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Conditionally Positive Definite Functions and Laplace–Stieltjes Integrals

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In this paper, we characterize those functions that are conditionally positive definite on Euclidean spaces $\mathbb{R}^d$ for all $d = 1, 2, \ldots$, as certain Laplace–Stieltjes integrals.

INTRODUCTION

Let $C(\mathbb{R}^d)$ denote the set of all continuous complex-valued functions on $\mathbb{R}^d$. A function $f \in C(\mathbb{R}^d)$ is said to be positive on $\mathbb{R}^d$ if for any n complex numbers $c_1, c_2, \ldots, c_n$ and any n points $x_1, x_2, \ldots, x_n$ in $\mathbb{R}^d$, we have

$$\sum_{i=1}^{n} \sum_{j=1}^{n} c_i \bar{c}_j f(x_i - x_j) \geqslant 0.$$

Let k be a nonnegative integer, and let $\Pi_k(\mathbb{R}^d)$ denote the set of all d-variable polynomials of degree k or less. A function $f \in C(\mathbb{R}^d)$ is said to be conditionally positive definite of order $k (k \geqslant 1)$ on $\mathbb{R}^d$, if for any n complex numbers $c_1, c_2, \ldots, c_n$ and any n points $x_1, x_2, \ldots, x_n$ in $\mathbb{R}^d$ satisfying

$$\sum_{i=1}^{n} c_i p(x_i) = 0 \qquad \text{for all} \quad p \in \Pi_{k-1}(\mathbb{R}^d),$$

we have

$$\sum_{i=1}^{n} \sum_{j=1}^{n} c_i \bar{c}_j f(x_i - x_j) \geqslant 0.$$

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We denote the set of all positive definite functions on $\mathbb{R}^d$ by $P(\mathbb{R}^d)$ and the set of all conditionally positive functions of order k on $\mathbb{R}^d$ by $CP_k(\mathbb{R}^d)$.

We recall that a function h defined on $(0, \infty)$ is said to be completely monotone on $(0, \infty)$ if $(-1)^m f^{(m)}(t) \geqslant 0$ for all $t>0$ and $m=0, 1, 2, \ldots$. The well-known Bernstein–Widder Theorem [W] asserts that a function h is completely monotone on $(0, \infty)$ if and only if h has the Laplace–Stieltjes integral representation

$$h(t)=\int_0^\infty e^{-tu}\, d\alpha(u), \qquad t>0,$$

where $\alpha(u)$ is a positive Borel measure on $(0, \infty)$. Following Schoenberg [S], we denote by $\mathcal{M}$ the set of functions which belong to $C[0, \infty)$ and are completely monotone on $(0, \infty)$.

Let $x := (x_1, \ldots, x_d) \in \mathbb{R}^d$, denote the Euclidean norm of x by $|x|$, i.e., $|x| = (x_1^2 + \cdots + x_d^2)^{1/2}$. It follows from the Bernstein–Widder Theorem that if $h \in \mathcal{M}$ then the function $H(x) := h(|x|^2)$ is positive definite on $\mathbb{R}^d$ for all $d=1, 2, \ldots$. Remarkably, Schoenberg [S] proved that the converse of this result is true. In the same paper, Schoenberg also proved the following result: In order that the functions $H(x)=h(|x|^2)$ be conditionally positive definite of order 1 on $\mathbb{R}^d$ for all $d=1, 2, \ldots$, it is necessary and sufficient that $(-1)\,h'$ be completely monotone on $(0, \infty)$.

Schoenberg's results find applications in a wide range of mathematics; see Berg *et al.* [BCR], Donoghue [D], and Wells and Williams [WW].

Michelli [M] proved that if $h \in C[0, \infty)$, and for some $k=1, 2, \ldots$, $(-1)^k h^{(k)}$ is completely monotone on $(0, \infty)$, then $H(x)=h(|x|^2) \in CP_k(\mathbb{R}^d)$ for all $d=1, 2, \ldots$. Michelli conjectured that the converse of this result is also true. Actually Michelli gave a simple proof of the converse for $k=1$. We note that while Michelli's results were established in an elegant way, the converse for the case $k>1$ has remained unsettled for the last several years. Careful examination reveals that some basic differences exist between the case $k=1$ and the case $k>1$. The lack of proof for this important case was also mentioned by Narcowich and Ward [NW].

The purpose of this paper is to give a complete proof to the converse of Micchelli's theorem. Thus, part of Schoenberg's beautiful theory of positive definite functions on metric spaces is extended to conditionally positive definite functions. We start in Section 1 with the development of integral representations for radial conditionally positive definite functions. The main result is proved in Section 2. In Section 3, we point out some distinctions between the cases $k=1$ and $k>1$.

1. Notations and Preliminaries

Let d be a positive integer, $x=(x_1, ..., x_d) \in \mathbb{R}^d$ and $\xi=(\xi_1, ..., \xi_d) \in \mathbb{R}^d$. Let $S(\mathbb{R}^d)$ denote the space of Schwartz class functions and $S'(\mathbb{R}^d)$ be the dual space of $S(\mathbb{R}^d)$. For $\varphi \in S(\mathbb{R}^d)$, we define its Fourier transform $\varphi(\xi)$ by the formula

$$\hat{\varphi}(\xi)=\frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{-i\xi x} \varphi(x)\, dx,$$

where ξx denotes the usual inner product on $\mathbb{R}^d$, i.e., $\xi x=\sum_{i=1}^d \xi_i x_i$. It is well-known that if $\varphi \in S(\mathbb{R}^d)$, then $\hat{\varphi} \in S(\mathbb{R}^d)$ and the following Fourier inversion formula holds:

$$\varphi(x)=\frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{ix\xi} \hat{\varphi}(\xi)\, d\xi.$$

Also, for $\varphi, \psi \in S(\mathbb{R}^d)$, we define the inner product of φ and ψ

$$\langle \varphi, \psi \rangle_d=\frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \varphi(x)\, \overline{\psi(x)}\, dx.$$

