Infinite-dimensional moment-SOS hierarchy for nonlinear partial differential equations

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December 12, 2024

Abstract

We formulate a class of nonlinear evolution partial differential equations (PDEs) as linear optimization problems on moments of positive measures supported on infinite-dimensional vector spaces. Using sums of squares (SOS) representations of polynomials in these spaces, we can prove convergence of a hierarchy of finite-dimensional semidefinite relaxations solving approximately these infinite-dimensional optimization problems. As an illustration, we report on numerical experiments for solving the heat equation subject to a nonlinear perturbation.

1 Introduction

The *moment-sum-of-squares (SOS) hierarchy* is a mathematical technology that consists of formulating a nonconvex nonlinear mathematical problem as a linear convex optimization problem on the cone of positive measures, and then solving approximately the infinite-dimensional linear problem on measures by a hierarchy of finite-dimensional convex (and typically semidefinite) optimization problems called moment relaxations. This hierarchy builds on the duality between the cone of positive moments and the cone of positive polynomials, and its convergence relies on SOS representations of positive polynomials. See [18] for a recent overview and applications.

The moment-SOS hierarchy, also known as the Lasserre hierarchy, [29, 20] was originally used in the early 2000s to solve globally finite-dimensional polynomial optimization problems [33], and then it was extended to optimal control of nonlinear ordinary differential equations [31, 21, 19]. It was later on extended to optimal control of linear partial differential equations

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(PDEs) [34]. More recently, it was further extended to nonlinear PDEs, for scalar hyperbolic conservation laws [37] as well as in a more general semialgebraic setting [28].

The approach followed in [37, 28] consists of introducing linear optimization problems with measure-valued solutions, with the aim that the measures are concentrated on the solution of the PDE. Concentration is achieved for scalar hyperbolic conservation laws using additional linear entropy inequalities [37]. In the more general setting of [28], concentration cannot be ensured, and there may be a relaxation gap between the nonlinear PDE and the linear problem on measures, unless the problem is convex [17].

Prior to these recent attempts, in [39] the authors discretized nonlinear PDEs in the time and space domain, producing a large-scale but sparse non-convex polynomial optimization problem that can be solved with the sparse moment-SOS hierarchy [46, 35]. In [34] the authors focused on the optimal control of linear evolution PDEs with Riesz spectral operators, i.e., with a discrete real spectrum. In this setting, the infinite-dimensional evolution equation was discretized and approximated with a finite-dimensional ordinary differential equation, and the standard finite-dimensional moment-SOS hierarchy is applied as in [31, 21, 19].

In this paper we follow a radically different route to solving nonlinear PDEs with the moment-SOS hierarchy. We use measures supported on infinite-dimensional vector spaces to formulate the nonlinear PDE as a moment problem. The vector space is chosen such that, on the one hand, we have a representation theorem to deal with the corresponding infinite-dimensional moment problem, and on the other hand, we can numerically solve the infinite-dimensional problem with finite-dimensional sections of the semidefinite cone. As a result, approximated moments (also called pseudo-moments) of the measure solution are obtained at the price of solving a hierarchy of semidefinite optimization problems of increasing size. If the linear moment problem has a unique solution, then we can prove that our pseudo-moments converge to it.

Measures supported on infinite-dimensional spaces can be used to formulate nonlinear PDEs as linear transport problems, but so far there has been very few attempts to deal numerically with these objects. Statistical solutions of nonlinear PDEs are modeled by measures on infinite-dimensional spaces, see [11] for Navier-Stokes equations and [9] for systems of hyperbolic conservation laws. The need for statistical solutions in numerical implementations is substantiated in [8, 10], also through concrete numerical computations. There is the potential of applying moment-SOS techniques in this context, as reported in the recent work [42], which presents itself as an infinite-dimensional extension of the finite-dimensional setup of [45] without attempting numerical implementation. While there are documented attempts to solve nonlinear PDEs with the finite-dimensional moment-SOS hierarchy, see e.g., [47, 13, 37, 28] and references therein, we are still missing a systematic extension to the infinite-dimensional setup.

The purpose of this paper is to fill this gap and to settle the ground for a genuine, systematic application of the moment-SOS hierarchy to numerically solve nonlinear PDEs as linear optimization problems on measures supported on infinite-dimensional spaces.

The outline of our paper is as follows. In Section 2 we introduce our functional analytic setting and the class of nonlinear evolution PDEs we consider. Then we describe our three step infinite-dimensional moment-SOS hierarchy approach:

Step 1 - *Reformulation*: we express in Section 3 the nonlinear PDE as a linear equation on an occupation measure supported on the solution. Under the assumption of non relaxation gap, this provides us with an equivalent linear reformulation of the nonlinear PDE. In turn, the linear measure equation is reformulated as a linear equation satisfied by the moment functions of the occupation measure;

Step 2 - *Representation*: in Section 4, positivity and analyticity conditions are enforced on the moment functions so that they uniquely represent the occupation measure. This allows for a mathematically sound application of the moment-SOS hierarchy;

Step 3 - *Implementation*: we use approximation properties of our solution space to formulate our moment function conditions in terms of scalar valued moments in Section 5.

This allows us to numerically approximate the solution of the nonlinear PDE as closely as desired at the price of solving a family of convex semidefinite optimization problems of increasing size, as explained in Section 5.2. In Section 6 we illustrate in detail our approach in the case of the heat equation, a well-studied evolution PDE. We start with the linear heat equation, so that we can check consistency of the numerical solution with the known analytic solution. Then we introduce quadratic nonlinear perturbations and we illustrate that the numerics behave consistently.

2 Nonlinear evolution PDE

Let $\mathcal{H}$ be a topological vector space of real valued functions in a real variable and let us denote by $\mathcal{H}'$ the topological dual of $\mathcal{H}$. Let $\mathcal{H}_0$ be a linear subspace of $\mathcal{H}$ endowed with a topology that makes the inclusion of $\mathcal{H}_0$ in $\mathcal{H}$ continuous and let $F : \mathcal{H}_0 \to \mathcal{H}_0$ be a continuous operator.

We consider the following PDE:

$$\frac{\partial u(t,x)}{\partial t} = F(u(t,x)), \quad t \in [0,1], \quad x \in [-\pi,\pi], \tag{1}$$

with given initial condition

$$u(0,.) = u_0 \in \mathcal{H}_0$$

and periodic boundary condition

$$u(t,-\pi) = u(t,\pi).$$

Let $\mathbb{T} := \mathbb{R}/2\pi\mathbb{Z}$ denote the torus, i.e., the interval $[-\pi,\pi]$ with identified end points. Here for each $t \in [0,1]$, the function $u(t,\cdot) : \mathbb{T} \to \mathbb{R}\,, x \mapsto u(t,x)$ belongs to $\mathcal{H}_0$.

Typical choices for $\mathcal{H}$ and $\mathcal{H}_0$ are the space of periodic distributions on $\mathbb{T}$ and a Sobolev space on $\mathbb{T}$, respectively.

The operator F is a polynomial function of u, its derivatives and integrals w.r.t. x. Typical examples are the viscous Burgers operator

$$F(u(t,x)) = -\frac{1}{2}\frac{\partial(u(t,x)^2)}{\partial x} + \varepsilon\frac{\partial^2 u(t,x)}{\partial x^2}$$

or the heat operator with a distributed nonlinearity

$$F(u(t,x)) = \frac{\partial^2 u(t,x)}{\partial x^2} + \varepsilon \int_T u(t,x) f_1(x) dx \int_T u(t,x) f_2(x) dx$$

for given $\varepsilon > 0$, $f_1 \in \mathcal{H}'$, $f_2 \in \mathcal{H}'$. More details on the choice of F will follow in Section 3.

Denoting by $\mathbf{u}$ the function $[0,1] \to \mathcal{H}_0$, $t \mapsto u(t,\cdot)$, we view PDE (1) as an *infinite-dimensional evolution equation*:

$$\frac{d\mathbf{u}(t)}{dt} = F(\mathbf{u}(t)). \tag{2}$$

Throughout the paper we assume that this equation has a well-defined unique solution.

Assumption 1 (Existence and uniqueness) *Given $u_0 \in \mathcal{H}_0$, evolution equation (2) has a unique solution $\mathbf{u} \in \mathcal{C}^1([0,1];\mathcal{H}_0)$ with $\mathbf{u}(0) = u_0$.*

3 Reformulation

3.1 Linear measure equation

Consider the time-dependent Dirac measure $\mu_t = \delta_{\mathbf{u}(t)}$ supported on the solution $\mathbf{u}$ of (2) and let $\phi\colon [0,1] \times \mathcal{H} \to \mathbb{R}$ be a test function in $\mathcal{C}^\infty([0,1] \times \mathcal{H}; \mathbb{R})$. Since $\mu_0 = \delta_{\mathbf{u}(0)}$ and $\mu_1 = \delta_{\mathbf{u}(1)}$, on the one hand we have

$$\int_0^1 \frac{d}{dt}\phi(t,\mathbf{u}(t))\,dt = \phi(1,\mathbf{u}(1)) - \phi(0,\mathbf{u}(0)) = \int_{\mathcal{H}} \phi(1,h)\,d\mu_1(h) - \int_{\mathcal{H}} \phi(0,h)\,d\mu_0(h). \tag{3}$$

On the other hand, using first the chain rule and then the fact that $\mu_t = \delta_{\mathbf{u}(t)}$, we obtain

$$\begin{aligned} \int_0^1 \frac{d}{dt}\phi(t,\mathbf{u}(t))\,dt &= \int_0^1 \left(\frac{\partial \phi}{\partial t}(t,\mathbf{u}(t)) + \frac{\partial \phi}{\partial h}(t,\mathbf{u}(t)) \frac{d}{dt}\mathbf{u}(t) \right) dt \\ &= \int_0^1 \int_{\mathcal{H}} \left(\frac{\partial \phi}{\partial t}(t,h) + \frac{\partial \phi}{\partial h}(t,h) F(h) \right) d\mu_t(h)\,dt, \end{aligned} \tag{4}$$

where $\frac{\partial \phi}{\partial h}$ is the Fréchet derivative of ϕ with respect to $h \in \mathcal{H}$, which is a linear functional on $\mathcal{H}$, and $\frac{d}{dt}\mathbf{u}(t) = \frac{\partial u}{\partial t}(t,x) = F(\mathbf{u}(t))$ by (2).

Comparing (3) and (4), we get the following linear measure reformulation of (2)

$$\int_{\mathcal{H}} \phi(1,h)\,d\mu_1(h) - \int_{\mathcal{H}} \phi(0,h)\,d\mu_0(h) = \int_0^1 \int_{\mathcal{H}} \left(\frac{\partial \phi}{\partial t}(t,h) + \frac{\partial \phi}{\partial h}(t,h) F(h) \right) d\mu_t(h)\,dt, \tag{5}$$

for any test function $\phi \in \mathcal{C}^\infty([0,1] \times \mathcal{H}; \mathbb{R})$. We therefore proved the following result.

Theorem 1 *Let $\mathbf{u} \in \mathcal{C}^1([0,1];\mathcal{H}_0)$ be a solution to evolution equation (2), then the measure $\mu_t = \delta_{\mathbf{u}(t)}$ on $\mathcal{H}_0$ satisfies linear equation (5). Conversely, if $\mu_t = \delta_{\mathbf{v}(t)}$ satisfies (5) for some $\mathbf{v} \in \mathcal{C}^1([0,1];\mathcal{H}_0)$, then setting $\mathbf{u} := \mathbf{v}$ gives a solution $\mathbf{u}$ of (2).*

The measure μ_t is referred to as *Young measure*, or parametrized measure. This class of measures is widely studied in convex relaxations of nonlinear calculus of variations and optimal control problems, see e.g. [48], [43] or [7, Part III]. The measure $dt\, d\mu_t$ is called *occupation measure*, because it measures the time a trajectory occupies a given set. It is classically used in Markov decision processes and dynamical systems, as well as, for the application of the moment-SOS hierarchy to nonlinear optimization and control problems, see e.g., [31, 21, 19, 34, 37, 18, 28, 17].

3.2 No relaxation gap

Theorem 1 establishes that a measure supported on a solution of evolution equation (2) solves linear equation (5). However, it may happen that a measure solving the linear equation (5) is not supported on a function in $\mathcal{C}^1([0,1];\mathcal{H}_0)$ and so not on a solution of evolution equation (2). To preclude this situation, we make the following assumption.

