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# About repulsiveness of determinantal point processes

Christophe Ange Napoléon Biscio<sup>1</sup> and Frédéric Lavancier<sup>1</sup>

<sup>1</sup> Laboratoire de Mathématiques Jean Leray, University of Nantes, France

#### Abstract

Determinantal point processes (DPPs) have recently proved to be a useful class of models in several areas of statistics, including spatial statistics, statistical learning or telecommunications networks. They are models for repulsive (or regular, or inhibitive) point processes, in the sense that nearby points of the process tend to repel each other. We consider two ways to quantify the repulsiveness of a point process, both based on its second order properties, and we address the question of how repulsive a stationary DPP can be. We exhibit the most repulsive stationary DPP, when the intensity is fixed. We investigate similarly the possible repulsiveness in the subclass of R-dependent stationary DPPs (for some fixed positive R), or equivalently DPPs with R-compactly supported kernels. Finally, in both the general case and the R-dependent case, we present some new parametric families of stationary DPPs that can cover all possible repulsiveness, from the homogeneous Poisson process (which induces no interaction) to the most repulsive DPP.

*Keywords:* regularity, inhibition, pair correlation function, *R*-dependent point process, covariance function, compactly supported covariance function.

## 1 Introduction

Determinant point processes (DPPs) were introduced in their general form by O. Macchi in 1975 [27] to model fermions in quantum mechanics, though some specific DPPs appeared much earlier in random matrix theory. DPPs actually arise in many fields of probability, see [19] and [32] for some examples, and for this reason have deserved a lot of attention from a theoretical point of view.

DPPs are repulsive (or regular, or inhibitive) point processes, meaning that nearby points of the process tend to repeal each other (this concept will be clearly described in the following). This property is adapted to many statistical problems where DPPs have been recently used : in biology to study the repartition of cells [25], in telecommunication to model the locations of network nodes [6, 28], in statistical learning to construct a dictionary of diverse sets [23].

The growing interest for DPPs in the statistical community is due to some appealing properties of this class of processes. To mention but a few : their moments are explicitly known, parametric families can easily been considered, their density on any compact set admits a close form expression making likelihood inference feasible, and they can be simulated easily and quickly. Section 2 summarizes some of these properties and we refer to [25] for a detailed presentation. These features make the class of DPPs a competitive alternative to the usual class of models for repulsiveness, namely the Gibbs point processes. In contrast, for Gibbs point processes, no close form expression are available for the moments, the likelihood involves an intractable normalizing constant and their simulation requires some Markov Chain Monte Carlo methods.

However, DPPs can not model any kind of repulsive point patterns. For instance, DPPs can not involve a hardcore distance between points, contrary to the Matérn's hardcore point process, or the RSA (random sequential absorption) model or some hardcore Gibbs models, see [20] Section 6.5. In this paper, we address the question of how repulsive a stationary DPP can be. We also investigate the repulsiveness in the subclass of R-dependent stationary DPPs, or equivalently DPPs with R-compactly supported kernels, that are of special interest for statistical inference in high dimension, see Section 4. In both cases, we present in Section 5 some parametric families of DPPs that cover all possible range of repulsiveness.

To quantify the repulsiveness of a point process, we consider its second-order properties. Let X be a stationary point process in  $\mathbb{R}^d$  with intensity (i.e. expected number of points per unit volume)  $\rho > 0$  and second order intensity function  $\rho^{(2)}(x, y)$ . Denoting dx an infinitesimal region around x and |dx| its Lebesgue measure, the second order intensity function of X is informally defined in [7] as

$$\rho^{(2)}(x,y) = \lim_{|dx| \to 0, |dy| \to 0} \frac{E[X(dx)X(dy)]}{|dx||dy|}, \quad x, y \in \mathbb{R}^d,$$

where X(dx) denotes the number of points of X in dx. A formal definition is given in Section 2. Note that  $\rho^{(2)}(x, y)$  only depends on y - x because of our stationarity assumption. In spatial statistics, the second order properties of X are generally studied through the pair correlation function (in short pcf), defined for any  $x \in \mathbb{R}^d$ ,  $x \neq 0$ , by

$$g(x) = \frac{\rho^{(2)}(0,x)}{\rho^2},$$

while g(0) = 0. Note that x in g(x) is to be interpreted as the difference between two points of X.

For  $x \neq y$ ,  $\rho^{(2)}(x, y)|dx||dy|$  may be viewed as the probability that X has a point in dx and another point in dy. Similarly  $\rho|dx|$  may be interpreted as the probability that X has a point in dx. Accordingly, it is commonly accepted, see for example [34], that if g(x) = 1 then there is no interaction between two points separated by x, whereas there is attraction if g(x) > 1 and repulsiveness if g(x) < 1.

Following this remark, we introduce below a way to compare the *global repulsive*ness of two stationary point processes with the same intensity.

**Definition 1.1.** Let X and Y be two point processes with the same intensity  $\rho$  and respective pair correlation function  $g_X$  and  $g_Y$ . Assuming that both  $(1 - g_X)$ 

and  $(1 - g_Y)$  are integrable, we say that X is globally more repulsive than Y if  $\int (1 - g_X) \ge \int (1 - g_Y)$ .

The quantity  $\int (1-g)$  is already considered in [25] as a measure for repulsiveness. It can be justified in several ways. First, it is a natural geometrical method to quantify the distance from g to 1 (corresponding to no interaction), where the area between g and 1 contributes positively to the measure of repulsiveness when g < 1 and negatively if g > 1. Second, as explained in [25], denoted P the law of X, and  $P_o^!$  its reduced Palm distribution,  $\rho \int (1-g)$  corresponds to the limit, when  $r \to \infty$ , of the difference between the expected number of points within distance r from the origin under P and under  $P_o^!$ . Recall that  $P_o^!$  can be interpreted as the distribution of X conditioned to have a point at the origin. Third, the variance of the number of points of X in a compact set D is  $Var(X(D)) = \rho |D| - \rho^2 \int_{D^2} (1-g(y-x)) dxdy$ , see [20]. Thus, the intensity  $\rho$  being fixed, maximizing  $\int (1-g)$  is equivalent to minimize Var(X(D))/|D| when  $D \to \mathbb{R}^d$ , provided D and g are sufficiently regular to apply the mean value theorem. Finally, it is worth mentioning that for any stationary point processes, we have  $\int (1-g) \leq 1/\rho$ , see (2.5) in [24].

In practice, repulsiveness is often interpreted in a local sense, as two neighbor points are expected to be not too close. This is the case for hardcore point processes, where a minimal distance  $\delta$  is imposed between points. If the latter property holds, then g(x) = 0 whenever  $|x| < \delta$ . A DPP can not involved any hardcore distance, but in the same spirit, we may ask its pcf to stay as close as possible to 0 near the origin. This leads to the following criteria to compare the *local repulsiveness* of two point processes. We denote by  $\nabla g$  and  $\Delta g$  the gradient and the Laplacian of grespectively.

**Definition 1.2.** Let X and Y be two point processes with the same intensity  $\rho$  and respective pair correlation function  $g_X$  and  $g_Y$ . Assuming that  $g_X$  is twice differentiable at 0, we say that X is more locally repulsive than Y if either  $g_Y$  is not twice differentiable at 0, or  $g_Y$  is twice differentiable at 0 with  $\Delta g_Y(0) \geq \Delta g_X(0)$ .

As suggested by this definition, a process is said locally repulsive only if its pcf is twice differentiable at 0. In this case g(0) = 0 by definition, and  $\nabla g(0) = 0$  because g(x) = g(-x). Therefore to compare the behavior of two twice differentiable pcfs near the origin, specifically the curvatures of their graphs near the origin, the Laplacian operator is involved in Definition 1.2. As an example, a hardcore process is locally more repulsive than any other process because  $\Delta g(0) = 0$  in this case. On the other hand, a concave pcf is not differentiable at the origin and for this reason the associated point process is less locally repulsive than any process with a twice differentiable pcf.

We recall the definition of a stationary DPP and some related basic results in Section 2. Section 3 is devoted to the study of DPP's repulsiveness, both in the sense of Definition 1.1 and Definition 1.2. While these definitions have two different viewpoints, they agree in the choice of what can be considered as the most repulsive DPP. In Section 4, we focus on the subclass of DPPs with compactly supported kernels and we investigate similarly their possible repulsiveness. Then, in Section 5, we present three parametric families of DPPs which cover all the possible range of repulsiveness, as revealed by the previous sections, and have further interesting properties. Section 6 gathers the proofs of our theoretical results.

## 2 Stationary DPPs

In this section, we review the basic definition and some properties of stationary DPPs. For a detailed presentation, including the non stationary case, we refer to the survey by Hough et al. [19].

Basics of point processes may be found in [4, 5]. Let us recall that a point process X is simple if two points of X never coincide, almost surely. The joint intensities of X are defined as follows.

**Definition 2.1.** If it exists, the joint intensity of order  $k \ (k \ge 1)$  of a simple point process X is the function  $\rho^{(k)} : \mathbb{R}^d \to \mathbb{R}^+$  such that for any family of mutually disjoint subsets  $D_1, \ldots, D_k$  in  $\mathbb{R}^d$ ,

$$E\prod_{i=1}^{k} X(D_i) = \int_{D_1} \dots \int_{D_k} \rho^{(k)}(x_1, \dots, x_k) dx_1 \dots dx_k,$$

where X(D) denotes the number of points of X in D and E is the expectation over the distribution of X. In addition, we shall require that  $\rho^{(k)}(x_1, \ldots, x_k) = 0$  if  $x_i = x_j$ for some  $i \neq j$ .

In the stationary case,  $\rho^{(k)}(x_1, \ldots, x_k) = \rho^{(k)}(0, \ldots, x_k - x_1)$ , so that the intensity  $\rho$  and the second order intensity function  $\rho^{(2)}$  introduced previously become the particular cases associated to k = 1 and k = 2 respectively.

**Definition 2.2.** Let  $C : \mathbb{R}^d \to \mathbb{R}$  be a function. A point process X on  $\mathbb{R}^d$  is a stationary DPP with kernel C, in short  $X \sim DPP(C)$ , if for all  $k \ge 1$ , its joint intensity of order k satisfies the relation:

$$\rho^{(k)}(x_1,\ldots,x_k) = \det[C](x_1,\ldots,x_k), \quad \forall (x_1,\ldots,x_k) \in (\mathbb{R}^d)^k,$$

where  $[C](x_1, \ldots, x_k)$  denotes the matrix with entries  $C(x_i - x_j), 1 \le i, j \le k$ .

A first example is the homogeneous Poisson process with intensity  $\rho$ . It corresponds to the DPP with kernel

$$C(x) = \rho \mathbf{1}_{\{x=0\}}, \ \forall x \in \mathbb{R}^d.$$

$$(2.1)$$

However, this example is very particular and represents in some sense the extreme case of a DPP without any interaction, while DPPs are in general repulsive as discussed at the end of this section.

Definition 2.2 does not ensure existence or unicity of DPP(C), given C. The following proposition claims that a DPP, if it exists, is unique.

**Proposition 2.3** ([19]). A kernel C defines at most one DPP.

Concerning existence, a general result, including the non stationary case, was proved by O. Macchi in [27]. It relies on the Mercer representation of C on any compact set. Unfortunately this representation is known only in a few cases, making the conditions impossible to verify in practice for most functions C. Nevertheless, the situation becomes simpler in our stationary framework, where the conditions only involve the Fourier transform of C.

**Definition 2.4.** We define the Fourier transform of a function  $h \in L^1(\mathbb{R}^d)$  as:

$$\mathcal{F}(h)(t) = \int_{\mathbb{R}^d} h(x) e^{2i\pi x \cdot t} dx, \quad \forall t \in \mathbb{R}^d.$$

By Plancherel's theorem, this definition is extended to  $L^2(\mathbb{R}^d)$ , see [33].

**Remark 2.5.** For symmetric kernels C, as assumed in the following, we have  $\mathcal{FF}(C) = C$ , so  $\mathcal{F}^{-1} = \mathcal{F}$  in this case.

**Proposition 2.6** ([25]). Assume C is a symmetric continuous real-valued function in  $L^2(\mathbb{R}^d)$ . Then DPP(C) exists if and only if  $0 \leq \mathcal{F}(C) \leq 1$ .