The following Parseval identity holds for all $\varphi, \psi \in S(\mathbb{R}^d)$

$$\langle \varphi, \psi \rangle_d=\langle \hat{\varphi}, \bar{\psi} \rangle_d.$$

Let $K(\mathbb{R}^d)$ denote the space of all infinitely differentiable functions on $\mathbb{R}^d$ with compact supports and $K'(\mathbb{R}^d)$ its dual space. Following Gelfand and Vilenkin [GV], we denote the image of $K(\mathbb{R}^d)$ under the Fourier transform by $\mathbb{Z}(\mathbb{R}^d)$, the dual space of $\mathbb{Z}(\mathbb{R}^d)$ by $\mathbb{Z}'(\mathbb{R}^d)$. An element of the spaces $K(\mathbb{R}^d)$, $S(\mathbb{R}^d)$, and $\mathbb{Z}(\mathbb{R}^d)$ is henceforth called a test function, and an element of their dual spaces called a distribution. We also use the notation $\langle T, \varphi \rangle_d$ to denote the action of a distribution T on a test function φ, as no confusion is likely to occur. For $T \in S'(\mathbb{R}^d)$, we define its Fourier transform according to the following equation

$$\langle \hat{T}, \hat{\varphi} \rangle_d=\langle T, \varphi \rangle_d, \qquad \varphi \in S(\mathbb{R}^d).$$

For $T \in K'(\mathbb{R}^d)$, the Fourier transform T is defined as an element of $\mathbb{Z}'(\mathbb{R}^d)$ according to the equation

$$\langle \hat{T}, \hat{\varphi} \rangle_d=\langle T, \varphi \rangle_d, \qquad \varphi \in K(\mathbb{R}^d).$$

The latter definition is justified by the well-known Paley–Weiner Theorems; see Yosida [Y, p. 166].

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The following lemma can be verified by using standard limit arguments.

LEMMA 1.1. *$f \in CP_k(\mathbb{R}^d)$ if and only if*

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f(x-y)\,\varphi(x)\,\overline{\varphi(y)}\,dx\,dy \geqslant 0$$

for all $\varphi \in K(\mathbb{R}^d)$ that satisfies $\int_{\mathbb{R}^d} \varphi(x)\,q(x)\,dx = 0$ for all $q \in \Pi_{k-1}(\mathbb{R}^d)$.

Let $j = (j_1, ..., j_d)$ be a nonnegative integer multi-index and denote the differential operator d^j/dx^j by D^j. Let $p(x) = \sum_{|j|=k} a_j x^j$ be a homogeneous polynomial of degree k. Then $p(D) = \sum_{|j|=k} a_j D^j$ is a linear homogeneous constant-coefficient differential operator of order k.

DEFINITION 1.2. A function $f(x)$ in $C(\mathbb{R}^d)$ is called k-positive definite if

$$\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f(x-y)\{p(D)\,\varphi(x)\}\{\overline{p(D)\,\varphi(y)}\}\,dx\,dy \geqslant 0$$

for all $\varphi \in K(\mathbb{R}^d)$ and all linear homogeneous constant-coefficient differential operators $p(D)$ of order k.

LEMMA 1.3. *If $f \in CP_k(\mathbb{R}^d)$, then f is k-positive definite.*

Proof. This follows from the simple fact that if $\varphi(x) = p(D)\,\psi(x)$ with $\psi \in K(\mathbb{R}^d)$ and $p(D)$ a linear homogeneous constant-coefficient differential operator of order k, then, an application of Fubini's theorem and integration by parts show that $\int_{\mathbb{R}^d} \varphi(x)\,q(x)\,dx = 0$ for all polynomials $q(x)$ of degree $\leqslant k-1$. ∎

Remark 1.4. Madych and Nelson [MN] proved the stronger result that $f \in CP_k(\mathbb{R}^d)$ if and only if f is k-positive definite. In this paper, we only need the sufficiently part of their result which is Lemma 1.3.

The following result can be found in Gelfand and Vilenkin [GV, Theorem 1′, p. 179].

LEMMA 1.5′. *Let f be k-positive definite. Then, for any $\varphi \in K(\mathbb{R}^d)$, the following identity is true:*

$$\langle f, \varphi\rangle_d = \langle \hat{f}, \varphi\rangle_d = \int_{\Omega_0}\left[\hat{\varphi}(\xi) - \alpha(\xi)\sum_{|j|=0}^{2k-1}\frac{\hat{\varphi}^{(j)}(0)}{j!}\,\xi^j\right]d\mu_d(\xi)$$
$$+\sum_{|j|=0}^{2k} a_j\,\frac{\hat{\varphi}^{(j)}(0)}{j!}, \tag{1}$$

where $\Omega_0 = \mathbb{R}^d \backslash \{0\}$, *and* μ_d *is a tempered positive Borel measure on* Ω_0, *independent of* φ, *such that* $\int_{0<|\xi|\leqslant 1} |\xi|^{2k}\, d\mu_d(\xi) < \infty$; $\alpha(\xi)$ *is a function in* $\mathbb{Z}(\mathbb{R}^d)$ *such that* $\alpha(\xi)-1$ *has a zero of order* $2k+1$ *at* $\xi = 0$; $a_j = \langle \hat{f}, \alpha(\xi)\, \xi^j \rangle_d$ *for* $|j| < 2k$; *the numbers* a_j, $|j| = 2k$, *are such that the Hermitian form* $\sum_{|i|=|j|=k} a_{i+j} \xi_i \bar{\xi}_j$ *is positive definite.*

For technical reasons, we need the following slightly different version of the above lemma, which can be proved by the same argument.