Assumption 2 (No relaxation gap) *Linear equation* (5) *with given initial data* $\mu_0 = \delta_{\mathbf{u}(0)}$ *has a unique solution* $\mu_t = \delta_{\mathbf{u}(t)}$.

Under Assumptions 1 and 2, it follows from Theorem 1 that the solution of linear equation (5) with given initial data $\mu_0 = \delta_{\mathbf{u}(0)}$ is concentrated on the solution of evolution equation (2) with $\mathbf{u}(0) = u_0$. In other words, solving (5) solves (2). If we cannot ensure Assumption 2 a priori, we can enforce the absence of a relaxation gap by one of the following approaches:

- formulating the PDE as a convex minimization problem, see, e.g., [3];
- adding (linear or convex) conditions, e.g., entropy inequalities [37];
- assume that F is convex, or consider its convex envelope [17].

3.3 Linear moment equation

We proceed now to rewrite (5) as a linear equation on the moments of the occupation measure so to be able to exploit a recent result on the infinite-dimensional moment problem (see Section 4). To this purpose let us define the concept of moment function for a measure supported on $\mathbb{R} \times \mathcal{H}_0$ where $\mathcal{H}_0$ is a Hilbert space in $\mathcal{H}$. For this, we adapt to our setting the notion of polynomials and then of moment function given in [27, 22, 24]. The infinite-dimensional moment problem has also been studied, e.g., in [44], [2], [5], [1], the survey [23] and references therein.

Let $\mathscr{P}$ be the set of all polynomials in the variables $t \in \mathbb{R}$ and $h \in \mathcal{H}_0$ of the form

$$P(t,h) := \sum_{\ell=0}^{N} \sum_{k=0}^{M} \langle t^{\otimes \ell}, c_\ell \rangle \langle h^{\otimes k}, f^{(k)} \rangle, \tag{6}$$

where $c_\ell, f^{(0)} \in \mathbb{R}$ and $f^{(k)} \in (\overline{\mathcal{H}_0^{\otimes k}})'$, for $\ell = 0, \ldots, N$ and $k = 0, \ldots, M$ with $N, M \in \mathbb{N}$. Here $\langle \cdot, \cdot \rangle$ denotes the duality between the considered vector spaces and their corresponding dual spaces. By convention, for all $c \in \mathbb{R}$, we set $\langle t^{\otimes 0}, c \rangle = c$ and $\langle h^{\otimes 0}, c \rangle = c$.

Note that here all tensor products are intended to be symmetric and that, since $\mathcal{H}_0$ is a Hilbert space, the completed tensor product always corresponds to the Hilbert space tensor norm.

Definition 1 (Moment function) *Let $\ell, k \in \mathbb{N}$ and μ a Radon measure defined on $\mathbb{R} \times \mathcal{H}$ and supported on $\mathbb{R} \times \mathcal{H}_0$. We say that μ has* $(\ell, k)-$th continuous (w.r.t. $\mathcal{H}_0 \subseteq \mathcal{H}$) local moment *if*

$$\int_{\mathbb{R}\times\mathcal{H}} |\langle t, 1\rangle|^\ell |\langle h, f\rangle|^k d\mu(t,h) < \infty, \ \forall f \in \mathcal{H}', \tag{7}$$

and the functional $f \mapsto \int_{\mathbb{R}\times\mathcal{H}} |\langle t, 1\rangle|^\ell |\langle h, f\rangle|^k d\mu(t,h)$ on $\mathcal{H}'$ is continuous in the topology induced by $\mathcal{H}_0'$. In this case the $(\ell, k)-$th moment function *of μ is the symmetric continuous multilinear functional $m^\mu_{\ell,k}$ on $\mathbb{R}^{\otimes\ell} \oplus (\overline{\mathcal{H}_0^{\otimes k}})'$ (see discussion before [24, Definition 1.3]) such that*

$$\langle m^\mu_{\ell,k}, 1 \oplus f^{(k)}\rangle = \int_{\mathbb{R}\times\mathcal{H}} \langle t, 1\rangle^\ell \langle h^{\otimes k}, f^{(k)}\rangle d\mu(t,h), \ \forall f^{(k)} \in (\overline{\mathcal{H}_0^{\otimes k}})'. \tag{8}$$

By convention, $m^\mu_{0,0} := \mu(\mathbb{R} \times \mathcal{H}_0)$.

Notice that if $\mathcal{H}_0$ is a Banach space and the measure μ is supported in a bounded subset of $\mathbb{R} \times \mathcal{H}_0$ then it necessarily has continuous local moments.

Definition 2 (Determinacy) *A Radon measure μ defined on $\mathbb{R} \times \mathcal{H}$ and supported on $\mathbb{R} \times \mathcal{H}_0$ is said to be* determinate *if for any other Radon measure ν defined on $\mathbb{R} \times \mathcal{H}$ and supported on $\mathbb{R} \times \mathcal{H}_0$ such that $m^\mu_{\ell,k} = m^\nu_{\ell,k}$ for all $\ell, k \in \mathbb{N}$, it holds $\nu = \mu$.*

In (5) let us now consider the test function

$$\phi(t,h) := t^\ell \lambda_1(h) \cdots \lambda_k(h), \tag{9}$$

where $\lambda_1, \ldots, \lambda_k \in \mathcal{H}'$, and $\ell, k \in \mathbb{N}$. Note that, since the measures in (5) are assumed to fulfill (7), the integrals appearing in (5) are all finite.

If $\mathcal{H}$ is the space of periodic distributions on $\mathbb{T}$, then

$$\lambda_j(h) = \langle h, \psi_j\rangle = \int_{\mathbb{T}} h(x)\psi_j(x)\, dx, \tag{10}$$

where ψ_j are C^∞ periodic functions on $\mathbb{T}$.

The Frechet derivative of ϕ with respect to h at the point $g \in \mathcal{H}$ is given by

$$\frac{\partial \phi}{\partial h}(t,h)(g) = t^\ell \sum_{j=1}^k \lambda_1(h) \cdots \widehat{\lambda_j(h)} \cdots \lambda_k(h)\lambda_j(g) \tag{11}$$

where we used the notation

$$\lambda_1(h) \cdots \widehat{\lambda_j(h)} \cdots \lambda_k(h) := \frac{\prod_{i=1}^k \lambda_i(h)}{\lambda_j(h)}.$$

Substituting (9) and (11) into the linear equation (5), we get:

$$1^\ell \int_{\mathcal{H}} \lambda_1(h)\cdots\lambda_k(h)\,d\mu_1(h) - 0^\ell \int_{\mathcal{H}} \lambda_1(h)\cdots\lambda_k(h)\,d\mu_0(h)$$
$$= \int_0^1 \int_{\mathcal{H}} \ell t^{\ell-1}\lambda_1(h)\cdots\lambda_k(h)\,d\mu_t(h)\,dt$$
$$+ \int_0^1 \int_{\mathcal{H}} t^\ell \sum_{j=1}^{k} \lambda_1(h)\cdots\widehat{\lambda_j(h)}\cdots\lambda_k(h)\lambda_j(F(h))\,d\mu_t(h)\,dt. \quad (12)$$

Choosing λ_k as in (10), we obtain the linear equation:

$$1^\ell \int_{\mathcal{H}} \langle h,\psi_1\rangle\cdots\langle h,\psi_k\rangle\,d\mu_1(h) - 0^\ell \int_{\mathcal{H}} \langle h,\psi_1\rangle\cdots\langle h,\psi_k\rangle\,d\mu_0(h)$$
$$= \int_0^1 \int_{\mathcal{H}} \ell t^{\ell-1}\langle h,\psi_1\rangle\cdots\langle h,\psi_k\rangle\,d\mu_t(h)\,dt$$
$$+ \int_0^1 \int_{\mathcal{H}} t^\ell \sum_{j=1}^{k} \langle h,\psi_1\rangle\cdots\widehat{\langle h,\psi_j\rangle}\cdots\langle h,\psi_k\rangle\langle F(h),\psi_j\rangle\,d\mu_t(h)\,dt. \quad (13)$$

In order to formulate this equation as a linear equation on moment functions, we make the following standing assumption on the structure of the nonlinear operator F appearing in evolution equation (2).

Assumption 3 (Polynomial operator) *The operator $F : \mathcal{H}_0 \to \mathcal{H}_0$ is of the form*

$$F(h) = \sum_{s=0}^{N} F_s(h^{\otimes s}),$$

where each $F_s : \overline{\mathcal{H}_0^{\otimes s}} \to \mathcal{H}_0$ is continuous. In other words, each F_s can be seen as a homogeneous polynomial in $\mathscr{P}$ which is independent of t.

The second summand of linear equation (13) can then be written as:

$$\int_0^1 \int_{\mathcal{H}} t^\ell \sum_{j=1}^{k}\sum_{s=0}^{N} \langle h,\psi_1\rangle\cdots\widehat{\langle h,\psi_j\rangle}\cdots\langle h,\psi_k\rangle\langle F_s(h^{\otimes s}),\psi_j\rangle\,d\mu_t(h)\,dt$$
$$= \int_0^1 \int_{\mathcal{H}} t^\ell \sum_{j=1}^{k}\sum_{s=0}^{N} \langle h,\psi_1\rangle\cdots\widehat{\langle h,\psi_j\rangle}\cdots\langle h,\psi_k\rangle\langle h^{\otimes s}, F_s^*(\psi_j)\rangle\,d\mu_t(h)\,dt$$
$$= \int_0^1 \int_{\mathcal{H}} t^\ell \sum_{j=1}^{k}\sum_{s=0}^{N} \langle h^{\otimes k-1+s}, \psi_1\otimes\cdots\otimes\widehat{\psi_j}\otimes\cdots\psi_k\otimes F_s^*(\psi_j)\rangle\,d\mu_t(h)\,dt$$
$$= \sum_{j=1}^{k}\sum_{s=0}^{N} \langle m_{\ell,k-1+s}^{dt\mu_t}, \psi_1\otimes\cdots\otimes\widehat{\psi_j}\otimes\cdots\psi_k\otimes F_s^*(\psi_j)\rangle \quad (14)$$

where $F_s^* : \mathcal{H}_0' \to \overline{\mathcal{H}_0^{\otimes s}}$ denotes the adjoint of F_s. Hence, equation (13) becomes a linear equation on moment functions:

$$\langle m_{\ell,k}^{\delta_1\mu_1}, 1 \oplus (\psi_1 \otimes \cdots \otimes \psi_k)\rangle - \langle m_{\ell,k}^{\delta_0\mu_0}, 1 \oplus (\psi_1 \otimes \cdots \otimes \psi_k)\rangle =$$
$$\langle m_{\ell-1,k}^{dt\mu_t}, \ell \oplus (\psi_1 \otimes \cdots \otimes \psi_k)\rangle + \sum_{j=1}^{k}\sum_{s=0}^{N}\langle m_{\ell,k-1+s}^{dt\mu_t}, \psi_1 \otimes \cdots \otimes \widehat{\psi_j} \otimes \cdots \psi_k \otimes F_s^*(\psi_j)\rangle. \quad (15)$$

We just proved the following reformulation of Theorem 1.

Theorem 2 *Equation* (5) *always implies equation* (15)*. The converse holds provided the measures* $dt\, d\mu_t$*,* $\delta_1\, \mu_1$ *and* $\delta_0\, \mu_0$ *are determinate.*

4 Representation

So far, we have reformulated linear measure equation (5) as linear moment function equation (15). Theorem 2 states that the two equations are equivalent provided all the involved measures are determinate, i.e., they are uniquely determined by their moment functions. In this section, we consider the case when $\mathcal{H}$ is the space $\mathscr{D}(\mathbb{T})$ of periodic distributions on $\mathbb{T}$ and $\mathcal{H}_0$ is a Sobolev space $W_2^{-k}(\mathbb{T})$ (see below). In Theorem 3 we provide conditions on a sequence of multilinear functionals to be the moment functions of some measure and to ensure its determinacy.

