W_s^j\Bigg].$$

On the other hand, from (3) we can write

$$J_{t,0}=J_{s,0}+\sum_{r=1}^d\Bigg[\int_s^t\frac{\partial a_i}{\partial x_r}(u,X_u)J_{u,0}\mathrm{d}u$$

$$+\sum_{k=1}^m\int_s^t\frac{\partial b_{\cdot,k}}{\partial x_r}(s,X_s)J_{u,0}\mathrm{d}W_u^k+\sum_{q=1}^l\int_s^t\frac{\partial c_{\cdot,q}}{\partial x_r}(s,X_s)J_{u,0}\mathrm{d}B_u^{H,q}\Bigg],$$

which, upon multiplying by $J_{s,0}^{-1}b_{\cdot,k}(s,X_s)$ on the right leads to the same equation on $J_{u,s}b_{\cdot,k}(s,X_s)$ as that on $\mathsf{D}_s^{W,k}X_u^r$. Hence, by uniqueness, we get the desired result. □

Further we establish a simple estimate on the Itô integral of a Hölder continuous integrand.

Lemma 3 *Let* $\{f(t),t\in[0,T]\}$ *be an* $\mathbf{F}$*-adapted stochastic process such that* $\mathsf{E}\left[\,\|f\|_\theta^p\,\right]<\infty$ *for all* $p\ge1$*, and* $0<\delta<\Delta\le T$*. Then for all* $s,t,u\in[0,T]$ *such*

that $u < s < t$, $t - s < \delta$, $t - u \le \Delta$ it holds

$$\left| \int_s^t \big(f(v) - f(u)\big) \mathrm{d}W_v \right| \le \Delta^{\theta} \delta^{1/2} \xi_{\Delta,\delta},$$

where $\mathsf{E}\left[\xi_{\Delta,\delta}^p \right] < C_p \mathsf{E}\left[\|f\|_{\theta}^p \right]$ *for all* $p \ge 1$.

Proof It suffices to establish the required result for p large enough, then one can get deduce it for all $p \ge 1$ with the help of Jensen's inequlaity.

By the Garsia–Rodemich–Rumsey inequality, we get

$$\left| \int_s^t \big(f(v) - f(u)\big) \mathrm{d}W_v \right| \le C|t-s|^{1/4} \left(\int_s^t \int_s^t \frac{\left| \int_x^y \big(f(v) - f(u)\big) \mathrm{d}W_v \right|^8}{|x-y|^4} \mathrm{d}x\mathrm{d}y \right)^{1/8}$$
$$\le C \Delta^{\theta} \delta^{1/2} \xi_{\Delta,\delta},$$

where

$$\xi_{\Delta,\delta} = \Delta^{-\theta} \delta^{-1/4} \left(\int_s^t \int_s^t \frac{\left| \int_x^y \big(f(v) - f(u)\big) \mathrm{d}W_v \right|^8}{|x-y|^4} \mathrm{d}x\mathrm{d}y \right)^{1/8}.$$

For $p > 8$ the Hölder inequality entails that

$$\mathsf{E}\left[\xi_{\Delta,\delta}^p \right] \le \Delta^{-\theta p} \delta^{-p/4} (t-s)^{2(p/8-1)} \int_s^t \int_s^t \mathsf{E}\left[\frac{\left| \int_x^y \big(f(v) - f(u)\big) \mathrm{d}W_v \right|^p}{|x-y|^{p/2}} \right] \mathrm{d}x\mathrm{d}y$$
$$\le C_p \Delta^{-\theta p} \delta^{-2} \int_s^t \int_s^t \mathsf{E}\left[\frac{\left(\int_x^y |f(v) - f(u)|^2 \mathrm{d}v \right)^{p/2}}{|x-y|^{p/2}} \right] \mathrm{d}x\mathrm{d}y$$
$$\le C_p \Delta^{-\theta p} \delta^{-2} \mathsf{E}\left[\|f\|_{\theta}^p \right] \Delta^{p\theta} \delta^2 = C_p \mathsf{E}\left[\|f\|_{\theta}^p \right].$$

Hence, we arrive at the desired statement. □

We also need the result concerning the pathwise regularity property of X. It establishes certain exponential integrability of the Hölder seminorm of X, so it is an interesting result on its own.