LEMMA 1.5. *Let f be k-positive definite, and let* $\alpha(\xi) \in \mathbb{Z}(\mathbb{R}^d)$ *be such that* $\alpha(\xi)-1$ *has a zero of order* $2k$ *at* $\xi = 0$. *Then, for any* $\varphi \in K(\mathbb{R}^d)$, *the following identity is true*:

$$\langle f, \varphi \rangle_d = \langle \hat{f}, \hat{\varphi} \rangle_d = \int_{\Omega_0} \left[\hat{\varphi}(\xi) - \alpha(\xi) \sum_{|j|=0}^{2k-1} \frac{\hat{\varphi}^{(j)}(0)}{j!}\, \xi^j \right] d\mu_d(\xi)$$
$$+ \sum_{|j|=0}^{2k-1} a_j \frac{\hat{\varphi}^{(j)}(0)}{j!} + \sum_{|j|=2k} a_j \frac{\hat{\varphi}^{(j)}(0) - \alpha^{(j)}(0)\, \hat{\varphi}(0)}{j!}, \tag{2}$$

where μ_d *is a tempered positive Borel measure on* Ω_0 *such that* $\int_{0<|\xi|\leqslant 1} |\xi|^{2k}\, d\mu_d(\xi) < \infty$; $a_j = \langle \hat{f}, \alpha(\xi)\, \xi^j \rangle_d$ *for* $|j| < 2k$; *the numbers* a_j, $|j| = 2k$, *are such that the Hermitian form* $\sum_{|i|=|j|=k} a_{i+j} \xi_i \bar{\xi}_j$ *is positive definite.*

LEMMA 1.6. *Let* a_j, $|j| = 2k$, *be the numbers in Lemma* 1.5. *Then the following relation holds true*:

$$\sum_{|j|=2k} a_j \frac{D^j(|x|^{2k})(0)}{j!} = \sum_{|i|=k} a_{2i} \frac{D^{2i}(|x|^{2k})(0)}{(2i)!} \geqslant 0. \tag{3}$$

Proof. The equality part is obvious. The inequality follows from the fact that for all $|i| = k$, a_{2i} are nonnegative since they are on the main diagonal of the semi-positive definite matrix $(a_{i+j})_{|i|=|j|=k}$. ∎

Let ω_{d-1} be the area of the unit sphere S_{d-1} of $\mathbb{R}^d$ and let

$$\Omega_d(x) = \frac{1}{\omega_{d-1}} \int_{S_{d-1}} e^{ix\sigma}\, d\sigma,$$

where $d\sigma$ denotes the usual measure on S_{d-1}. Then Ω_d is radial and hence we can write $\Omega_d(t) = 1/\omega_{d-1} \int_{S_{d-1}} e^{itx_0\sigma}\, d\sigma$, where x_0 is a fixed unit vector in $\mathbb{R}^d$ and $t = |x|$.

LEMMA 1.7. *The following results about the function Ω_d are true*:

(i) $\Omega_d(t)=\sum_{l=0}^{\infty}\frac{(-1)^l t^{2l}}{(2l)!!\prod_{s=0}^{l-1}(d+2s)}, \qquad t\in[0,\infty),$

(ii) $\lim_{d\to\infty}\Omega_d(t\sqrt{2d})=e^{-t^2}$ *uniformly for* $t\in[0,\infty)$,

(iii) $|\Omega_d^{(m)}(t)|\leqslant C(d,m)(1+t)^{-(d-1)/2}, \qquad t\in(0,\infty), m=0,1,2,\ldots.$

$C(d,m)$ is some constant depending only on d and m.

Proof. Parts (i) and (ii) were proved by Schoenberg [S]. Part (iii) follows from a smooth partition of unity for S_{d-1} and integration by parts; see Littman [L]. ∎

Lemma 1.5 gives a distributional expression for k-positive definite functions. In the proof of our main result, we need the following integral representation of k-positive definite radial functions.

THEOREM 1.8. *If g is k-positive definite and radial on $\mathbb{R}^d$, then for each $x\in\mathbb{R}^d$, we have*

$$g(|x|)=\int_0^{\infty}\left(\Omega_d(|x|\,r)-\alpha(r)\sum_{l=0}^{k-1}\frac{(-1)^l r^{2l}|x|^{2l}}{(2l)!!\prod_{s=0}^{l-1}(d+2s)}\right)r^{-2k}\,d\beta_d(r)$$

$$+\sum_{l=0}^{k-1}\frac{(-1)^l}{(2l)!!\prod_{s=0}^{l-1}(d+2s)}\langle\hat{g},\alpha(r)\,r^{2l}\rangle_d\,|x|^{2l}, \tag{4}$$

where

$$\alpha(r)=e^{-r^2}\sum_{l=0}^{k-1}\frac{r^{2l}}{l!}, \qquad \beta_d(r)$$

is an increasing function on $[0,\infty)$ satisfying $\int_1^{\infty}r^{-2k}\,d\beta_d(r)<\infty$, and $(2l)!!=2l(2l-2)\cdots 2$.

Proof. Select $\psi\in K(\mathbb{R}^d)$ such that $\hat{\psi}(0)=1$. Let $\delta>0$. We choose $\hat{\varphi}(\xi)=\hat{\varphi}_\delta(\xi)=e_{-ix\xi}\hat{\psi}(\delta\xi)$ in Eq. (2). Then we have the following:

(i) $\lim_{\delta\to 0}\langle g,\varphi_\delta\rangle_d=\lim_{\delta\to 0}\langle\hat{g},\hat{\varphi}_\delta\rangle_d=g(x),$

(ii) $\lim_{\delta\to 0}\hat{\varphi}_\delta^{(j)}(0)=(e^{-ix\xi})^{(j)}(\xi)|_{\xi=0}$ for all j, with $|j|=0,1,\ldots,2k,$

$$\text{(iii)}\quad \lim_{\delta\to 0}\frac{1}{|\xi|^{2k}}\left(\hat{\varphi}_\delta(\xi)-\alpha(\xi)\sum_{|j|=0}^{2k-1}\frac{\hat{\varphi}_\delta^{(j)}(0)}{j!}\xi^j\right)$$
$$=\frac{1}{|\xi|^{2k}}\left[e^{-ix\xi}-\alpha(\xi)\sum_{|j|=0}^{2k-1}((e^{-ix\xi})^{(j)}(\xi)|_{\xi=0})\frac{\xi^j}{j!}\right].$$

The limit in Part (iii) is uniform for $|\xi|\leqslant 1$.

