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Time-dependent moments from partial differential equations and the time-dependent set of atoms

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Abstract

We study the time-dependent moments $s_\alpha(t) = \int x^\alpha \cdot f(x,t)\ \mathrm{d}x$ of the solution f of the partial differential equation $\partial_t f = \nu\Delta f + g \cdot \nabla f + h \cdot f$ with initial Schwartz function data $f_0 \in \mathcal{S}(\mathbb{R}^n)$. At first we describe the dual action on the polynomials, i.e., the time-evolution of f is completely moved to the polynomial side $s_\alpha(t) = \int p(x,t) \cdot f_0(x)\ \mathrm{d}x$. We investigate the special case of the heat equation. We find that several non-negative polynomials which are not sums of squares become sums of squares under the heat equation in finite time. Finally, we solve the problem of moving atoms under the equation $\partial_t f = g \cdot \nabla f + h \cdot f$ with $f_0 = \mu_0$ being a finitely atomic measure. We find that in the time evolution $\mu_t = \sum_{i=1}^k c_i(t) \cdot \delta_{x_i(t)}$ the atom positions $x_i(t)$ are governed only by the transport term $g \cdot \nabla$ and that the time-dependent coefficients $c_i(t)$ have an analytic solution depending on $x_i(t)$.

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1. Introduction

1.1. Static Moments

Let μ be a Borel measure on $\mathbb{R}^n$ for some $n \in \mathbb{N}$ and $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}_0^n$. The α-moment s_α of μ is

$$s_\alpha = \int_{\mathbb{R}^n} x^\alpha \, \mathrm{d}\mu(x) \tag{1}$$

with $x^\alpha := x_1^{\alpha_1} \cdots x_n^{\alpha_n}$. The *classical moment problem* is: Given finitely or infinitely many real numbers s_α in a sequence $s = (s_\alpha)_{\alpha \in \mathsf{A} \subseteq \mathbb{N}_0^n}$, does there exist a Borel measure μ such that (1) holds for all $\alpha \in \mathsf{A}$? If the answer to this question is affirmative, then μ is called a *representing measure* of s and s is called a *moment sequence*. If A is finite, then s is a *truncated* moment sequence, and if $\mathsf{A} = \mathbb{N}_0^n$, then s is called *full* moment sequence. Additionally, if $\operatorname{supp} \mu \subseteq K$ for some $K \subseteq \mathbb{R}^n$, then s is called a *K-moment sequence*. A classical tool to investigate moment sequences is the *Riesz functional* $L = L_s : \mathbb{R}[x_1, \dots, x_n] \to \mathbb{R}$ defined by $L_s(x^\alpha) := s_\alpha$ and linearly extended to $\mathbb{R}[x_1, \dots, x_n]$ if s is full or linearly extended to $\{x^\alpha \mid \alpha \in \mathsf{A}\}$ if s is truncated. $L : \mathbb{R}[x_1, \dots, x_n] \to \mathbb{R}$ is called a *moment functional* if it is represented by some Borel measure μ. We always assume measures to be non-negative unless specifically denoted as *signed* measures.

Moments are a classical field of research [Akh65, BPT13, dDS22, Sch17, Fia16, Hav35, Hav36, IKLS17, Kem68, Kem71, Kem87, KN77, Lan80b, Lan80a, Las15, Lau05, Lau09, LM09, ST43, Sti94, Sto01, IK20, IKKM22] and in modern times they are still of interest, e.g. because of the following application in optimization. Let $p \in \mathbb{R}[x_1, \dots, x_n]$ be a polynomial. Then

$$\min_{x_0 \in K \subseteq \mathbb{R}^n} p(x_0) = \min_{\substack{\mu : \operatorname{supp} \mu \subseteq K, \\ \mu(K) = 1}} \int p(x) \, \mathrm{d}\mu(x) = \min_{\substack{s \ K\text{-moment} \\ \text{sequence}, \ s_0 = 1}} L_s(p), \tag{2}$$

since for the first equality we have that for any $x_0 \in \mathbb{R}^n$ the Dirac measure δ_{x_0} acts as a point evaluation in (1) and the second formulation holds by linearity of the integral using the s_α definition in (1). See e.g. [Las15] for more.

A classical result for truncated moment sequences is the *Richter* [Ric57] (or *Richter–Rogosinski–Rosenbloom* [Ric57, Rog58, Ros52]) *Theorem*; see [dDS22] for a detailed discussion about the historical development.

Theorem 1.1 (Richter Theorem 1957 [Ric57, Satz 4]). *Let $d \in \mathbb{N}$, $\mathcal{V}$ be a d-dimensional real vector space of measurable real functions $f : \mathcal{X} \to \mathbb{R}$ on a measurable space $\mathcal{X}$, and $L : \mathcal{V} \to \mathbb{R}$ be a moment functional, i.e., there exists a measure μ on $\mathcal{X}$ such that*

$$L(f) = \int_{\mathcal{X}} f(x) \, \mathrm{d}\mu(x)$$

for all $f \in \mathcal{V}$. Then there are $c_1, \ldots, c_k > 0$ and $x_1, \ldots, x_k \in \mathcal{X}$ with $k \leq d$ such that

$$L(f) = \sum_{i=1}^{k} c_i \cdot f(x_i)$$

for all $f \in \mathcal{V}$, i.e., we always find a k-atomic representing measure $\nu = \sum_{i=1}^{k} c_i \cdot \delta_{x_i}$ of L with $k \leq d$.

The points x_i in the k-atomic representing measure ν are called *atoms* and the minimal number k of atoms for fixed L is called *Carathéodory number* $\mathcal{C}(L)$ resp. $\mathcal{C}(s)$ for truncated moment sequences. A k-atomic representing measure is also called a (*Gauss*) *quadrature rule* [Gau15]. Two questions arise naturally in theory and applications:

(a) How many atoms $\mathcal{C}(L)$ are required to represent L?

(b) Where are the atoms x_i located in a representation of L?

Very recent studies about the Carathéodory number $\mathcal{C}(L)$ are [RS18, dDS18b, dDK21] and the *set of atoms* (or *core variety*) is studied in [Fia17, dDS18a, BF20].

All the studies and references given so far have one thing in common: They study *static* moments, i.e., s is fixed in these studies and properties are only derived from and for s. Hence, the study of the *moment cone* $\mathcal{S}_{\mathsf{A}}$ (= set of all moment sequences s) is only pointwise and collecting or even connecting moment sequences with the same properties in the moment cone is difficult and does not arise naturally.

1.2. Time-dependent Moments

Let $n, m \in \mathbb{N}$. We denote by $C_b^\infty(\mathbb{R}^n, \mathbb{R}^m)$ the set of *smooth bounded functions*

$$C_b^\infty(\mathbb{R}^n, \mathbb{R}^m) := \{f \in C^\infty(\mathbb{R}^n, \mathbb{R}^m) \mid \|\partial^\alpha f\|_\infty < \infty \text{ for all } \alpha \in \mathbb{N}_0^n\}$$

and by $\mathcal{S}(\mathbb{R}^n, \mathbb{R}^m)$ the *Schwartz functions*

$$\mathcal{S}(\mathbb{R}^n, \mathbb{R}^m) := \left\{f \in C^\infty(\mathbb{R}^n, \mathbb{R}^m) \,\middle|\, \|x^\alpha \partial^\beta f\|_\infty < \infty \text{ for all } \alpha, \beta \in \mathbb{N}_0^n\right\}.$$

By $C^d([0, \infty), C_b^\infty(\mathbb{R}^n, \mathbb{R}^m))$ we denote all functions $f : \mathbb{R}^n \times [0, \infty) \to \mathbb{R}^m$ such that

(i) $f(\,\cdot\,,t), \partial_t f(\,\cdot\,,t), \ldots, \partial_t^d f(\,\cdot\,,t) \in C_b^\infty(\mathbb{R}^n, \mathbb{R}^m)$ for all $t \geq 0$ and

(ii) $\partial^\alpha f(x,\,\cdot\,) \in C^d([0,\infty), \mathbb{R}^m)$ for all $x \in \mathbb{R}^n$ and $\alpha \in \mathbb{N}_0^n$.

Let $d \in \mathbb{N}_0$, $\nu = (\nu_1, \ldots, \nu_n)^T \in [0,\infty)^n$, $\nu \cdot \Delta = \nu_1 \cdot \partial_1^2 + \cdots + \nu_n \cdot \partial_n^2$ be the anisotropic Laplace operator, $g = (g_1, \ldots, g_n) \in C^d([0,\infty), C_b^\infty(\mathbb{R}^n, \mathbb{R}^n))$ be a smooth bounded vector field, $h = (h_{i,j})_{i,j=1}^m \in C^d([0,\infty), C_b^\infty(\mathbb{R}^n, \mathbb{R}^{m\times m}))$ be a smooth bounded matrix function, $k = (k_1, \ldots, k_m)^T \in \mathcal{S}(\mathbb{R}^n, \mathbb{R}^m)$ be a Schwartz function vector-valued function, and $a \in \mathbb{R}^n$ be a vector.

Then by [dD19, Thm. 2.10] the initial value problem

$$\begin{aligned} \partial_t f(x,t) &= \nu \Delta f(x,t) + [ax + g(x,t)] \cdot \nabla f(x,t) + h(x,t) \cdot f(x,t) + k(x,t) \\ f(x,0) &= f_0(x) \in \mathcal{S}(\mathbb{R}^n, \mathbb{R}^m) \end{aligned} \tag{3}$$

with $(ax+g)\cdot\nabla := (a_1x_1+g_1)\cdot\partial_1 + \cdots + (a_nx_n+g_n)\cdot\partial_n$ has a unique solution $f \in C^{d+1}([0,\infty), \mathcal{S}(\mathbb{R}^n, \mathbb{R}^m))$. Additionally, for $m = 1$ and $f_0 \geq 0$ we have that $f(\,\cdot\,,t) \geq 0$ for all $t \geq 0$.