Theorem 4 *Let* $\{X_t, t \in [0,T]\}$ *be the solution to* (4). *Assume that* a, b, c *satisfy the assumption* C1. *Then* $X \in C^{\theta}[0,T]$ *for* $\theta \in (0, 1/2)$ *and* $\mathsf{E}\left[\exp\left\{ K \|X\|_{\theta}^q \right\} \right] < \infty$ *for all* $q \in \big(0, q^*\big)$, $K > 0$, *where*

$$q^* = \frac{4H}{2(H+\theta)+1} \wedge \frac{2H+1}{4H}.$$

In particular, $\mathsf{E}\left[\|X\|_{\theta}^p \right] < \infty$ *for all* $p > 0$.

Proof Define for $\varepsilon \in (0, T]$

$$\|X\|_{\theta,\varepsilon} = \sup_{0\le t-\varepsilon\le s<t\le T} \frac{|X_t - X_s|}{(t-s)^\theta}.$$

Clearly, $\|X\|_\theta \le \|X\|_{\theta,\varepsilon} + 2\varepsilon^{-\theta}\|X\|_\infty$. It follows from [11, equation (4)] that

$$\|X\|_{\theta,\varepsilon} \le C_1\left(\left\|I^b\right\|_\theta + \Lambda_\mu\left(1 + \|X\|_\infty \varepsilon^{\mu-\theta}\right)\right),$$

for any $\varepsilon \in (0, C_2\Lambda_\mu^{-1/\mu}]$ where C_1, C_2 are some positive constants, $\mu \in (1/2, H)$, $\Lambda_\mu = \|B_H\|_\mu + 1$, $I_t^b = \int_0^t b(X_s)dW_s$. Therefore, setting $\varepsilon = C_2\Lambda_\mu^{-1/\mu}$, we obtain

$$\|X\|_\theta \le C_1\left(\left\|I^b\right\|_\theta + \Lambda_\mu + 2\|X\|_\infty \Lambda^{\theta/\mu}\right) \le C\left(\left\|I^b\right\|_\theta + \Lambda_\mu + \|X\|_\infty^{p'} + \Lambda^{q'\theta/\mu}\right),$$

where $p' > 1$, and $q' = p'/(p'-1)$ is the exponent conjugate to p'. Therefore,

$$\|X\|_\theta^q \le C\left(\left\|I^b\right\|_\theta^q + \Lambda_\mu^q + \|X\|_\infty^{p'q} + \Lambda^{qq'\theta/\mu}\right).$$

Evidently, $q^* < 1$, so it follows from [13, Lemma 1] that $\mathsf{E}\left[\exp\left\{K\left\|I^b\right\|_\theta^q\right\}\right] < \infty$ for all $K > 0$. Further, Λ_μ is an almost surely finite supremum of a centered Gaussian family, so by Fernique's theorem $\mathsf{E}\left[\exp\left\{K\Lambda_\mu^z\right\}\right] < \infty$ for any $K > 0$, $z \in (0, 2)$. Finally, by [11, Corollary 4], $\mathsf{E}\left[\exp\left\{K\|X\|_\infty^z\right\}\right] < \infty$ for all $K > 0, z < 4H/(2H+1)$. Now if $p' > 1$ is close to $4Hq^{-1}(2H+1)^{-1}$ (thanks to the bound on q such choice is possible) and μ is close to H, then q' is close to $4H/(4H - q(2H+1))$, and $qq'\theta/\mu$ is close to $4q\theta/(4H - q(2H+1))$, which is less than 2. Indeed, the last statement is equivalent to $q(2\theta + 2H + 1) < 4H$, which is true thanks to the restriction on q. Thus, we get the desired integrability. □

The following result is a Norris type lemma for mixed SDEs. It is a crucial result to prove existence of density under the Hörmander condition. Loosely speaking, this statement says that if

$$Y_t = Y_0 + \int_0^t a(s)\mathrm{d}s + \int_0^t b(s)\mathrm{d}W_s + \int_0^t c(s)\mathrm{d}B_s^H, \tag{9}$$

$\|Y\|_\infty = \|Y\|_{\infty;[0,T]}$ is small, then $\|b\|_\infty$ and $\|c\|_\infty$ can not be large. This means that the integral w.r.t. W and w.r.t. B^H can not compensate each other well. The rigorous formulation is as follows.