Since μ_d is a tempered Borel measure and $\alpha\in\mathbb{Z}(\mathbb{R}^d)$, we see that

$$\text{(iv)}\quad \lim_{\delta\to 0}\int_{|\xi|\geqslant 1}\alpha(\xi)\sum_{|j|=0}^{2k-1}\frac{\hat{\varphi}_\delta^{(j)}(0)}{j!}\xi^j\,d\mu_d(\xi)$$
$$=\int_{|\xi|\geqslant 1}\alpha(\xi)\sum_{|j|=0}^{2k-1}(e^{-ix\xi})^{(j)}(\xi)\Big|_{\xi=0}\frac{\xi^j}{j!}\,d\mu_d(\xi),$$

$$\text{(v)}\quad \lim_{\delta\to 0}\int_{|\xi|\geqslant 1}\hat{\varphi}_\delta(\xi)\,d\mu_d(\xi)=\int_{|\xi|\geqslant 1}e^{-ix\xi}\,d\mu_d(\xi)$$

for every x, and $\int_{|\xi|\geqslant 1}e^{-ix\cdot\xi}\,d\mu_d(\xi)$ is finite for each $x\in\mathbb{R}^d$.

We point out that (v) is true since

$$\int_{|\xi|\geqslant 1}d\mu_d(\xi)<\infty$$

Here follows a proof of this fact. Take $\psi(x)=\theta(\cdot)*\overline{\theta(-\cdot)}$ for some $\theta\in K(\mathbb{R}^d)$, then $\hat{\psi}\geqslant 0$. Let $\hat{\varphi}_\delta(\xi)=\hat{\psi}(\delta\xi)$. Then we have

$$g(0)=\lim_{\delta\to 0}\langle\hat{g},\hat{\varphi}_\delta\rangle=\lim_{\delta\to 0}\left(\sum_{i=1}^{5}I_i\right),$$

where

$$I_1=\int_{0<|\xi|\leqslant 1}\left[\hat{\varphi}_\delta(\xi)-\alpha(\xi)\sum_{|j|=0}^{2k-1}\frac{\hat{\varphi}_\delta^{(j)}(0)}{j!}\xi^j\right]d\mu_d(\xi),$$

$$I_2=\int_{|\xi|\geqslant 1}\hat{\varphi}_\delta(\xi)\,d\mu_d(\xi),$$

$$I_3=\int_{|\xi|\geqslant 1}\alpha(\xi)\sum_{|j|=0}^{2k-1}\frac{\hat{\varphi}_\delta^{(j)}(0)}{j!}\xi^j\,d\mu_d(\xi),$$

and I_4, I_5 are the corresponding last two terms in (2) with φ replaced by φ_δ. It is easy to check that

$$\left|\hat{\varphi}_\delta(\xi)-\alpha(\xi)\sum_{|j|=0}^{2k-1}\frac{\hat{\varphi}_\delta^{(j)}(0)}{j!}\xi^j\right|\leqslant C\,|\xi|^{2k}$$

for all $|\xi|\leqslant 1$, and some constant C independent of δ.

Therefore, I_1 has a finite limit as $\delta \to 0$, so do I_3, I_4, and I_5 as can be proved easily. Consequestly, $\lim_{\delta \to 0} \int_{|\xi| \geq 1} \hat{\varphi}_\delta(\xi)\, d\mu_d(\xi)$ is finite. Since $\hat{\varphi}_\delta \to 1$ and is positive, we have

$$\int_{|\xi| \geq 1} d\mu_d(\xi) < \infty$$

$$\text{(vi)} \quad \lim_{\delta \to 0} \int_{|\xi| \geq 1} \hat{\varphi}_\delta(\xi)\, d\mu_d(\xi) = \int_{|\xi| \geq 1} e^{-ix\xi}\, d\mu_d(\xi)$$

for every x, and $\int_{|\xi| \geq 1} e^{-ix \cdot \xi}\, d\mu_d(\xi)$ is finite for each $x \in \mathbb{R}^d$.

From the above limit relations we see that if we choose $\hat{\varphi} = \hat{\varphi}_\delta$ in Eq. (2) and let $\delta \to 0^+$, then we get

$$\begin{aligned} g(x) = &\int_{\Omega_0} \left(e^{-ix\xi} - \alpha(\xi) \sum_{|j|=0}^{2k-1} (e^{-ix\xi})^{(j)}(\xi) \Big|_{\xi=0} \frac{\xi^j}{j!} \right) d\mu_d(\xi) \\ &+ \sum_{|j|=0}^{2k-1} \langle \hat{g}, \alpha(\xi)\, \xi^j \rangle (e^{-ix\xi})^{(j)}(\xi) \Big|_{\xi=0} \frac{1}{j!} \\ &+ \sum_{|j|=2k} a_j \frac{(e^{-ix\xi})^{(j)}(\xi=0) - \alpha^{(j)}(0)}{j!}. \end{aligned} \tag{5}$$