For $f_0 \in \mathcal{S}(\mathbb{R}^n)$ with $f_0 \geq 0$ we can calculate the moments

$$s_\alpha(0) := \int_{\mathbb{R}^n} x^\alpha \cdot f_0(x) \,\mathrm{d}x$$

for all $\alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbb{N}_0^n$. Since the time-dependent solution f of (3) is unique, Schwartz function valued, and non-negative for $m = 1$ and $f_0 \geq 0$, we find that the solution f induces unique time-dependent moments

$$s_\alpha(t) := \int_{\mathbb{R}^n} x^\alpha \cdot f(x,t) \,\mathrm{d}x \tag{4}$$

for all $t \geq 0$.

The time-dependent moments can be defined for nonlinear partial differential equations as well. Let us look at a (non-linear) example. In [dD19, Lem. 3.6] for Burgers' equation

$$\partial_t f(x,t) = -f(x,t) \cdot \partial_x f(x,t)$$

we calculated the time-dependent moments

$$s_{k,p}(t) := \int_{\mathbb{R}} x^k \cdot f(x,t)^p \,\mathrm{d}x$$

of $f(x,t)^p$ for all $k, p \in \mathbb{N}_0$ and found the explicit expression

$$s_{k,p}(t) = \sum_{i=0}^{k} \frac{s_{k-i,p+i}(0)}{i!} \cdot t^i \cdot \prod_{j=0}^{i-1} \frac{(p+j)\cdot(k-j)}{1+(p+j)^2} \quad \in \mathbb{R}[t] \tag{5}$$

which depends only on the initial values $s_{k-i,p+i}(0)$ of f_0. Hence, despite the fact that for any non-constant $f_0 \in \mathcal{S}(\mathbb{R})$ the classical solution of Burgers' equation

breaks down in finite time, the moments are *a priori* known for all times $t \in \mathbb{R}$. In [dD19, Exm. 3.7] we then calculate for the one-tooth-function

$$f_0(x) := \begin{cases} 1+x & \text{for } x \in [-1,0], \\ 1-x & \text{for } x \in [0,1] \\ 0 & \text{else} \end{cases} \qquad \geq 0$$

the time-dependent moments $s_{0,1}(t)$, $s_{1,1}(t)$, and $s_{2,1}(t)$ to find

$$\int_{\mathbb{R}} (x-t)^2 \cdot f(x,t) \, \mathrm{d}x = L_{s(t)}((x-t)^2) = \frac{1}{6} - \frac{2}{15}t^2 \quad \xrightarrow{t \to \pm\infty} \quad -\infty. \tag{6}$$

Applying a molifier S_ε to f_0 gives $S_\varepsilon f_0 \in \mathcal{S}(\mathbb{R})$ for all $\varepsilon > 0$ and (6) changes continuously with $\varepsilon > 0$. Then (6) holds at least for the time of the existence of the classical solution. But the classical solution remains non-negative which contradicts (6), i.e., Burgers' equation breaks down in finite time. In other words, Burgers' equation as a (non-linear) transport equation, starting with a non-negative f_0 means that the classical solution is also non-negative as long as it exist. While from (5) we see that *a priori* the moments might exist for all times, the derivation of (5) requires that $f(x,t)$ is a classical solution, i.e., smooth and even Schwartz. The break down of the classical solution of Burgers' equation in finite time is therefore not observed through the moments becoming infinite (i.e., they stop to exist), but through the non-negativity property of the representing measure which is encoded in the moments. For some $t > 0$ we find a non-negative polynomial $p \in \mathbb{R}[x]$ such that $L_{s(t)}(p) < 0$, i.e., (6) shows that non-negativity is not preserved for all times and therefore the classical solution u does not exist for all times.

The Burgers' equation example has two nice features:

(a) the time-dependent moments are polynomial in time: $s_{k,p}(t) \in \mathbb{R}[t]$, and

(b) the example to contradict non-negativity of the moments only needs moment up to degree 2, i.e., 0th, 1st, and 2nd moments.

Studying (3) with general $\nu = (\nu_1, \ldots, \nu_n) \in [0,\infty)^n$, C_b^∞-functions g_i and $h_{i,j}$, and Schwartz functions k_i it is evident that neither (a) nor (b) need to be satisfied anymore. I.e. we can in general not hope for the time-dependent moments $s_\alpha(t)$ to be polynomial in time, depending only on the initial values $s_\alpha(0)$, and to observe certain properties we no longer can rely on finitely many moments $s_\alpha(t)$. We have to explore the computational and theoretical limits of time-dependent moments $s_\alpha(t)$. That is, among other things, one purpose of this study. We say that a (moment) sequence s *evolves with respect to* or *along the partial differential equation (3)* if a representing measure of s evolves with respect to (3). Hence, in principle the time-evolution $s(t)$ depends on the choice of representing measure μ_0 of $s(0)$ if $s(0)$ is *indeterminate*, i.e., $s(0)$ has more than one representing measure.

The time-dependent moments $s(t)$ from the heat equation $\partial_t f = \Delta f$ were studied extensively in [CdD22]. In [MP20, MWHL20, KHL22, KRZ22] moments

also have been applied to (non-linear) PDEs. In the present work we proceed the study [CdD22] and go beyond the heat equation. The paper is structured as follows.

In the next section (Section 2) we describe for (3) with $k = 0$ the dual action on the polynomials. We describe the dual action by the dual operator of (3) and show that polynomials in general are no longer polynomials for $t > 0$ but at least remain in an algebra $\mathrm{Pol}(\mathbb{R}^n)$ (see (7) for the definition). For $\nu\Delta + g\nabla + h$ with $g(x,t) = g(t)$ and $h(x,t) = h(t)$ we can solve the dual action analytically (see Corollary 2.6). We find that g and h have no effect on non-negativity and therefore study the (dual) action of the Laplace operator on polynomials in Section 3 more closely. We give a simple way to solve the polynomial heat equation in Theorem 3.3. We collect several results of this action and also present several specific results on non-negative polynomials. We show several examples where non-negative polynomials become sums of squares under the heat equation and also give counter examples, when a non-negative polynomial which is not a sum of squares does not become a sum of squares. Our observations lead to two open problems (Open Problem 5.1 and 5.2). In Section 4 we investigate the application of (3) with $\nu = 0$ and $k = 0$ to atomic measures. We find that since $g(x,t) \cdot \nabla$ and $h(x,t)$ in general do not commute and therefore a solution can not be constructed from solutions of the individual operators, for atomic measures we can at first solve the time-evolution with respect to the transport operator $g(x,t) \cdot \nabla$ and then apply the scaling operator $h(x,t)$. We find that the number of atoms is unchanged. We describe the time-evolution of $\mu_t = \sum_{i=1}^{k} c_i(t) \cdot \delta_{x_i(t)}$ in Lemma 4.1 and Theorem 4.2. For the full moment problem we show that the time-dependent moment sequence (functional) remains a boundary of the moment cone for all times. For the truncated moment problem we show that we can enter the interior of the moment cone and that the time-evolution in general depends on the representing measure. In Section 5 we summarize the results, give final discussions, and state the open problem.

2. The dual of a partial differential equation acting on polynomials

By [dD19, Thm. 2.10] we know that (3) has a unique solution $f \in C^{d+1}([0,\infty), \mathcal{S}(\mathbb{R}^n, \mathbb{R}^m))$ and therefore the time-dependent moments $s_\alpha(t)$ in (4) exist for all times $t \in [0,\infty)$. In this section we show that like in the heat equation [CdD22] the action of the operator $A = \nu \cdot \Delta + g(x,t)\nabla + h(x,t)$ has a dual action A^* acting on the polynomials, i.e., the time-dependency of the solution $f(x,t)$ is moved to a time-dependency of $p(x,t)$:

$$\int p_0(x) \cdot f(x,t) \, \mathrm{d}x = \int p(x,t) \cdot f_0(x) \, \mathrm{d}x$$

for all $t \in [0,\infty)$. We will see in Theorem 2.2 that while $p(x,0) \in \mathbb{R}[x_1,\ldots,x_n]$, we have in general $p(x,t) \notin \mathbb{R}[x_1,\ldots,x_n]$ for any $t \neq 0$. We have to introduce

the following space of *at most polynomially increasing functions* $\mathrm{Pol}(\mathbb{R}^n)$ on $\mathbb{R}^n$:

$$\mathrm{Pol}(\mathbb{R}^n) := \{f \in C^\infty(\mathbb{R}^n) \,|\, \text{for all } \alpha \in \mathbb{N}_0^n \text{ there exists } p_\alpha \in \mathbb{R}[x] \text{ such that } |\partial^\alpha f(x)| \le p_\alpha(x) \text{ for all } x \in \mathbb{R}^n\}. \tag{7}$$

We collect some simple properties of $\mathrm{Pol}(\mathbb{R}^n)$.

Lemma 2.1. *Let $n \in \mathbb{N}$. Then the following hold:*

i) $\mathrm{Pol}(\mathbb{R}^n)$ *is an algebra.*

ii) $\mathcal{S}(\mathbb{R}^n) \subsetneq \mathrm{Pol}(\mathbb{R}^n)$.

iii) $\mathbb{R}[x_1, \dots, x_n] \subsetneq \mathbb{R}[x_1, \dots, x_n] + C_b^\infty(\mathbb{R}^n) \subsetneq \mathrm{Pol}(\mathbb{R}^n) \subsetneq \mathcal{S}(\mathbb{R}^n)'$.