In the following all the functions spaces are real vector spaces of real valued functions unless explicitly stated. The space $\mathcal{C}^\infty(\mathbb{T})$ can be constructed as the projective limit of Sobolev spaces $W_2^\alpha(\mathbb{T})$ for all $\alpha \in \mathbb{N}$ (see [12, Thm 9.0.1] and note that the torus is there defined as $\mathbb{R}/\mathbb{Z}$), where the Sobolev space $W_2^\alpha(\mathbb{T})$ is defined as the completion of $\mathcal{C}^\infty(\mathbb{T})$ w.r.t. the following norm (see e.g., [41, p.156-159])

$$\|\varphi\|_{W_2^\alpha(\mathbb{T})} := \left(\sum_{n\in\mathbb{Z}}(1+n^2)^\alpha \left|\frac{1}{\sqrt{2\pi}}\int_{\mathbb{T}}\varphi(x)e^{-inx}dx\right|^2\right)^{\frac{1}{2}}.$$

This construction induces a natural projective limit topology on $\mathcal{C}^\infty(\mathbb{T})$, which makes it a separable nuclear space, as by [38, Lemma 33] for any $\alpha \in \mathbb{N}$ there exists $\beta \in \mathbb{N}$ such that the embedding $W_2^\beta(\mathbb{T}) \hookrightarrow W_2^\alpha(\mathbb{T})$ is Hilbert-Schmidt. In fact, this holds for all $\beta > \alpha + \frac{1}{2}$. (This can be also derived by the more general results in [41, pp.162-172]). Let us denote by $\mathscr{D}(\mathbb{T})$ the space $\mathcal{C}^\infty(\mathbb{T})$ equipped with the projective limit topology, and let us denote its dual by $\mathscr{D}'(\mathbb{T})$. Then we can define $W_2^s(\mathbb{T})$ for any $s \in \mathbb{R}$ (see [12, Section 10]) as follows

$$W_2^s(\mathbb{T}) := \left\{f \in \mathscr{D}'(\mathbb{T}) : \|f\|_{W_2^s(\mathbb{T})} < \infty\right\}.$$

In the following we identify the dual of $W_2^s(\mathbb{T})$ with $W_2^{-s}(\mathbb{T})$.

Theorem 3 *Let* $m := (m_{\ell,k})_{\ell,k\in\mathbb{N}}$ *be such that each* $m_{\ell,k}$ *is a multilinear functional on* $\mathbb{R}^\ell \times (\mathcal{C}^\infty(\mathbb{T}))^k$ *symmetric in the first* ℓ *variables as well as in the second* k *variables. If*

1. $\sum_{\ell,k,\ell',k'} \langle m_{\ell+\ell',k+k'}, (c_\ell c_{\ell'}) \oplus (f^{(k)} \otimes f^{(k')})\rangle \geq 0,$

   $\sum_{\ell,k,\ell',k'} \langle m_{\ell+\ell'+1,k+k'} - m_{\ell+\ell'+2,k+k'}, (c_\ell c_{\ell'}) \oplus (f^{(k)} \otimes f^{(k')})\rangle \geq 0,$

   $\forall c_\ell, c_{\ell'} \in \mathbb{R}, f^{(k)} \in \mathcal{C}^\infty(\mathbb{T}^k), f^{(k')} \in \mathcal{C}^\infty(\mathbb{T}^{k'}),$

2. $$\sum_{\ell=1}^{\infty} \frac{1}{\sqrt[2\ell]{\langle m_{2\ell,0}, 1^{\otimes 2\ell} \oplus 0\rangle}} = \infty$$

   and there exists a countable total subset E of $\mathcal{C}^\infty(\mathbb{T})$ such that

   $$\sum_{k=1}^{\infty} \frac{1}{\sqrt[2k]{\langle m_{0,2k}, 0 \oplus f^{\otimes 2k}\rangle}} = \infty, \quad \forall\ f \in E,$$

3. *for each $\ell, k \in \mathbb{N}$, there exists $j_{\ell,k} \in \mathbb{N}$ such that $m_{\ell,k}$ is $\|\cdot\|^\ell \times \|\cdot\|^k_{W_2^{j_{\ell,k}}(\mathbb{T})}-$continuous,*

then there exists a unique Radon measure μ which is supported in $[0,1]\times W_2^{-\beta}(\mathbb{T}) \subseteq \mathbb{R}\times\mathscr{D}'(\mathbb{T})$ for some $\beta > \max\{j_{0,2}, j_{1,1}, j_{2,0}\} + \frac{1}{2}$, and whose sequence of moment functions is m.

Equivalently, if we denote by L_m the Riesz functional associated to the sequence m, i.e.,,

$$\begin{aligned} L_m : \quad \mathscr{P} \quad &\to \mathbb{R} \\ a(t,h) = \sum_{\ell=0}^{N}\sum_{k=0}^{M} \langle t^{\otimes\ell}, c_\ell\rangle\langle h^{\otimes k}, f^{(k)}\rangle \quad &\mapsto L_m(a) := \sum_{\ell=0}^{N}\sum_{k=0}^{M} \langle m_{\ell,k}, c_\ell \oplus f^{(k)}\rangle \end{aligned}$$

then the conditions of Theorem 3 can be written in the following more concise form as:

1. $L_m(a^2) \geq 0, L_m(b\,a^2) \geq 0,\ \forall a \in \mathscr{P},\ b(t,h) := \langle t^{\otimes 1}, 1\rangle(1 - \langle t^{\otimes 1}, 1\rangle)\langle h^{\otimes 0}, 1\rangle,$
2. $$\sum_{\ell=1}^{\infty} \frac{1}{\sqrt[2\ell]{L_m(\langle t^{\otimes 2\ell}, 1^{\otimes 2\ell}\rangle\langle h^{\otimes 0}, 0\rangle)}} = \infty$$

   and there exists a countable total subset E of $\mathcal{C}^\infty(\mathbb{T})$ such that

   $$\sum_{k=1}^{\infty} \frac{1}{\sqrt[2k]{L_m(\langle t^{\otimes 0}, 1\rangle\langle h^{\otimes 2k}, f^{\otimes 2k}\rangle)}} = \infty, \quad \forall\ f \in E,$$

3. for each $\ell, k \in \mathbb{N}$, there exist $j_{\ell,k} \in \mathbb{N}$ and $Q_{\ell,k} > 0$ such that

   $$\left|L_m(\langle t^{\otimes\ell}, c_\ell\rangle\langle h^{\otimes k}, f^{\otimes k)}\rangle)\right| \leq Q_{\ell,k}|c_\ell|\|f\|^k_{W_2^{j_{\ell,k}}(T)},\ \forall c_\ell \in \mathbb{R}, f \in \mathcal{C}^\infty(\mathbb{T}).$$

Proof: In [26, Theorem 3.3] the authors establish solvability conditions for the moment problem on the symmetric tensor algebra $S(V)$ of a nuclear space V and so for measures supported on the topological dual of V. Applying this general result for $V = \mathbb{R} \oplus \mathcal{C}^\infty(\mathbb{T})$ endowed with the product topology given by the euclidean topology on $\mathbb{R}$ and the projective topology on $\mathcal{C}^\infty(\mathbb{T})$ mentioned above, we obtain the desired conclusion. Note the $d-$th homogeneous component $S(V)_d$ of $S(V)$ is given by $S(V)_d = \bigoplus_{\ell+k=d} S(\mathbb{R})_\ell \otimes S(\mathcal{C}^\infty(\mathbb{T}))_k$. $\square$

Note that in Theorem 3-3 the boundedness is imposed for every $\ell, k \in \mathbb{N}$, while the support of the representing measure is contained in $[0,1] \times W_2^{-\beta}(\mathbb{T})$, i.e., the support is controlled by the bound for $\ell, k \in \mathbb{N}$ such that $\ell + k = 2$ (for further details see the proof of [26, Theorem 3.3-(4)]). Also notice that, since the support of the representing measure is in $[0,1] \times W_2^{-\beta}(\mathbb{T})$, the positivity conditions in Theorem 3-1 in the t variable are in accordance with the representability conditions in Hausdorff Theorem [14], i.e., a linear $L : \mathbb{R}[X] \to \mathbb{R}$ has a $[0,1]-$representing measure if and only if $L(p^2) \geq 0$ and $L(X(1-X)p) \geq 0$ for any $p \in \mathbb{R}[X]$.

5 Implementation

5.1 Discretization

Theorem 3 and linear equation (15) are formulated in terms of the moment functions. Now we proceed towards a computer implementation by replacing the moment functions by scalar valued moments. Note that in the following definition the moment functions are applied to complex valued test functions, resulting in complex valued functionals which are invariant under complex conjugation. It is straightforward that the complex version of Theorem 3 holds, where in condition 1 for the Riesz functional a^2 is replaced by $a\bar{a}$ and in condition 2 for the Riesz' functional $f^{\otimes 2k}$ is replaced by $f^{\otimes k} \otimes \bar{f}^{\otimes k}$.

Definition 3 (Moment) *Given a Radon measure μ on $\mathbb{R} \times \mathscr{D}'(\mathbb{T})$ with $(\ell, k)-$th continuous local moment for any $\ell, k \in \mathbb{N}$ and moment function sequence $m := (m^\mu_{\ell,k})_{\ell,k\in\mathbb{N}}$, its* moment *indexed by $\ell \in \mathbb{N}, n_1, \ldots, n_k \in \mathbb{Z}$ for $k \in \mathbb{N}$ is the complex number*

$$y^\mu_{\ell,n_1,\ldots,n_k} := \langle m^\mu_{\ell,k}, 1 \oplus (\psi_{n_1} \otimes \cdots \otimes \psi_{n_k}) \rangle = \int_{\mathbb{R}} \int_{\mathscr{D}'(\mathbb{T})} t^\ell \langle h, \psi_{n_1} \rangle \cdots \langle h, \psi_{n_k} \rangle \, d\mu(h,t) \qquad (16)$$

where the test functions $\psi_{n_j} \in \mathcal{C}^\infty(\mathbb{T}; \mathbb{C})$ are set to the complex exponentials

$$\psi_{n_j}(x) := \frac{1}{\sqrt{2\pi}} e^{-i\, n_j x}. \qquad (17)$$

By convention, for $k = 0$ we set $y^\mu_{\ell,n_1,\ldots,n_k} = y^\mu_{\ell,\emptyset}$.

This particular class of test functions is dense in $\mathcal{C}^\infty(\mathbb{T}; \mathbb{C})$. The complex exponentials are the eigenfunctions of the Laplacian operator on $\mathbb{T}$. There may be other choices more adapted to the other operators. For example, if the linear part of the polynomial operator F is a

second order differential operator (with appropriate self-adjoint boundary conditions), we can replace the complex exponentials by the eigenfunctions of the corresponding Sturm-Liouville problem.

In the above definition each

$$h_{n_j} := \langle h, \psi_{n_j} \rangle$$

is a Fourier coefficient of the periodic distribution h expressed with its Fourier series

$$h(x) = \frac{1}{\sqrt{2\pi}} \sum_{n \in \mathbb{Z}} h_n e^{\mathbf{i}nx}. \tag{18}$$

In the moment index $\ell, n_1, \ldots, n_k$, the integer ℓ is called the *time degree*, the integer k is called the *algebraic degree*, whereas the integer $\max_{j=1,\ldots,k} |n_j|$ is called the *harmonic degree*.

Notice that the moment sequence y satisfies the following symmetry properties:

$$\overline{y^{\mu}_{\ell,n_1,\ldots,n_k}} = y^{\mu}_{\ell,-n_1,\ldots,-n_k}, \tag{19}$$

$$y^{\mu}_{\ell,n_{\sigma(1)},\ldots,n_{\sigma(k)}} = y^{\mu}_{\ell,n_1,\ldots,n_k} \quad \forall \sigma \in S_k, \tag{20}$$

where the bar denotes the complex conjugate and S_k denotes the symmetric group, the set of all permutations of k elements.