Theorem 5 *Assume that* $H \in (1/2, 2/3)$, $\theta \in (\theta_*, 1/2)$, *where*

$$\theta_* = \frac{H - \frac{1}{2}}{3 - 4H},$$

and that a, b, c *in* (9) *are* $\mathbf{F}$*-adapted processes satisfying* $\mathsf{E}\left[\|a\|_\infty^p + \|b\|_\theta^p + \|c\|_\theta^p \right] < \infty$ *for all* $p \geq 1$. *Then exists* $q > 0$ *such that for all* $p \geq 1, \varepsilon > 0$

$$\mathsf{P}\left\{ \|Y\|_\infty < \varepsilon \text{ and } \|b\|_\infty + \|c\|_\infty > \varepsilon^q \right\} \leq C_p \varepsilon^p.$$

Proof Here we imitate the proof of in [1, Proposition 3.4]. For notational simplicity, we assume that $T = 1$. For some positive integers M and r denote $\Delta = 1/M$, $\delta = \Delta/r$ and define the following uniform partitions of $[0, 1]$: $T_N = N\delta$, $N = 0, \ldots, M$; $t_n = \delta n$, $n = 0, \ldots, Mr$. Further, fix some $\breve{H} \in (1/2, H)$ and write for $N = 0, \ldots, M-1$, $n = Nr, \ldots, (N+1)r - 1$ (so that $t_n \in [T_N, T_{N+1})$), $i = 1, \ldots, d$

$$\begin{aligned} &\left\langle c_i(T_N), B^H_{t_{n+1}} - B^H_{t_n} \right\rangle + \left\langle b_i(T_N), W_{t_{n+1}} - W_{t_n} \right\rangle \leq |Y^i_{t_{n+1}} - Y^i_{t_n}| + \delta \|a\|_\infty \\ &\quad + \left| \int_{t_n}^{t_{n+1}} \langle b_i(s) - b_i(T_N), \mathrm{d}W_s \rangle \right| + \left| \int_{t_n}^{t_{n+1}} \langle c_i(s) - c_i(T_N), \mathrm{d}B^H_s \rangle \right| \qquad (10) \\ &\quad \leq 2 \|Y\|_\infty + \delta \|a\|_\infty + C\Delta^\theta \delta^{\breve{H}} \|c\|_\theta \left\|B^H\right\|_{\breve{H}} + \Delta^\theta \delta^{1/2} \xi_{\Delta,\delta} =: S, \end{aligned}$$

where in the last step we have used the Young–Love inequality (see e.g. [9, Proposition 1]) and Lemma 3.

For processes ξ, ζ denote

$$V_N(\xi, \zeta) = \sum_{n=Nr}^{(N+1)r-1} \left(\xi_{t_{n+1}} - \xi_{t_n}\right)\left(\zeta_{t_{n+1}} - \zeta_{t_n}\right); \qquad (11)$$

we remind that the summation is in fact over $t_n \in [T_N, T_{N+1})$. Squaring the both sides of (10), summing over $n = Nr, \ldots, (N+1)r - 1$ and then taking the square root we get

$$\begin{aligned} &\Bigg(\sum_{u,v=1}^m b_{i,u}(T_N) b_{i,v}(T_N) V_N(W^u, W^v) + \sum_{u,v=1}^l c_{i,u}(T_N) c_{i,v}(T_N) V_N(B^{H,u}, B^{H,v}) \qquad (12) \\ &\quad + \sum_{u=1}^m \sum_{v=1}^l b_{i,u}(T_N) c_{i,v}(T_N) V_N(W^u, B^{H,v}) \Bigg)^{1/2} \leq C\Delta^{1/2}\delta^{-1/2} S. \qquad (13) \end{aligned}$$

Therefore,

$$\begin{aligned}
&\sum_{u=1}^{m} |b_{i,u}(T_N)|\, V_N(W^u, W^u)^{1/2} + \sum_{v=1}^{l} |c_{i,v}(T_N)|\, V_N(B^{H,v}, B^{H,v}) \\
&\quad \le C\Bigg(\sum_{1\le u<v\le m} |b_{i,u}(T_N)|^{1/2} |b_{i,v}(T_N)|^{1/2} |V_N(W^u, W^v)|^{1/2} \\
&\qquad + \sum_{1\le u<v\le l} |c_{i,u}(T_N)|^{1/2} |c_{i,v}(T_N)|^{1/2} |V_N(B^{H,u}, B^{H,v})|^{1/2} \\
&\quad + \sum_{u=1}^{m}\sum_{v=1}^{l} |b_{i,u}(T_N)|^{1/2} |c_{i,v}(T_N)|^{1/2} |V_N(W^u, B^{H,v})|^{1/2} + \Delta^{1/2}\delta^{-1/2} S\Bigg).
\end{aligned} \tag{14}$$