In other words, Proposition 2.6 ensures existence of DPP(C) if C is a continuous real-valued covariance function in  $L^2(\mathbb{R}^d)$  with  $\mathcal{F}(C) \leq 1$ . Henceforth, we assume the following condition:

**Condition**  $\mathcal{K}$ . A kernel C is said to verify condition  $\mathcal{K}$  if:

(i) C is a symmetric continuous real-valued function,

(ii) 
$$C \in L^2(\mathbb{R}^d)$$
,

(iii)  $0 \leq \mathcal{F}(C) \leq 1.$ 

Let us note that the third assumption in Condition  $\mathcal{K}$  is necessary for existence, while the two others are satisfied by most statistical models of covariance functions, the main counterexample being (2.1). Standard parametric families of kernels include the Gaussian, the Whittle-Matérn and the generalized Cauchy covariance functions, where the condition  $\mathcal{F}(C) \leq 1$  implies some restriction on the parameters space, see [25].

From Definition 2.2, all DPP's moments are explicitly known. In particular, denoting  $\rho$  and g the intensity and the pcf of DPP(C), we have

- for all  $x \in \mathbb{R}^d$ ,  $\rho(x) = \rho = C(0)$ ,
- for all  $x, y \in \mathbb{R}^d$ ,  $\rho^{(2)}(x, y) = \rho^2 C(x y)^2$ , so that for all  $x \in \mathbb{R}^d$

$$1 - g(x) = \frac{C(x)^2}{\rho^2}.$$
(2.2)

From this relation, we see that any stationary DPP satisfies  $g \leq 1$ , proving that it induces repulsiveness. Moreover, the study of repulsiveness of stationary DPPs, as defined in Definitions 1.1 and 1.2, reduces to considerations on the kernel C.

Another pleasant feature of DPPs is that their probability density function on any compact set admits a close form expression, as presented in the following. From a statistical point of view, this property is crucial, as it makes maximum likelihood inference feasible.

Let S be a compact subset of  $\mathbb{R}^d$  and C a kernel satisfying condition  $\mathcal{K}$ . Define for all  $x, y \in S$ 

$$\tilde{C}_S(x,y) = \sum_{k=1}^{\infty} C_S^k(x,y), \qquad D = \sum_{k=1}^{\infty} \frac{1}{k} \int_S C_S^k(x,x) dx,$$
(2.3)

where for all  $x, y \in S$ ,  $C_S^1(x, y) = C(y - x)$  and for  $k \ge 2$ 

$$C_S^k(x,y) = \int_S C_S^{k-1}(x,z)C_S(z,y) \,\mathrm{d}z, \quad \forall x,y \in S.$$

Set  $det[\tilde{C}](x_1,\ldots,x_n) = 1$  if n = 0. Then we have the following result.

**Theorem 2.7** ([27]). Assume C verifies condition  $\mathcal{K}$  with  $\mathcal{F}(C) < 1$ , then  $DPP(C) \cap S$  is absolutely continuous with respect to the homogeneous Poisson process on S with unit intensity, and has density

$$f(\{x_1, \dots, x_n\}) = \exp(|S| - D) \det[\tilde{C}](x_1, \dots, x_n)$$
(2.4)

for all  $(x_1, ..., x_n) \in S^n$  and n = 0, 1, ...

## 3 Most repulsive DPPs

We first present the most globally repulsive DPPs, in the sense of Definition 1.1. They were briefly introduced in [25] and are given by the following proposition.

**Proposition 3.1.** In the sense of Definition 1.1, DPP(C) is the most globally repulsive DPP among all DPPs with intensity  $\rho$  and kernel satisfying condition  $\mathcal{K}$  if and only if  $\mathcal{F}(C)$  is even and equals almost everywhere an indicator function of a Borel set with volume  $\rho$ .

According to Proposition 3.1, there exists an infinity of choices to the most globally repulsive DPP in the sense of Definition 1.1. Figure 1 shows the pcf of three examples of DPPs in dimension d = 1 given by Proposition 3.1 when  $\rho = 1$ . Precisely, they correspond to DPPs with kernels  $C_1 = \mathcal{F}(\mathbf{1}_{[-\frac{1}{2},\frac{1}{2}]}), C_2 = \mathcal{F}(\mathbf{1}_{[-\frac{3}{4},-\frac{1}{4}]} + \mathbf{1}_{[\frac{1}{4},\frac{3}{4}]})$  and  $C_3 = \mathcal{F}(\mathbf{1}_{[-\frac{2}{3},-\frac{1}{3}]} + \mathbf{1}_{[-\frac{1}{6},\frac{1}{6}]} + \mathbf{1}_{[\frac{1}{3},\frac{2}{3}]}).$ 

Figure 1: Comparison between the pcfs of  $DPP(C_1)$ ,  $DPP(C_2)$  and  $DPP(C_3)$  denoted  $g_1, g_2$  and  $g_3$  respectively



Clearly,  $DPP(C_1)$  is the most natural choice among all solutions provided by Proposition 3.1 in dimension d = 1. This choice seems confirmed in Figure 1, if we favor repulsiveness at small distances.

Similarly, in dimension d, the natural choice is  $DPP(C_B)$  where  $C_B = \mathcal{F}(\mathbf{1}_{|\cdot|^d \le \rho \tau^d})$ and  $\tau^d = \Gamma(d/2 + 1)/\pi^{\frac{d}{2}}$  is the radius of the ball with unit volume. The explicit expression of  $C_B$  is given by (see appendix B.5 in [17])

$$C_B(x) = \mathcal{F}(\mathbf{1}_{|\cdot|^d \le \rho \tau^d})(x) = \frac{\sqrt{\rho \Gamma(\frac{d}{2}+1)}}{\pi^{d/4}} \frac{J_{\frac{d}{2}}\left(2\sqrt{\pi} \Gamma(\frac{d}{2}+1)^{\frac{1}{d}} \rho^{\frac{1}{d}} |x|\right)}{|x|^{\frac{d}{2}}}, \ \forall x \in \mathbb{R}^d, \ (3.1)$$

where  $J_{\underline{d}}$  is the Bessel function of the first kind. For example, we have:

- for d = 1,  $C_B = C_1 = sinc(x) = \frac{\sin(\pi \rho |x|)}{\pi |x|}$ ,
- for d = 2,  $C_B = jinc(x) = \sqrt{\rho} \frac{J_1(2\sqrt{\pi\rho}|x|)}{\sqrt{\pi}|x|}$ .

This choice was already favored in [25]. However, there is no indication from Proposition 3.1 to suggest  $C_B$  instead of another kernel given by the proposition. This choice becomes clear if we look at the local repulsiveness as defined in Definition 1.2.

**Proposition 3.2.** In the sense of Definition 1.2, the most locally repulsive DPP among all DPPs with intensity  $\rho$  and kernel satisfying condition  $\mathcal{K}$  is  $DPP(C_B)$ .

Thus, from Propositions 3.1 and 3.2, we deduce the following corollary:

**Corollary 3.3.** The kernel  $C_B$  is the unique kernel C verifying condition  $\mathcal{K}$  such that DPP(C) is both the most globally and the most locally repulsive DPP among all DPPs with intensity  $\rho$ .

**Remark 3.4.** In [3], A. Borodin and S. Serfaty characterize the disorder of a point process by its "renormalized energy". Accordingly, the smaller the renormalized energy, the more repulsive the point process. In their Theorem 3, A. Borodin and S. Serfaty show that  $DPP(C_B)$  minimizes the renormalized energy among the most globally repulsive DPPs given by Proposition 3.1. This result confirms Corollary 3.3, that the most repulsive stationary DPP, if any has to be chosen, is  $DPP(C_B)$ . However, except when the DPPs are given by Proposition 3.1, all stationary DPPs have an infinite renormalized energy (see Theorem 1 in [3]), which indicates that the renormalized energy is not of practical use to compare the repulsiveness between two arbitrary DPPs.

# 4 Most repulsive DPPs with compactly supported kernels

In this section, we assume that the kernel C is compactly supported, i.e. there exists R > 0 such that C(x) = 0 if |x| > R. In this case, DPP(C) is an R-dependent point process in the sense that if A and B are two sets separated by a distance larger than R, then  $DPP(C) \cap A$  and  $DPP(C) \cap B$  are independent. This property is a straightforward consequence of Theorem 2.7. In particular, the matrix  $[\tilde{C}]$  involved in the density of DPP(C), see Theorem 2.7, becomes sparse. This is particularly convenient for likelihood inference in high dimension when fitting parametric models.

We are thus interested by the repulsiveness properties of DPPs with kernels satisfying the following condition.

**Condition**  $\mathcal{K}_c(\rho, R)$ . A kernel C or DPP(C) is said to verify condition  $\mathcal{K}_c(\rho, R)$  if:

- (i) C verifies condition  $\mathcal{K}$ ,
- (ii) C is compactly supported with range R, i.e C(x) = 0 for  $|x| \ge R$ ,
- (iii)  $C(0) = \rho$ , in others words,  $\rho$  is the intensity of DPP(C).

The following proposition shows that any kernel satisfying condition  $\mathcal{K}$  can be arbitrarily approximated by kernels verifying  $\mathcal{K}_c(\rho, r)$  for r large enough.

Let us define the function h by

$$h(x) = \exp\left(\frac{1}{|x|^2 - 1}\right) \mathbf{1}_{|x|<1}, \quad \forall x \in \mathbb{R}^d.$$
(4.1)

Denote  $||h||^2 = \int |h(t)|^2 dt$  and [h \* h] the self-convolution product of h.

**Proposition 4.1.** Let C be a kernel verifying condition  $\mathcal{K}$  with  $C(0) = \rho$  and h be defined by (4.1). Then, for all r > 0, the function  $C_r$  defined by:

$$C_r(x) = \frac{1}{\|h\|^2} [h * h] \left(\frac{2x}{r}\right) C(x), \quad \forall x \in \mathbb{R}^d,$$
(4.2)

verifies  $\mathcal{K}_c(\rho, r)$ . Moreover we have:

$$\lim_{r \to +\infty} C_r = C, \tag{4.3}$$

uniformly on all compact sets.

In particular, by taking  $C = C_B$  in Proposition 4.1, it is always possible to find a kernel  $C_r$  verifying  $\mathcal{K}_c(\rho, r)$  that yields a repulsiveness (local or global) as close as we wish to the repulsiveness of  $C_B$ , provided that r is large enough. However, given a maximal range of interaction R, it is clear that the maximal repulsiveness implied by kernels verifying  $\mathcal{K}_c(\rho, R)$  can not reach the one of  $C_B$ . In the following, we study the DPP's repulsiveness when the range R is fixed.

In comparison with condition  $\mathcal{K}$ , the compactly supported assumption in condition  $\mathcal{K}_c(\rho, R)$  makes the optimization problems raised in Definition 1.1 and Definition 1.2 much more difficult to investigate. As a negative result, we know very little about the most globally repulsive DPP, in the sense of Definition 1.1, under condition  $\mathcal{K}_c(\rho, R)$ . From relation (2.2), this is equivalent to find a kernel C with maximal  $L^2$ -norm under the constraint that C verifies  $\mathcal{K}_c(\rho, R)$ . Without the constraint  $\mathcal{F}(C) \leq 1$ , this problem is known as the square-integral Turán problem with range R, see for example [22]. For this less constrained problem, only the following existence result is proved and no explicit formula of the solution is known.

**Theorem 4.2** ([8]). A solution to the square-integral Turán problem with range R exists.

In dimension d = 1, it has been proved that the solution is unique and there exists an algorithm to approximate it, see [14]. In this case, numerical approximations show that the solution with range R verifies condition  $\mathcal{K}_c(\rho, R)$  only if  $R \leq 1.02/\rho$ . This gives the most globally repulsive DPP verifying  $\mathcal{K}_c(\rho, R)$  in dimension d = 1, when  $R \leq 1.02/\rho$ , albeit without explicit formula. For other values of R, or in dimension  $d \geq 2$ , no results are available, to the best of our knowledge.

Let us now turn to the investigation of the most locally repulsive DPP, in the sense of Definition 1.2, under condition  $\mathcal{K}_c(\rho, R)$ . Recall that without the compactly supported constraint of the kernel, we showed in Section 3 that the most locally repulsive DPP, namely  $DPP(C_B)$ , is also (one of) the most globally repulsive DPP.

For  $\nu > 0$ , we denote by  $j_{\nu}$  the first positive zero of the Bessel function  $J_{\nu}$  and by  $J'_{\nu}$  the derivative of  $J_{\nu}$ . We refer to [1] for a survey about Bessel functions and their zeros. Let us further define the constant M as

$$M^{d} = \frac{2^{d-2} j_{\frac{d-2}{2}}^{2} \Gamma\left(\frac{d}{2}\right)}{\rho \pi^{\frac{d}{2}}}$$

We have in particular  $M\rho = \pi^2/8 \approx 1.234$  when d = 1,  $M\rho^{1/2} = j_0/\pi^{1/2} \approx 1.357$  when d = 2, and  $M\rho^{1/3} = \pi^{1/3} \approx 1.465$  when d = 3.