Proof. (i) and (ii) follow immediately from the definition of $\mathrm{Pol}(\mathbb{R}^n)$ in (7). For (iii) all inclusions $\subseteq$ are clear, it remains to show that the inclusions are proper $\subsetneq$. For the first $\subsetneq$ we have $\sin x_1 \in [\mathbb{R}[x_1, \dots, x_n] + C_b^\infty(\mathbb{R}^n)] \setminus \mathbb{R}[x_1, \dots, x_n]$, for the second $\subsetneq$ we have $x_1^2 \cdot \sin x_1 \in \mathrm{Pol}(\mathbb{R}^n) \setminus [\mathbb{R}[x_1, \dots, x_n] + C_b^\infty(\mathbb{R}^n)]$, and the last $\subsetneq$ is clear. □

Let $p \in \mathrm{Pol}(\mathbb{R}^n)$ and f be the unique solution of

$$\begin{aligned} \partial_t f(x,t) &= \nu \Delta f(x,t) + g(x,t) \cdot \nabla f(x,t) + h(x,t) \cdot f(x,t) \\ f(x,0) &= f_0(x) \end{aligned}$$

with $f_0 \in \mathcal{S}(\mathbb{R}^n)$, $g = (g_1, \dots, g_n)^T \in C([0,\infty), C_b^\infty(\mathbb{R}^n, \mathbb{R}))$, and $h \in C([0,\infty), C_b^\infty(\mathbb{R}^n, \mathbb{R}))$. Then

$$\begin{aligned} &\partial_t \int p(x) \cdot f(x,t) \, \mathrm{d}x \\ &\quad = \int p(x) \cdot [\nu \Delta + g(x,t) \cdot \nabla + h(x,t)] f(x,t) \, \mathrm{d}x \end{aligned}$$

is by partial integration (since $p \in \mathrm{Pol}(\mathbb{R}^n)$ and $f \in \mathcal{S}(\mathbb{R}^n)$)

$$= \int f(x,t) \cdot [\nu \Delta + g(x,t) \cdot \nabla - \operatorname{div} g(x,t) + h(x,t)] p(x) \, \mathrm{d}x$$

The following result shows, that the time evolution of f can be shifted to p. The proof uses techniques of the semi-group approximations of the solution f.

Theorem 2.2. *Let $d \in \mathbb{N}_0$, $\nu \ge 0$, $g = (g_1, \dots, g_n)^T \in C^d([0,\infty), C_b^\infty(\mathbb{R}^n)^n)$, and $h \in C^d([0,\infty), C_b^\infty(\mathbb{R}^n))$. Let $f \in C^{d+1}([0,\infty), \mathcal{S}(\mathbb{R}^n))$ be the unique solution of*

$$\begin{aligned} \partial_f(x,t) &= \nu \Delta f(x,t) + g(x,t) \cdot \nabla f(x,t) + h(x,t) \cdot f(x,t) \\ f(x,0) &= f_0(x) \end{aligned} \tag{8}$$

with $f_0 \in \mathcal{S}(\mathbb{R}^n)$. Let $T > 0$. Then the unique solution p_T of

$$\begin{aligned} \partial_t p_T(x,t) &= \nu \Delta p_T(x,t) - g(x, T-t) \cdot \nabla p_T(x,t) \\ &\qquad + (h(x,T-t) - \operatorname{div} g(x,T-t)) \cdot p_T(x,t) \\ p(x,0) &= p_0(x) \in \operatorname{Pol}(\mathbb{R}^n) \end{aligned} \tag{9}$$

fulfills $p_T \in C^{d+1}([0,T], \operatorname{Pol}(\mathbb{R}^n))$, and we have

$$\int p_0(x) \cdot f(x,T) \, \mathrm{d}x = \int p_T(x,T) \cdot f_0(x) \, \mathrm{d}x. \tag{10}$$

Proof. Note, the solution f of (8) is unique since it is unique on any open bounded set $U \subset \mathbb{R}^n$, see e.g. [Eva10, Ch. 7], and we have $f \in C^{d+1}([0,\infty), \mathcal{S}(\mathbb{R}^n))$, see e.g. [dD19]. Let $N \in \mathbb{N}$ and $\mathcal{Z}_N = \{t_0 = 0 < t_1 < \cdots < t_N = T\}$ be a decomposition of $[0,T]$. Then for the operator

$$A(x,t) = \nu \Delta + g(x,t) \cdot \nabla + h(x,t)$$

we have the dual operator

$$A^*(x,t) = \nu \Delta - g(x,t) \cdot \nabla - \operatorname{div} g(x,t) + h(x,t).$$

Note, of course, we actually also have to give the domain of the operators A and A^*. We are working for A on $\mathcal{S}(\mathbb{R}^n)$ and for A^* it is therefore sufficient to work on $\operatorname{Pol}(\mathbb{R}^n)$. We only have to ensure that $p_T \in \operatorname{Pol}(\mathbb{R}^n)$.

The unique solution f can be approximated in $\mathcal{S}(\mathbb{R}^n)$ by the semigroup approach (Trotter [Tro59])

$$f(x,T) = \lim_{N \to \infty} \prod_{i=1}^{N} \exp\left(\int_{t_{i-1}}^{t_i} A(x,s) \, \mathrm{d}s \right) f_0(x). \tag{11}$$

For any operator B we have for the dual B^* the relation $\langle f, Bg \rangle = \langle B^* f, g \rangle$ and for exponentials $\exp(B)$ we have $\langle f, \exp(B) g \rangle = \langle \exp(B^*) f, g \rangle$. When we apply these to (11) we have to pay attention at the order of the operators, since in general they do not commute and are additionally time-dependent. We use the order $\prod_{i=1}^{N} B_i = B_N B_{N-1} \cdots B_1$ in this formulas. Hence, we get

$$\begin{aligned} \int_{\mathbb{R}^n} p_0(x) \cdot f(x,T) \, \mathrm{d}x &= \lim_{N \to \infty} \int_{\mathbb{R}^n} p_0(x) \cdot \prod_{i=1}^{N} \exp\left(\int_{t_{i-1}}^{t_i} A(x,s) \, \mathrm{d}s \right) f_0(x) \, \mathrm{d}x \\ &= \lim_{N \to \infty} \int_{\mathbb{R}^n} \left[\prod_{i=N}^{1} \exp\left(\int_{t_{i-1}}^{t_i} A^*(x,s) \, \mathrm{d}s \right) p_0(x) \right] \cdot f_0(x) \, \mathrm{d}x \\ &= \int_{\mathbb{R}^n} p_T(x,T) \cdot f_0(x) \, \mathrm{d}x. \end{aligned}$$

The last equality holds in the same way as (11). We set

$$p_T(x,T) := \lim_{N \to \infty} \prod_{i=N}^{1} \exp\left(\int_{t_{i-1}}^{t_i} A^*(x,s) \, \mathrm{d}s \right) p_0(x)$$

and see that p_T solves (10) since the last equality holds for all $f_0 \in \mathcal{S}(\mathbb{R}^n)$, i.e., especially for all test functions $f_0 \in C_0^\infty(\mathbb{R}^n) \subset \mathcal{S}(\mathbb{R}^n)$. This indeed shows that $p_T \in \mathrm{Pol}(\mathbb{R}^n)$ and the time-dependency of $A(x,t)$ combined with the fact that $A(x,t)$ and $A(x,t')$ for $t \neq t'$ in general do not commute shows that we have to take the reverse order in the operator product, i.e., $p_T(x,t)$ solves by substituting $t \mapsto T-t$ in A^* the equation $\partial_t p_T(x,t) = A^*(x,T-t)p_T(x,t)$. $\square$

Remark 2.3. Theorem 2.2 holds with the same proof also for the anisotropic Laplace operator $\nu \cdot \Delta = \nu_1 \partial_1^2 + \cdots + \nu_n \partial_n^2$ with $\nu = (\nu_1, \ldots, \nu_n) \in [0,\infty)^n$. Additionally, let $M \in \mathbb{R}^{n\times n}$ be a symmetric positive-definite matrix. Then by a change of coordinates the operator $(\partial_1, \ldots, \partial_n)M(\partial_1, \ldots, \partial_n)$ can be diagonalized to the anisotropic Laplace operator $\nu \cdot \Delta$. ∘

Remark 2.4. In Theorem 2.2 we have seen that the action of (3) on f_0 is shifted to p_0. But since the dual action on p_0 is independent on f_0, it also provides the action (3) on measures μ_0 instead of functions f_0. This provides a way to study the set of atoms in Section 4. ∘

Remark 2.5. In the proof of Theorem 2.2 note that $A = \nu\Delta + g\nabla + h$ is in general an unbounded operator, i.e., it is not defined on all $L^2(\mathbb{R}^n)$. Since $\partial_t f = Af$ with $f_0 \in \mathcal{S}(\mathbb{R}^n)$ has a unique Schwartz function solution it is therefore sufficient to take the domain of A as $\mathcal{D}(A) = \mathcal{S}(\mathbb{R}^n)$. This very restrictive domain enables us in Theorem 2.2 to have $\mathrm{Pol}(\mathbb{R}^n) \subseteq \mathcal{D}(A^*)$. Here, the restriction that g and h are C_b^∞-functions is essential. It is not sufficient to have A such that $Af \in \mathcal{S}(\mathbb{R}^n)$ for any $f \in \mathcal{S}(\mathbb{R}^n)$. E.g. take $\nu = 0$, $g = 0$ and $h = x^4$ with $f_0(x) = e^{-x^2}$. Then $\partial_t f(x,t) = x^4 \cdot f(x,t)$ has as an ordinary differential equation in t with fixed x the unique solution $f(x,t) = e^{-x^2 + t\cdot x^4}$, i.e., $f(\,\cdot\,,t) \notin \mathcal{S}(\mathbb{R}^n)$ for any $t > 0$. Additionally note, that in [DH19, Thm. 2.2] a condition on the generator A is given such that the semi-group e^{At} maps the Schwartz class $\mathcal{S}$ to the Schwartz class $\mathcal{S}$. ∘

We have seen in the previous proof that the time-reversal for the dual equation acting on p_0 appears because Δ, $g(x,t)\nabla$, and $h(x,t)$ do not commute (pairwise) in general. If g and h are time-independent, then of course the time-reversal disappears naturally since no time-dependency exists. Another way the time-reversal disappears is, when Δ, $g(x,t)\nabla$, and $h(x,t)$ commute (pairwise), e.g. when g and h do not depend on x. We then have the following explicit solution for $p_t(x,t)$. We denote by Θ_t the heat kernel, i.e.,

$$\Theta_t(x) = \frac{1}{(4\pi t)^{n/2}} \cdot \exp\left(\frac{-\|x\|^2}{4t}\right)$$

for all $t > 0$.