It follows from Proposition 2.2 in [MN] that $|g(x)| \leq M(|x|^{2k}+1)$ for some $M>0$ and all $x \in \mathbb{R}^d$. Hence, $g \in S'(\mathbb{R}^d)$. Since $\mathbb{Z}(\mathbb{R}^d)$ is dense in $S'(\mathbb{R}^d)$, it is not difficult to see that Eq. (2) still holds true for functions $\alpha(x)$ and $\varphi(x)$ in $S(\mathbb{R}^d)$ as long as $g \in S'(\mathbb{R}^d)$ and $\alpha(x)-1$ has a zero of order $2k$ at $x=0$. Therefore, we may choose

$$\alpha(x) = e^{-x^2} \sum_{l=0}^{k-1} \frac{x^{2l}}{l!},$$

which is radial and $\alpha(x)-1$ has a zero of order $2k$ at $x=0$. The fact that g is radial implies

$$\frac{1}{\omega_{d-1}} \int_{S^{d-1}} g(|x|\, w)\, dw = g(|x|).$$

Therefore, by Eq. (5) and series expansion of the function Ω_d in (1) of Lemma 1.7, we have

$$\begin{aligned} g(|x|) = &\int_{0^+}^{\infty} \left(\Omega_d(|x|\, r) - \alpha(r) \sum_{l=0}^{k-1} \frac{(-1)^l r^{2l} |x|^{2l}}{(2l)!! \prod_{s=0}^{l-1} (d+2s)} \right) r^{-2k}\, d\beta_d(r) \\ &+ \sum_{l=0}^{k-1} \frac{(-1)^l}{(2l)!! \prod_{s=0}^{l-1} (d+2s)} \langle \hat{g}, \alpha(r)\, r^{2l} \rangle_d\, |x|^{2l} \\ &+ \sum_{|j|=2k} a_j \frac{(r^{2k})^{(j)}(0)}{j!} \left(\frac{(-1)^k |x|^{2k}}{(2l)!! \prod_{s=0}^{k-1} (d+2s)} + 1 \right) \end{aligned} \tag{6}$$

where $\beta_d(r) = \int_{0<|\xi| \leq r} |\xi|^{2k}\, d\mu_d(\xi)$ for $r>0$.

Let

$$A_d = \sum_{|j| = 2k} a_j \frac{(r^{2k})^{(j)}(0)}{j!}.$$

Then $A_d \geqslant 0$ by Lemma 1.6. Define $\beta_d(0) := \lim_{r \to 0^+} \beta r(r) - A_d$. Then $\beta_d(r)$ is increasing on $[0, \infty)$, and we can rewrite Equation (6) as

$$g(|x|) = \int_0^\infty \left(\Omega_d(|x|\, r) - \alpha(r) \sum_{l=0}^{k-1} \frac{(-1)^l r^{2l} |x|^{2l}}{(2l)!! \prod_{s=0}^{l-1} (d+2s)} \right) r^{-2k}\, d\beta_d(r)$$

$$+ \sum_{l=0}^{k-1} \frac{(-1)^l}{(2l)!! \prod_{s=0}^{l-1} (d+2s)} \langle \hat{g}, \alpha(r)\, r^{2l} \rangle_d\, |x|^{2l}. \tag{7}$$

Here the last term in Eq. (6) is incorporated in the integral in Eq. (7) by the mass of $d\beta_d$ at $r = 0$.

By the facts that $\int_{0 < |\xi| \leqslant 1} |\xi|^{2k}\, d\mu_d(\xi) < \infty$ and that μ_d is a tempered measure, we see that $\beta_d(r)$ is finite for each $r > 0$. The conclusion $\int_1^\infty r^{-2k}\, d\beta_d(r) < \infty$ follows from the fact that $\int_{|\xi| \geqslant 1} d\mu_d(\xi) < \infty$. This finishes the proof of the theorem. ∎

2. The Main Theorem

Theorem 2.1. *Given a continuous function $f(t)$ on $[0, +\infty)$, let $g(t) = f(t^2)$. The following two statements are equivalent.*

(a) *$g(|x|) \in CP_k(\mathbb{R}^d)$ for all positive integers d.*

(b) *$f^{(m)}(t)$ exists for all positive integers m and all $t \in (0, +\infty)$, and furthermore, $(-1)^k f^{(k)}(t)$ is completely monotone on $(0, +\infty)$.*

Remark 2.2. (b) $\Rightarrow$ (a) was proved by Micchelli [M] and the case $k = 1$ of the part (a) $\Rightarrow$ (b) was done by Schoenberg [S].

We need to establish several lemmas, which require d be relatively large. But for the convenience of presentation, we take $d = 8k + 1$.

Lemma 2.3. *Let g be k-positive definite and radial on R^{8k+1}. Then for each positive integer m with $0 \leqslant m \leqslant 4k$, $g^{(m)}(t)$ exists and satisfies*

$$|g^{(m)}(t)| \leqslant C(m)(1 + t^{-4k} + t^{2k}), \; t \in (0, +\infty), \tag{8}$$

where $C(m)$ is a constant depending only on m.

Proof. We will use the same letter C to stand for different constants depending on m. Here we give the proof only for $0 \leqslant m \leqslant 2k$. The case $2k < m \leqslant 4k$ can be treated in the same way.

In Eq. (6), we replace $|x|$ by t. Then from Part (iii) of Lemma 1.7, we have $|g^{(m)}(t)| \leqslant C(1+t^{2k-m})$ for $t \in [1, +\infty)$. So, Inequality (8) will be proved if we can show that $|g^{(m)}(t)| \leqslant Ct^{-4k}$ for $t \in (0, 1)$. For this purpose, we write

$$\begin{aligned} g^{(m)}(t) &= \int_0^1 \frac{d^m}{dt^m}\left(\Omega_d(tr) - \alpha(r) \sum_{l=0}^{k-1} \frac{(-1)^l r^{2l} |t|^{2l}}{(2l)!! \prod_{s=0}^{l-1} (d+2s)}\right) r^{-2k}\, d\beta_d(r) \\ &\quad + \int_1^\infty \frac{d^m}{dt^m}\left(\Omega_d(tr) - \alpha(r) \sum_{l=0}^{k-1} \frac{(-1)^l r^{2l} t^{2l}}{(2l)!! \prod_{s=0}^{l-1} (d+2s)}\right) r^{-2k}\, d\beta_d(r) \\ &\quad + \frac{d^m}{dt^m}\left(\sum_{l=0}^{k-1} \frac{(-1)^l}{(2l)!! \prod_{s=0}^{l-1} (d+2s)} \langle g, \alpha(r) r^{2l} \rangle_d\, t^{2l}\right) \\ &= I_1 + I_2 + I_3. \end{aligned}$$