**Proposition 4.3.** If  $R \leq M$ , then, in the sense of Definition 1.2, there exists an unique isotropic kernel  $C_R$  such that  $DPP(C_R)$  is the most locally repulsive DPP among all DPPs with kernel verifying  $\mathcal{K}_c(\rho, R)$ . It is given by  $C_R = u * u$  where

$$u(x) = \kappa \; \frac{J_{\frac{d-2}{2}}\left(2j_{\frac{d-2}{2}}\frac{|x|}{R}\right)}{|x|^{\frac{d-2}{2}}} \; \mathbf{1}_{|x|<\frac{R}{2}},\tag{4.4}$$

with  $\kappa^2 = \frac{4\Gamma(d/2)}{\rho \pi^{d/2} R^2} \left( J'_{\frac{d-2}{2}}(j_{\frac{d-2}{2}}) \right)^{-2}$ .

In this proposition  $C_R$  is only given as a convolution product. Nonetheless, an explicit expression  $C_R$  is known in dimension d = 1 and d = 3, see [9]. On the other hand, the Fourier transform is known in any dimension since  $\mathcal{F}(C_R) = \mathcal{F}(u)^2$ . We get from the proof of Proposition 4.3, for all  $x \in \mathbb{R}^d$ ,

$$\mathcal{F}(C_R)(x) = \rho \pi^{d/2} R^d j_{\frac{d-2}{2}}^2 \Gamma\left(\frac{d}{2}\right) \left(\frac{J_{\frac{d-2}{2}}(\pi R|x|)}{(\pi R|x|)^{\frac{d-2}{2}} \left(j_{\frac{d-2}{2}}^2 - (\pi R|x|)^2\right)}\right)^2.$$
(4.5)

If  $R \ge M$ , we do not have any close form expression of the most locally repulsive DPP. However, under some extra regularity assumptions, we can state the following general result about its existence and the form of the solution.

**Condition**  $\mathcal{M}(\rho, R)$ . A function u is said to verify condition  $\mathcal{M}(\rho, R)$  if u(x) = 0 for  $|x| > \frac{R}{2}$ , u is a radial function and  $u \in L^2$  with  $||u||^2 = \rho$ .

**Proposition 4.4.** For any R > 0, there exists an isotropic kernel  $C_R$  such that  $DPP(C_R)$  is the most locally repulsive DPP among all DPPs with kernel C verifying  $\mathcal{K}_c(\rho, R)$ . It can be expressed as  $C_R = u * u$  where u satisfies  $\mathcal{M}(\rho, R)$ . Furthermore, if we assume that  $\sup_{x \in \mathbb{R}^d} \mathcal{F}(C)(x) = \mathcal{F}(C)(0)$  and u is twice differentiable on its support, then u is of the form

$$u(x) = \left(\beta + \gamma \frac{J_{\frac{d-2}{2}}(\sqrt{\alpha}|x|)}{|x|^{\frac{d-2}{2}}}\right) \mathbf{1}_{|x| < \frac{R}{2}},\tag{4.6}$$

where  $\alpha > 0, \beta \ge 0$  and  $\gamma$  are three constants linked by the conditions  $\mathcal{M}(\rho, R)$  and  $\int_{\mathbb{R}^d} u(x) dx \le 1$ .

In the case  $R \leq M$ , this proposition is a consequence of Proposition 4.3 where  $\beta = 0$ ,  $\alpha = \frac{4}{R^2} j_{\frac{d-2}{2}}^2$ , and  $\gamma = \kappa$ . When R > M, it is an open problem to find an explicit expression to the kernel  $C_R$  without any extra regularity assumptions. Even in this case, (4.6) only gives the form of the solution and the constants  $\alpha$ ,  $\beta$  and  $\gamma$  are not explicitly known. In particular the choice  $\beta = 0$  does not lead to the most locally repulsive DPP when R > M, contrary to the case  $R \leq M$ . In fact, the condition  $\mathcal{M}(\rho, R)$  allows us to express  $\beta$  and  $\gamma$  as functions of  $\alpha$ , R and  $\rho$ , but then some numerical approximation are needed to find the value of  $\alpha$  in (4.6), given R and  $\rho$ , such that  $DPP(C_R)$  is the most locally repulsive DPP. We detail these relations in Section 5.3, where we start from (4.6) to suggest a new parametric family of compactly supported kernels.

Contrary to what happens in the non compactly supported case of Section 3, the most locally repulsive DPP is not the most globally repulsive DPP under  $\mathcal{K}_c(\rho, R)$ . This is easily checked in dimension d = 1 when  $R \leq 1.02/\rho$  implying  $R \leq M$ : In this case the most globally repulsive DPP under  $\mathcal{K}_c(\rho, R)$  is  $DPP(T_R)$ , where  $T_R$  is the solution of the square-integral Turán problem with range R, and the most locally repulsive DPP is  $DPP(C_R)$  where  $C_R$  is given by (4.4). However, according to the results of Section 3 corresponding to  $R = \infty$ , we expect that  $DPP(C_R)$  has a strong global repulsiveness even for moderate values of R. This is confirmed in Figure 2, that shows the pcf of  $DPP(C_R)$  when  $d = 1, \rho = 1$ , and  $R = 1.02, R = M \approx 1.234$ and R = 2M, where in this case we take  $C_R = u * u$  with u given by (4.6) and the constants are obtained by numerical approximations. The pcfs of  $DPP(T_{1.02})$  and  $DPP(C_B)$  are added for sake of comparison. We also note from the behavior of the pcf near the origin, that even if  $DPP(T_{1.02})$  is the most globally repulsive DPP under  $\mathcal{K}_c(\rho, R)$  when  $R \leq 1.02/\rho$ , its local repulsiveness is not very strong. On the other hand,  $DPP(C_R)$  seems to present strong global repulsiveness for the values of R considered in the figure.

Figure 2: In dimension d = 1, comparison between the pcf of  $DPP(T_{1.02})$ ,  $DPP(C_B)$  and  $DPP(C_R)$  for R = 1.02, M, 2M.



# 5 Parametric families of DPP kernels

A convenient parametric family of kernels  $\{C_{\theta}\}_{\theta\in\Theta}$ , where  $\Theta \subset \mathbb{R}^{q}$  for some  $q \geq 1$ , should ideally :

- (a) provide a close form expression for  $C_{\theta}$ , for any  $\theta$ ,
- (b) provide a close form expression for  $\mathcal{F}(C_{\theta})$ , for any  $\theta$ ,
- (c) be flexible enough to cover all the possible range of repulsiveness of DPPs, that goes from the Poisson point process to  $DPP(C_B)$ .

The second property above is needed to check the condition of existence  $\mathcal{F}(C_{\theta}) \leq 1$ , but it is also useful for some approximations in practice. Indeed, the algorithm for simulating DPP(C) on a compact set S, as presented in [19], relies on the Mercer representation of C on S, which is rarely known in practice. In [25], this decomposition is simply approximated by the Fourier series of C, where the k-th Fourier coefficients is replaced by  $\mathcal{F}(C)(k)$ , up to some rescaling. The same approximation is used to compute  $\tilde{C}$  involved in the likelihood in Theorem 2.7. This Fourier approximation proved to be accurate in most cases, both from a practical and a theoretical point of view, provided  $\rho$  is not too small, and to be computationally efficient, see [25].

In addition to (a)-(c), we may also require that  $C_{\theta}$  be compactly supported with maximal range R, following the motivation explained in Section 4, in which case the maximal possible repulsiveness is given by  $DPP(C_R)$ . Or we may require that  $\mathcal{F}(C_{\theta})$  be compactly supported, in which case the Fourier series mentioned in the previous paragraph becomes a finite sum and no truncation is needed in practice. Note however that  $C_{\theta}$  and  $\mathcal{F}(C_{\theta})$  can not be both compactly supported.

Several standard parametric families of kernels are available, including the wellknown Whittle-Matérn and the generalized Cauchy covariance functions, where the condition  $\mathcal{F}(C_{\theta}) \leq 1$  implies some restriction on the parameter space, see [25]. Although they encompass a close form expression for both  $C_{\theta}$  and  $\mathcal{F}(C_{\theta})$ , they do not cover all possible range of repulsiveness. Another family of parametric kernels is considered in [25], namely the power exponential spectral model, that contains as a limiting case  $C_B$  and the Poisson kernel (2.1). For this reason this family covers all possible range of repulsiveness, but then only  $\mathcal{F}(C_{\theta})$  is given and no close expression is available for  $C_{\theta}$ . For all these families, none of  $C_{\theta}$  and  $\mathcal{F}(C_{\theta})$  is compactly supported.

Below, we present alternative families of parametric kernels. The first one is the Laguerre-Gaussian family and fulfills the three requirements (a)-(c) above. The second family follows (a)-(c) too, and additionally the Fourier transform of the kernels is compactly supported. We finally introduce new families of compactly supported kernels, inspired by Proposition 4.1 and Proposition 4.4.

#### 5.1 Laguerre-Gaussian family

Let us first recall the definition of the Laguerre polynomials. We denote by  $\mathbb{N}$  the set  $\{0, 1, 2, ...\}$  and by  $\mathbb{N}^*$  the set  $\mathbb{N} \setminus \{0\}$ .

**Definition 5.1.** The Laguerre polynomials are defined for all  $m \in \mathbb{N}$  and  $\alpha \in \mathbb{R}$  by:

$$L_m^{\alpha}(x) = \sum_{k=0}^m \binom{m+\alpha}{m-k} \frac{(-x)^k}{k!}.$$

For all  $m \in \mathbb{N}^*$ ,  $\alpha > 0$ ,  $\rho > 0$  and  $x \in \mathbb{R}^d$ , we consider the Laguerre-Gaussian function

$$C(x) = \frac{\rho}{\binom{m-1+\frac{d}{2}}{m-1}} L_{m-1}^{\frac{d}{2}} \left(\frac{1}{m} \left|\frac{x}{\alpha}\right|^2\right) e^{-\frac{1}{m}\left|\frac{x}{\alpha}\right|^2}.$$
(5.1)

This kernel already appears in the literature, see e.g. [11] for an application in approximation theory. The following proposition summarizes the properties that are relevant for its use as a DPP kernel.

**Proposition 5.2.** Let C be given by (5.1), then its Fourier transform is, for all  $x \in \mathbb{R}^d$ ,

$$\mathcal{F}(C)(x) = \frac{\rho}{\binom{m-1+\frac{d}{2}}{m-1}} \alpha^d (m\pi)^{\frac{d}{2}} e^{-m(\pi\alpha|x|)^2} \sum_{k=0}^{m-1} \frac{(\pi\sqrt{m}|\alpha x|)^{2k}}{k!}$$
(5.2)

and DPP(C) exists if and only if  $\alpha \leq \alpha_{\max}$  where

$$\alpha_{\max}^d = \frac{\binom{m-1+\frac{d}{2}}{m-1}}{\rho(m\pi)^{\frac{d}{2}}}.$$

In this case, DPP(C) is stationary and isotropic with intensity  $\rho$ . Moreover, we have the convergence, for any  $\rho > 0$  and  $\alpha > 0$ ,

$$\lim_{m \to +\infty} C(x) = \rho \Gamma\left(\frac{d}{2} + 1\right) \frac{J_{\frac{d}{2}}\left(2|\frac{x}{\alpha}|\right)}{|\frac{x}{\alpha}|^{\frac{d}{2}}}$$
(5.3)

uniformly on all compact sets. In particular, for  $\alpha = \alpha_{max}$  we have :

$$\lim_{m \to +\infty} C(x) = C_B(x) \tag{5.4}$$

uniformly on all compact sets and where  $C_B$  is defined in (3.1).

This family of kernels contains the Gaussian kernel, being the particular case m = 1, and covers all range of repulsiveness from the Poisson kernel (2.1) (when  $\alpha \to 0$ ) to  $C_B$ , in view of (5.4).

For instance, in dimension d = 2, we have  $\alpha_{\max} = \frac{1}{\sqrt{\rho\pi}}$ , which does not depend of *m* in this case. Figure 3 shows, when d = 2, the behavior of the pcf of DPP(C)with respect to  $\alpha$ . Figure 4 illustrates, when  $\alpha$  is fixed to  $\alpha = \alpha_{\max}$ , the convergence result (5.4).