Corollary 2.6. *Let $n \in \mathbb{N}_0$, $\nu \geq 0$, $g = (g_1, \ldots, g_n)$, and $g_1, \ldots, g_n, h \in C^d([0,\infty), \mathbb{R})$. Then for the dual action (9) and (10) in Theorem 2.2 we have*

$$p_t(x,t) = e^{H(t)} \cdot [\Theta_{\nu t} * p_0](x + G(t))$$

with $\Theta_{\nu t}$ the heat kernel, $G(t) := \int_0^t g(t)\,\mathrm{d}s$, and $H(t) := \int_0^t h(s)\,\mathrm{d}s$.

In [CdD22] the first and the second author studied the time-dependent moments from the heat equation in more detail. For the dual action it was especially found that

$$p_0 \in \mathbb{R}[x_1, \dots, x_n]_{\leq d} \qquad \Rightarrow \qquad [\Theta_{\nu t} * p_0](x) \in \mathbb{R}[x_1, \dots, x_n]_{\leq d}$$

for all $t \geq 0$ and additionally of course because of the convolution with the non-negative heat kernel

$$p_0 \geq 0 \qquad \Rightarrow \qquad [\Theta_{\nu t} * p_0](x) \geq 0$$

for all $t \geq 0$. Hence, with $p_0 \in \mathbb{R}[x_1, \dots, x_n]$ in Corollary 2.6 we have $p_t(x,t) \in \mathbb{R}[x_1, \dots, x_n]$ for all $t \in [0, \infty)$ (and even for all $t \in \mathbb{R}$, see [CdD22]). In the general case of Theorem 2.2 we only can ensure $p_t(x,t) \in \mathrm{Pol}(\mathbb{R}^n)$, but not $p_t(x,t) \in \mathbb{R}[x_1, \dots, x_n]$. To see that, let e.g. $\nu = 0$ and $g = 0$, i.e., we have the explicit solution

$$p_t(x,t) = \exp\left(\int_0^t h(x,s)\ \mathrm{d}s\right) \cdot p_0(x)$$

and with $h(x) = \sin(x)$ we have that $p_t(x,t) \notin \mathbb{R}[x_1, \dots, x_n]$ for all $t \neq 0$.

Therefore, in case of Corollary 2.6 we have that g and h do not alter the properties of p_0 (significantly), but the group action induced by the Laplace operator might give changes. We will see that in the next section.

3. Non-negative polynomials and the heat equation

Time-dependent moments induced by the heat equation were already studied in [CdD22]. There also the dual action on the polynomials was observed. We continue this investigation. We repeat the essential definitions and results for the convenience of the reader.

Definition 3.1. Let $d \in \mathbb{N}_0$. We define $\mathfrak{p}_{2d}, \mathfrak{p}_{2d+1} \in \mathbb{R}[x,t]$ by

$$\mathfrak{p}_{2d}(x,t) := \sum_{j=0}^{d} \frac{(2d)!}{(2d-2j)! \cdot j!} \cdot t^j \cdot x^{2d-2j}$$

and

$$\mathfrak{p}_{2d+1}(x,t) := \sum_{j=0}^{d} \frac{(2d+1)!}{(2d+1-2j)! \cdot j!} \cdot t^j \cdot x^{2d+1-2j}.$$

Example 3.2. We have

$$\begin{aligned}
\mathfrak{p}_0(x,t) &= 1 \\
\mathfrak{p}_1(x,t) &= x \\
\mathfrak{p}_2(x,t) &= 2t + x^2
\end{aligned}$$

$$
\begin{aligned}
\mathfrak{p}_3(x,t) &= 6tx + x^3 \\
\mathfrak{p}_4(x,t) &= 12t^2 + 12tx^2 + x^4 \\
\mathfrak{p}_5(x,t) &= 60t^2x + 20tx^3 + x^5 \\
\mathfrak{p}_6(x,t) &= 120t^3 + 180t^2x^2 + 30tx^4 + x^6 \\
&\vdots
\end{aligned}
$$

∘

Straightforward calculations show that $\mathfrak{p}_k$, $k \in \mathbb{N}_0$, solve the initial value heat equation

$$
\begin{aligned}
\partial_t \mathfrak{p}_k(x,t) &= \partial_x^2 \mathfrak{p}_k(x,t) \\
\mathfrak{p}_k(x,0) &= x^k.
\end{aligned}
\tag{12}
$$

Hence, by linearity of the heat equation we have the following extension of Definition 3.1 and the observation (12).

Theorem 3.3. *Let $d \in \mathbb{N}_0$, $n \in \mathbb{N}$, and $f_0(x) = \sum_{\alpha \in \mathbb{N}_0^n} c_\alpha \cdot x^\alpha \in \mathbb{R}[x_1, \dots, x_n]$. Then*

$$
\mathfrak{p}_{f_0}(x,t) := \sum_{\alpha \in \mathbb{N}_0^n} c_\alpha \cdot \mathfrak{p}_{\alpha_1}(x_1,t) \cdots \mathfrak{p}_{\alpha_n}(x_n,t) \quad \in \mathbb{R}[x_1, \dots, x_n, t] \tag{13}
$$

with $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}_0^n$ solves the initial value heat equation

$$
\begin{aligned}
\partial_t f(x,t) &= \Delta f(x,t) \\
f(x,0) &= f_0(x).
\end{aligned}
$$

Proof. By linearity of the Laplace operator Δ it is sufficient to look at $f_0(x) = x^\alpha$ for $\alpha \in \mathbb{N}_0^n$. By (12) we already have $\partial_t \mathfrak{p}_{\alpha_i}(x_i) = \partial_i^2 \mathfrak{p}_{\alpha_i}(x)$ and hence

$$
\begin{aligned}
\partial_t \mathfrak{p}_{f_0}(x,t) &= \partial_t [\mathfrak{p}_{\alpha_1}(x_1,t) \cdots \mathfrak{p}_{\alpha_n}(x_n,t)] \\
&= [\partial_t \mathfrak{p}_{\alpha_1}(x_1,t)] \cdot \mathfrak{p}_{\alpha_2}(x_2,t) \cdots \mathfrak{p}_{\alpha_n}(x_n,t) \\
&\qquad + \cdots + \mathfrak{p}_{\alpha_1}(x_1,t) \cdots \mathfrak{p}_{\alpha_{n-1}}(x_{n-1},t) \cdot [\partial_t \mathfrak{p}_{\alpha_n}(x_n,t)] \\
&= [\partial_1^2 \mathfrak{p}_{\alpha_1}(x_1,t)] \cdot \mathfrak{p}_{\alpha_2}(x_2,t) \cdots \mathfrak{p}_{\alpha_n}(x_n,t) \\
&\qquad + \cdots + \mathfrak{p}_{\alpha_1}(x_1,t) \cdots \mathfrak{p}_{\alpha_{n-1}}(x_{n-1},t) \cdot [\partial_n^2 \mathfrak{p}_{\alpha_n}(x_n,t)] \\
&= \Delta \mathfrak{p}_{f_0}(x,t).
\end{aligned}
$$

□

Note, in Definition 3.1 we defined $\mathfrak{p}$ for the monomials x^d, $d \in \mathbb{N}_0$, and in (13) we define $\mathfrak{p}$ by linearity for any $f_0 \in \mathbb{R}[x]$. Hence, if $f_0(x) = x^d$ then both definitions coincide: $\mathfrak{p}_{f_0} = \mathfrak{p}_d$. The same shall hold for the multivariate case to keep the notation simple.

Example 3.4 (Motzkin polynomial [Mot67])**.** Let

$$
f_{\text{Motz}}(x,y) = 1 - 3x^2y^2 + x^4y^2 + x^2y^4 \in \mathbb{R}[x,y]
$$

be the Motzkin polynomial. Then by Definition 3.1 (resp. Example 3.2) we have the substitutions

$$\begin{aligned} x^2 &\mapsto 2t + x^2, \qquad & x^4 &\mapsto 12t^2 + 12tx^2 + x^4, \\ y^2 &\mapsto 2t + y^2, \qquad & y^4 &\mapsto 12t^2 + 12ty^2 + y^4 \end{aligned}$$

and get

$$\begin{aligned} \mathfrak{p}_{\mathrm{Motz}}(x,y,t) &= 1 - 3(2t + x^2)(2t + y^2) + (12t^2 + 12tx^2 + x^4)(2t + y^2) \\ &\quad + (2t + x^2)(12t^2 + 12ty^2 + y^4) \\ &= 1 - 12t^2 + 48t^3 + 6t(-1 + 6t)(x^2 + y^2) + (-3 + 24t)x^2y^2 \\ &\quad + 2t(x^4 + y^4) + x^4y^2 + x^2y^4 \end{aligned}$$

for all $t \in \mathbb{R}$. ∘

Since the heat kernel is a Schwartz function the convolution with polynomials is well-defined and uniqueness of the solution of the heat equation shows that

$$(\Theta_t * f_0)(x) = \mathfrak{p}_{f_0}(x,t) \tag{14}$$

holds for all $f_0 \in \mathbb{R}[x_1, \ldots, x_n]$. That the heat kernel preserves polynomials holds for all convolution kernels which are integrable with respect to polynomials. To make the paper self-contained, let us briefly state and prove this known fact.