It is easy to see that $|I_1| \leqslant C$, and $|I_3| \leqslant C$ for $t \in (0, 1)$. To control I_2, it suffices to control

$$\int_1^\infty \frac{d^m}{dt^m} [\Omega_d(tr)]\, r^{-2k}\, d\beta_d(r).$$

By Part (iii) of Lemma 1.7 again, we have for, $t \in (0, 1)$,

$$\begin{aligned} \int_1^\infty \frac{d^m}{dt^m} [\Omega_d(tr)]\, r^{-2k}\, d\beta_d(r) &\leqslant C \int_1^\infty (tr)^{-4k} r^m r^{-2k}\, d\beta_d(r) \\ &= Ct^{-4k} \int_1^\infty r^{-(4k-m)} r^{-2k}\, d\beta_d(r) \leqslant Ct^{-4k}. \quad \blacksquare \end{aligned}$$

LEMMA 2.4. *Let g be as in Lemma 2.3 and let $f(t) = g(t^{1/2})$. Then for $0 \leqslant m \leqslant 4k$, we have*

$$|f^{(m)}(t)| \leqslant C(m)(1 + t^{-6k} + t^k) \tag{9}$$

Proof. Write $f(t^2) = g(t)$. Then Inequality (9) follows from Lemma 2.3 with a simple calculation. $\blacksquare$

The following lemma can also be verified by a simple calculation which we omit.

LEMMA 2.5. *Let f and g be functions of t such that $g(t)=f(t^2)$. Assume that $f\in C^\infty[0,+\infty)$. For $d=1, 2, \ldots$, $x\in\mathbb{R}^d$, let $t=|x|$. Denote $f^{(j)}(s)|_{s=t^2}$ as $f^{(j)}(t^2)$. Then, for each positive integer l,*

$$(\Delta^l g)(|x|)=(2d)^l f^{(l)}(t^2)+\sum_{j=1}^{2l} q_j(d, t^2)\, f^{(j)}(t^2), \tag{10}$$

where for each $1\leqslant m\leqslant 2l$, $q_j(d, t^2)$ satisfies

$$|q_j(d, t^2)/(2d)^{l-1}|\leqslant C_j(t^{2l}+1),$$

where C_j depends only on m.

From Eqs. (9) and (10), we get the following important estimate.

LEMMA 2.6. *Let g be k-positive definite and radial on $\mathbb{R}^d$ for all integer d. Then, for $0\leqslant l\leqslant 2k$, $x\in\mathbb{R}^d$, and $d\geqslant 8k+1$, we have*

$$\left|\frac{(\Delta^l g)(|x|)}{(2d)^l}\right|\leqslant C_l(1+|x|^{-12k}+|x|^{6k}),$$

where C_l can be chosen to be independent of the space dimension d.

LEMMA 2.7. *Let g be as in Lemma 2.6, and*

$$\alpha(r)=e^{-r^2}\sum_{l=0}^{k-1}\frac{r^{2l}}{l!}.$$

Set

$$\alpha_d(r)=\alpha\left(\frac{r}{\sqrt{2d}}\right)=e^{-(r^2/2d)}\sum_{l=0}^{k-1}\frac{r^{2l}}{l!(2d)^l}.$$

Then, for each integer $l, 0\leqslant l\leqslant k-1$, the following numerical sequence is bounded:

$$\left\{\frac{1}{(2d)^l}\langle g, \alpha_d(r)\, r^{2l}\rangle_d;\, d=1, 2, \ldots\right\}.$$

Proof.

$$\begin{aligned}\frac{1}{(2d)^l}\langle \hat{g}, \alpha_d(r)\, r^{2l}\rangle_d &=\frac{1}{(2d)^l}\left\langle r^{2l}\sum_{j=0}^{k-1}\frac{r^{2j}}{j!(2d)^j}\,\hat{g}, e^{-r^2/2d}\right\rangle_d\\
&=\frac{d^{d/2}}{(2\pi)^{d/2}}\int_{\mathbb{R}^d}\left[\sum_{j=0}^{k-1}\frac{(-1)^{l+j}\Delta^{l+j}g(|x|)}{j!(2d)^{l+j}}\right]e^{-d|x|^2}\,dx\\
&=\sum_{j=0}^{k-1}\frac{d^{d/2}\omega_{d-1}}{(2\pi)^{d/2}j!}\int_0^\infty\frac{(-1)^{l+j}\Delta^{l+j}g(r)}{(2d)^{l+j}}e^{-dr^2/2}r^{d-1}\,dr.\end{aligned}$$

Note that $l+j \leqslant 2k$. So by Lemma 2.6, it suffices to show

$$I_d = \frac{d^{d/2}\omega_{d-1}}{(2\pi)^{d/2}} \int_0^\infty (1 + r^{-12k} + r^{6k})\, e^{-dr^2/2} r^{d-1}\, dr \leqslant M < \infty$$

for all $d \geqslant 12k+1$.

Using the change of variable $(d/2)\, r^2 = t$, we get

$$\begin{aligned} F_d &= \frac{d^{d/2}\omega_{d-1}}{(2\pi)^{d/2}} \frac{1}{2} \left(\frac{2}{d}\right)^{d/2} \int_0^\infty \left(1 + \left(\frac{2}{d} t\right)^{-6k} + \left(\frac{2}{d} t\right)^{3k}\right) e^{-t} t^{d/2-1}\, dt \\ &= \frac{1}{\Gamma(1/2)} \left(\Gamma\left(\frac{d}{2}\right) + \left(\frac{2}{d}\right)^{-6k} \Gamma\left(\frac{d}{2} - 6k\right) + \left(\frac{2}{d}\right)^{3k} \Gamma\left(\frac{d}{2} + 3k\right)\right). \end{aligned} \tag{11}$$

Here we used the formula

$$\omega_{d-1} = \frac{2\pi^{d/2}}{\Gamma(d/2)}.$$

We see immediately from Eq. (11) that I_d is uniformly bounded for all $d \geqslant 12k+1$. ∎

We are now in the position to prove the main theorem.