Further, for arbitrary $f \in C^\theta[0,1]$,

$$\left| \Delta \sum_{N=0}^{M-1} |f(T_N)| - \|f\|_{L^1[0,1]} \right| \le \|f\|_\theta \, \Delta^\theta,$$

which yields

$$\begin{aligned}
&\sum_{u=1}^{m} \|b_{i,u}\|_{L^1[0,1]} + \sum_{v=1}^{l} \|c_{i,v}\|_{L^1[0,1]} \\
&\le \sum_{u=1}^{m} \left(\Delta^\theta \|b_{i,u}\|_\theta + \Delta \sum_{N=0}^{M-1} |b_{i,u}(T_N)| \right) + \sum_{v=1}^{l} \left(\Delta^\theta \|c_{i,v}\|_\theta + \Delta \sum_{N=0}^{M-1} |c_{i,v}(T_N)| \right) \\
&\le \sum_{u=1}^{m} \Bigg(\Delta^\theta \|b\|_\theta + \Delta^{1/2} \|b\|_\infty \sum_{N=0}^{M-1} \left| \Delta^{1/2} - V_N(W^u, W^u)^{1/2} \right| \\
&\qquad + \Delta^{1/2}\delta^{1/2-H} \sum_{N=0}^{M-1} |b_{i,u}(T_N)|\, V_N(W^u, W^u)^{1/2} \Bigg) \\
&\quad + \sum_{v=1}^{l} \Bigg(\Delta^\theta \|c\|_\theta + \Delta^{1/2}\delta^{1/2-H} \|c\|_\infty \sum_{N=0}^{M-1} \left| \Delta^{1/2}\delta^{H-1/2} - V_N(B^{H,v}, B^{H,v})^{1/2} \right| \\
&\qquad + \Delta^{1/2}\delta^{1/2-H} \sum_{N=0}^{M-1} |c_{i,v}(T_N)|\, V_N(B^{H,v}, B^{H,v})^{1/2} \Bigg).
\end{aligned}$$

Therefore, using (14), we arrive at

$$\begin{aligned}
\|b\|_{L^1[0,1]} + \|c\|_{L^1[0,1]} &\le C\Bigg(\Delta^{\theta}\big(\|b\|_{\theta} + \|c\|_{\theta} \big) \\
&+ \Delta^{1/2}\delta^{1/2-H} \|b\|_{\infty} \sum_{N=0}^{M-1} \sum_{u,v=1}^{m} \left| \Delta^{1/2}\delta_{u,v} - |V_N(W^u, W^v)|^{1/2} \right| \\
&+ \Delta^{1/2}\delta^{1/2-H} \|c\|_{\infty} \sum_{N=0}^{M-1} \sum_{u,v=1}^{l} \left| \Delta^{1/2}\delta^{H-1/2}\delta_{u,v} - \left| V_N(B^{H,u}, B^{H,v}) \right|^{1/2} \right| \\
&+ \Delta^{1/2}\delta^{1/2-H} \|c\|_{\infty}^{1/2} \|b\|_{\infty}^{1/2} \sum_{N=0}^{M-1} \sum_{u=1}^{m} \sum_{v=1}^{l} \left| V_N(W^u, B^{H,v}) \right|^{1/2} + \delta^{-H} S \Bigg) \\
&\le C\Bigg(\|b\|_{\theta} + \|c\|_{\theta} + \Delta^{-1/4}\delta^{3/4-H} \|b\|_{\infty} R^W \\
&+ \Delta^{H-1}\delta^{1-H} \|c\|_{\infty} R^B + \Delta^{-1/4}\delta^{(1-H)/2} \left(\|c\|_{\infty} + \|b\|_{\infty} \right) R^{W,B} + \delta^{-H} S \Bigg),
\end{aligned}$$

where

$$\begin{aligned}
R^W &= \Delta^{3/4}\delta^{-1/4} \sum_{N=0}^{M-1} \sum_{u,v=1}^{m} \left| \Delta^{1/2}\delta_{u,v} - |V_N(W^u, W^v)|^{1/2} \right|, \\
R^B &= \Delta^{H-3/2}\delta^{1/2} \sum_{N=0}^{M-1} \sum_{u,v=1}^{l} \left| \Delta^{1/2}\delta^{H-1/2}\delta_{u,v} - \left| V_N(B^{H,u}, B^{H,v}) \right|^{1/2} \right|, \qquad (15) \\
R^{W,B} &= \Delta^{3/4}\delta^{-H/2} \sum_{N=0}^{M-1} \sum_{u=1}^{m} \sum_{v=1}^{l} \left| V_N(W^u, B^{H,v}) \right|^{1/2}.
\end{aligned}$$