Figure 3: Pcf's of DPP(C) and  $DPP(C_B)$  where C is given by (5.1), and when  $d = 2, \rho = 1, m = 1$  and different values of  $\alpha$  from 0.1 to  $\alpha_{\max} \approx 0.56$ .



Figure 4: Pcf's of DPP(C) and  $DPP(C_B)$  where C is given by (5.1), and when  $d = 2, \rho = 1, \alpha = \alpha_{\max} \approx 0.56$  and different values of m.



### 5.2 Bessel-type family

For all  $\sigma \ge 0$ ,  $\alpha > 0$ ,  $\rho > 0$ , we consider the Bessel-type kernel

$$C(x) = \rho \, 2^{\frac{\sigma+d}{2}} \Gamma\left(\frac{\sigma+d+2}{2}\right) \frac{J_{\frac{\sigma+d}{2}}\left(2|\frac{x}{\alpha}|\sqrt{\frac{\sigma+d}{2}}\right)}{\left(2|\frac{x}{\alpha}|\sqrt{\frac{\sigma+d}{2}}\right)^{\frac{\sigma+d}{2}}}, \quad x \in \mathbb{R}^d.$$
(5.5)

This positive definite function first appears in [30], where it is called the Poisson function. It has been further studied in [12] and [13], where it is called the Bessel-type function. For obvious reasons, we prefer the second terminology when applied to point processes. For any  $x \in \mathbb{R}$ , we denote by  $x_+$  its positive part, i.e.  $x_+ = \max(x, 0)$ .

**Proposition 5.3.** Let C be given by (5.5), then its Fourier transform is, for all  $x \in \mathbb{R}^d$ ,

$$\mathcal{F}(C)(x) = \rho \, \frac{(2\pi)^{\frac{d}{2}} \alpha^d \Gamma(\frac{\sigma+d+2}{2})}{(\sigma+d)^{\frac{d}{2}} \Gamma(\frac{\sigma+2}{2})} \left(1 - \frac{2\pi^2 \alpha^2 |x|^2}{\sigma+d}\right)_+^{\frac{\sigma}{2}} \tag{5.6}$$

and DPP(C) exists if and only if  $\alpha \leq \alpha_{\max}$  where

$$\alpha_{\max}^{d} = \frac{(\sigma+d)^{\frac{d}{2}}\Gamma(\frac{\sigma+2}{2})}{\rho(2\pi)^{\frac{d}{2}}\Gamma(\frac{\sigma+d+2}{2})}$$

In this case, DPP(C) defines a stationary and isotropic DPP with intensity  $\rho$ . Moreover, if  $\sigma = 0$  and  $\alpha = \alpha_{\max}$ , then  $C = C_B$  where  $C_B$  is defined in (3.1). In addition, we have the convergence, for any  $\rho > 0$  and  $\alpha > 0$ ,

$$\lim_{\sigma \to +\infty} C(x) = \rho \, e^{-\left(\frac{|x|}{\alpha}\right)^2},\tag{5.7}$$

uniformly on all compact sets.

The Bessel-type family contains  $C_B$  as a particular case and the Poisson kernel as a limiting case, when  $\alpha \to 0$ . Hence this family covers all range of repulsiveness. Moreover,  $\mathcal{F}(C)$  is compactly supported, see (5.6).

Figure 5 shows the behavior of the pcf of DPP(C) with respect to  $\sigma$ , while Figure 6 illustrates the convergence result (5.7).

Figure 5: Pcf's of DPP(C) where C is given by (5.5), when d = 2,  $\rho = 1$ ,  $\sigma = 0$  and different values of  $\alpha$ . The case  $\alpha = \alpha_{\max} = 1/\sqrt{\pi} \approx 0.56$  corresponds to  $C = C_B$ .



Figure 6: Pcf's of DPP(C) where C is given by (5.5), when d = 2,  $\rho = 1$ ,  $\alpha = \alpha_{\max}$ , and different values of  $\sigma$ . The case  $\sigma = 0$  corresponds to  $C = C_B$ .



#### 5.3 Families of compactly supported kernels

As suggested by Proposition 4.1, we can consider the following family of compactly supported kernels, parameterized by the range R > 0,

$$C_1(x) = \frac{1}{\|h\|^2} [h * h] \left(\frac{2x}{R}\right) C_B(x), \quad \forall x \in \mathbb{R}^d,$$
(5.8)

where h is given by (4.1). The Poisson kernel (2.1) and  $C_B$  are two limiting cases, when respectively  $R \to 0$  and  $R \to +\infty$ . However this family of kernels has several drawbacks : no close form expression are available for  $C_1$ , nor for  $\mathcal{F}(C_1)$ ; Moreover, at range R fixed,  $DPP(C_1)$  is not the most repulsive DPP, see Proposition 4.4 and Figure 7. This is the reason why we turn ourselves to another family of compactly supported kernels.

Following Proposition 4.4, we introduce a new family of compactly supported kernel with range R, given as a convolution product of functions as in (4.6). Specifically, let R > 0,  $\rho > 0$  and  $\alpha > 0$  such that  $\frac{R\sqrt{\alpha}}{2}$  is not a zero of the Bessel function  $J_{\frac{d-2}{2}}$ , then we consider the kernel  $C_2 = u * u$  with

$$u(x) = \sqrt{\rho} \ \beta(R,\alpha) \left( 1 - \frac{R^{\frac{d}{2}-1}}{2^{\frac{d}{2}-1}J_{\frac{d}{2}-1}(\frac{R\sqrt{\alpha}}{2})} \frac{J_{\frac{d}{2}-1}(\sqrt{\alpha}|x|)}{|x|^{\frac{d}{2}-1}} \right) \mathbf{1}_{|x| \le \frac{R}{2}}, \tag{5.9}$$

where

$$\beta(R,\alpha) = \left[\frac{R^{d-1}\pi^{d/2}}{2^{d-1}\Gamma\left(\frac{d}{2}\right)} \left(\frac{R}{d} - \frac{4}{\sqrt{\alpha}} \frac{J_{\frac{d}{2}}\left(\frac{R\sqrt{\alpha}}{2}\right)}{J_{\frac{d}{2}-1}\left(\frac{R\sqrt{\alpha}}{2}\right)} + \frac{R}{2} \left(1 - \frac{J_{\frac{d}{2}-2}\left(\frac{R\sqrt{\alpha}}{2}\right)J_{\frac{d}{2}}\left(\frac{R\sqrt{\alpha}}{2}\right)}{J_{\frac{d}{2}-1}^{2}\left(\frac{R\sqrt{\alpha}}{2}\right)}\right)\right)\right]^{-\frac{1}{2}}$$

**Proposition 5.4.** Let  $C_2 = u * u$  where u is given by (5.9), then its Fourier transform is  $\mathcal{F}(u)^2$  where for all  $x \in \mathbb{R}^d$ 

$$\begin{aligned} \mathcal{F}(u)(x) &= \sqrt{\rho} \ \beta(R,\alpha) \left(\frac{R}{2|x|}\right)^{\frac{d}{2}-1} \left(\frac{R}{2|x|} J_{\frac{d}{2}}(\pi R|x|) \right. \\ &+ \frac{\pi}{J_{\frac{d-2}{2}}(\frac{R\sqrt{\alpha}}{2})} \frac{R\sqrt{\alpha} J_{\frac{d-2}{2}}'(\frac{R\sqrt{\alpha}}{2}) J_{\frac{d-2}{2}}(\pi R|x|) - 2\pi R J_{\frac{d-2}{2}}(\frac{R\sqrt{\alpha}}{2}) |x| J_{\frac{d-2}{2}}'(\pi R|x|)}{\alpha - 4\pi^2 |x|^2} \right). \end{aligned}$$

Moreover  $DPP(C_2)$  exists if and only if  $\alpha$  is such that  $|\mathcal{F}(u)| \leq 1$ . In this case,  $DPP(C_2)$  defines a stationary and isotropic R-dependent DPP with intensity  $\rho$ .

The choice of u in (5.9) comes from (4.6) where  $\gamma$  has been fixed to let u continuous at |x| = R/2, and where  $\beta$  is deduced from the relation  $C_2(0) = ||u||^2 = \rho$ . Given  $\rho$  and R, the remaining free parameter in this parametric family becomes  $\alpha$ . The restriction that  $\frac{R\sqrt{\alpha}}{2}$  must not be a zero of  $J_{\frac{d-2}{2}}$  can be alleviated by setting in these cases  $\beta = 0$  in (4.6) and fix  $\gamma$  so that  $C_2(0) = \rho$ . Then the most locally repulsive DPP (4.4) when  $R \leq M$  would be part of the parametric family. However, these kernels can be arbitrarily approximated by some kernel given by (5.9) for some value of  $\alpha$ , so we do not include these particular values of  $\alpha$  in the family above.

The condition  $|\mathcal{F}(u)| \leq 1$  on  $\alpha$ , given R and  $\rho$ , must be checked numerically. In most cases, the maximal value of  $\mathcal{F}(u)$  holds at the origin and we simply have to check whether  $|\mathcal{F}(u)(0)| \leq 1$ . No theoretical results are available to claim the existence of an admissible  $\alpha$ , but from our experience, it seems to exist an infinity of admissible  $\alpha$  for any R and  $\rho$ . Moreover, while the most locally repulsive DPP when  $R \leq M$  is known and corresponds to (4.4), the most repulsive DPP when R > Min the above parametric family seems to correspond to the minimal value of  $\alpha$  such that  $|\mathcal{F}(u)| \leq 1$ , denoted  $\alpha_{\min}$ .

The main interest of the parametric family given by  $C_2$  is that it covers a large range of repulsiveness, as shown in Figure 8, whereas the kernels are compactly supported. Moreover the close form expression of  $\mathcal{F}(C_2)$  is available and this family contains the most locally repulsive DPP with range R, in view of Proposition 4.4, at least when  $R \leq M$ . As an illustration, Figure 7 shows that  $DPP(C_2)$  is more repulsive than  $DPP(C_1)$  for moderate values of R. However,  $C_2$  does not converge to  $C_B$  when R tends to infinity, contrary to  $C_1$ . Figure 9 illustrates the effect of  $\alpha$ on  $C_2$ , given  $\rho$  and R.

Figure 7: Pcf's of  $DPP(C_1)$ ,  $DPP(C_2)$  and  $DPP(C_B)$  when d = 2,  $\rho = 1$ ,  $\alpha = \alpha_{\min}$  for  $C_2$  and different values of R.



Figure 8: Pcf's of  $DPP(C_2)$  and  $DPP(C_B)$  when d = 2,  $\rho = 1$ ,  $\alpha = \alpha_{\min}$  and different values of R.



Figure 9: Pcf's of  $DPP(C_2)$  and  $DPP(C_B)$  when d = 2,  $\rho = 1$ , R = 3 and different values of  $\alpha$ .



## 6 Proofs

#### 6.1 **Proof of Proposition 3.1**

This result was already observed in [25]. According to Definition 1.1, we seek to maximizing  $\int_{\mathbb{R}^d} 1 - g(x) dx$  where g is the pcf of a DPP with intensity  $\rho$  and kernel C verifying condition  $\mathcal{K}$ . By (2.2) the kernel C of a DPP with intensity  $\rho$  and pcf g is:

$$C(x) = \rho \sqrt{1 - g(x)}, \quad \forall x \in \mathbb{R}^d,$$

and it verifies  $C(0) = \rho$ . Therefore, this optimization problem is equivalent to maximizing  $\int_{\mathbb{R}^2} C^2$  under the constraints that C verifies condition  $\mathcal{K}$  and  $C(0) = \rho$ . By Parseval's equality, this is equivalent to maximizing  $\int \mathcal{F}(C)^2$  under the same constraints. First, let us notice the following Lemma.

**Lemma 6.1.** If C verifies condition  $\mathcal{K}$  then  $\mathcal{F}(C)$  is in  $L^1(\mathbb{R}^d)$ .

*Proof.* This lemma is proved by the same arguments as in Theorem 1.8.13 in [29]. Since the Fourier transform preserves inner product in  $L^2$ , we have:

$$\int_{\mathbb{R}^d} \mathcal{F}(C)(x) e^{-\frac{\pi |x|^2}{n^2}} dx = \int_{\mathbb{R}^d} C(x) n^d e^{-|nx|^2} dx.$$

Then, by the substitution u = nx, we have:

$$\int_{\mathbb{R}^d} \mathcal{F}(C)(x) e^{-\frac{|\pi x|^2}{n^2}} dx = \int_{\mathbb{R}^d} C\left(\frac{u}{n}\right) e^{-|u|^2} du.$$
(6.1)

Note that C can be viewed as a covariance function, thereby  $|C(x)| \leq C(0)$ . Therefore we have from (6.1):

$$\int_{\mathbb{R}^d} \mathcal{F}(C)(x) e^{-\frac{|\pi x|^2}{n^2}} dx \le C(0) \int_{\mathbb{R}^d} e^{-|u|^2} du = \frac{\sqrt{\pi}C(0)}{2}.$$
 (6.2)

Since  $\mathcal{F}(C) \geq 0$ , Beppo Levi's theorem applies in the left-hand side of (6.2). So by letting *n* tends to infinity, we obtain:

$$0 \le \int_{\mathbb{R}^d} \mathcal{F}(C)(x) dx \le \frac{\sqrt{\pi}C(0)}{2},$$

which shows that  $\mathcal{F}(C)$  is in  $L^1(\mathbb{R}^d)$ .