Proof of Theorem 2.1. We only need to show that (a) implies (b). Since $g \in CP_k(\mathbb{R}^d)$ implies that g is k-positive on $\mathbb{R}^d$, g has the integral representation as in Eq. (4). Now we choose $\alpha_d(r) = \alpha(r/\sqrt{2d})$ to replace $\alpha(r)$ in Eq. (4). Then, at $x = 0$, we have

$$g(0) = \int_0^\infty (1 - \alpha_d(r))\, r^{-2k}\, d\beta_d(r) + \langle \hat{g}, \alpha_d(r) \rangle_d. \tag{12}$$

By Lemma 2.7, we see that

$$\int_0^\infty (1 - \alpha_d))\, r^{-2k}\, d\beta_d(r) = \int_0^\infty (1 - \alpha(r))\, r^{-2k} \frac{d\beta_d(r\sqrt{2d}}{(2d)^k}$$

is uniformly bounded for all d.

Recall that

$$\alpha(r) = e^{-r^2} \sum_{l=0}^{k-1} \frac{r^{2l}}{l!}.$$

It is easy to check the following properties of $\alpha(r)$:

$$\text{(i)}\quad 1-\alpha(r)\geqslant 0 \text{ on } [0,+\infty),$$

$$\text{(ii)}\quad \min_{r\in(0,1)}[(1-\alpha(r))\,r^{-2k}]>0,$$

$$\text{(iii)}\quad \min_{r\in[1,+\infty)}(1-\alpha(r))>0.$$

It follows that both

$$\int_0^\infty \frac{d\beta_d(r\sqrt{2d})}{(2d)^k} \quad \text{and} \quad \int_1^\infty r^{-2k}\frac{d\beta_d(r\sqrt{2d})}{(2d)^k}$$

are uniformly bounded for all d. Helly's compactness theorem (see [Z, p. 137]) insures the existence of a nonnegative and nondecreasing function $\beta(r)$, and of a subsequence of $\{\beta_d(r\sqrt{2d})/(2d)^k\}$ converging to the function $\beta(r)$ on $[0,+\infty)$ at all points of continuity of $\beta(r)$. Consequently, $\int_1^\infty r^{-2k}\,d\beta(r)<\infty$.

We claim that for $t\in(0,+\infty)$,

$$g(t)=\int_0^\infty\left(e^{-t^2r^2}-\alpha(r)\sum_{l=0}^{k-1}\frac{(-1)^l r^{2l}t^{2l}}{l!}\right)r^{-2k}\,d\beta(r)+\sum_{l=0}^{k-1}a_l t^{2l}, \tag{13}$$

where a_l are some constants for $l=0,1,...,k-1$.

Once Eq. (13) is established, it is clear from the relation $f(t^2)=g(t)$ that

$$f(t)=\int_0^\infty\left(e^{-tr^2}-\alpha(r)\sum_{l=0}^{k-1}\frac{(-1)^l r^{2l}t^{l}}{l!}\right)r^{-2k}\,d\beta(r)+\sum_{l=0}^{k-1}\alpha_l t^{l}.$$

Hence, $f^{(m)}(t)$ exists for each $m\geqslant 1$ and $t\in(0,+\infty)$, and $(-1)^k f^{(k)}(t)$ is completely monotone on $(0,+\infty)$. So, in order to prove the theorem, it remains to verify Eq. (13).

Returning to Eq. (4) with $\alpha(r)$ replaced by $\alpha_d(r)$, we have, for $t\in(0,+\infty)$,

$$\begin{aligned} g(t)=&\int_0^\infty\left(\Omega_d(tr)-\alpha_d(r)\sum_{l=0}^{k-1}\frac{(-1)^l r^{2l}t^{2l}}{(2l)!!\prod_{s=0}^{l-1}(d+2s)}\right)r^{-2k}\,d\beta_d(r)\\ &+\sum_{l=0}^{k-1}\frac{(-1)^l}{(2l)!!\prod_{s=0}^{l-1}(d+2s)}\langle \hat{g},\alpha_d(r)\,r^{2l}\rangle_d\,t^{2l} \end{aligned} \tag{14}$$

By Lemma 2.7, we may assume (passing to a subsequence if necessary) that

$$\frac{(-1)^l}{(2l)!!\prod_{s=0}^{l-1}(d+2s)}\langle \hat{g},\alpha_d(r)\,r^{2l}\rangle_d\to a_l,$$

for some finite number a_l. Thus it suffices to show that for any fixed $t \in (0, +\infty)$, there is a subsequence of $\{d\}_{d=1}^{\infty}$ such that as $d \to \infty$, the integral

$$\int_0^{\infty} \left(\Omega_d(tr\sqrt{2d}) - \alpha(r) \sum_{l=0}^{k-1} \frac{(-1)^l r^{2l} t^{2l} (2d)^l}{(2l)!! \prod_{s=0}^{l-1} (d+2s)} \right) r^{-2k} \frac{d\beta_d(r\sqrt{2d})}{(2d)^k}$$

converges to the integral

$$\int_0^{\infty} \left(e^{-t^2 r^2} - \alpha(r) \sum_{l=0}^{k-1} \frac{(-1)^l r^{2l} t^{2l}}{l!} \right) r^{-2k} \, d\beta(r).$$