More specifically, for our evolution problem we respectively call *initial moments*, *terminal moments*, and *occupation moments* the following scalar moments:

$$y^{0}_{\ell,n_1,\ldots,n_k} := y^{\delta_0 \mu_0}_{\ell,n_1,\ldots,n_k} = 0^{\ell} \int_{\mathscr{D}'(\mathbb{T})} h_{n_1} \cdots h_{n_k} \, d\mu_0(h), \tag{21}$$

$$y^{1}_{\ell,n_1,\ldots,n_k} := y^{\delta_1 \mu_1}_{\ell,n_1,\ldots,n_k} = 1^{\ell} \int_{\mathscr{D}'(\mathbb{T})} h_{n_1} \cdots h_{n_k} \, d\mu_1(h), \tag{22}$$

$$y^{[0,1]}_{\ell,n_1,\ldots,n_k} := y^{dt\mu_t}_{\ell,n_1,\ldots,n_k} = \int_0^1 t^{\ell} \int_{\mathscr{D}'(\mathbb{T})} h_{n_1} \cdots h_{n_k} \, d\mu_t(h) \, dt. \tag{23}$$

For each $s = 1, \ldots, N$, the adjoint homogeneous operator appearing in the linear moment function equation (15) takes the concrete form:

$$F^*_s(\psi_{n_j}) = \sum_{r_1,\ldots,r_s \in \mathbb{Z}} a^{s,j}_{r_1,\ldots,r_s} \psi_{r_1} \ldots \psi_{r_s} \tag{24}$$

for some $a^{s,j}_{r_1,\ldots,r_s} \in \mathbb{R}$ and $r_1, \ldots, r_s \in \mathbb{Z}$. With these notations, the linear moment function equation (15) becomes the linear moment equation:

$$y^{1}_{\ell,n_1,\ldots,n_k} - y^{0}_{\ell,n_1,\ldots,n_k} = \ell y^{[0,1]}_{\ell-1,n_1,\ldots,n_k} + \sum_{j=1}^{k} \sum_{s=0}^{N} \sum_{r_1,\ldots,r_s \in \mathbb{Z}} a^{s,j}_{r_1,\ldots,r_s} y^{[0,1]}_{\ell,n_1,\ldots,n_{j-1},r_1,\ldots,r_s,n_{j+1},\ldots,n_k} \tag{25}$$

where $\ell, k \in \mathbb{N}, n_1, \ldots, n_k \in \mathbb{Z}$.

Let us now reformulate the conditions on a sequence of moment functions $m := (m^{\mu}_{\ell,k})_{\ell,k \in \mathbb{N}}$ given by Theorem 3 in terms of the associated sequence $y := (y^{\mu}_{\ell,n_1,\ldots,n_k})_{\ell,k \in \mathbb{N}}$ of scalar moments.

Given $\ell \in \mathbb{N}$, let us construct the following Hermitian matrix

$$\mathbf{M}_\ell(y) := \left[y^\mu_{\ell,n_1,\ldots,n_k,-n'_1,\ldots,-n'_{k'}} \right]_{k,k' \in \mathbb{N}, n_1,\ldots,n_k,n'_1,\ldots,n'_{k'} \in \mathbb{Z}}.$$

Then consistently with [29, 30] or [18, Chapter 1] we define the *moment matrix*

$$\mathbf{M}(y) := [\mathbf{M}_{\ell+\ell'}(y)]_{\ell,\ell' \in \mathbb{N}}$$

and the *localizing matrix*

$$\mathbf{M}(t(1-t)y) = [\mathbf{M}_{\ell+\ell'+1}(y) - \mathbf{M}_{\ell+\ell'+2}(y)]_{\ell,\ell' \in \mathbb{N}}.$$

Then the positivity conditions Theorem 3-1 for the choice of test functions in (17) become the positive semidefiniteness conditions $\mathbf{M}(y) \succeq 0$ and $\mathbf{M}(t(1-t)y) \succeq 0$, which are infinite-dimensional linear matrix inequalities in the moment sequence y (compare with e.g., [30, Theorem 3.2]).

Next we turn to the two growth conditions appearing in Theorem 3-2. By definition of $y^\mu_{\ell,\emptyset}$ is clear that the first becomes

$$\sum_{\ell=1}^{\infty} \frac{1}{\sqrt[2\ell]{y^\mu_{2\ell,\emptyset}}} = \infty$$

while for the second taking $E := \left(\frac{1}{\sqrt{2\pi}} e^{-\mathbf{i}nx} \right)_{n \in \mathbb{Z}}$ we obtain that

$$\forall\, n \in \mathbb{Z}, \quad \sum_{k=1}^{\infty} \frac{1}{\sqrt[2k]{y^\mu_{0,n,\cdots,n,-n,\cdots,-n}}} = \infty$$

where for each k, in the expression under the root, the term n and $-n$ appear k times each. The latter condition can be interpreted as an infinite-dimensional generalization of the multivariate Carleman condition, see e.g., [6] and [40].

Finally, we deal with the growth condition appearing in Theorem 3-3, which for the special choice of test functions in (17) becomes: For each $\ell, k \in \mathbb{N}$, there exist $j_{\ell,k} \in \mathbb{N}$ such that

$$\sum_{n_1,\ldots,n_k \in \mathbb{Z}} (1+n_1^2)^{-j_{\ell,k}} \cdots (1+n_k^2)^{-j_{\ell,k}} |y^\mu_{\ell,n_1,\ldots,n_k}|^2 < \infty.$$

We prove now that imposing those conditions on a generic $y := (y_{\ell,n_1,\ldots,n_k})_{\ell,k \in \mathbb{N}} \subset \mathbb{C}$ is enough to construct a sequence $(m_{\ell,k})_{\ell,k \in \mathbb{N}}$ fulfilling the assumptions of Theorem 3 and so to ensure the existence of a representing measure for y.

Theorem 4 *Let $y := (y_{\ell,n_1,\ldots,n_k})_{\ell,k \in \mathbb{N}} \subset \mathbb{C}$ be a sequence indexed by $\ell \in \mathbb{N}, n_1, \ldots, n_k \in \mathbb{Z}$ for $k \in \mathbb{N}$ such that* (19) *and* (20) *hold. If*

1. *a)* $\mathbf{M}(y) \succeq 0$,
   b) $\mathbf{M}(t(1-t)y) \succeq 0$,

2. a) $\sum_{\ell=1}^{\infty} \frac{1}{\sqrt[2\ell]{y_{2\ell,\emptyset}}} = \infty$

b) $\forall n \in \mathbb{Z}, \quad \sum_{k=1}^{\infty} \frac{1}{\sqrt[2k]{y_{0,n,\cdots,n,-n,\cdots,-n}}} = \infty$ *where for each* k*, in the expression under the root, the term* n *and* $-n$ *appear* k *times each,*

3. for each $\ell, k \in \mathbb{N}$*, there exist* $j_{\ell,k} \in \mathbb{N}$ *such that*

$$\sum_{n_1,\ldots,n_k \in \mathbb{Z}} (1+n_1^2)^{-j_{\ell,k}} \cdots (1+n_k^2)^{-j_{\ell,k}} |y_{\ell,n_1,\ldots,n_k}|^2 < \infty$$

then there exists a unique Radon measure μ *which is supported in* $[0,1] \times W_2^{-\beta}(\mathbb{T}) \subseteq \mathbb{R} \times \mathscr{D}'(\mathbb{T})$ *for some* $\beta > \max\{j_{0,2}, j_{1,1}, j_{2,0}\} + \frac{1}{2}$*, and whose scalr moment sequence is* y*.*

Proof: For any $\ell, k \in \mathbb{N}$, we use (16) to define the linear functional $m_{\ell,k}$ on the linear span in $\mathbb{C}^{\otimes \ell} \otimes (\mathcal{C}^\infty(\mathbb{T};\mathbb{C}))^{\otimes k}$ of all $1 \oplus \psi_{n_1} \otimes \cdots \otimes \psi_{n_k}$ for $\psi_1, \ldots, \psi_k$ as in (17) ($n_1, \ldots, n_k \in \mathbb{Z}$). By condition 3 and using the canonical identifications

$$\left(W_2^{j_{\ell,k}}(\mathbb{T};\mathbb{C}))^{\otimes k}\right)' \cong \left(W_2^{j_{\ell,k}}(\mathbb{T};\mathbb{C}))'\right)^{\otimes k} \cong \left(W_2^{-j_{\ell,k}}(\mathbb{T};\mathbb{C}))\right)^{\otimes k},$$

$m_{\ell,k}$ extends to a continuous linear functional on $\mathbb{C}^{\otimes \ell} \otimes W_2^{j_{\ell,k}}(\mathbb{T};\mathbb{C}))^{\otimes k}$. By (20), $m_{\ell,k}$ is a multilinear functional on $\mathbb{C}^\ell \times \left(W_2^{j_{\ell,k}}(\mathbb{T};\mathbb{C}))\right)^k$ symmetric in the first ℓ variables as well as in the second k variables. By (19), $m_{\ell,k}$ is invariant under complex conjugation, i.e., it defines a real valued multilinear functional on $\mathbb{R}^\ell \times \left(W_2^{j_{\ell,k}}(\mathbb{T})\right)^k$. Using the density of the complex exponentials and the continuity of $m_{\ell,k}$, conditions 1.a and 1.b imply that Theorem 3-1 holds. By condition 2.a and 2.b, Theorem 3-2 holds for $E := \left(\frac{1}{\sqrt{2\pi}} e^{-\mathbf{i}nx}\right)_{n \in \mathbb{Z}}$. Hence, Theorem 3 gives the desired conclusion. □

Remark 1 *In Theorem 4, the condition 2.a is actually already implied by conditions 1.a and 1.b, because the submatrices of* $\mathbf{M}(y)$ *and* $\mathbf{M}(t(1-t)y)$ *corresponding to* $k = 0$ *and* $k' = 0$ *are positive-semidefinite and so* $(y_{\ell,\emptyset})_{\ell \in \mathbb{N}}$ *is the moment sequence of a unique Radon measure* ν *supported in* $[0,1]$*, which in particular fulfills condition 2.a.*

Notice that the representing measure μ *provided by Theorem 4 can be disintegrated as* $d\mu(t,h) = d\nu(t)\, d\mu_t(h)$ *with* μ_t *probability measure on* $\mathscr{D}'(\mathbb{T})$ *supported in* $W_2^{-\beta}(\mathbb{T})$ *(see e.g. [15], [4, Section 10.6]).*

Remark 2 *If* $d\mu(t,h) := d\nu(t)\, d\mu_t(h)$ *with* ν *(finite) Borel measure on* $[0,1]$ *and* μ_t *probability measure on* $\mathscr{D}'(\mathbb{T})$*, then the corresponding moment sequence* $y := (y^\mu_{\ell,n_1,\ldots,n_k})_{\ell,k \in \mathbb{N}_0}$ *is such that* $y^\mu_{\ell,\emptyset} = \int_0^1 t^\ell \, d\nu(t)$*. Conversely, assume that conditions 1.a, 2.b and 3 in Theorem 4 hold for a sequence of complex numbers* $y := (y_{\ell,n_1,\ldots,n_k})$ *and that* $y_{\ell,\emptyset} = \int_0^1 t^\ell \, d\nu(t)$ *for a given (finite) Borel measure on* $[0,1]$*. Then of course condition 2.a holds as well and, arguing as in the proofs of Theorem 4 and of Theorem 3 and using [26, Theorem 3.3], it is possible to show that there exists a representing measure* μ *for* y *supported in* $\mathbb{R} \times \mathscr{D}'(\mathbb{T})$*. While we*

cannot claim a priori that μ is supported in $[0,1]\times\mathscr{D}'(\mathbb{T})$, disintegrating as in Remark 1 shows that in fact $d\mu(t,h)=d\nu(t)\,d\mu_t(h)$ with μ_t probability measure on $\mathscr{D}'(\mathbb{T})$. This allows us to avoid testing the positivity of the localizing matrix $\mathbf{M}(t(1-t)y)$ when applying Theorem 4 to the initial, terminal, and occupation moments (21)–(23), i.e., respectively for $\nu=\delta_0$ and $y_{\ell,\emptyset}=\delta_{\ell,0}$, $\nu=\delta_1$ and $y_{\ell,\emptyset}=1$, and $d\nu(t)=\chi_{[0,1]}(t)dt$ and $y_{\ell,\emptyset}=\frac{1}{\ell+1}$.