Theorem 3.5. *Let $d \in \mathbb{N}_0$ and ρ be a kernel such that $\int_{\mathbb{R}^n} y^\alpha \cdot \rho(y)\ \mathrm{d}y$ is finite for all $\alpha \in \mathbb{N}_0^n$ with $|\alpha| \leq d$, then*

$$\cdot * \rho : \mathbb{R}[x_1, \ldots, x_n]_{\leq d} \to \mathbb{R}[x_1, \ldots, x_n]_{\leq d}.$$

Proof. Let $p \in \mathbb{R}[x_1, \ldots, x_n]_{\leq d}$. Then from

$$(p * \rho)(x) = \int_{\mathbb{R}^n} p(x - y) \cdot \rho(y)\ \mathrm{d}y$$

and expanding $p(x-y)$ in the right side gives the assertion including the degree bound $\deg(p * \rho) \leq d$. □

Since the heat kernel is non-negative, the convolution of the heat kernel with a non-negative polynomial gives again a non-negative polynomial. Denote by $\mathrm{Pos}(n,d)$ the set of all non-negative polynomials on $\mathbb{R}^n$ with degree at most $d \in \mathbb{N}_0$:

$$\mathrm{Pos}(n,d) := \{p \in \mathbb{R}[x_1, \ldots, x_n]_{\leq d} \,|\, p(x) \geq 0 \text{ for all } x \in \mathbb{R}^n\}.$$

Non-negativity and Theorem 3.5 gives the following.

Corollary 3.6. *Let $n \in \mathbb{N}$, $d \in \mathbb{N}_0$, and $f_0 \in \mathrm{Pos}(n,d)$. Then*

$$\mathfrak{p}_{f_0}(\,\cdot\,,t) \in \mathrm{Pos}(n,d)$$

for all $t \geq 0$. Especially, if $f_0 \neq 0$ then $\mathfrak{p}_{f_0}(\,\cdot\,,t) > 0$ on $\mathbb{R}^n$ for all $t > 0$.

Corollary 3.7. *Let $n \in \mathbb{N}$ and $f_0 \in \mathbb{R}[x_1,\ldots,x_n]$. Assume there exist $t > 0$ and a point $\xi \in \mathbb{R}^n$ such that $\mathfrak{p}_{f_0}(\xi,t) < 0$. Then $f_0 \notin \mathrm{Pos}(n,d)$.*

Hence, recalling the Motzkin polynomial in Example 3.4 we find that $\mathfrak{p}_{\mathrm{Motz}}(\,\cdot\,,t) \in \mathrm{Pos}(2,6)$ for all $t \geq 0$. In the usual case (e.g. $f_0 \in L^2(\mathbb{R}^n)$) the convolution with the heat kernel has a smoothing effect on f_0, i.e., the regularity increases and $\Theta_t * f_0$ is a C^∞-function. But in the polynomial case we already started with a C^∞-function and this kind of regularity does not change. We have even seen that for $f_0 \in \mathbb{R}[x_1,\ldots,x_n]$ the function $\mathfrak{p}_{f_0}$ remains a polynomial for all $t \in \mathbb{R}$. But from the Motzkin polynomial in Example 3.4 we observe something additional. The Motzkin polynomial was of course the first non-negative polynomial found that is not a sum of squares. However, the heat kernel has another "smoothing effect" for this polynomial, as seen in the following continuation. We denote by $\mathrm{SOS}(n,d)$ the set of all sums of squares in $n \in \mathbb{N}$ variables of degree less or equal to $d \in \mathbb{N}_0$:

$$\mathrm{SOS}(n,d) := \{p \in \mathbb{R}[x_1,\ldots,x_n]_{\leq d} \,|\, p \text{ is a sum of squares}\}.$$

Example 3.8 (Motzkin polynomial, Example 3.4 continued)**.** We have

$$\begin{aligned}\mathfrak{p}_{\mathrm{Motz}}(x,y,1) = {} & 37 \cdot \left(1 - \frac{11}{148}x^2 - \frac{11}{148}y^2\right)^2 + \frac{71}{2} \cdot \left(x - \frac{4}{71}xy^2\right)^2 \\ & + \frac{71}{2} \cdot \left(y - \frac{4}{71}x^2y\right)^2 + \frac{57}{2}x^2y^2 + \frac{1063}{592} \cdot \left(x^2 + \frac{27}{1063}y^2\right)^2 \\ & + \frac{3815}{2126} \cdot y^4 + \frac{63}{71} \cdot x^4y^2 + \frac{63}{71}x^2y^4 \quad \in \mathrm{SOS}(2,6)\end{aligned}$$

i.e., $\mathfrak{p}_{\mathrm{Motz}}(\,\cdot\,,1)$ is by Corollary 3.6 not just non-negative, but in fact a sum of squares. This relation can easily be obtained e.g. by the use of Macaulay2 [GS] and the SumsOfSquares package [CKP20]. In fact, additional calculations indicate that

$$\mathfrak{p}_{\mathrm{Motz}}(\,\cdot\,,t) \in \begin{cases} \mathrm{Pos}(2,6) \setminus \mathrm{SOS}(2,6) & \text{for } t \in [0, T_{\mathrm{Motz}}), \text{ and} \\ \mathrm{SOS}(2,6) & \text{for } t \in [T_{\mathrm{Motz}}, \infty), \end{cases}$$

with

$$\frac{31\,998}{1\,000\,000} \quad < \quad T_{\mathrm{Motz}} \quad < \quad \frac{31\,999}{1\,000\,000}.$$

The choice of the intervals $[0, T_{\mathrm{Motz}})$ and $[T_{\mathrm{Motz}}, \infty)$ is clear since $\mathrm{SOS}(2,6)$ is closed and $\mathfrak{p}_{f_0}(\,\cdot\,,t)$ continuous in t, i.e., $\mathfrak{p}_{\mathrm{Motz}}(\,\cdot\,,T_{\mathrm{Motz}}) \in \mathrm{SOS}(2,6)$. ∘

$\mathfrak{p}_{\mathrm{Motz}} : [0,\infty) \ni t \mapsto \mathfrak{p}_{\mathrm{Motz}}(\,\cdot\,,t) \in \mathrm{Pos}(2,6)$ is a continuous path through the cone of non-negative polynomials. The following result shows that once $\mathfrak{p}_{f_0}$ enters $\mathrm{SOS}(n,d)$ e.g. at time $t_0 \geq 0$, then it stays in $\mathrm{SOS}(n,d)$ for all $t \geq t_0$.

Theorem 3.9. *Let $\rho \geq 0$ be a kernel such that $\int_{\mathbb{R}^n} y^\alpha \cdot \rho(y)\ \mathrm{d}y$ is finite for all $\alpha \in \mathbb{N}_0^n$ with $|\alpha| \leq d$, then*

$$\cdot * \rho : \mathrm{SOS}(n,d) \to \mathrm{SOS}(n,d).$$

Proof. Let $p \in \mathrm{SOS}(n,d)$, i.e., there exists a symmetric $Q \in \mathbb{R}^{N\times N}$ with $N = \binom{n+d}{d}$ such that $p(x) = (x^\alpha)_\alpha^T \cdot Q \cdot (x^\alpha)_\alpha$ where $(x^\alpha)_\alpha$ is the vector of all monomials x^α with $|\alpha| \leq d$. We then have

$$\begin{aligned}(p*\rho)(x) &= \int_{\mathbb{R}^n} p(x-y)\cdot\rho(y)\ \mathrm{d}y \\ &= \int_{\mathbb{R}^n} ((x-y)^\alpha)_\alpha^T \cdot Q \cdot ((x-y)^\alpha)_\alpha \cdot \rho(y)\ \mathrm{d}y\end{aligned}$$

and by Richter's Theorem [Ric57] we can replace $\rho(y)\ \mathrm{d}y$ by a finitely atomic representing measure $\mu = \sum_{i=1}^k c_i \cdot \delta_{y_i}$ with $c_i > 0$ and get

$$= \sum_{i=1}^k c_i \cdot ((x-y_i)^\alpha)_\alpha^T \cdot Q \cdot ((x-y_i)^\alpha)_\alpha \in \mathrm{SOS}(n,d). \qquad \square$$

Besides sums of squares, other non-negative polynomials are linear combinations of even powers of linear forms, i.e., they have a *Waring decomposition*

$$p(x) = \sum_{i=1}^k (a_i \cdot x)^d$$

with even $d \in \mathbb{N}$, $a_i \in \mathbb{R}^{n+1}$, and $a_i \cdot x := a_{i,0} + a_{i,1}x_1 + \cdots + a_{i,n}x_n$ [Rez92]. We denote by $\mathrm{War}(n,d)$ the (Waring) cone of all these polynomials, i.e., we have the proper inclusions

$$\mathrm{War}(n,d) \quad \subsetneq \quad \mathrm{SOS}(n,d) \quad \subsetneq \quad \mathrm{Pos}(n,d).$$

In Theorem 3.5 we have seen that convolution preserves being a polynomial, in Theorem 3.9 we have seen that convolution preserves being a sum of squares, and the next result shows that convolution also preserves being in the Waring cone.

Theorem 3.10. *Let $\rho \geq 0$ be a kernel such that $\int_{\mathbb{R}^n} y^\alpha \cdot \rho(y)\ \mathrm{d}y$ is finite for all $\alpha \in \mathbb{N}_0^n$, then $\cdot * \rho : \mathrm{War}(n,d) \to \mathrm{War}(n,d)$.*

Proof. Let $p \in \mathrm{War}(n,d)$, i.e., $p(x) = \sum_{i=1}^k (a_i \cdot x)^d$. Then

$$(p*\rho)(x) = \int_{\mathbb{R}^n} p(x-y)\cdot\rho(y)\ \mathrm{d}y$$

$$= \int_{\mathbb{R}^n} \sum_{i=1}^{k} (a_i \cdot (x-y))^d \cdot \rho(y) \, \mathrm{d}y$$

and by Richter's Theorem [Ric57] we can replace $\rho(y)\,\mathrm{d}y$ by a finitely atomic representing measure $\mu = \sum_{j=1}^{l} c_j \cdot \delta_{y_j}$ with $c_j > 0$ and get

$$= \sum_{j=1}^{l} \sum_{i=1}^{k} c_j \cdot (a_i \cdot (x - y_j))^d \in \mathrm{War}(n,d). \qquad \square$$

The Motzkin polynomial was the first polynomial found to be a non-negative polynomial which is not a sum of squares. But others have been identified [Mar08]. We want to investigate some of these in chronological order.