Under condition  $\mathcal{K}$  we have  $0 \leq \mathcal{F}(C) \leq 1$ , so  $\mathcal{F}(C)^2 \leq \mathcal{F}(C)$  where  $\mathcal{F}(C)$  is in  $L^1(\mathbb{R}^d)$  by Lemma 6.1. Hence:

$$\int_{\mathbb{R}^d} \mathcal{F}(C)^2(x) dx \le \int_{\mathbb{R}^d} \mathcal{F}(C)(x) dx.$$
(6.3)

Since  $0 \leq \mathcal{F}(C) \leq 1$ , this inequality becomes an equality if and only if  $\mathcal{F}(C)(x) \in \{0,1\}$  for almost every  $x \in \mathbb{R}^d$ . Moreover, since C is real and

$$\int_{\mathbb{R}^d} \mathcal{F}(C)(x) dx = C(0) = \rho,$$

the equality holds if and only if  $\mathcal{F}(C)$  is an even function that equals almost everywhere an indicator function of a Borel set with volume  $\rho$ . Note that in this case C follows condition  $\mathcal{K}$  because  $\mathcal{F}(C) \in L^1$  implies that  $C = \mathcal{FF}(C)$  is continuous and  $\mathcal{F}(C) \in L^2$  implies that  $C \in L^2$ . Thus, these kernels solve our optimization problem.

#### 6.2 **Proof of Proposition 3.2**

We notice that the kernel  $C_B$  verifies condition  $\mathcal{K}$  and  $C_B(0) = \rho$ , so it defines a DPP with intensity  $\rho$ . By analytic definition of Bessel functions, see (9.1.10) in [1], we have:

$$C_B(x) = \frac{\sqrt{\rho\Gamma(\frac{d}{2}+1)}}{\pi^{d/4}} \sum_{n=0}^{+\infty} \frac{(-1)^n \left(\sqrt{\pi}\Gamma(\frac{d}{2}+1)^{\frac{1}{d}}\rho^{\frac{1}{d}}\right)^{2n}}{2^{2n}n!\Gamma(n+1+d/2)} |x|^{2n}.$$

Thus  $C_B$  is twice differentiable at 0 and by (2.2), the associated pcf  $g_B$  is twice differentiable at 0 too. By Definition 1.2, any DPP having a pcf g that is not twice differentiable at 0 is less locally repulsive than  $DPP(C_B)$ . Consequently we assume in the following of the proof that g is twice differentiable at 0. The problem therefore reduces to minimize  $\Delta g(0)$  under the constraint that g is the pcf of a DPP with intensity  $\rho$  and kernel C verifying condition  $\mathcal{K}$ .

According to condition  $\mathcal{K}$ , the Fourier transform of the kernel C is well defined and belongs to  $L^1(\mathbb{R}^d)$  by Lemma 6.1. Therefore, we can define the function  $f = \frac{\mathcal{F}(C)}{\|\mathcal{F}(C)\|_1}$  and consider it as a density function of a random variable X =

 $(X_1, \cdots, X_d) \in \mathbb{R}^d.$ 

The kernel C being symmetric, we have  $\mathcal{FF}(C) = C$ , see Remark 2.5. Let us denote by  $\hat{f}$  the characteristic function of the random variable X with density f, i.e.  $\hat{f}(t) = \mathbb{E}(e^{it \cdot X})$ . We have the relation:

$$\widehat{f}(t) = \frac{C\left(\frac{t}{2\pi}\right)}{\|\mathcal{F}(C)\|_1}, \quad \forall t \in \mathbb{R}^d.$$
(6.4)

Thus, the characteristic function  $\hat{f}$  shares the same regularity as C. In particular,  $\hat{f}$  is twice differentiable at 0, so by usual properties of the characteristic function (see [31]), X has finite second order moments and:

$$E(X_i^2) = -\frac{\partial^2 \widehat{f}}{\partial x_i^2}(0) + \left(\frac{\partial \widehat{f}}{\partial x_i}(0)\right)^2, \quad \forall i = 1 \dots d.$$
(6.5)

On the other hand, as already noticed in introduction,  $\nabla g(0) = 0$  and so  $\frac{\partial C}{\partial x_i}(0) = 0$  for all  $i = 1, \ldots, d$ . By differentiating both sides of Equation (6.4), we obtain:

$$\frac{\partial \widehat{f}}{\partial x_i}(0) = \frac{1}{2\pi \|\mathcal{F}(C)\|_1} \frac{\partial C}{\partial x_i}(0) = 0, \quad \forall i = 1 \dots d$$
(6.6)

and

$$\frac{\partial^2 \widehat{f}}{\partial x_i^2}(0) = \frac{1}{4\pi^2 \|\mathcal{F}(C)\|_1} \frac{\partial^2 C}{\partial x_i^2}(0), \quad \forall i = 1 \dots d.$$
(6.7)

Then, we can deduce from (6.5), (6.6) and (6.7):

$$E(|X|^2) = E\left(\sum_{i=1}^d X_i^2\right) = -\Delta\hat{f}(0) = -\frac{1}{4\pi^2 \|\mathcal{F}(C)\|_1} \Delta C(0).$$

Moreover, since  $f = \frac{\mathcal{F}(C)}{\|\mathcal{F}(C)\|_1}$ :

$$E(|X|^2) = \int_{\mathbb{R}^d} |x|^2 f(x) dx = \int_{\mathbb{R}^d} |x|^2 \frac{\mathcal{F}(C)}{\|\mathcal{F}(C)\|_1} (x) dx.$$

Hence, the Laplacian of C at 0 is:

$$\Delta C(0) = -4\pi^2 \int_{\mathbb{R}^d} |x|^2 \mathcal{F}(C)(x) dx.$$
(6.8)

By Relation (2.2) and since  $\nabla C(0) = 0$ , we have:

$$\Delta g(0) = \Delta \left(1 - \frac{C^2}{\rho^2}\right)(0) = -\frac{1}{\rho^2} \left(\sum_{i=1}^d 2C(0) \frac{\partial^2 C}{\partial x_i^2}(0) + 2\left(\frac{\partial C}{\partial x_i}(0)\right)^2\right)$$
$$= -\frac{2}{\rho} \sum_{i=1}^d \frac{\partial^2 C}{\partial x_i^2}(0)$$
$$= -\frac{2}{\rho} \Delta C(0). \tag{6.9}$$

Finally, we deduce from (6.8) and (6.9) the relation:

$$\Delta g(0) = \frac{8\pi^2}{\rho} \int_{\mathbb{R}^d} |x|^2 \mathcal{F}(C)(x) dx.$$

Thus the two following optimization problems are equivalent.

Problem 1: Minimizing  $\Delta g(0)$  under the constraint that g is the pcf of a DPP with intensity  $\rho$  and kernel C satisfying condition  $\mathcal{K}$ .

Problem 2: Minimizing  $\int_{\mathbb{R}} |x|^2 \mathcal{F}(C)(x) dx$  under the constraint that C is a kernel twice differentiable at 0, verifying the condition  $\mathcal{K}$  and  $\int_{\mathbb{R}^d} \mathcal{F}(C)(x) dx = C(0) = \rho$ .

The latter optimization problem is a special case of Theorem 1.14 in [26], named bathtub principle, which gives the unique solution:

$$\mathcal{F}(C) = \mathbf{1}_{|\cdot|^d \le \rho \tau^d}$$

where we recall that  $\tau^d = \Gamma(d/2 + 1)/\pi^{\frac{d}{2}}$ .

#### 6.3 **Proof of Proposition 4.1**

First let notice that h is symmetric, real-valued, infinitely differentiable and verifies h(x) = 0 for  $x \ge 1$ , see Section 3.2 in [29]. Thus, ||h|| is finite and  $||h|| \ne 0$ , so  $C_r$  is well-defined.

Since  $h * h(0) = ||h||^2$ , we have  $C_r(0) = \rho$ . By product convolution properties, h \* h is symmetric, real-valued, infinitely differentiable and compactly supported with range 2. Thus, by (4.2),  $C_r$  is symmetric, real-valued, infinitely differentiable and compactly supported with range r. Then,  $C_r$  belongs to  $L^1 \cap L^2$ . In particular,  $\mathcal{F}(C_r)$  is well-defined pointwise. By Fourier transform properties, we have for all  $x \in \mathbb{R}^d$ :

$$\mathcal{F}(C_r)(x) = \frac{r^d}{2^d \|h\|^2} \left[ \mathcal{F}(h)^2 \left(\frac{r}{2} \cdot\right) * \mathcal{F}(C)(\cdot) \right](x).$$
(6.10)

Since h is symmetric,  $\mathcal{F}(h)$  is real valued so  $\mathcal{F}(h)^2 \geq 0$ . Thus, as  $\mathcal{F}(C) \geq 0$  by condition  $\mathcal{K}$ , we have  $\mathcal{F}(C_r) \geq 0$ . It remains to verify that  $\mathcal{F}(C_r) \leq 1$ . By condition  $\mathcal{K}$  we have  $0 \leq \mathcal{F}(C) \leq 1$  so:

$$\frac{r^d}{2^d \|h\|^2} \int_{\mathbb{R}^d} \mathcal{F}(h)^2 \left(\frac{rt}{2}\right) \mathcal{F}(C)(x-t) dt \le \frac{r^d}{2^d \|h\|^2} \int_{\mathbb{R}^d} \mathcal{F}(h)^2 \left(\frac{rt}{2}\right) dt.$$
(6.11)

By the substitution u = rt/2 and Parseval's equality, the right-and side of Relation (6.11) equals 1. Thus we obtain with Relations (6.10) and (6.11):

$$\mathcal{F}(C_r) \le 1.$$

It remains to show the convergence result (4.3), which reduces to prove that  $\frac{1}{\|h\|^2}[h*h]\left(\frac{2}{r}\cdot\right)$  tends to 1 uniformly on all compact sets when  $r \to \infty$ . But this follows from the uniform continuity of h\*h on every compact sets, implied by its continuity, and the fact that  $h*h(0) = \|h\|^2$ .

#### 6.4 **Proof of Proposition 4.3**

The proof is based on a theorem from Ehm et al. [9] recalled below with only slight changes in the presentation.

We say that  $C_1 = C_2$  up to a radialization if  $rad(C_1) = rad(C_2)$  where rad is the transformation defined as follows.

**Definition 6.2.** Let H denote the normalized Haar measure on the group SO(d) of rotations in  $\mathbb{R}^d$  and let C be a kernel verifying condition  $\mathcal{K}_c(\rho, R)$ . The radialization of the kernel C is the kernel  $\operatorname{rad}(C)$  defined by:

$$\operatorname{rad}(C)(x) = \int_{SO(d)} C(j(x)) H(dj).$$

Note that for any isotropic kernel C, C = rad(C).

Let us denote  $\gamma_d^2 = \frac{4j_{(d-2)/2}^{d-2}}{\pi^{\frac{d}{2}}\Gamma(\frac{d}{2})J_{\frac{d}{2}}^2(j_{(d-2)/2})}$  and  $c_d = \frac{4j_{\frac{d-2}{2}}^2}{4^d\pi^{\frac{d}{2}}\Gamma(\frac{d}{2})}$ .