Remark 3 *Assume that μ is a probability measure on $\mathbb{R}\times\mathscr{D}'(\mathbb{T})$ supported in $[0,1]\times B_R$ where B_R is a ball of radius R in $W_2^{-\beta_0}(\mathbb{T})$. Then μ has continuous local moments with respect to $W_2^{-\beta_0}(\mathbb{T})\subseteq\mathscr{D}'(\mathbb{T})$ (for a more detailed account on compactness and continuity in the moment problem see e.g. [25]). Using the inequality $\|\cdot\|_{\ell_2}\le\|\cdot\|_{\ell_1}$, we have that for all $\ell,k\in\mathbb{N}$ and $j_{\ell,k}\in\mathbb{N}$:*

$$\begin{aligned}
&\left(\sum_{n_1,\dots,n_k\in\mathbb{Z}}(1+n_1^2)^{-j_{\ell,k}}\cdots(1+n_k^2)^{-j_{\ell,k}}|y_{\ell,n_1,\dots,n_k}|^2\right)^{1/2}\\
&\le\sum_{n_1,\dots,n_k\in\mathbb{Z}}(1+n_1^2)^{-j_{\ell,k}/2}\cdots(1+n_k^2)^{-j_{\ell,k}/2}|y_{\ell,n_1,\dots,n_k}|\\
&\le\int_0^1\int_{B_R}t^\ell\sum_{n_1,\dots,n_k\in\mathbb{Z}}(1+n_1^2)^{-j_{\ell,k}/2}\cdots(1+n_k^2)^{-j_{\ell,k}/2}|h_{n_1}\cdots h_{n_k}|\,d\mu(t,h).
\end{aligned}$$

Notice that for $h\in B_R$ we have that:

$$\begin{aligned}
\sum_{n\in\mathbb{Z}}(1+n^2)^{-j_{\ell,k}/2}|h_n|&=\sum_{n\in\mathbb{Z}}(1+n^2)^{-j_{\ell,k}/2+\beta_0/2}(1+n^2)^{-\beta_0/2}|h_n|\\
&\le\left(\sum_{n\in\mathbb{Z}}(1+n^2)^{-j_{\ell,k}+\beta_0}\right)^{1/2}\left(\sum_{n\in\mathbb{Z}}(1+n^2)^{-\beta_0}|h_n|^2\right)^{1/2}\\
&\le\left(\sum_{n\in\mathbb{Z}}(1+n^2)^{-j_{\ell,k}+\beta_0}\right)^{1/2}\|h\|_{W_2^{-\beta_0}(\mathbb{T})}\le C_{j_{\ell,k}}R
\end{aligned}$$

for all $j_{\ell,k}-\beta_0>\frac{1}{2}$, i.e., for all $j_{\ell,k}>\beta_0+\frac{1}{2}$, where we have used the Cauchy–Schwartz inequality in ℓ_2 and $C_{j_{\ell,k}}$ is a positive constant depending on $j_{\ell,k}$.

Combining these estimates, we see that for the sequence of scalar moments $(y_{\ell,n_1,\dots,n_k})$ of μ the following holds for any $\ell,k\in\mathbb{N}$ and all $j_{\ell,k}>\beta_0+\frac{1}{2}$:

$$\sum_{n_1,\dots,n_k\in\mathbb{Z}}(1+n_1^2)^{-j_{\ell,k}}\cdots(1+n_k^2)^{-j_{\ell,k}}|y_{\ell,n_1,\dots,n_k}|^2\le C_{j_{\ell,k}}^{2k}R^{2k}.\tag{26}$$

Hence, if we fix $\gamma\in\mathbb{N}$ such that $\gamma>\beta_0+\frac{1}{2}$ and for each $\ell,k\in\mathbb{N}$ we choose $j_{\ell,k}=\gamma$, we easily see that (26) ensures that condition 3 in Theorem 4 holds. In particular, this implies that $(1+n^2)^{-2k\gamma}y^2_{0,\underbrace{n,\cdots,n}_{k\text{times}},\underbrace{-n,\cdots,-n}_{k\text{times}}}\le C_\gamma^{4k}R^{4k}$ and therefore

$$\sqrt[2k]{y_{0,n,\cdots,n,-n,\cdots,-n}}\le(1+n^2)^\gamma C_\gamma^2R^2,\tag{27}$$

so that condition 2.b in Theorem 4 holds automatically.

This remark will be essential for the choice of the objective functional for solving finite-dimensional optimization problems and proving the convergence of the moment–SOS hierarchy, see Theorem 5 below.

5.2 Approximation with the moment-SOS hierarchy

Let us summarize our developments so far. We have shown that under Assumptions 1, 2 and 3, given the moments y^0 of an initial measure $\delta_0\mu_0$ concentrated on an initial data, if there are sequences $y^{[0,1]}$ and y^1 solving linear equation (25) and satisfying the conditions of Theorem 4, then they are the sequences of moments of an occupation measure $dt\mu_t$ and a terminal measure $\delta_1\mu_1$ concentrated on the solution of PDE (1).

In order to implement the moment-SOS hierarchy on a computer, we proceed as in the finite-dimensional case, see e.g., [18, Chapter 2]. We just truncate the sequences up to a given time degree, algebraic degree and harmonic degree. The resulting conditions on the truncated sequences provide a finite-dimensional *semidefinite optimization* problem that can be solved on a computer with, e.g., interior-point algorithms. Since the moment problem is truncated, there are less variables and constraints, and we speak of a *moment relaxation*.

The solution to the moment relaxation are truncated sequences of *pseudo-moments*, in the sense that they are not necessarily moments of measures: the truncated semidefinite constraints are necessary, but not sufficient conditions for the sequences to have representing measures. However, when the truncation degrees go to infinity, the conditions become necessary and sufficient, and we speak of *convergence* of the moment-SOS hierarchy. Quantifying the speed of convergence, as a function of the time degree, algebraic degree and harmonic degree, is an interesting open research question.

There is a fundamental new feature in the infinite-dimensional setting that does not appear in the finite-dimensional case: typically the sums in (24) are infinite, so that we cannot write the linear constraints (25) for the truncated sequence of pseudo-moments. More precisely, finite sums correspond to distributed nonlinearities whereas infinite sums correspond to local nonlinearities using the convolution theorem for Fourier series, see Sections 6.2.1–6.2.2 for an example. We can remedy the situation by splitting the infinite sum into a finite sum involving only pseudo-moments up to a given harmonic degree and the remainder, or the residual, that we view as an additional modelling variable that we can estimate. We refer to Section 6.2.2 for details and an adaptation of the convergence theorem (Theorem 5) to this setting.

5.2.1 Optimization

In this paper we are only interested in solving nonlinear PDEs, there is no functional to be minimized. In practice, we can however control the growth of the pseudo-moment sequences in each moment relaxation by minimizing a particular convex functional of the moment matrices of the occupation measure and terminal measure.

An appropriate choice of functional to be minimized is the convex quadratic functional

appearing in the growth condition 3 of Theorem 4, since this choice will allow us to apply Theorem 4 for proving the convergence of the resulting moment-SOS hierarchy.

More explicitly, the quadratic functionals that we will minimize are of the form

$$q^\gamma(w) = \sum_{k,l\in\mathbb{N}} a_k b_\ell q^\gamma_{k,\ell}(w), \quad q^\gamma_{k,\ell}(w) = \sum_{n_1,\ldots,n_k\in\mathbb{Z}} (1+n_1^2)^{-\gamma}\cdots(1+n_k^2)^{-\gamma}|w_{\ell,n_1,\ldots,n_k}|^2 \tag{28}$$

with $\gamma \in \mathbb{N}$, a_k, b_ℓ strictly positive real numbers such that

$$\limsup_{k\to\infty} \sqrt[k]{a_k} = 0, \ \sum_{k=1}^{\infty} \sqrt[4k]{a_{2k}} = \infty, \ \sum_{\ell=0}^{\infty} b_\ell < \infty. \tag{29}$$

For instance, we take

$$a_k = \frac{1}{k^k}, \ b_\ell = \frac{1}{2^\ell}.$$

Expressed with moments, the optimization problem reads

$$\begin{array}{rll} p^* = & \inf\limits_{w^{[0,1]},w^1} & q^\gamma(w^{[0,1]}) + q^\gamma(w^1) \\ & \text{s.t.} & w^1_{\ell,n_1,\ldots,n_k} - w^0_{\ell,n_1,\ldots,n_k} = \\ & & \ell w^{[0,1]}_{\ell-1,n_1,\ldots,n_k} + \sum\limits_{j=1}^{k}\sum\limits_{s=0}^{N}\sum\limits_{r_1,\ldots,r_s\in\mathbb{Z}} a^{s,j}_{r_1,\ldots,r_s} w^{[0,1]}_{\ell,n_1,\ldots,n_{j-1},r_1,\ldots,r_s,n_{j+1},\ldots,n_k} \\ & & w^1_{\ell,\emptyset} = 1^\ell \\ & & \mathbf{M}(w^{[0,1]}) \succeq 0, \\ & & \mathbf{M}(w^1) \succeq 0, \end{array} \tag{30}$$

In this problem, the constraint $w^1_{\ell,\emptyset} = 1^\ell$ implies that $w^{[0,1]}_{\ell,\emptyset} = \frac{1}{\ell+1}$ since $w^0_{\ell,\emptyset} = 0^\ell$. Indeed, $w^0_{\ell,\emptyset}$, $w^1_{\ell,\emptyset}$ resp. $w^{[0,1]}_{\ell,\emptyset}$ are the moments of marginals with respect to time, which are respectively the Dirac measures at 0 and 1, and the Lebesgue measure on $[0,1]$. Notice that the constraints $\mathbf{M}(t(1-t)\, w^{[0,1]}) \succeq 0$ and $\mathbf{M}(t(1-t)\, w^1) \succeq 0$ do not appear because of Remark 2.

The infinite-dimensional problem (30) is truncated to pseudo-moments of time degree at most L, algebraic degree at most K, and harmonic degree at most N. The truncated quadratic functionals are

$$q^\gamma_{L,K,N}(w) = \sum_{l\le L, k\le K} a_k b_\ell \sum_{|n_1|,\ldots,|n_k|\le N} (1+n_1^2)^{-\gamma}\cdots(1+n_k^2)^{-\gamma}|w_{\ell,n_1,\ldots,n_k}|^2.$$

As we already remarked in the paragraph preceeding Section 5.2, the adjoint of the polynomial operator F often involves infinitely many terms when expressed in terms of complex exponentials (e.g., products of function and its derivatives w.r. to x leading to convolution of their Fourier series), resulting in infinitely many terms in the linear constraints for the moments and the need to introduce additional modelling variables for the residual when we truncate the infinite sum. See Section 6.2.2 below for more details.

For problem (30) this results in a hierarchy of finite-dimensional semidefinite *moment relaxations* with values $p^*_{L,K,N}$. Problem (30) has a dual, that we do not detail here, and which is

approximately solved with a hierarchy of finite-dimensional semidefinite *SOS strengthenings*, as in the finite-dimensional case, see e.g., [30, Chapter 2] or [18, Chapter 2].

For proving the convergence of this moment-SOS hierarchy, we will need the following additional assumption.

Assumption 4 *There exists $\mathcal{H}_1 \supseteq \mathcal{H}_0$ linear subspace of $\mathcal{H}$ such that $F : \mathcal{H}_1 \to \mathcal{H}_1$ is continuous and the unique solution $\mathbf{u}$ provided by Assumption 1 is also the unique solution of (2) in $\mathcal{C}^1([0,1];\mathcal{H}_1)$ with $\mathbf{u}(0) = u_0$.*

Indeed, fixing $\mathcal{H} = \mathscr{D}'(\mathbb{T})$, $\mathcal{H}_0 = W_2^{-\beta_0}(\mathbb{T})$ and $\mathcal{H}_1 = W_2^{-(\beta_0+2)}(\mathbb{T})$ for some $\beta_0 \in \mathbb{N}$, we can show the following convergence result.

Theorem 5 (Convergence of the moment-SOS hierarchy) *Under Assumptions 1, 2, 3, and 4, for all relaxation orders $L' \geq L > 0, K' \geq K > 0, N' \geq N > 0$ we get*

$$p^*_{L,K,N} \leq p^*_{L',K',N'} \leq p^*_{\infty,\infty,\infty} = p^*.$$

Proof: We only need to prove that $\lim_{L,K,N\to\infty} p^*_{L,K,N} = p^*$, where L, K, N respectively denote the time degree, the algebraic degree, and the harmonic degree of the truncated problem, i.e., we consider the initial, terminal, and occupation moments (21)–(23) with $\ell = 0, \ldots, L$, $k = 0, \ldots, K$, and $|n_j| \leq N, j = 1, \ldots, k$.