Example 3.11 (Robinson polynomial [Rob69])**.** Let

$$f_{\mathrm{Rob}}(x,y) = 1 - x^2 - y^2 - x^4 + 3x^2y^2 - y^4 + x^6 - x^4y^2 - x^2y^4 + y^6$$

be the Robinson polynomial, i.e., $f_{\mathrm{Rob}} \in \mathrm{Pos}(2,6) \setminus \mathrm{SOS}(2,6)$. Then by a direct calculation using Macaulay2 with the SumsOfSquares package similar to the Motzkin polynomial we find $\mathfrak{p}_{\mathrm{Rob}}(\,\cdot\,,1) \in \mathrm{SOS}(2,6)$ and by Theorem 3.9 we have

$$\mathfrak{p}_{\mathrm{Rob}}(\,\cdot\,,t) \in \begin{cases} \mathrm{Pos}(2,6) \setminus \mathrm{SOS}(2,6) & \text{for } t \in [0, T_{\mathrm{Rob}}), \text{ and} \\ \mathrm{SOS}(2,6) & \text{for } t \in [T_{\mathrm{Rob}}, \infty), \end{cases}$$

with

$$\frac{20\,946}{1\,000\,000} \quad < \quad T_{\mathrm{Rob}} \quad < \quad \frac{20\,947}{1\,000\,000}. \qquad \circ$$

Example 3.12 (Choi–Lam polynomial [CL77])**.** Let

$$f_{\mathrm{CL}}(x,y,z) = 1 - 4xyz + x^2y^2 + x^2z^2 + y^2z^2$$

be the Choi–Lam polynomial, i.e., $f_{\mathrm{CL}} \in \mathrm{Pos}(3,4) \setminus \mathrm{SOS}(3,4)$. We have

$$\begin{aligned} \mathfrak{p}_{\mathrm{CL}}(x,y,z,t) &= 1 - 4xyz + (2t + x^2)(2t + y^2) + (2t + x^2)(2t + z^2) \\ &\quad + (2t + y^2)(2t + z^2) \\ &= 1 + 12t^2 - 4xyz + 4t(x^2 + y^2 + z^2) + x^2y^2 + x^2z^2 + y^2z^2 \\ &= f_{\mathrm{CL}}(x,y,z) + 12t^2 + 4t(x^2 + y^2 + z^2) \end{aligned}$$

for all $t \in \mathbb{R}$ and for $t = \frac{1}{9}$ we have

$$\mathfrak{p}_{\mathrm{CL}}(x,y,z,1/9) = \frac{31}{27} + \left(xy - \frac{2}{3}z\right)^2 + \left(xz - \frac{2}{3}y\right)^2 + \left(yz - \frac{2}{3}x\right)^2. \qquad \circ$$

Macaulay2 calculations with the SumsOfSquares package suggest that for

$$T_{\mathrm{CL}} := \min\{t \geq 0 \mid \mathfrak{p}_{\mathrm{CL}}(\,\cdot\,,t) \in \mathrm{SOS}(3,4)\}$$

we have

$$\frac{1}{9} - 7 \cdot 10^{-9} \quad < \quad T_{\mathrm{CL}} \quad < \quad \frac{1}{9} - 6 \cdot 10^{-9}.$$

Example 3.13 (Schmüdgen polynomial [Sch79])**.** The polynomial

$$\begin{aligned} f_{\mathrm{Schm}}(x,y) &= (y^2-x^2)x(x+2)[x(x-2)+2(y^2-4)] \\ &\quad + 200[(x^3-4x)^2+(y^3-4y)^2] \quad \in \mathrm{Pos}(2,6)\setminus \mathrm{SOS}(2,6) \end{aligned}$$

is the Schmüdgen polynomial and we find $\mathfrak{p}_{\mathrm{Schm}}(\,\cdot\,,1) \in \mathrm{SOS}(2,6)$. In fact, Macaulay2 calculations with the SumsOfSquares package and Theorem 3.9 shows that $\mathfrak{p}_{\mathrm{Schm}}(\,\cdot\,,t) \in \mathrm{SOS}(2,6)$ for all $t \geq 2\cdot 10^{-4}$. ∘

Example 3.14 (Berg–Christensen–Jensen polynomial [BCJ79])**.** The Berg–Christensen–Jensen polynomial

$$f_{\mathrm{BCJ}}(x,y) = 1 - x^2y^2 + x^4y^2 + x^2y^4 \in \mathrm{Pos}(2,6)\setminus \mathrm{SOS}(2,6)$$

is connected to the Motzkin polynomial f_{Motz} (Example 3.4) by

$$f_{\mathrm{BCJ}}(x,y) = f_{\mathrm{Motz}}(x,y) + 2x^2y^2$$

and hence from Theorem 3.9 we see that

$$\mathfrak{p}_{\mathrm{BCJ}}(\,\cdot\,,t) \in \mathrm{SOS}(2,6)$$

for all $t \geq \frac{1}{6}$. ∘

After all these historic examples let us have a look at a more modern example from the vast literature of non-negative polynomials which are not sums of squares.

Example 3.15 (Harris polynomial [Har99, $R_{2,0}$ in Lem. 5.1 and 6.8])**.** Let

$$\begin{aligned} f_{\mathrm{Har}}(x,y) = \quad & 16x^{10} - 36x^8y^2 + 20x^6y^4 + 20x^4y^6 - 36x^2y^8 + 16y^{10} \\ & - 36x^8 \ + 57x^6y^2 - 38x^4y^4 + 57x^2y^6 - 36y^8 \\ & + 20x^6 \ - 38x^4y^2 - 38x^2y^4 + 20y^6 \\ & + 20x^4 \ + 57x^2y^2 + 20y^4 \\ & - 36x^2 \ - 36y^2 \\ & + 16 \end{aligned}$$

be the Harris polynomial, i.e., $f_{\mathrm{Har}} = R_{2,0} \in \mathrm{Pos}(2,10)\setminus \mathrm{SOS}(2,10)$. With Example 3.2,

$$\mathfrak{p}_8(x,t) = 1680t^4 + 3360t^3x^2 + 840t^2x^4 + 56tx^6 + x^8,$$

and

$$\mathfrak{p}_{10}(x,t) = 30240t^5 + 75600t^4x^2 + 25200t^3x^4 + 2520t^2x^6 + 90tx^8 + x^{10}$$

we calculate $\mathfrak{p}_{\mathrm{Har}}$ and find $\mathfrak{p}_{\mathrm{Har}}(\,\cdot\,,1) \in \mathrm{SOS}(2,10)$. In fact, Macaulay2 calculations and Theorem 3.9 show that $\mathfrak{p}_{\mathrm{Har}}(\,\cdot\,,t) \in \mathrm{SOS}(2,10)$ for all $t \geq 8\cdot 10^{-4}$. ∘

All examples so far become a sum of squares for large t. However, this is not in general true.

Lemma 3.16. *Let $n, d \in \mathbb{N}$ and*

$$f(x) = \sum_{|\alpha| \leq 2d} a_\alpha \cdot x^\alpha \in \mathrm{Pos}(n, 2d)$$

such that

$$f_{2d}(x) := \sum_{|\alpha| = 2d} a_\alpha \cdot x^\alpha \notin \mathrm{SOS}(n, 2d),$$

then $\mathfrak{p}_f(\,\cdot\,, t) \in \mathrm{Pos}(n, 2d) \setminus \mathrm{SOS}(n, 2d)$ for all $t \geq 0$.

Proof. Assume there is a $t \geq 0$ such that

$$\mathfrak{p}_f(x, t) = \sum_{i=1}^{k} \left(\sum_{|\alpha| \leq d} c_{i,\alpha}(t) \cdot x^\alpha \right)^2 = \sum_{|\alpha| \leq 2d} a_\alpha(t) \cdot x^\alpha \in \mathrm{SOS}(n, 2d).$$

Since by Definition 3.1 we have $a_\alpha(t) = a_\alpha(0)$ for all $\alpha \in \mathbb{N}_0^n$ with $|\alpha| = 2d$ the sum of squares decomposition of $\mathfrak{p}_f(\,\cdot\,, t)$ gives

$$f_{2d}(x) = \sum_{i=1}^{k} \left(\sum_{|\alpha| = d} c_{i,\alpha}(t) \cdot x^\alpha \right)^2 \in \mathrm{SOS}(n, 2d)$$

which contradicts the assumption $f_{2d} \notin \mathrm{SOS}(n, 2d)$. □

The following example shows that the condition $f_{2d} \in \mathrm{SOS}(n, 2d)$ in Lemma 3.16 is necessary, but not sufficient. Just take the polynomial $f(w, x, y, z) = z^6 - 3x^2y^2z^2 + x^4y^2 + x^2y^4 + w^8 \in \mathrm{Pos}(3, 8) \setminus \mathrm{SOS}(3, 8)$.