Further we use the following interpolation inequality, valid for any $f \in C^{\theta}[0,1]$ and $\gamma < 1$:

$$\|f\|_{\infty} \le C\big(\gamma \|f\|_{\theta} + \gamma^{-1/\theta} \|f\|_{L^1[0,1]} \big).$$

for any $\gamma \le 1$. Thus,

$$\|b\|_\infty + \|c\|_\infty \le C\big(\|b\|_\theta + \|c\|_\theta\big)\gamma + C\gamma^{-1/\theta}\Big(\big(\|b\|_\theta + \|c\|_\theta\big)\Delta^\theta$$
$$+(\|b\|_\infty + \|c\|_\infty)\Big[\Delta^{-1/4}\delta^{3/4-H}R^W + \Delta^{H-1}\delta^{1-H}R^B + \Delta^{-1/4}\delta^{(1-H)/2}R^{W,B}\Big]$$
$$+\delta^{-H}\|Y\|_\infty + \delta^{1-H}\|a\|_\infty + \Delta^\theta\delta^{\check{H}-H}\|c\|_\theta\left\|B^H\right\|_{\check{H}} + \Delta^\theta\delta^{1/2-H}\xi_{\Delta,\delta}\Big). \tag{16}$$

Now we want to put

$$\Delta^\beta \sim \varepsilon^\beta, \delta \sim \varepsilon^\alpha, \gamma \sim \varepsilon^\eta, \alpha > \beta > 0, \eta > 0,$$

so that in the right-hand side of (16), the exponents of ε are positive for all terms except $\|Y\|_\infty$. Since $(H-1/2)/\theta \le (3-4H) < 1$, it is possible to take $\beta/\alpha \in \big((H-1/2)/\theta, (3-4H)\big)$ so that both $\theta\beta + (1/2-H)\alpha$ and $-\beta/4 + (3/4-H)\alpha$ are positive. Also $(H-1)\beta + (1-H)\alpha = (1-H)(\alpha-\beta) > 0$, $-\beta/4 + (1-H)\alpha/2 > -\beta/4 + (3/4-H)\alpha > 0$, $\theta\beta + (\check{H}-H)\alpha > \theta\beta + (1/2-H)\alpha > 0$. Therefore, by choosing η small enough we can make all needed exponents positive.

Thus, for some $\kappa > 0$ and $C_1 > 0$ we have

$$\|b\|_\infty + \|c\|_\infty \le C_1\|Y\|_\infty\varepsilon^{-\lambda} + C_1\varepsilon^\kappa\Big((\|b\|_\infty + \|c\|_\infty)\big[R^W + R^B + R^{W,B}\big]$$
$$+ \|b\|_\theta + \|c\|_\theta + \|a\|_\infty + \|c\|_\theta\left\|B^H\right\|_{\check{H}} + \xi_{\Delta,\delta}\Big),$$

where $\lambda = H\alpha + \eta/\theta$. Consequently, for ε small enough

$$\mathsf{P}\left\{\|b\|_\infty + \|c\|_\infty > \varepsilon^{\kappa/2} \text{ and } \|Y\|_\infty < \varepsilon^{\lambda+\kappa}\right\}$$
$$\le \mathsf{P}\left\{R^W \ge \varepsilon^{-\kappa/3}\right\} + \mathsf{P}\left\{R^B \ge \varepsilon^{-\kappa/3}\right\} + \mathsf{P}\left\{R^{W,B} \ge \varepsilon^{-\kappa/3}\right\}$$
$$+\mathsf{P}\left\{\|b\|_\theta + \|c\|_\theta + \|c\|_\theta\left\|B^H\right\|_{\check{H}} + \xi_{\Delta,\delta} \ge \varepsilon^{-\kappa/3}\right\}.$$

Now the statement follows by applying Lemmas 3 and 6 and the Chebyshev inequality. □

Lemma 6 *Let R^W, R^B and $R^{W,B}$ be given by (15) and (11). Then we have for any $h > 1$ the following concentration inequalities*

$$\mathsf{P}\left\{R^W \ge h\right\} \le \frac{C}{\Delta}\exp(-Ch^2), \tag{17}$$

$$\mathsf{P}\left\{R^B \ge h\right\} \le \frac{C}{\Delta}\exp(-Ch^2), \tag{18}$$

$$\mathsf{P}\left\{R^{W,B} \ge h\right\} \le \frac{C}{\Delta}\exp(-Ch^2). \tag{19}$$