**Theorem 6.3** ([9]). Let  $\Psi$  be a twice differentiable characteristic function of a probability density f on  $\mathbb{R}^d$  and suppose that  $\Psi(x) = 0$  for  $|x| \ge 1$ . Then

$$-\Delta\Psi(0) = \int |x|^2 f(x) dx \ge 4j_{(d-2)/2}^2$$

with equality if and only if, up to a radialization,  $\Psi = \omega_d * \omega_d$ , where  $\omega_d(x) = \gamma_d \frac{\Gamma(\frac{d}{2})}{\frac{J(d-2)/2}{J(d-2)/2}} \frac{J_{\frac{d-2}{2}}(2j_{\frac{d-2}{2}}|x|)}{|x|^{\frac{d-2}{2}}}$  for  $|x| \leq \frac{1}{2}$  and  $\omega_d(x) = 0$  for  $|x| \geq \frac{1}{2}$ . The corresponding minimum variance density is

$$f(x) = c_d \Gamma\left(\frac{d}{2}\right)^2 \left(\frac{2^{\frac{d-2}{2}} J_{\frac{d-2}{2}}\left(\frac{|x|}{2}\right)}{\left|\frac{x}{2}\right|^{\frac{d-2}{2}} \left(j_{(d-2)/2}^2 - \left(\frac{|x|}{2}\right)^2\right)}\right)^2.$$

According to Definition 1.2 and by the same arguments as in the proof of Proposition 3.2 and Relation (6.9), we seek a kernel C twice differentiable at 0 such that  $\Delta C(0)$  is maximal among all kernels verifying condition  $\mathcal{K}_c(\rho, R)$ .

In a first step, we exhibit a candidate for the solution to this optimization problem and in a second step we check that it verifies all required conditions.

Step 1. We say that a function C verifies  $\widetilde{\mathcal{K}_c}(\rho, R)$  if it verifies  $\mathcal{K}_c(\rho, R)$  without necessarily verifying  $\mathcal{F}(C) \leq 1$ . We notice that a function C verifies  $\widetilde{\mathcal{K}_c}(\rho, R)$  if and only if the function  $\Psi$  defined by:

$$\Psi(x) = \frac{C(Rx)}{\rho}, \ x \in \mathbb{R}^d, \tag{6.12}$$

verifies  $\widetilde{\mathcal{K}_c}(1,1)$ . Therefore, we have a one-to-one correspondence between  $\widetilde{\mathcal{K}_c}(\rho, R)$  and  $\widetilde{\mathcal{K}_c}(1,1)$ .

On the other hand, if a function  $\Psi$  verifies condition  $\widetilde{\mathcal{K}_c}(1,1)$ , it is by Bochner's Theorem the characteristic function of a random variable X. Moreover, the function  $\Psi$ is continuous and compactly supported so it is in  $L^1(\mathbb{R}^d)$  and the random variable X has a density f, see [31]. Thus, by Theorem 6.3, any function  $\Psi$  twice differentiable at 0 and verifying condition  $\widetilde{\mathcal{K}_c}(1,1)$  satisfies:

$$\Delta \Psi(0) \le -4j_{(d-2)/2}^2. \tag{6.13}$$

By differentiating both sides of Equation (6.12), we have:

$$\Delta\Psi(0) = \frac{R^2}{\rho} \Delta C(0), \qquad (6.14)$$

where we recall that the function C is twice differentiable at 0 and verifies  $\widetilde{\mathcal{K}_c}(\rho, R)$ . Thus, by Equations (6.13) and (6.14), for all kernels C twice differentiable at 0 and verifying  $\widetilde{\mathcal{K}_c}(\rho, R)$  we have:

$$\Delta C(0) = \frac{\rho \Delta \Psi(0)}{R^2} \le -\frac{4\rho j_{(d-2)/2}^2}{R^2}.$$
(6.15)

By Theorem 6.3, equality holds in (6.15) if and only if  $\Psi = \omega_d * \omega_d$  and we name  $C_R$  the corresponding kernel C given by relation (6.12). This kernel is the candidate to our optimization problem, however it remains to prove that it verifies condition  $\mathcal{K}_c(\rho, R)$ .

Step 2. Let us prove that  $C_R$  verifies  $\mathcal{K}_c(\rho, R)$ . We have seen in Step 1 that  $C_R$  verifies  $\widetilde{\mathcal{K}_c}(\rho, R)$  and is twice differentiable at 0. Thus, it remains to verify that  $\mathcal{F}(C_R) \leq 1$ . By Theorem 6.3, the function  $\Psi = \omega_d * \omega_d$  is the characteristic function of a probability density f. Thus, we have:

$$\mathcal{F}(\Psi)(x) = (2\pi)^d f(2\pi x), \quad \forall x \in \mathbb{R}^d,$$
(6.16)

so by Theorem 6.3 we deduce:

$$\mathcal{F}(\Psi)(x) = (2\pi)^d c_d \Gamma\left(\frac{d}{2}\right)^2 \left(\frac{2^{\frac{d-2}{2}}J_{\frac{d-2}{2}}(|\pi x|)}{|\pi x|^{\frac{d-2}{2}}\left(j_{(d-2)/2}^2 - (|\pi x|)^2\right)}\right)^2.$$
(6.17)

By (6.12) and Fourier transform dilatation we obtain the expression (4.5) of  $\mathcal{F}(C_R)$ .

Moreover, the Bessel functions are non-negative up to their first non-negative zero so  $\omega_d \geq 0$ , which implies that  $\Psi \geq 0$ . Hence by (6.17),

$$\mathcal{F}(\Psi)(x) = \left| \int_{\mathbb{R}^d} \Psi(t) e^{2i\pi x \cdot t} dt \right| \le \int_{\mathbb{R}^d} \Psi(t) dt = \mathcal{F}(\Psi)(0) = \frac{2^d \pi^d c_d}{j_{\frac{d-2}{2}}^4}.$$
 (6.18)

Thus, by (6.12) and Fourier transform dilatation, we have:

$$\mathcal{F}(C_R)(x) \le \mathcal{F}(C_R)(0) = \frac{2^d R^d \rho \pi^d c_d}{j_{\frac{d-2}{2}}^4} = \frac{R^d}{M^d}.$$
(6.19)

Since by hypothesis  $R \leq M$ , we have  $\mathcal{F}(C_R) \leq 1$ .

#### 6.5 **Proof of Proposition 4.4**

According to Definition 1.2 and by the same arguments as in the proof of Proposition 3.2 and Relation (6.9), we seek a kernel C twice differentiable at 0 such that  $\Delta C(0)$  is maximal among all kernels verifying condition  $\mathcal{K}_c(\rho, R)$ . By relation (6.8), this is equivalent to solve the following problem A.

**Problem A:** Minimize  $\int_{\mathbb{R}^d} |x|^2 \mathcal{F}(C)(x) dx$  under the constraints that C is twice differentiable at 0 and verifies  $\mathcal{K}_c(\rho, R)$ .

The proof of Proposition 4.4 is based on three lemmas proved in the following.

As a first preliminary result, the following lemma shows that C solves Problem A if C is the auto-convolution of a certain function. In its statement the gradient  $\nabla u$  has to be considered in the sense of distribution when  $u \in L^2$  is not differentiable.

**Lemma 6.4.** A kernel  $C_R$  is solution to Problem A if and only if there exists a function u such that, up to a radialization,  $C_R = u * u$  where u minimizes  $\int_{\mathbb{R}^d} |\nabla u(x)|^2 dx$ among all functions u verifying  $\mathcal{M}(\rho, R)$  and  $\mathcal{F}(u)^2 \leq 1$ .

The existence statement in Proposition 4.4 is given by the following lemma.

**Lemma 6.5.** There exists a solution to Problem A.

By Lemma 6.4,  $C_R = u * u$  where u is the solution of an optimization problem. Then, under the additional constraint  $\sup_{x \in \mathbb{R}^d} \mathcal{F}(C)(x) = \mathcal{F}(C)(0)$ , we have by Fourier transform properties  $\sup_{x \in \mathbb{R}^d} (\mathcal{F}(u)(x))^2 = (\mathcal{F}(u)(0))^2$ . Since  $\mathcal{F}(u)^2(0) = (\int_{\mathbb{R}^d} u(t)dt)^2$ , the constraint  $\mathcal{F}(u)^2 \leq 1$  in Lemma 6.4 becomes  $(\int_{\mathbb{R}^d} u(t)dt)^2 \leq 1$ . Moreover, we notice that if u is a solution of the optimization problem, so is -u. Thus, we can assume without loss of generality that  $\int_{\mathbb{R}^d} u(t)dt \geq 0$ , so that the constraint  $(\int_{\mathbb{R}^d} u(t)dt)^2 \leq 1$  becomes  $\int_{\mathbb{R}^d} u(t)dt \leq 1$ . In this situation, the optimization problem addressed in Lemma 6.4 can be solved by variational calculus. However an explicit form of the solution is available only if we assume that  $u \in \mathcal{C}^2(B(0, \frac{R}{2}))$ , meaning that u is twice continuously differentiable on its support. It is given by the following lemma, which completes the proof of Proposition 4.4.

**Lemma 6.6.** If a function u minimizes  $\int_{\mathbb{R}^d} |\nabla u(x)|^2 dx$  among all functions u verifying  $\mathcal{M}(\rho, R)$ ,  $u \in \mathcal{C}^2(B\left(0, \frac{R}{2}\right))$  and  $\int_{\mathbb{R}^d} u(x) dx \leq 1$ , then u is of the form :

$$u(x) = \left(\beta + \gamma \frac{J_{\frac{d-2}{2}}\left(\sqrt{\alpha}|x|\right)}{|x|^{\frac{d-2}{2}}}\right) \mathbf{1}_{|x| < \frac{R}{2}},$$

with  $\alpha > 0, \beta \ge 0$  and  $\gamma$  are three constants linked by the conditions  $\mathcal{M}(\rho, R)$  and  $\int_{\mathbb{R}^d} u(x) dx \le 1$ .

#### Proof of Lemma 6.4

Let C be a kernel twice differentiable at 0, verifying the condition  $\mathcal{K}_c(\rho, R)$ . In particular, the kernel C is a covariance function twice differentiable at 0, so it is of regularity at least  $\mathcal{C}^2$  on  $\mathbb{R}^d$ . Moreover, the quantity  $\int_{\mathbb{R}^d} |x|^2 \mathcal{F}(C)(x) dx$  is invariant under radialization of the kernel C, see relation (44) in [9]. Thus, we can consider C as a radial function. Then, by Theorem 3.8 in [9], there exists a countable set A and a sequence of real valued functions in  $L^2$ ,  $\{u_k\}_{k \in A}$ , such that:

$$C(x) = \sum_{k \in A} u_k * u_k(x).$$
 (6.20)

Moreover, the convergence of the series is uniform and for each  $k \in A$ , the support of  $u_k$  lies in  $B\left(0, \frac{R}{2}\right)$ . Thus, by uniform convergence of the series we have :

$$\int_{\mathbb{R}^d} |x|^2 \mathcal{F}(C)(x) dx = \int_{\mathbb{R}^d} |x|^2 \sum_{k \in A} |\mathcal{F}(u_k)(x)|^2 dx$$
$$= \sum_{k \in A} \int_{\mathbb{R}^d} |x \mathcal{F}(u_k)(x)|^2 dx$$
$$= \sum_{k \in A} \sum_{j=1}^d \int_{\mathbb{R}^d} |x_j \mathcal{F}(u_k)(x)|^2 dx$$
(6.21)

where  $x_j$  denotes the j - th coordinates of the vector x. In addition, we note that  $u_k \in L^2$  so  $|\cdot|\mathcal{F}(u_k)(\cdot) \in L^2$  by (6.21). Then by Theorem 7.9 in [26]  $\nabla u_k \in L^2$ , where  $\nabla u_k$  has to be viewed in the distributional sense, and we have:

$$\mathcal{F}(\partial_j u_k)(x) = 2i\pi x_j \mathcal{F}(u_k)(x).$$
(6.22)

Thus, we have:

$$\int_{\mathbb{R}^d} |x|^2 \mathcal{F}(C)(x) dx = \sum_{k \in A} \sum_{j=1}^d \int_{\mathbb{R}^d} \left| \frac{\mathcal{F}(\partial_j u_k)(x)}{2i\pi} \right|^2 dx.$$

According to Parseval equality, it follows that:

$$\int_{\mathbb{R}^d} |x|^2 \mathcal{F}(C)(x) dx = \sum_{k \in A} \sum_{j=1}^d \int_{\mathbb{R}^d} \left| \frac{\partial_j u_k(x)}{2i\pi} \right|^2 dx \qquad (6.23)$$
$$= \sum_{k \in A} \int_{\mathbb{R}^d} \frac{|\nabla u_k(x)|^2}{4\pi^2} dx.$$

As every term in the sum (6.23) is positive and since this inequality holds for every kernel C, the minimum of  $\int_{\mathbb{R}^d} |x|^2 \mathcal{F}(C)(x) dx$  is reached if and only if this sum reduces to one term where  $u_k = u$ . Then we have C = u \* u and

$$\int_{\mathbb{R}^d} |x|^2 \mathcal{F}(C)(x) dx = \int_{\mathbb{R}^d} \frac{|\nabla u(x)|^2}{4\pi^2} dx.$$
(6.24)

Therefore, minimizing  $\int_{\mathbb{R}^d} |x|^2 \mathcal{F}(C)(x) dx$  is equivalent to minimize  $\int_{\mathbb{R}^d} |\nabla u(x)|^2 dx$ . It remains to translate the constraints on the kernel C as constraints on u.