Example 3.17. Let $f(x, y, z) = z^6 - 3x^2y^2z^2 + x^4y^2 + x^2y^4 \in \mathrm{Pos}(3, 6) \setminus \mathrm{SOS}(3, 6)$ be the homogeneous Motzkin polynomial. Then $\mathfrak{p}_f(\,\cdot\,, t) \in \mathrm{Pos}(3, 6) \setminus \mathrm{SOS}(3, 6)$ for all $t \geq 0$. ∘

Remark 3.18. The result in Lemma 3.16 also holds for $f_{2d} \notin \mathrm{War}(n, 2d)$, i.e., $\mathfrak{p}_f(\,\cdot\,, t) \in \mathrm{Pos}(n, 2d) \setminus \mathrm{War}(n, 2d)$. ∘

While we have seen in Lemma 3.16 and Example 3.17 that there are non-negative polynomials which do not become sum of squares under the heat equation, the following result shows that any non-negative polynomial becomes asymptotically close to $\mathrm{SOS}(\mathbb{R}^n)$ under the heat equation, that is, the constant polynomial becomes an attractor of the polynomial heat equation.

Lemma 3.19. *Let $n \in \mathbb{N}$ and $f \in \mathrm{Pos}(\mathbb{R}^n)$ with $\deg f = 2d$ for some $d \in \mathbb{N}$. Then*

$$\lim_{t \to \infty} \mathfrak{p}_f(x, t) \cdot t^{-d} = c > 0.$$

Proof. Let $k \in \mathbb{N}$. It is easy to see that $\Delta^k g$ is constant on $\mathbb{R}^n$ for all $g \in \mathbb{R}[x_1, \ldots, x_n]_{\leq 2k}$ and even equal to zero for all $g \in \mathbb{R}[x_1, \ldots, x_n]_{\leq 2k-1}$.

Since $f \in \mathrm{Pos}(\mathbb{R}^n)$ with $\deg f = 2d$ we have that the homogeneous part f_{2d} of f of degree $2d$ is non-zero and non-negative on $\mathbb{R}^n$. Let S be the unit sphere in $\mathbb{R}^n$. Since $f_{2d} \in \mathrm{Pos}(\mathbb{R}^n) \setminus \{0\}$ we have

$$\int_S f_{2d}(x) \, \mathrm{d}x > 0$$

and by [Ilt98, Cor. 1] we have $\Delta^m f_{2d} \neq 0$ for all $m = 1, \ldots, d$. Hence, $\partial_t^d \mathfrak{p}_f(x,t) = \Delta^d \mathfrak{p}_f(x,t) = \Delta^d f_{2d}(x) = c > 0$ which proves the statement. □

Lemma 3.16 and Example 3.17 have only been proven here for $n \geq 3$, but for $n = 2$ no counterexample has been found. In fact, every time evolution of the polynomials $f \in \mathrm{Pos}(\mathbb{R}^2) \setminus \mathrm{SOS}(\mathbb{R}^2)$ in the Examples 3.8, 3.11, 3.13, and 3.14 enters $\mathrm{SOS}(\mathbb{R}^2)$ and by Theorem 3.9 never leaves $\mathrm{SOS}(\mathbb{R}^2)$ again. It is open if for $n = 2$ every time evolution of a non-negative polynomial becomes a sum of squares; see Open Problem 5.1.

4. Time-dependent set of atoms

4.1. Coefficients in C_b^∞

Let $L : \mathbb{R}[x_1, \ldots, x_n]_{\leq d} \to \mathbb{R}$ with $d \in \mathbb{N}_0 \cup \{\infty\}$ be a (truncated) moment functional. When a $p_0 \in \mathbb{R}[x_1, \ldots, x_n]_{\leq d}$ with $p_0 \geq 0$ exists with $L(p_0) = 0$, then $\operatorname{supp} \mu \subseteq \mathcal{Z}(p_0)$ for any representing measure μ of L.

In Section 2 we calculated the dual action of (3) on $p_0 \in \mathrm{Pol}(\mathbb{R}^n)$. It is easy to see that with $\nu > 0$ and $p_0 \geq 0$, then $p_t > 0$ for all $t > 0$. Therefore for a moment functional L we always have $L(p_t) > 0$ and no restriction of the support of the representing measure is possible. Therefore, we can only study the time-dependent set of atoms for $\nu = 0$.

Let us remind the reader, that for any time-dependent vector field g and starting point $x_0 \in \mathbb{R}^n$ the system of ordinary differential equations

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} G(x,t) &= g(x,t) \\ G(x_0, 0) &= x_0 \end{aligned} \tag{15}$$

has by the Picard–Lindelöff Theorem a unique solution $G : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$. That means a particle located at $x_0 \in \mathbb{R}^n$ for time $t_0 = 0$ has the trajectory $G(x_0, t)$ when it experiences the force field g, i.e., at time $t \in \mathbb{R}$ is has the position $G(x_0, t) \in \mathbb{R}^n$.

The initial value problem (3) acts only on functions f_0. But by duality in Section 2 also the action of (3) on a measure μ_0 is well-defined. The following solves the problem for a Dirac measure.

Lemma 4.1. *Let $g \in C(\mathbb{R}, C_b^\infty(\mathbb{R}^n))^n$ be a time-dependent vector field and $G : \mathbb{R}^n \times [0,\infty) \to \mathbb{R}^n$ be the unique solution of (15). Additionally, let $h \in C(\mathbb{R}, C_b^\infty(\mathbb{R}^n))$, $x_0 \in \mathbb{R}^n$, and $c_0 > 0$. Then the measure valued differential equation*

$$\begin{aligned} \partial_t \mu_t(x) &= -g(x,t)\nabla\mu_t(x) + h(x,t)\cdot\mu_t(x) \\ \mu_0(x) &= c_0 \cdot \delta_{x_0}(x) \end{aligned} \tag{16}$$

has the unique solution

$$\mu_t(x) = c_0 \cdot \exp\left(\int_0^t h(G(x_0,s),s)\ \mathrm{d}s\right) \cdot \delta_{G(x_0,t)}(x)$$

for all $t \in \mathbb{R}$.

Proof. Let $A(x,t) = -g(x,t)\nabla$ and $B(x,t) = h(x,t)$ be the two operators in (16), i.e., (16) reads $\partial_t\mu_t = A\mu_t + B\mu_t$. Then by Trotters approach we have

$$\mu_t(x) = \lim_{N\to\infty}\left[\prod_{i=1}^N \exp\left(\int_{t_{i-1}}^{t_i} B(x,s)\ \mathrm{d}s\right)\exp\left(\int_{t_{i-1}}^{t_i} A(x,s)\ \mathrm{d}s\right)\right]\mu_0(x)$$

for any decompositions $\mathcal{Z}_N = \{t_0 = 0 < t_1 < \cdots < t_N = t\}$ with $\Delta\mathcal{Z}_N \to 0$ as $N \to \infty$.

But A is the transport operator and hence when acting on $c_0 \cdot \delta_{x_0}(x)$ we can use the approximation

$$\begin{aligned} \exp\left(\int_{t_0}^{t_1} A(x,s)\ \mathrm{d}s\right) c_0 \cdot \delta_{x_0}(x) &\approx c_0 \cdot \delta_{x_0}\left(x - \int_{t_0}^{t_1} g(x,s)\ \mathrm{d}s\right) \\ &\approx c_0 \cdot \delta_{x_0 + \int_{t_0}^{t_1} g(x_0,s)\ \mathrm{d}s}(x) \end{aligned}$$

on the interval $[t_0, t_1]$ (and similarly by induction on all $[t_{i-1}, t_i]$ for $i = 1, \ldots, N$) which gives for $N \to \infty$ with $\Delta\mathcal{Z}_N \to 0$ the same result $\mu_t(x)$. On the other hand the operator B acts only as multiplication and hence does not affect the transport of the Dirac measure by A. The point x_0 is therefore transported by A, which is seen by the approximation $x_i := x_{i-1} + \int_{t_{i-1}}^{t_i} g(x_{i-1},s)\ \mathrm{d}s$. We therefore have $\mu_t(y) = c(t)\cdot\delta_{x(t)}(y)$ with $x(t) = G(x_0,t)$.

Since now the Dirac measure $\delta_{G(x_0,t)}$ moves along the vector field g starting at x_0, it experiences at time t the multiplication operator $B(x(t),t) = h(G(x_0,t),t)$ and therefore we have

$$c(t) = c_0 \cdot \exp\left(\int_0^t h(G(x_0,s),s)\ \mathrm{d}s\right) \tag{$*$}$$

which proves the statement. Uniqueness follows either by the uniqueness of the dual problem or directly by uniqueness of G and $(*)$. □

The solution of (16) for $\mathrm{d}\mu_0(x) = f_0(x)\,\mathrm{d}x$ with $f_0 \in \mathcal{S}(\mathbb{R}^n)$ can in general not be written down explicitly. But for the case of $\mu_0 = c_0 \cdot \delta_{x_0}$ Lemma 4.1 shows that (16) is simply solved since the transport term $g(x,t)\cdot\nabla$ acts only on the point $x_0 = x(0)$ to get $x(t)$ and the multiplication $h(x,t)$ only acts on the coefficient $c_0 = c(0)$ to get $c(t)$. This simplifies the description of the solution immensely and provides in the following result a way to trace the Carathéodory number $\mathcal{C}(s)$.

Theorem 4.2. *Let $n \in \mathbb{N}$, $s(0) = (s_\alpha(0))_{\alpha\in\mathbb{N}^n} \in \mathcal{S}_{n,\infty}$ be a n-dimensional moment sequence with finite rank Hankel matrix $\mathcal{H}(s(0))$, $g \in C(\mathbb{R}, C(\mathbb{R}^n, \mathbb{R}^n))$, and $h \in C(\mathbb{R}, C(\mathbb{R}, \mathbb{R}))$. Then there is a unique time evolution $s : \mathbb{R} \to \mathcal{S}_{n,\infty}$ of $s(0)$ with respect to*

$$\partial_t f(x,t) = -g(x,t)\nabla f(x,t) + h(x,t)\cdot f(x,t).$$

Additionally, for all $t \in \mathbb{R}$ we have

$$\operatorname{rank}\mathcal{H}(s(t)) = \operatorname{rank}\mathcal{H}(s(0))$$

and therefore the Carathéodory number is constant, i.e., $\mathcal{C}(s(t)) = \mathcal{C}(s(0))$.