Proof By [1, Lemma 3.1] we have for $h > 0$

$$\mathsf{P}\left\{\left|\Delta^{1/2} - V_N(W^u, W^u)^{1/2}\right|\Delta^{-1/4}\delta^{-1/4} \geq h\right\} \leq C\exp\left(-Ch^2\right). \tag{20}$$

Further, let $u \neq v$. Since W^u and W^v are independent, and W^v has independent increments, then conditional on W^v, $V_N(W^w, W^u)\Delta^{-1/2}\delta^{-1/2}$ has a centered Gaussian distribution with the variance $V_N(W^v, W^v)\Delta^{-1}$. Therefore,

$$\begin{aligned}
&\mathsf{P}\left\{|V_N(W^u, W^v)|^{1/2}\Delta^{-1/4}\delta^{-1/4} \geq h\right\} \\
&= \mathsf{E}\left[\,\mathsf{P}\left\{|V_N(W^u, W^v)|\Delta^{-1/2}\delta^{-1/2} \geq h^2\right\} \,\middle|\, W^v\,\right] \leq C\,\mathsf{E}\left[\exp\left\{-\frac{h^4\Delta}{4V_N(W^v, W^v)}\right\}\right] \\
&\leq C\exp\left\{-\frac{h^4\Delta}{4(\Delta^{1/2} + v)^2}\right\} + \mathsf{P}\left\{\left|\Delta^{1/2} - V_N(W^v, W^v)^{1/2}\right| \geq v\right\} \\
&\leq C\exp\left\{-\frac{h^4\Delta}{8(\Delta + v^2)}\right\} + C\exp\left\{-C\frac{v^2}{\Delta^{1/2}\delta^{1/2}}\right\},
\end{aligned}$$

where we have used (20). Setting $v^2 = h^2\Delta$ and recalling that $\Delta \geq \delta$ we get

$$\mathsf{P}\left\{|V_N(W^u, W^v)|^{1/2}\Delta^{-1/4}\delta^{-1/4} \geq h\right\} \leq C\exp\left(-Ch^2\right).$$

Combining this with (20), we get

$$\begin{aligned}
\mathsf{P}\left\{R^W \geq h\right\} &\leq \sum_{N=0}^{M-1}\sum_{u,v=1}^{m}\mathsf{P}\left\{\Delta^{-1/4}\delta^{-1/4}\left|\Delta^{1/2}\delta_{u,v} - |V_N(W^u, W^v)|^{1/2}\right| \geq hm^2\right\} \\
&\leq \frac{C}{\Delta}\exp\left\{-Ch^2\right\}.
\end{aligned}$$

Using the inequalities from [1, Lemma 3.2] and repeating the last step, we get (18).

The estimate (19) is proved similarly to (17), so we omit some details. Write

$$\begin{aligned}
&\mathsf{P}\left\{|V_N(W^u, B^{H,v})|^{1/2}\Delta^{-1/4}\delta^{-H/2} \geq h\right\} \\
&= \mathsf{E}\left[\,\mathsf{P}\left\{|V_N(W^u, B^{H,v})|\Delta^{-1/2}\delta^{-H} \geq h^2\right\} \,\middle|\, B^{H,v}\,\right] \leq C\,\mathsf{E}\left[\exp\left\{-\frac{h^4\Delta\delta^{2H-1}}{4V_N(B^{H,v}, B^{H,v})}\right\}\right] \\
&\leq C\exp\left\{-\frac{h^4\Delta\delta^{2H-1}}{4(\Delta^{1/2}\delta^{H-1/2} + v)^2}\right\} + \mathsf{P}\left\{\left|\Delta^{1/2}\delta^{H-1/2} - V_N(B^{H,v}, B^{H,v})^{1/2}\right| \geq v\right\} \\
&\leq C\exp\left\{-\frac{h^4\Delta\delta^{2H-1}}{8(\Delta\delta^{2H-1} + v^2)}\right\} + C\exp\left\{-C\frac{v^2}{4\Delta^{2H-1}\delta}\right\}.
\end{aligned}$$

Setting $v^2 = h^2 \Delta \delta^{2H-1}$ and taking into account that $\Delta \geq \delta$, we arrive at

$$\mathsf{P}\left\{|V_N(W^u, B^{H,v})|^{1/2} \Delta^{-1/4} \delta^{-H/2} \geq h\right\} \leq C \exp\left\{-Ch^2\right\}.$$

From here (19) is deduced similarly to (17). □

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