Without loss of generality, we may assume that the whole sequence of $d\beta_d(r\sqrt{2d})/(2d)^k$ converges to $\beta(r)$ on $[0, +\infty)$ at all points where the function $\beta(r)$ is continuous. Set

$$h_d(r) = \Omega_d(tr\sqrt{2d}) - \alpha(r) \sum_{l=0}^{k-1} \frac{(-1)^l r^{2l} t^{2l} (2d)^l}{(2l)!! \prod_{s=0}^{l-1} (d+2s)},$$

and

$$h(r) = e^{-t^2 r^2} - \alpha(r) \sum_{l=0}^{k-1} \frac{(-1)^l r^{2l} t^{2l}}{l!}.$$

In order to prove the above limit relation, we need only to show that for every $\varepsilon > 0$, there is an $N_\varepsilon > 0$ such that

$$\left| \int_0^{\infty} h_d(r)\, r^{-2k} \frac{d\beta_d(r\sqrt{2d})}{(2d)^k} - \int_0^{\infty} h(r)\, r^{-2k} \, d\beta(r) \right| \leqslant \varepsilon \tag{15}$$

for all $d \geqslant N_\varepsilon$. Here N_ε depends on ε and the fixed t.

Using Part (i) of Lemma 1.7 and the fact that

$$\frac{(2d)^l}{(2l)!! \prod_{s=0}^{l-1} (d+2s)} \to \frac{1}{l!} \quad \text{as} \quad d \to \infty,$$

we see that $\lim_{d \to \infty} h_d(r)\, r^{-2k}$, uniformly for $r \in [0, 1]$. Also, from Part (ii) of Lemma 1.7, it is easy to check that $\lim_{d \to \infty} h_d(r) = h(r)$ uniformly for $r \in [1, +\infty)$. Since both

$$\int_0^1 \frac{d\beta_d(r\sqrt{2d}}{(2d)^k} \quad \text{and} \quad \int_1^{\infty} r^{-2k} \frac{d\beta_d(r\sqrt{2d}}{(2d)^k}$$

are uniformly bounded for all d, it follows that for the given $\varepsilon > 0$, there is an $N_1 > 0$ such that

$$\left| \int_0^\infty h_d(r)\, r^{-2k} \frac{d\beta_d(r\sqrt{2d}}{(2d)^k} - \int_0^\infty h(r)\, r^{-2k} \frac{d\beta_d(r\sqrt{2d})}{(2d)^k} \right| \leqslant \frac{\varepsilon}{4} \tag{16}$$

for all $d \geqslant N_1$.

Note that for the fixed $t \in (0, +\infty)$, $\lim_{r\to\infty} h(r) = 0$, we see that there is an $M > 0$ such that

$$\left| \int_R^\infty h(r)\, r^{-2k} \frac{d\beta_d(r\sqrt{2d})}{(dd)^k} \right| \leqslant \frac{\varepsilon}{4} \tag{17}$$

for all $R \geqslant M$ and $d \geqslant N_1$. By taking limit in Inequality (17), we get

$$\left| \int_R^\infty h(r)\, r^{-2k}\, d\beta(r) \right| \leqslant \frac{\varepsilon}{4}, \tag{18}$$

for all $R \geqslant M$.

In Inequalities (17) and (18), if we choose R to be a point of continuity of $\beta(r)$, then the Helly's Theorem implies

$$\lim_{d\to\infty} \int_0^R h(r)\, r^{-2k} \frac{d\beta_d(r\sqrt{2d})}{(2d)^k} = \int_0^R h(r)\, r^{-2k}\, d\beta(r).$$

Hence, for the given $\varepsilon > 0$, there is an $N_2 > 0$ such that

$$\left| \int_0^R h(r)\, r^{-2k} \frac{d\beta_d(r\sqrt{2d})}{(2d)^k} - \int_0^R h(r)\, r^{-2k}\, d\beta(r) \right| \leqslant \frac{\varepsilon}{4} \tag{19}$$

for all $d \geqslant N_2$.

Thus, Inequality (15) follows from Inequalities (16), (17), (18), and (19) by choosing $N_\varepsilon = \max\{N_1, N_2\}$. This verifies Identity (13), and therefore the proof of Theorem 2.1 is complete. ∎

3. Concluding Remarks

There are some intimate relationships between positive definite functions and conditionally negative definite functions of degree 1 (a function f is called conditionally negative definite of degree 1 if $-f$ is conditionally positive definite of degree 1). We refer to [BCR, Chap. 3] for a beautiful illustration of these results. It is very natural to expect that similar relationships exist between conditionally positive (negative) definite functions of degree k and degree $k+1$ for $k \geqslant 1$. Unfortunately, the attempt was in vain since there are counter-examples. By direct differentiation, one can show the well-known result that if $f \in \mathcal{M}$ and if $g \in C[0, \infty)$ and g' is completely monotone on $(0, \infty)$, then $f \circ g \in \mathcal{M}$; see Sun [SX, p. 23]. In particular, for such function g and a number $a > 0$, the function e^{-ag} belongs to $\mathcal{M}$. Using this remarkable result, Schoenberg [S] characterized the class of functions which are conditionally negative definite of degree 1 on all the Euclidean spaces $\mathbb{R}^d$, $d = 1, 2, \ldots$. (Schoenberg did not use the phrase "conditionally negative definite," but his "imbedding" language carries the same meaning). This naturally leads us to consider the following general setting: If $f \in \mathcal{M}$ and $g \in C[0, \infty)$ such that $g^{(k)}$ is completely monotone on $(0, \infty)$, then $h^{(k-1)}$ is completely monotone on $(0, \infty)$ for $h = f \circ g$. Unfortunately, this is not true even for $k = 2$. In fact, for $f(t) = e^{-t}$, and $g(t) = t^\alpha$, with $1 < \alpha < 2$, we have $f \in \mathcal{M}$ and $g^{(2)}$ is completely monotone, but h' is not completely monotone for $h = f \circ g$.

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