By Assumptions 1, 2 and Theorem 1 for $\mathcal{H} = \mathscr{D}'(\mathbb{T})$ and $\mathcal{H}_0 = W_2^{-\beta_0}(\mathbb{T})$, we have that there exist unique Radon measures μ_t on $\mathscr{D}'(\mathbb{T})$ supported on $\mathbf{u}(t) \in W_2^{-\beta_0}(\mathbb{T})$ satisfying the linear equation (5) with initial data $\mu_0 = \delta_{\mathbf{u}(0)}$, where $\mathbf{u}$ is the unique solution of (2) with $\mathbf{u}(0) = u_0$. By Assumption 3 and Theorem 2, the moment functions corresponding to $\delta_0\mu_0$, $\delta_1\mu_1$ and $dt\mu_t$ satisfy the linear equation (15) and their scalar moments $y^0 := (y^0_{\ell,n_1,\ldots,n_k}), y^1 := (y^1_{\ell,n_1,\ldots,n_k}), y^{[0,1]} := (y^{[0,1]}_{\ell,n_1,\ldots,n_k})$ satisfy the linear equation (25).

Notice that since the solution $\mathbf{u}(t)$ of (2) is a continuous function on $[0,1]$ by Assumption 1, it is contained in some ball B_R of radius R in $W_2^{-\beta_0}(\mathbb{T})$. Therefore, by Remark 3, we get that for each $s \in \{0, 1, [0,1]\}$, all $\ell, k \in \mathbb{N}$ and $\gamma \in \mathbb{N}$ with $\gamma > \beta_0 + \frac{1}{2}$:

$$q^\gamma_{\ell,k}(y^s) = \sum_{n_1,\ldots,n_k\in\mathbb{Z}} (1+n_1^2)^{-\gamma} \cdots (1+n_k^2)^{-\gamma} |y^s_{\ell,n_1,\ldots,n_k}|^2 \leq C^{2k}_\gamma R^{2k}. \tag{31}$$

Then (28) and (29) imply that for each $s \in \{0, 1, [0,1]\}$ we have:

$$q^\gamma(y^s) \leq \mathbf{C} := \sum_{\ell=0}^{\infty}\sum_{k=0}^{\infty} b_\ell a_k C^{2k}_\gamma R^{2k} < \infty. \tag{32}$$

Now, in the truncated finite-dimensional optimization programs computing $p^*_{L,K,N}$, given y^0, we minimize the truncated versions of the convex quadratic functionals $q^\gamma_{L,L,K}(w^s) \leq q^\gamma(w^s)$ over a truncated feasibility set containing the truncation of y^s and, hence, the minimum is still less then or equal to $\mathbf{C}$. Notice that it follows that an argmin $w_{L,K,N}$ satisfies

$$|w^s_{L,K,N;\ell,n_1,\ldots,n_k}| \leq (1+n_1^2)^{\gamma/2} \cdots (1+n_k^2)^{\gamma/2} \frac{\sqrt{\mathbf{C}}}{\sqrt{a_k b_\ell}}. \tag{33}$$

Then, for each $\ell, n_1, \ldots, n_k$, the pseudo moments of the truncated optimization programs $w^s_{L,K,N;\ell,n_1,\ldots,n_k}$ are bounded in L, K, N, and we can assume after passing to a subsequence that all the pseudo-moments converge with $w^s_{\ell,n_1,\ldots,n_k} = \lim_{L,K,N\to\infty} w^s_{L,K,N;\ell,n_1,\ldots,n_k}$. The limit pseudo moments w^s still satisfy the estimates (33) and in particular for all $n \in \mathbb{N}$ we have:

$$|w^s_{0,n,\ldots,n,-n,\ldots,-n}| \leq (1+n^2)^{k\gamma} \frac{\sqrt{\mathbf{C}}}{\sqrt{a_{2k} b_0}} \tag{34}$$

where n and $-n$ respectively appear k times in $w^s_{0,n,\ldots,n,-n,\ldots,-n}$. Therefore,

$$\sum_{k=1}^{\infty} \frac{1}{\sqrt[2k]{w^s_{0,n,\ldots,n,-n,\ldots,-n}}} \geq \sum_{k=1}^{\infty} (1+n^2)^{-\gamma/2} \frac{\sqrt[4k]{a_{2k}}\,\sqrt[4k]{b_0}}{\sqrt[4k]{\mathbf{C}}} = \infty, \tag{35}$$

because of (29) (since $\lim_{k\to\infty} \frac{\sqrt[4k]{b_0}}{\sqrt[4k]{\mathbf{C}}} = 1$). It follows now from Theorem 4 that the limit pseudo-moments $w^{[0,1]}$ and w^1 are respectively the scalar moment sequence of unique Radon measures supported on $[0,1] \times W_2^{-\beta}(\mathbb{T})$ for some $\beta > \gamma + \frac{1}{2}$ and so for some $\beta > \beta_0 + 1$. Since the limit pseudo-moments satisfy all the linear equations (25), Assumption 2, Remark 2, and Assumption 4 for $\mathcal{H}_1 = W_2^{-(\beta_0+2)}(\mathbb{T})$ ensures that these measures coincide with the occupation measure $dt\mu_t$ and the terminal measure $\delta_1\mu_1$ corresponding to the unique solution $\mathbf{u}(t)$ of (2) in $W_2^{-\beta_0}(\mathbb{T})$. □

5.2.2 Symmetry and sparsity

It was already observed that the moment sequences satisfy symmetry properties (19) and (20). Symmetries can be exploited to reduce to size of the semidefinite relaxations, and hence to improve scalability of the approach when the truncation degrees increase, see [35]. Sparsity of the moment and localizing matrices, with their specific Hankel and Toeplitz structure, as well sparsity of the linear moment equation, can also be exploited by semidefinite programming solvers.

5.2.3 Recovering the solution

Finally, once pseudo-moments are available, it is desirable to recover approximately the graph of the solution of the PDE. For that purpose, we can use the Christoffel-Darboux kernel [32]: this SOS polynomial constructed from the pseudo-moments has small values on the graph of the function to be recovered. Good approximations of the functions can be obtained from small value sets of the kernel, with convergence guarantees for increasing degree. This graph recovery technique was studied in detail in [36] for measures supported on finite-dimensional spaces. An infinite-dimensional extension of the Christoffel-Darboux kernel was recently described in [16]. In the context of PDE solving, it would be interesting to construct this kernel and study its convergence properties.

6 Case study: the heat equation

6.1 Linear heat equation

Let us first consider the linear heat equation (1) with $F(u(t,x)) = \frac{\partial^2 u(t,x)}{\partial x^2}$.

6.1.1 Linear moment equation

Using the duality pairing (10) and noticing that

$$\langle h'', \psi \rangle = \langle h, \psi'' \rangle, \tag{36}$$

linear equation (13) reads

$$\begin{aligned} 1^\ell \int_{\mathcal{H}} \langle h, \psi_{n_1} \rangle \cdots \langle h, \psi_{n_k} \rangle \, d\mu_1(h) - 0^\ell \int_{\mathcal{H}} \langle h, \psi_{n_1} \rangle \cdots \langle h, \psi_{n_k} \rangle \, d\mu_0(h) \\ = \int_0^1 \int_{\mathcal{H}} \ell t^{\ell-1} \langle h, \psi_{n_1} \rangle \cdots \langle h, \psi_{n_k} \rangle \, d\mu_t(h) \, dt \\ + \int_0^1 \int_{\mathcal{H}} t^\ell \sum_{j=1}^k \langle h, \psi_{n_1} \rangle \cdots \widehat{\langle h, \psi_{n_j} \rangle} \cdots \langle h, \psi_{n_k} \rangle \langle h, \psi''_{n_j} \rangle \, d\mu_t(h) \, dt. \end{aligned}$$

In the duality pairing, we choose complex exponentials $\psi_{n_j}(x) = \frac{1}{\sqrt{2\pi}} e^{-\mathbf{i} n_j x}$, where $n_1, \ldots, n_k \in \mathbb{Z}$ so that corresponding linear functionals are the Fourier coefficients of $h \in \mathcal{H}$ denoted by $h_n := \langle h, \frac{1}{\sqrt{2\pi}} e^{-\mathbf{i} n x} \rangle$. Since $\left(e^{-\mathbf{i} n x}\right)'' = -n^2 e^{-\mathbf{i} n x}$, the linear equation becomes

$$\begin{aligned} 1^\ell \int_{\mathcal{H}} h_{n_1} \cdots h_{n_k} \, d\mu_1(h) - 0^\ell \int_{\mathcal{H}} h_{n_1} \cdots h_{n_k} \, d\mu_0(h) \\ = \int_0^1 \int_{\mathcal{H}} \ell t^{\ell-1} h_{n_1} \cdots h_{n_k} \, d\mu_t(h) \, dt - \sum_{j=1}^k n_j^2 \int_0^1 \int_{\mathcal{H}} t^\ell \; h_{n_1} \cdots h_{n_k} \, d\mu_t(h) \, dt. \end{aligned} \tag{37}$$

Following Definition 3 and notation (21)–(23), the initial, terminal and occupation moments are given by

$$\begin{aligned} y^0_{\ell,n_1,\ldots,n_k} &= 0^\ell \int_{\mathcal{H}} h_{n_1} \cdots h_{n_k} \, d\mu_0(h), \\ y^1_{\ell,n_1,\ldots,n_k} &= 1^\ell \int_{\mathcal{H}} h_{n_1} \cdots h_{n_k} \, d\mu_1(h), \\ y^{[0,1]}_{\ell,n_1,\ldots,n_k} &= \int_0^1 \int_{\mathcal{H}} t^\ell \, h_{n_1} \cdots h_{n_k} \, d\mu_t(h) \, dt, \end{aligned}$$

and we can rewrite the linear moment equation (25) as

$$y^1_{\ell,n_1,\ldots,n_k} - y^0_{\ell,n_1,\ldots,n_k} = \ell y^{[0,1]}_{\ell-1,n_1,\ldots,n_k} - \sum_{j=1}^k n_j^2 \; y^{[0,1]}_{\ell,n_1,\ldots,n_k}. \tag{38}$$

Here $\ell, k = 0, 1, 2, \ldots,\ n_1, \ldots, n_k = 0, \pm 1, \pm 2, \ldots$.

Notice that in the case $\ell = 0$, the first term on the right hand side does not appear since the test function does not depend on t. Notice also that $y^0_{\ell,n_1,\ldots,n_k} = 0$ for $\ell > 0$ and that $y^1_{\ell,n_1,\ldots,n_k}$ is independent of ℓ.