Since C = u \* u, where u is one of the function in the decomposition (6.20), u is a so-called real valued Boas-Kac root of C, see [9]. Thus, since C is radial, we have by Theorem 3.1 in [9] and the discussion below that u is radial and verifies u(x) = 0for  $|x| \geq \frac{R}{2}$ . Since C verifies  $\mathcal{K}_c(\rho, R)$ , we have  $C(0) = \rho$  and  $0 \leq \mathcal{F}(C) \leq 1$ . By product convolution properties, those constraints are respectively equivalent on uto:  $\int_{\mathbb{R}^d} u(x)^2 dx = \rho$  and  $\mathcal{F}(u)^2 \leq 1$ . Therefore, u verifies condition  $\mathcal{M}(\rho, R)$  and  $\mathcal{F}(u)^2 \leq 1$ .

#### Proof of Lemma 6.5

According to Lemma 6.4,  $C_R$  is solution to Problem A if and only if  $C_R = u * u$  where u minimizes  $\int_{\mathbb{R}^d} |\nabla u(x)|^2 dx$  among all functions u verifying  $\mathcal{M}(\rho, R)$  and  $\mathcal{F}(u)^2 \leq 1$ . We prove the existence of this minimum u.

Let  $\Omega$  denote the set  $B\left(0, \frac{R}{2}\right)$ . We recall that  $H^1(\Omega)$  is the Sobolev space defined by:

$$H^1(\Omega) = \left\{ f: \Omega \to \mathbb{R}^d, \ f \in L^2, \ \nabla f \in L^2 \right\},$$

with the norm  $||f||_{H^1(\Omega)} = (||f||^2 + ||\nabla f||^2)^{\frac{1}{2}}$ . For a review on Sobolev spaces, see for example [10] or [26]. Let us further denote  $\mathcal{E}$  the set of functions  $f \in H^1(\Omega)$ verifying  $\mathcal{M}(\rho, R)$  and  $\mathcal{F}(f)^2 \leq 1$ .

If the minimum u above exists but  $u \notin H^1(\Omega)$ , then  $\int_{\Omega} |\nabla u(x)|^2 dx = \infty$ , which means that  $\mathcal{E}$  is empty, otherwise u would not be the solution of our optimization problem. But  $\mathcal{E}$  is not empty, see for instance the functions in Section 5.3, so if uexists,  $u \in H^1(\Omega)$ . Let  $(w_k)_{k \in \mathbb{N}}$  be a minimizing sequence in  $\mathcal{E}$ , i.e.

$$\int_{\Omega} |\nabla w_k(x)|^2 dx \underset{k \to +\infty}{\longrightarrow} \inf_{v \in \mathcal{E}} \int_{\Omega} |\nabla v(x)|^2 dx, \qquad (6.25)$$

where for all  $k, w_k \in \mathcal{E}$ . By (6.25) and since for all  $k, \int_{\Omega} |w_k(x)|^2 dx = \rho$ , the sequence  $\{w_k\}$  is bounded in  $H^1(\Omega)$ . Then, by Rellich-Kondrachov compactness Theorem (see [10]), it follows that, up to a subsequence,  $\{w_k\}$  converges in  $L^2$  to a certain function  $w \in L^2$  verifying:

$$\int_{\Omega} |\nabla w(x)|^2 dx = \inf_{v \in \mathcal{E}} \int_{\Omega} |\nabla v(x)|^2 dx.$$
(6.26)

Let us prove that  $w \in \mathcal{E}$ , so that u = w is the solution of our optimization problem. First  $w \in H^1(\Omega)$  as justified earlier. Second, as rotations are isometric functions and since any  $w_k$  is radial by hypothesis, we have for any  $j \in SO(d)$ :

$$\left\{ \int_{\mathbb{R}^d} |w(x) - w_k(x)|^2 \, dx \to 0 \right\} \Leftrightarrow \left\{ \int_{\mathbb{R}^d} |w(j(x)) - w_k(j(x))|^2 \, dx \to 0 \right\},$$
$$\Leftrightarrow \left\{ \int_{\mathbb{R}^d} |w(j(x)) - w_k(x)|^2 \, dx \to 0 \right\}.$$

Hence, by uniqueness of the limit, the function w is radial and in particular, its Fourier transform is real. Third, since w is the  $L^2$  limit of  $w_k$ , w verifies the following properties:

- w is compactly supported in  $B\left(0, \frac{R}{2}\right)$ , because  $w_k \in \mathcal{E}$  for all k.
- $w \in L^2$  by Rellich-Kondrachov Theorem.
- $\int_{\mathbb{R}^d} |w(x)|^2 dx = \int_{\mathbb{R}^d} |w_k(x)|^2 dx = \rho$  since a sphere in  $L^2$  is closed.

Therefore, w verifies  $\mathcal{M}(\rho, R)$ . Finally, let us prove that  $\mathcal{F}(w)^2 \leq 1$ . For every  $k, w_k$  belongs to  $L^2$  and is compactly supported in  $\Omega$ . Thus by Cauchy-Schwartz inequality it is easily checked that  $w_k \in L^1$ , so we can consider  $\mathcal{F}(w_k)(x)$  for every  $x \in \mathbb{R}^d$ , and

$$|\mathcal{F}(w)(x) - \mathcal{F}(w_k)(x)| \le a \sqrt{\int_{\mathbb{R}^d} |w(t) - w_k(t)|^2 dt}, \quad \forall x \in \mathbb{R}^d,$$

where a is a positive constant. Thereby the convergence of  $w_k$  to w in  $L^2$  implies the pointwise convergence of  $\mathcal{F}(w_k)$  to  $\mathcal{F}(w)$ . Thus, from the relation

$$\mathcal{F}(w_k)(x) \le 1, \quad \forall x \in \mathbb{R}^d, \quad \forall k \in \mathbb{N},$$

we deduce  $\mathcal{F}(w) \leq 1$ .

#### Proof of Lemma 6.6

We denote as before  $\Omega = B\left(0, \frac{R}{2}\right)$ . The optimization problem in Lemma 6.6 is a variational problem with isoperimetric constraints. By Theorem 2, Chapter 2 from [15], every solution must solve the following boundary problem:

$$\Delta u + \alpha u - \frac{\lambda}{2} = 0, \text{ on } \Omega,$$
  

$$u = 0, \text{ on } \partial \Omega.$$
(6.27)

In equation (6.27),  $\alpha$  and  $\lambda$  are the Lagrange multipliers respectively associated to the constraints  $\int u^2 = \rho$  and  $\int u \leq 1$ . By Karush-Kuhn-Tucker Theorem, see Section VII in [18],  $\lambda \geq 0$ . Moreover, a solution to the partial differential equation with boundary condition (6.27) is obtained by linear combination of a homogeneous solution and a particular solution. By Theorem 2 Section 6.5 in [10], the Laplacian operator  $-\Delta$  has only positive eigenvalues. Hence the associated homogeneous equation  $\Delta u + \alpha u = 0$  can have a solution only if  $\alpha > 0$ .

In addition, the function u is radial by hypothesis, so there exists a function  $\tilde{u}$  on  $\mathbb{R}$  such that:

$$\forall x \in \mathbb{R}^d, \ u(x) = \tilde{u}(|x|).$$

The partial differential equation (6.27) then becomes:

$$\tilde{u}''(t) + \frac{d-1}{t}\tilde{u}'(t) + \alpha\tilde{u}(t) - \frac{\lambda}{2} = 0, \quad \forall t \in \left]0, \frac{R}{2}\right[,$$
$$\tilde{u}\left(\frac{R}{2}\right) = 0.$$

As  $\alpha$  is positive, we obtain from relations (3) and (4), Section 4.31 in [36] that a solution to this equation is of the form:

$$\tilde{u}(t) = \left(\frac{\lambda}{2\alpha} + c_1 \frac{J_{(d-2)/2}(\sqrt{\alpha}t)}{t^{(d-2)/2}} + c_2 \frac{Y_{(d-2)/2}(\sqrt{\alpha}t)}{t^{(d-2)/2}}\right) \mathbf{1}_{0 < t < \frac{R}{2}}, \tag{6.28}$$

where  $Y_{(d-2)/2}$  denotes the Bessel function of the second kind. By hypothesis, the function u is continuous on  $\Omega$  so in particular at 0. Since  $Y_{(d-2)/2}$  has a discontinuity at 0, see for example [1], and the remaining terms in (6.28) are continuous, we must have  $c_2 = 0$ . Then, by renaming the constant  $c_1$  by  $\gamma$  and letting  $\beta = \lambda/(2\alpha)$ , we obtain that if u is solution to the optimization problem of Lemma 6.6, then u writes

$$u(x) = \left(\beta + \gamma \frac{J_{(d-2)/2}(\sqrt{\alpha}|x|)}{|x|^{(d-2)/2}}\right) \mathbf{1}_{x \in \Omega},$$
(6.29)

where  $\alpha$  and  $\beta$  verify  $\alpha > 0$  and  $\beta \ge 0$ .

#### 6.6 Proof of Proposition 5.2

Let the function  $f_m$  be defined for all  $m \in \mathbb{N}$  by

$$f_m(x) = L_m^{d/2} \left( |x|^2 \right) e^{-|x|^2}, \quad \forall x \in \mathbb{R}^d.$$
 (6.30)

This function is radial, thus by Appendix B.5 in [17] we have:

$$\mathcal{F}(f_m)(x) = \frac{2\pi}{|x|^{\frac{d-2}{2}}} \int_0^{+\infty} r^{\frac{d}{2}} L_m^{\frac{d}{2}}(r^2) e^{-r^2} J_{\frac{d-2}{2}}(2\pi r|x|) dr.$$

According to [21], we have  $\forall t > 0$ ,  $\forall n, m \in \mathbb{N}$ ,  $\forall \sigma \in \mathbb{R}$ ,  $\operatorname{Re}(\alpha) > 0$ ,  $\operatorname{Re}(\nu) > -1$ :

$$\int_{0}^{+\infty} r^{\nu+1} e^{-\alpha r^2} L_m^{\nu-\sigma}(\alpha r^2) L_n^{\sigma}(\alpha r^2) J_{\nu}(rt) dr = \frac{(-1)^{m+n}}{2\alpha} \left(\frac{t}{2\alpha}\right)^{\nu} e^{-\frac{t^2}{4\alpha}} L_m^{\sigma-m+n}\left(\frac{t^2}{4\alpha}\right) L_n^{\nu-\sigma+m-n}\left(\frac{t^2}{4\alpha}\right). \quad (6.31)$$

By taking  $\nu = \frac{d-2}{2}$ ,  $\alpha = 1$ , n = 0,  $\sigma = -1$ , we obtain:

$$\mathcal{F}(f_m)(x) = \frac{2\pi}{|x|^{\frac{d-2}{2}}} \frac{(-1)^m}{2} \left(\frac{|2\pi x|}{2}\right)^{\frac{d-2}{2}} e^{-\frac{|2\pi x|^2}{4}} L_m^{-1-m} \left(\frac{|2\pi x|^2}{4}\right)$$
$$= \pi^{\frac{d}{2}} (-1)^m e^{-|\pi x|^2} \sum_{k=0}^m \binom{-1}{m-k} \frac{(-1)^k |\pi x|^{2k}}{k!}$$
$$= \pi^{\frac{d}{2}} (-1)^m e^{-|\pi x|^2} \sum_{k=0}^m (-1)^{m-k} \frac{(-1)^k |\pi x|^{2k}}{k!}.$$

Therefore, we have:

$$\mathcal{F}(f_m)(x) = \pi^{\frac{d}{2}} e^{-|\pi x|^2} \sum_{k=0}^m \frac{|\pi x|^{2k}}{k!}.$$

As  $C(x) = \frac{\rho}{\binom{m-1+\frac{d}{2}}{m-1}} f_{m-1}(\frac{1}{\sqrt{m}}\frac{x}{\alpha})$ , we obtain by dilatation and linearity of the Fourier transform the formula (5.2).