Proof. Since $K := \operatorname{rank}\mathcal{H}(s(0))$ is finite, there exists a unique K-atomic representing measure $\mu_0 = \sum_{i=0}^{K} c(0)\cdot\delta_{x_i(0)}$ of $s(0)$. By linearity of the time-evolution and Lemma 4.1 we have the unique time-evolution of $\mu_t = \sum_{i=1}^{K} c_i(t)\cdot\delta_{x_i(t)}$ and therefore the unique time-evolution of $s(t)$.

It remains to show that $\mathcal{C}(s(t)) = \operatorname{rank}\mathcal{H}(s(t)) = \operatorname{rank}\mathcal{H}(s(0)) = \mathcal{C}(s(0))$. While the first and the third equality is clear from the rank, see e.g. [Sch17, Prop. 17.21], we have to show the second equality. For that it is sufficient to show that the path of $x_k(t)$ never splits or two paths $x_j(t)$ and $x_k(t)$ $(j \neq k)$ intersect for any $t \in \mathbb{R}$. But this follows from Lemma 4.1 and the uniqueness of the solution $x_j(t) = G(x_j(0), t)$ of (15) by Peano's Theorem, i.e., when two integral curves $x_j(t)$ and $x_k(t)$ of (15) coincide for some $t' \in \mathbb{R}$, i.e., $x_j(t') = x_k(t')$, then $x_j(t) = x_k(t)$ for all $t \in \mathbb{R}$, especially for $t = 0$ which contradicts the minimal choice of $K = \operatorname{rank}\mathcal{H}(s(0))$. □

In the univariate case the previous result also holds for the truncated moment problem.

Example 4.3. Let $s(0) = (s_k(0))_{k=0}^{2d}$ with $d \in \mathbb{N}$ be a moment sequence on the boundary of the moment cone, i.e., s is represented by $\mu_0 = \sum_{k=1}^{l\leq d} c_k(0)\cdot\delta_{x_k(0)}$ with $c_1(0),\dots,c_l(0) > 0$ and $x_1(0),\dots,x_l(0)$ pairwise different and the non-negative polynomial $p_0(x) = (x - x_1(0))^2\cdots(x - x_l(0))^2$ fulfills $L_{s(0)}(p_0) = 0$. Let $s(t)$ evolve with respect to $\partial_t f = -g\partial_x f + h\cdot f$. By Lemma 4.1 we have $\mu_t = \sum_{k=1}^{l\leq d} c_k(t)\cdot\delta_{x_k(t)}$ and therefore $L_{s(t)}(p_t) = 0$ for the non-negative polynomial $p_t(x) = (x - x_1(t))^2\cdots(x - x_l(t))^2$. Hence, the boundary moment sequence remains a boundary sequence for all times. ∘

Remark 4.4. In the previous example we have seen that for univariate truncated moment moment sequences on the boundary the time evolution with respect to (3) with $\nu = 0$ remains a boundary truncated moment sequence for all times. And additionally, the time evolution is unique, depending only on the initial moments. For multivariate moment sequences this no longer holds. Firstly, multivariate (truncated) moment sequences on the boundary can be indeterminate [dDS22] and the time evolution then depends on the choice of the representing measure μ_0. And secondly, even if the truncated boundary moment sequence is determinate, it can immediately enter the interior of the moment cone. To see this, take an example from optimal design [Rez92] where the isolated zeros of a non-negative polynomial is maximal. For example take 10 projective zeros of the Robinson polynomial [Rob69] after rotation of the projective space such that no zero lies at infinity (all 10 zeros are then in the affine space $\mathbb{R}^2$). Since the zeros are isolated we find a vector field $g : \mathbb{R}^2 \to \mathbb{R}^2$ such that these points are in general position for $t \neq 0$. Then by the Alexander–Hirschowitz theorem [AH95] there is no non-negative polynomial of degree 6 vanishing on all these 10 points, i.e., the truncated moment sequence from the measure μ_t with $t \neq 0$ belongs to an interior moment sequence. ◦

4.2. Extension to C^∞

We have so far treated $g \in C_b^\infty(\mathbb{R}^n, \mathbb{R}^n)$. We want to see what happens when we extend this class. In [CdD22] we calculated the explicit time-evolution of the moments for $\partial_t f(x,t) = x \cdot \partial_x f(x,t)$ and we got

$$s_k(t) = s_k(0) \cdot e^{-(k+1)\cdot t}.$$

Also for $k = 0$ the moments can be calculated only from the initial values $s(0)$ by solving $\partial_t s_0(t) = 0$ and $\partial_t s_k(t) = -k \cdot s_{k-1}(t)$ for $k \in \mathbb{N}$ by induction.

When we have $\partial_t f = x^k \partial_x f$ with $k \geq 2$, it is in general not possible to calculate the time-dependent moments. For moment sequences with finite rank we can at least ensure the existence of the time-evolution $s(t)$ for small times and we observe a finite break down in time.

Example 4.5. Let $k = 2$ and $x_0 = 1$. Then to solve

$$\begin{aligned} \partial_t \mu_t &= -x^2 \cdot \partial_x \mu_t \\ \mu_0 &= \delta_1 \end{aligned}$$

we have by Lemma 4.1 to solve

$$\begin{aligned} \partial_t x(t) &= a \cdot x(t)^2 \\ x(0) &= 1, \end{aligned}$$

i.e., we have

$$t = \int_1^x y^{-k} \, \mathrm{d}y = (k-1) \cdot \left[1 - x^{1-k}\right]$$

and hence $x(t) = (1-t)^{-1}$. Since $\lim_{t \nearrow 1} x(t) = \infty$, we have that the time-dependent moments $s_l(t)$ for $\partial_t f = -x^2 \cdot \partial_x f$ exist only for $t < 1$ and $s_l(1) = \infty$ for all $l \in \mathbb{N}$. ◦

The previous example demonstrates why we have to restrict to $g \in C_b^\infty$.

5. Summary and open questions

We investigated time-dependent moments from partial differential equations. At first we gave the dual action on the polynomials (Theorem 2.2). While for general coefficients g and h we leave $\mathbb{R}[x_1, \ldots, x_n]$ in general, for coefficients independent on x we remain in $\mathbb{R}[x_1, \ldots, x_n]$. We investigated the action of the heat equation on non-negative polynomials more deeply. In Examples 3.8, 3.11, and 3.13 to 3.15 we have collected examples of non-negative polynomials on $\mathbb{R}^2$ which are not sums of squares. But under the action of the heat equation after finite time they become sums of squares. The highest degree part is a non-negative homogeneous polynomial in two variables and hence a sum of squares [Hil88]. If this holds for all bivariate non-negative polynomials is still open.

Open Problem 5.1. *Let $f \in \mathrm{Pos}(\mathbb{R}^2) \setminus \mathrm{SOS}(\mathbb{R}^2)$. Is it true that there always is a $T = T(f) > 0$ such that $\mathfrak{p}_f(x,t) \in \mathrm{SOS}(\mathbb{R}^2)$ for all $t \geq T$?*

By Theorem 3.9 Open Problem 5.1 reduces to the questions that $\mathfrak{p}_f(x,T) \in \mathrm{SOS}(\mathbb{R}^2)$ holds for at least one $T > 0$.

On $\mathbb{R}^n$ with $n \geq 3$ this in general no longer holds and the heat equation fails to produce sum of squares from non-negative polynomials in three or more variables, see Lemma 3.16 and Example 3.17. Note, the Choi–Lam polynomial (Example 3.12) is a non-negative polynomial in 3 variables, not a sum of squares, but becomes a sum of squares under the heat equation. From the counterexamples in Lemma 3.16 and Example 3.17 we see that it is necessary that the highest degree part is a sum of squares. And from the calculations we get the impression that the SOS-property is pushed from the highest degree part to the lower degree parts. Supported by Example 3.12, Hilbert's Theorem [Hil88] then implies the second open question.

Open Problem 5.2. *Let $f \in \mathrm{Pos}(\mathbb{R}^3) \setminus \mathrm{SOS}(\mathbb{R}^3)$ with $\deg f \leq 4$. Is it true that there always is a $T = T(f) > 0$ such that $\mathfrak{p}_f(x,t) \in \mathrm{SOS}(\mathbb{R}^3)$ for all $t \geq T$?*

The third possibility in Hilbert's Theorem [Hil88] is $\deg f = 2$. But then $\mathfrak{p}_f(x,t) = f(x) + c \cdot t$ with $c > 0$ [Ilt98], i.e., homogenization shows already $f \in \mathrm{SOS}(n,2)$.

In Lemma 3.19 we show that under the heat equation any non-negative polynomial in $\mathbb{R}[x_1, \ldots, x_n]$ gets close to the constant polynomial

$$\lim_{t \to \infty} \mathfrak{p}_f(x,t) \cdot t^{-d} = c > 0,$$

i.e., the positive constant polynomials are attractors of the polynomial heat equation.

For the equation $\partial_t f = g \cdot \nabla f + h \cdot f$ we calculate the time-dependent set of atoms, i.e., we solve the problem of how the atoms of a finitely atomic representing measure $\mu_t = \sum_{i=1}^k c_i(t) \cdot \cdot \delta_{x_i(t)}$ evolve in time. We find that the

atom positions $x_i(t)$ are governed by the transport term $g \cdot \nabla$ but are unaffected by the scaling with h. The coefficients (masses) $c_i(t)$ can then be analytically solved from the $x_i(t)$, see Lemma 4.1 and Theorem 4.2.

We also extended the treatment beyond smooth and bounded coefficients and found that atoms under the transport term $-x^2 \cdot \partial_x$ move to infinity in finite time, i.e., a finite break down of the moments (and the measure solution) appears even for linear partial differential equations, see Example 4.5.

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