6.1.2 Analytic solution

The solution u can be expressed as a Fourier series:

$$u(t,x) = \frac{1}{\sqrt{2\pi}} \sum_{n\in\mathbb{Z}} u_n(t) e^{\mathbf{i}nx}.$$

From the linear heat equation

$$\frac{\partial u(t,x)}{\partial t} = \frac{\partial^2 u(t,x)}{\partial x^2}$$

it follows that

$$\frac{d}{dt} u_n(t) = -n^2 u_n(t)$$

for any n, which yields

$$u_n(t) = u_n(0) e^{-n^2 t}.$$

Therefore the solution reads

$$u(t,x) = \frac{1}{\sqrt{2\pi}} \sum_{n\in\mathbb{Z}} u_n(0) e^{-n^2 t} e^{\mathbf{i}nx}.$$

Lemma 1 *Given $\ell, k \in \mathbb{N}$ and $n_1, \ldots, n_k \in \mathbb{Z}$, let $N := n_1^2 + \cdots + n_k^2$. The initial, terminal and occupation moments solving the linear equation (38) can be expressed in closed-form as follows:*

$$\begin{aligned}
y^0_{\ell,n_1,\ldots,n_k} &= 0^\ell u_{n_1}(0) \cdots u_{n_k}(0), \\
y^1_{\ell,n_1,\ldots,n_k} &= 1^\ell u_{n_1}(0) \cdots u_{n_k}(0) e^{-N}, \\
y^{[0,1]}_{\ell,n_1,\ldots,n_k} &= \begin{cases} \frac{u_0(0)^k}{\ell+1} & \text{if } (n_1,\ldots,n_k) = (0,\ldots,0) \\ u_{n_1}(0)\cdots u_{n_k}(0) \left(\frac{\ell!}{N^{\ell+1}} - e^{-N} \sum_{j=1}^{\ell+1} \frac{\ell!}{N^j (\ell-j+1)!} \right) & \text{if } (n_1,\ldots,n_k) \neq (0,\ldots,0). \end{cases}
\end{aligned}$$

Proof: The initial and terminal moments readily follow from the Fourier series expansion. The occupation moments are given by

$$y^{[0,1]}_{\ell,n_1,\ldots,n_k} = u_{n_1}(0) \cdots u_{n_k}(0) \int_0^1 t^\ell e^{-Nt} dt.$$

First consider the case $(n_1,\ldots,n_k) = (0,\ldots,0)$. Then, using the definiton of $y_{\ell,0,\ldots,0}$ and observing that in this case $N = 0$, we easily get:

$$y^{[0,1]}_{\ell,0,\ldots,0} = \underbrace{u_0(0)\cdots u_0(0)}_{k \text{ times}} \int_0^1 t^\ell dt = \frac{u_0(0)^k}{\ell+1}.$$

For the case $(n_1, \dots, n_k) \neq (0, \dots, 0)$, we set for convenience $I_\ell := \int_0^1 t^\ell e^{-Nt} dt$. Then the conclusion will follow at once by

$$I_\ell = \frac{\ell!}{N^{\ell+1}} - e^{-N} \sum_{j=1}^{\ell+1} \frac{\ell!}{N^j(\ell - j + 1)!}, \tag{39}$$

which by induction holds for all $\ell \in \mathbb{N}$. Indeed, a direct computation of the integral I_ℓ provides the base case, that is,

$$I_0 = \int_0^1 e^{-Nt} dt = -\frac{e^{-Nt}}{N}\Big|_{t=0}^{t=1} = \frac{1}{N} - \frac{e^{-N}}{N},$$

i.e., (39) holds for $\ell = 0$. Suppose now that (39) holds for $\ell = l$ with $l \geq 0$ and let us prove it for $\ell = l + 1$. Integrating by parts and using the definition of I_l we obtain that

$$\begin{aligned} I_{l+1} &= \int_0^1 t^{l+1} e^{-Nt} dt \\ &= -\frac{t^{l+1} e^{-Nt}}{N}\Big|_{t=0}^{t=1} + \int_0^1 (l+1) t^l \frac{e^{-Nt}}{N} dt \\ &= \frac{1}{N}\left((l+1) I_l - e^{-N}\right). \end{aligned}$$

This by inductive assumption becomes

$$\begin{aligned} I_{l+1} &= \frac{1}{N}\left(\frac{l!(l+1)}{N^{l+1}} - e^{-N} \sum_{j=1}^{l+1} \frac{l!(l+1)}{N^j(l-j+1)!} - e^{-N}\right) \\ &= \frac{(l+1)!}{N^{l+2}} - e^{-N} \sum_{j=1}^{l+1} \frac{(l+1)!}{N^{j+1}(l-j+1)!} - \frac{e^{-N}}{N} \\ &= \frac{(l+1)!}{N^{l+2}} - e^{-N} \sum_{j=0}^{l+1} \frac{(l+1)!}{N^{j+1}(l-j+1)!} \\ &= \frac{(l+1)!}{N^{l+2}} - e^{-N} \sum_{r=1}^{l+2} \frac{(l+1)!}{N^r(l+1-r+1)!}, \end{aligned}$$

where in the last step we used the change of variable $r = j + 1$. Hence, by induction, (39) holds for all $\ell \in \mathbb{N}$, which yields the conclusion. □

6.2 Nonlinear heat equation

6.2.1 Distributed nonlinearity

Consider a nonlinear heat PDE (1) with a distributed quadratic nonlinearity, e.g.,

$$F(u(t,x)) = \frac{\partial^2 u(t,x)}{\partial x^2} + \epsilon \int_{-\pi}^{\pi} u(t,x) f_1(x) dx \int_{-\pi}^{\pi} u(t,x) f_2(x) dx \tag{40}$$

where $f_1, f_2 \in \mathcal{C}^\infty(T)$ are given functions, and $\epsilon \in \mathbb{R}$ is a given small number.

Let us choose e.g., the real valued functions $f_1 = \psi_{m_1} + \psi_{-m_1}$, $f_2 = \psi_{m_2} + \psi_{-m_2}$ for $m_1, m_2 \in \mathbb{N}$ and $\psi_{m_j}(x) = \frac{1}{\sqrt{2\pi}} e^{-\mathbf{i} m_j x}$ as in Section 5.

In linear moment equation (13) we substitute $F(h) = h'' + \epsilon(h_{m_1} + h_{-m_1})(h_{m_2} + h_{-m_2}) \cdot 1$ (we could in principle replace the constant function 1 by any real valued trigonometric polynomial). Using (36) we have

$$\langle F(h), \psi_j \rangle = \langle h, \psi_j'' \rangle + \epsilon(h_{m_1} + h_{-m_1})(h_{m_2} + h_{-m_2}) \langle 1, \psi_j \rangle.$$

Using further $\psi_n'' = -n^2 \psi_n$ and $\langle 1, \psi_n \rangle = \delta_{n0}$ (the orthogonality of the complex exponentials) we obtain instead of (37) the following:

$$\begin{aligned} 1^\ell \int_{\mathcal{H}} h_{n_1} \cdots h_{n_k} \, d\mu_1(h) - 0^\ell \int_{\mathcal{H}} h_{n_1} \cdots h_{n_k} \, d\mu_0(h) \\ = \int_0^1 \int_{\mathcal{H}} \ell t^{\ell-1} h_{n_1} \cdots h_{n_k} \, d\mu_t(h) \, dt - \sum_{j=1}^k n_j^2 \int_0^1 \int_{\mathcal{H}} t^\ell \; h_{n_1} \cdots h_{n_k} \, d\mu_t(h) \, dt \\ - \epsilon \int_0^1 \int_{\mathcal{H}} t^\ell \; \sum_{j=1}^k \delta_{n_j 0} h_{n_1} \cdots \widehat{h_{n_j}} \cdots h_{n_k} (h_{m_1} + h_{-m_1})(h_{m_2} + h_{-m_2}) \, d\mu_t(h) \, dt. \end{aligned} \quad (41)$$

In terms of moments, we obtain finally instead of (38) the following:

$$\begin{aligned} y^1_{\ell,n_1,\ldots,n_k} - y^0_{\ell,n_1,\ldots,n_k} = \ell y^{[0,1]}_{\ell-1,n_1,\ldots,n_k} - \sum_{j=1}^k n_j^2 \; y^{[0,1]}_{\ell,n_1,\ldots,n_k} \\ - \epsilon \sum_{j=1}^k \delta_{n_j 0} \Big(y^{[0,1]}_{\ell,n_1,\ldots,\widehat{n_j},\ldots,n_k,m_1,m_2} + y^{[0,1]}_{\ell,n_1,\ldots,\widehat{n_j},\ldots,n_k,m_1,-m_2} \\ + y^{[0,1]}_{\ell,n_1,\ldots,\widehat{n_j},\ldots,n_k,-m_1,m_2} + y^{[0,1]}_{\ell,n_1,\ldots,\widehat{n_j},\ldots,n_k,-m_1,-m_2} \Big) \end{aligned} \quad (42)$$

for $\ell, k = 0, 1, 2, \ldots$, $n_1, \ldots, n_k = 0, \pm 1, \pm 2, \ldots$ (and again, for $\ell = 0$ the first term on the right hand side does not appear).

6.2.2 Local nonlinearity

Let us consider now a nonlinear heat PDE (1) with a distributed quadratic nonlinearity, e.g.,

$$F(u(t,x)) = \frac{\partial^2 u(t,x)}{\partial x^2} + \epsilon u(t,x)^2 \quad (43)$$

where $\epsilon \in \mathbb{R}$ is a given small number.

In linear moment equation (13) we substitute $F(h) = h'' + \epsilon h^2$. Using (36) we have

$$\langle F(h), \psi_j \rangle = \langle h, \psi_j'' \rangle + \epsilon \langle h^2, \psi_j \rangle.$$

Using the Fourier series expansion (18), by convolution we get

$$h^2 = \frac{1}{2\pi} \sum_{n,m\in\mathbb{Z}} h_m h_{n-m} e^{\mathbf{i}nx}. \tag{44}$$

Using this together with $\psi_n'' = -n^2\psi_n$ we obtain instead of (37) the following:

$$\begin{aligned} 1^\ell \int_{\mathcal{H}} h_{n_1}\cdots h_{n_k}\, d\mu_1(h) - 0^\ell \int_{\mathcal{H}} h_{n_1}\cdots h_{n_k}\, d\mu_0(h) \\ = \int_0^1 \int_{\mathcal{H}} \ell t^{\ell-1} h_{n_1}\cdots h_{n_k}\, d\mu_t(h)\, dt - \sum_{j=1}^k n_j^2 \int_0^1 \int_{\mathcal{H}} t^\ell\ h_{n_1}\cdots h_{n_k}\, d\mu_t(h)\, dt \\ - \epsilon \int_0^1 \int_{\mathcal{H}} t^\ell \sum_{j=1}^k h_{n_1}\cdots \widehat{h_{n_j}} \cdots h_{n_k} \left(\frac{1}{\sqrt{2\pi}} \sum_{m\in\mathbb{Z}} h_m h_{n_j-m} \right) d\mu_t(h)\, dt. \end{aligned} \tag{45}$$

In terms of moments, we obtain finally instead of (38) the following:

$$y^1_{\ell,n_1,\dots,n_k} - y^0_{\ell,n_1,\dots,n_k} = \ell y^{[0,1]}_{\ell-1,n_1,\dots,n_k} - \sum_{j=1}^k n_j^2\ y^{[0,1]}_{\ell,n_1,\dots,n_k} - \frac{\epsilon}{\sqrt{2\pi}} \sum_{j=1}^k \sum_{m\in\mathbb{Z}} y^{[0,1]}_{\ell,n_1,\dots,\widehat{n_j},\dots,n_k,m,n_j-m} \tag{46}$$

for $\ell, k = 0, 1, 2, \dots$, $n_1, \dots, n_k = 0, \pm 1, \pm 2, \dots$ (and again, for $\ell = 0$ the first term on the right hand side does not appear).

As announced in Section 5.2 we explain now how to truncate this infinite sum and control the residual so that we can produce a convergent hierarchy of finite dimensional problems. Let us rewrite (46) in the form

$$\begin{aligned} y^1_{\ell,n_1,\dots,n_k} - y^0_{\ell,n_1,\dots,n_k} = \ell y^{[0,1]}_{\ell-1,n_1,\dots,n_k} - \sum_{j=1}^k n_j^2\ y^{[0,1]}_{\ell,n_1,\dots,n_k} \\ - \frac{\epsilon}{\sqrt{2\pi}} \sum_{j=1}^k \left(\sum_{|m|\le M, |n_j-m|\le M} y^{[0,1]}_{\ell,n_1,\dots,\widehat{n_j},\dots,n_k,m,n_j-m} + z_{\ell,n_1,\dots,\widehat{n_j},\dots,n_k;n_j,M} \right) \end{aligned} \tag{47}$$

Notice that $|m| \le M, |n_j - m| \le M \iff m \in [-M, M] \cap [n_j - M, n_j + M] \iff \max\{-M, n_j - M\} \le m \le \min\{M, n_j + M\}$ (also note that $-M \le n_j \le M$). Here the remainders

$$z_{\ell,n_1,\dots,\widehat{n_j},\dots,n_k;n_j,M} = \left(\sum_{m=-\infty}^{\max\{-M,n_j-M\}} + \sum_{m=\min\{M,n_j+M\}} \right) y^{[0,1]}_{\ell,n_1,\dots,\widehat{n_j},\dots,n_k,m,n_j-m} \tag{48}$$

are seen as additional modelling variables, for which we are going to obtain an estimate going to zero (quickly) as $M \to \infty$.