Clearly  $\mathcal{F}(C) \geq 0$ , let us investigate the condition  $\mathcal{F}(C) \leq 1$  for the existence of DPP(C). We notice from (5.2) that:

$$\mathcal{F}(C)(x) = ae^{-b|x|^2} \sum_{k=0}^{m-1} \frac{b^k |x|^{2k}}{k!},$$
(6.32)

where a and b are positive constants. Since  $\mathcal{F}(C)$  depends on the variable x only through its norm, we consider the function h define for all  $r \ge 0$  by:

$$h(r) = \mathcal{F}(C) \left( (r, 0, \cdots, 0) \right)$$

so that for all  $x \in \mathbb{R}^d$ ,  $\mathcal{F}(C)(x) = h(|x|)$ . For every r > 0, h is derivable at r and a straightforward calculation leads to:

$$h'(r) = ae^{-br^2} \left( -2br \sum_{k=0}^{m-1} \frac{b^k r^{2k}}{k!} + \sum_{k=1}^{m-1} 2k \frac{b^k r^{2k-1}}{k!} \right)$$
$$= -2ae^{-br^2} \frac{b^m r^{2m-1}}{(m-1)!}.$$

Then, the function h is decreasing on  $(0, +\infty)$ . Since h is continuous on  $\mathbb{R}^+$ , its maximum is attained at zero and so is the maximum of  $\mathcal{F}(C)$ . Therefore, for every  $x \in \mathbb{R}^d$ , we have:

$$\mathcal{F}(C)(x) \le \mathcal{F}(C)(0) = \frac{\rho(m\pi)^{\frac{d}{2}}}{\binom{m-1+\frac{d}{2}}{m-1}} \alpha^d.$$

Then,  $\mathcal{F}(C) \leq 1$  if and only if  $\alpha^d \leq \frac{\binom{m-1+\frac{d}{2}}{m-1}}{\rho(m\pi)^{\frac{d}{2}}}$ . In this case, C verifies the condition  $\mathcal{K}$ . By proposition 2.6, DPP(C) exists and is stationary. Moreover C is radial and since  $L_{m-1}^{d/2}(0) = \binom{m-1+\frac{d}{2}}{m-1}$ , see (22.4.7) in [1], we have  $C(0) = \rho$ , meaning that the intensity of DPP(C) is  $\rho$ .

It remains to prove the convergence results (5.3) and (5.4). An immediate application of Theorem 8.1.3 in [35] gives the convergence (5.3), see also Proposition 1 in [2]. Moreover, we have:

$$\lim_{m \to +\infty} \alpha_{\max} = \frac{1}{\sqrt{\pi} \Gamma\left(\frac{d}{2} + 1\right)^{\frac{1}{d}} \rho^{\frac{1}{d}}}.$$
(6.33)

Hence, by (6.33) and (5.3), we obtain the convergence (5.4).

#### 6.7 Proof of Proposition 5.3

By Equation (9.1.7) in [1], we have  $C(0) = \rho$ . So, if DPP(C) exists, its intensity is  $\rho$ . According to Proposition 2.6, DPP(C) exists if C verifies the condition  $\mathcal{K}$ . It is immediate that C is a symmetric continuous real-valued function. Since Bessel functions are analytic and by the asymptotic form (9.2.1) in [1], it is clear that Cbelongs to  $L^2$ . It remains to obtain  $\mathcal{F}(C)$  and verify the condition  $0 \leq \mathcal{F}(C) \leq 1$ . We define the family of functions  $p_{\sigma}$  by:

$$p_{\sigma}(x) = \frac{J_{\frac{\sigma+d}{2}}(|x|)}{|x|^{\frac{\sigma+d}{2}}}.$$
(6.34)

As  $p_{\sigma}$  is radial, by formula in Appendix B.5 in [17] we have:

$$\mathcal{F}(p_{\sigma})(x) = \frac{2\pi}{|x|^{\frac{d-2}{2}}} \int_{0}^{+\infty} r^{\frac{d}{2}} p_{\sigma}(r) J_{\frac{d-2}{2}}(2\pi r|x|) dr$$

By using 6.575 in [16] with the correspondence  $\mu \leftarrow \frac{d-2}{2}$ ,  $\nu \leftarrow \frac{\sigma+d-2}{2}$ ,  $\beta \leftarrow |2\pi x|$ ,  $\alpha \leftarrow 1$ , we have for  $\sigma > -2$ :

$$\mathcal{F}(p_{\sigma})(x) = \frac{2\pi}{|2\pi x|^{\frac{d-2}{2}}} \frac{(1 - |2\pi x|^2)^{\frac{1}{2}} |2\pi x|^{\frac{d-2}{2}}}{2^{\frac{\sigma}{2}} \Gamma(\frac{\sigma}{2} + 1)}$$
$$= 2^{\frac{d}{2} - \frac{\sigma}{2}} \pi^{\frac{d}{2}} \frac{(1 - |2\pi x|^2)^{\frac{\sigma}{2}}}{\Gamma(\frac{\sigma+2}{2})}.$$

Since  $C(x) = \rho 2^{\frac{\sigma+d}{2}} \Gamma\left(\frac{\sigma+d+2}{2}\right) p_{\sigma}\left(2\frac{x}{\alpha}\sqrt{\frac{\sigma+d}{2}}\right)$ , we obtain by dilatation of the Fourier transform the formula (5.6).

We have obviously  $\mathcal{F}(C) \geq 0$ . Since  $\sigma \geq 0$ ,  $\mathcal{F}(C)$  attains its maximum at 0. Thus  $\mathcal{F}(C) \leq 1$  if and only if:

$$\mathcal{F}(C)(0) = \frac{\rho(2\pi)^{\frac{d}{2}} \alpha^d \Gamma(\frac{\sigma+d+2}{2})}{(\sigma+d)^{\frac{d}{2}} \Gamma(\frac{\sigma+2}{2})} \le 1,$$

which is equivalent to  $\alpha^d \leq \frac{(\sigma+d)^{\frac{d}{2}}\Gamma\left(\frac{\sigma+2}{2}\right)}{\rho(2\pi)^{\frac{d}{2}}\Gamma\left(\frac{\sigma+d+2}{2}\right)}.$ 

Finally, when  $\sigma = 0$  and  $\alpha = \alpha_{\text{max}}$ , DPP(C) exists and a straightforward calculation gives  $C = C_B$ . The convergence result (5.7) may be found in [12] and is a direct application of (1.8) in [30].

#### 6.8 **Proof of Proposition 5.4**

By the discussion in Section 4, DPP(C) exists and is an *R*-dependent DPP with intensity  $\rho$  if *C* verifies  $\mathcal{K}_c(\rho, R)$ . Since  $u \in L^2$ , the kernel *C* is continuous by Theorem 2.20 in [26]. Moreover, *u* verifies u(x) = 0 for  $|x| > \frac{R}{2}$ , so by product convolution properties, *C* verifies C(x) = 0 for |x| > R. Then *C* belongs to  $L^2$ . Since *u* is radial, so is *C*. It remains to verify that  $0 \leq \mathcal{F}(C) \leq 1$  and  $C(0) = \rho$ .

By product convolution properties, we have  $C(0) = \int_{\mathbb{R}^d} u(x)^2 dx$ . From the definition of u in (5.9), we have

$$\frac{\int_{\mathbb{R}^d} u^2(x) dx}{\rho \beta(R,\alpha)^2} = \int_{\mathbb{R}^d} \left( 1 - 2\left(\frac{R}{2}\right)^{\frac{d}{2}-1} \frac{J_{\frac{d-2}{2}}(\sqrt{\alpha}|x|)}{J_{\frac{d-2}{2}}(\frac{R\sqrt{\alpha}}{2})|x|^{\frac{d-2}{2}}} + \left(\frac{R}{2}\right)^{d-2} \frac{J_{\frac{d-2}{2}}^2(\sqrt{\alpha}|x|)}{J_{\frac{d-2}{2}}^2(\frac{R\sqrt{\alpha}}{2})|x|^{d-2}} \right) \mathbf{1}_{|x| \le \frac{R}{2}} dx \\
= \frac{2\pi^{\frac{d}{2}}}{\Gamma(d/2)} \int_0^{\frac{R}{2}} \left( r^{d-1} - 2\left(\frac{R}{2}\right)^{\frac{d-2}{2}} \frac{J_{\frac{d-2}{2}}(\sqrt{\alpha}r)}{J_{\frac{d-2}{2}}(\frac{R\sqrt{\alpha}}{2})} r^{\frac{d}{2}} + \left(\frac{R}{2}\right)^{d-2} \frac{J_{\frac{d-2}{2}}^2(\sqrt{\alpha}r)}{J_{\frac{d-2}{2}}^2(\frac{R\sqrt{\alpha}}{2})} r \right) dr.$$

By derivation of Bessel functions, see [1], we notice that for all  $b \in \mathbb{R}$ , a primitive of  $xJ_{\frac{d-2}{2}}^2(bx)$  is given by  $\frac{x^2}{2}\left(J_{\frac{d-2}{2}}^2(xb) - J_{\frac{d}{2}-2}(xb)J_{\frac{d}{2}}(xb)\right)$ . It follows from Appendix B.3 in [17] that:

$$\begin{split} \frac{\int_{\mathbb{R}^d} u^2(x) dx}{\rho \beta(R,\alpha)^2} &= \frac{\pi^{d/2} R^d}{d \ \Gamma(\frac{d}{2}) 2^{d-1}} - 4 \left(\frac{R}{2}\right)^{d-1} \frac{\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} \frac{J_{\frac{d}{2}}(\frac{R\sqrt{\alpha}}{2})}{\sqrt{\alpha} J_{\frac{d}{2}-1}(\frac{R\sqrt{\alpha}}{2})} \\ &+ \left(\frac{R}{2}\right)^d \frac{\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})} \left(1 - \frac{J_{\frac{d}{2}-2}(\frac{R\sqrt{\alpha}}{2}) J_{\frac{d}{2}}(\frac{R\sqrt{\alpha}}{2})}{J_{\frac{d}{2}-1}^2(\frac{R\sqrt{\alpha}}{2})}\right). \end{split}$$

Thus, by the definition of  $\beta(R, \alpha)$ , we obtain that  $\int_{\mathbb{R}^d} u(x)^2 dx = \rho$ .

Let us now calculate  $\mathcal{F}(C)$ . We have  $\mathcal{F}(C) = \mathcal{F}(u)^2$ . Since *u* is radial,  $\mathcal{F}(u)$  is real valued and so  $\mathcal{F}(C) \geq 0$ . In addition, we have by Appendix B.5 in [17] and Relation (5.9):

$$\begin{aligned} \mathcal{F}(u)(x) &= \sqrt{\rho}\beta(R,\alpha) \frac{2\pi}{|x|^{\frac{d-2}{2}}} \left( \int_0^{\frac{R}{2}} r^{\frac{d}{2}} J_{\frac{d-2}{2}}(2\pi r|x|) dr \right. \\ &\left. - \frac{R^{\frac{d}{2}-1}}{2^{\frac{d}{2}-1} J_{\frac{d}{2}-1}(\frac{R\sqrt{\alpha}}{2})} \int_0^{\frac{R}{2}} r J_{\frac{d-2}{2}}(\sqrt{\alpha}r) J_{\frac{d-2}{2}}(2\pi r|x|) dr \right). \end{aligned}$$

Since  $\alpha > 0$ , we have by Appendix B.3 in [17] and Formula 6.521 in [16] :

$$\mathcal{F}(u)(x) = \sqrt{\rho}\beta(R,\alpha)\frac{2\pi}{|x|^{\frac{d-2}{2}}} \left(\frac{R^{\frac{d}{2}}}{\pi 2^{\frac{d}{2}+1}} \frac{J_{\frac{d}{2}}(\pi R|x|)}{|x|} + \frac{R^{\frac{d}{2}-1}}{2^{\frac{d}{2}}J_{\frac{d}{2}-1}(\frac{R\sqrt{\alpha}}{2})}\frac{R\sqrt{\alpha}J_{\frac{d-2}{2}}'(\frac{R\sqrt{\alpha}}{2})J_{\frac{d-2}{2}}(\pi R|x|) - 2\pi RJ_{\frac{d-2}{2}}(\frac{R\sqrt{\alpha}}{2})|x|J_{\frac{d-2}{2}}'(\pi R|x|)}{\alpha - 4\pi^{2}x^{2}}\right)$$

$$(6.35)$$

from which we deduce the Fourier transform of u in Proposition 5.4. Therefore, if  $\alpha$  is such that  $\mathcal{F}(u)^2 \leq 1$ , then  $\mathcal{F}(C) \leq 1$  and so C verifies  $\mathcal{K}_c(\rho, R)$ .

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