Lemma 2 *Assume that the measures μ_t are supported in a ball B_R of radius R in $W_2^{-\beta_0}(\mathbb{T})$ (where $\beta_0 < -\frac{1}{2}$). Then*

$$|z_{\ell,n_1,\dots,\widehat{n_j},\dots,n_k;n_j,M}| \le \frac{1}{\ell+1} 2R^{k+1} \sqrt{-\frac{M^{2\beta_0+1}}{2\beta_0+1}}. \tag{49}$$

Proof: Denote by $(h) := (h_m)_{m\in\mathbb{Z}}$ the sequence of Fourier coefficients of h, by $(h)_M$ its truncation to $[-M, M]$, and by $*$ the convolution over $\mathbb{Z}$, and notice that

$$\left(\sum_{m=-\infty}^{\max\{-M,n_j-M\}} + \sum_{m=\min\{M,n_j+M\}}^{\infty}\right) h_m h_{n_j-m} \tag{50}$$

is the n_j element in the sequence

$$(h) * (h) - (h)_M * (h)_M = ((h) - (h)_M) * (h) + (h)_M * ((h) - (h)_M).$$

We have

$$\begin{aligned}\left|((h) * (h) - (h)_M * (h)_M)_{n_j}\right| &\le \left|(((h) - (h)_M) * (h))_{n_j}\right| + \left|((h)_M * ((h) - (h)_M))_{n_j}\right| \\ &\le \|(h) - (h)_M\|_2 \|(h)\|_2 + \|(h)_M\|_2 \|(h) - (h)_M\|_2 \le 2\|(h) - (h)_M\|_2 \|(h)\|_2. \end{aligned}\tag{51}$$

If $h \in W_2^{-\beta_0}(\mathbb{T})$, then clearly

$$|h_n| \le (1+n^2)^{\beta_0/2} \|h\|_{W_2^{-\beta_0}(\mathbb{T})}. \tag{52}$$

Combining (51) and (52) and noticing that, since $\beta_0 < -\frac{1}{2}$, $2\beta_0 + 1 < 0$ and also $\|(h)\|_2 \le \|h\|_{W_2^{-\beta_0}(\mathbb{T})}$, we obtain that

$$\begin{aligned}\left|\left(\sum_{m=-\infty}^{\max\{-M,n_j-M\}} + \sum_{m=\min\{M,n_j+M\}}^{\infty}\right) h_m h_{n_j-m}\right| &\le 2\|(h)\|_2 \left(\sum_{|m|>M} |h_m|^2\right)^{1/2} \\ &\le 2\|h\|^2_{W_2^{-\beta_0}(\mathbb{T})} \left(\sum_{|m|>M} (1+n^2)^{\beta_0}\right)^{1/2} \le 2\|h\|^2_{W_2^{-\beta_0}(\mathbb{T})} \left(\int_{M-1}^{\infty} x^{2\beta_0}\, dx\right)^{1/2} \\ &\le 2\|h\|^2_{W_2^{-\beta_0}(\mathbb{T})} \sqrt{-\frac{M^{2\beta_0+1}}{2\beta_0+1}}. \end{aligned}\tag{53}$$

Let us now assume that the support of μ_t is contained in $\|h\|_{W_2^{-\beta_0}(\mathbb{T})} \le R$ for all $t \in [0,1]$. Using (52) for $h_{n_1}, \ldots, \widehat{h_{n_j}}, \ldots, h_{n_k}$ and (53) for the truncated convolution (50), multiplying by t^ℓ and integrating with respect to $d\mu_t(h)\, dt$ we finally obtain (49). □

We see now from Lemma 2, cf. the proof of Theorem 5, that $z_{\ell,n_1,\ldots,\widehat{n_j},\ldots,n_k;n_j,N} \to 0$ for $N \to \infty$ so that as the relaxation order r of the truncated problem goes to infinity, the truncated linear constraints (47) on the moments give us the true linear constraints (46). Now, if we have an a priori estimate of R, we can simply add the resulting inequalities (49) as a linear constraint to the finite dimensional truncated problems and Theorem 5 holds with the same proof. Otherwise, we can recover the conclusion of the theorem by adding an appropriate weighted sum of the residual modelling variables to the convex quadratic functionals $q^\gamma_{N,L,K}$ that we optimize, e.g., we optimize instead the functional

$$\tilde{q}^\gamma_{L,K,N}(y) = q^\gamma_{L,K,N}(y) + \sum_{l\le L, k\le K, |n_1|,\ldots,|n_k|\le N} \frac{1}{k!}\frac{1}{2^l}\frac{1}{(1+n_1)^2\cdots(1+n_k)^2} z_{\ell,n_1,\ldots,\widehat{n_j},\ldots,n_k;n_j,N}. \tag{54}$$

6.3 Numerical experiments

We developed Matlab codes to generate the semidefinite moment relaxations in YALMIP dual format and call the external semidefinite solver Mosek for solving the nonlinear heat PDE. The main files `heatmom_qd.m` for quadratic distributed nonlinearity and `heatmom_ql.m` for quadratic local nonlinearity, as well as their dependencies, can be downloaded at

`homepages.laas.fr/henrion/software/heatmom/`

The moment relaxations are generated by various values of the time degree, algebraic degree and harmonic degree, as defined in Section 5. Decision variables are the occupation moment vector $y^{[0,1]}$ and the terminal moment vector y^1. The initial moment vector y^0 is given, and it is computed from an initial condition

$$u(0,x) = \sum_{k\in\mathbb{Z}} u_k(0) e^{\mathbf{i}kx}$$

with finitely many nonzero Fourier coefficients. For our experiments we took

$$u_{-1}(0) = u_0(0) = u_1(0) = 1.$$

In Table 1 we report sizes of the moment vector and moment matrix for various degrees. General purpose semidefinite solvers on a standard computer can deal with semidefinite matrices of size of a few hundreds and a few tens of thousands of variables. For example, on our laptop, for degrees (4,2,4) and (4,4,2) the semidefinite relaxation is solved in less than 0.5 sec. For degrees (4,4,4), (6,4,4) resp. (6,4,6) it takes approx. 13, 24 resp. 544 secs.

For the linear heat PDE ($\epsilon = 0$) we can compare the pseudo-moments obtained by optimization and the analytic moments calculated in Lemma 1. We report in Figure 1 the relative accuracy between the pseudo-moments and the analytic occupation moments. When all the degrees are equal to 4, we can see that approx. 95% of the pseudo-moments are approximating the exact moments with relative accuracy 10^{-5}.

For the heat PDE with distributed nonlinearity, we do not have the analytic moments, but in Figure 2 we report on the discrepancy between the computed pseudo-moments and the analytic moments for $\epsilon = 0$, for distinct values of ϵ. Similarly, for the hear PDE with local nonlinearity, we report in Figure 3 on the discrepancy between the computed pseudo-moments and the analytic moments for $\epsilon = 0$, for distinct values of ϵ.

Acknowledgements

This work benefited from feedback from Giovanni Fantuzzi, David Goluskin and Victor Magron. This research was supported through the program "Oberwolfach Research Fellows" by the Mathematisches Forschungsinstitut Oberwolfach in 2023. The last three authors wish to thank the Banff International Research Station for the opportunity to work on this project during the workshop 23w5033 and the research in teams 23rit010. M. Infusino is indebted

to the Baden–Württemberg Stiftung for the financial support to this work by the Eliteprogramme for Postdocs and is a member of GNAMPA group of INdAM. S. Kuhlmann was partially supported by the Ausschuss für Forschungsfragen (AFF) from the University of Konstanz. V. Vinnikov would like to thank Milken Families Foundation Chair in Mathematics for a partial support of his research.

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7 Tables and Figures

(time, algebraic, harmonic) degrees	moment vector size	moment matrix size
(2, 2, 2)	63	12
(4, 2, 2)	105	18
(6, 2, 2)	147	24
(6, 2, 4)	385	40
(2, 4, 2)	378	42
(4, 4, 2)	630	63
(6, 4, 2)	882	84
(4, 4, 4)	3575	165
(6, 4, 4)	5005	220
(6, 4, 6)	16660	420
(6, 6, 4)	35035	880
(6, 6, 6)	189924	2240

Table 1: Moment vector and matrix sizes for various degrees.

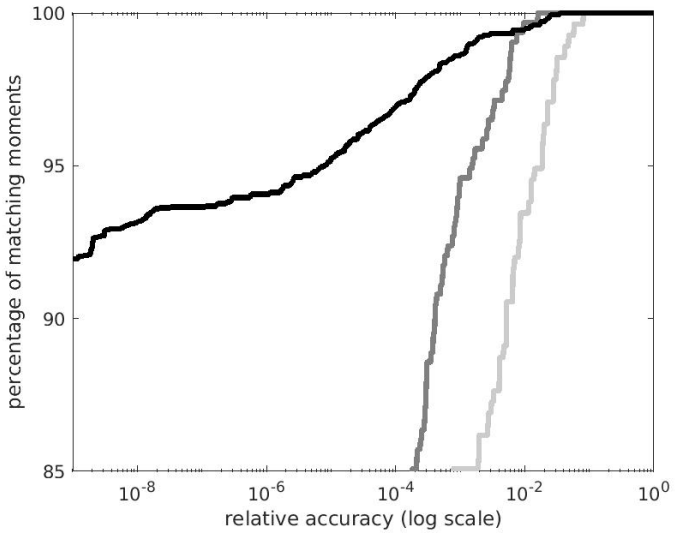

Figure 1: Percentage of matching occupation moments versus relative accuracy for distinct time, algebraic and harmonic degrees: (4,2,4) light gray, (4,4,2) dark gray, (4,4,4) black.

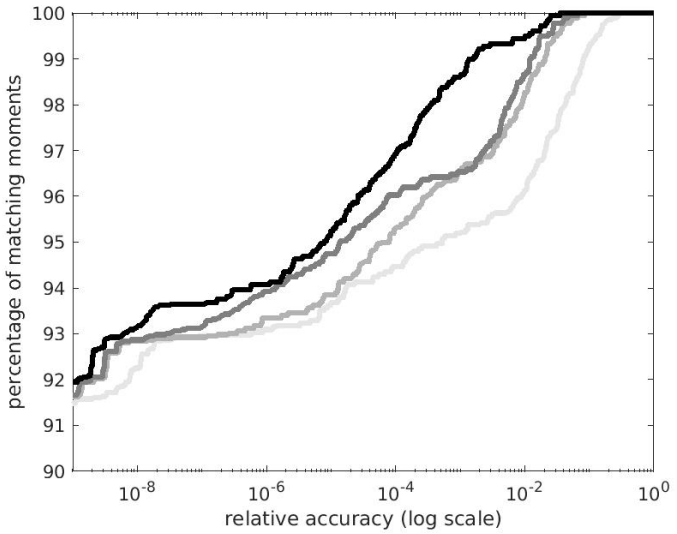

Figure 2: Distributed nonlinearity: percentage of matching occupation moments versus relative accuracy for distinct values of ϵ: 0 black, 10^{-6} dark gray, 10^{-3} gray, 1 light gray.

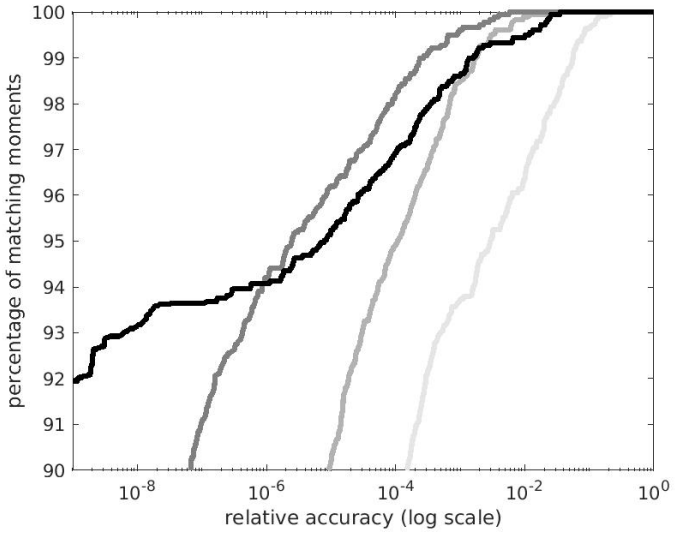

Figure 3: Local nonlinearity: percentage of matching occupation moments versus relative accuracy for distinct values of ϵ: 0 black, 10^{-6} dark gray, 10^{-3} gray, 1 light gray.