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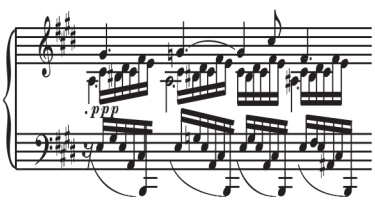

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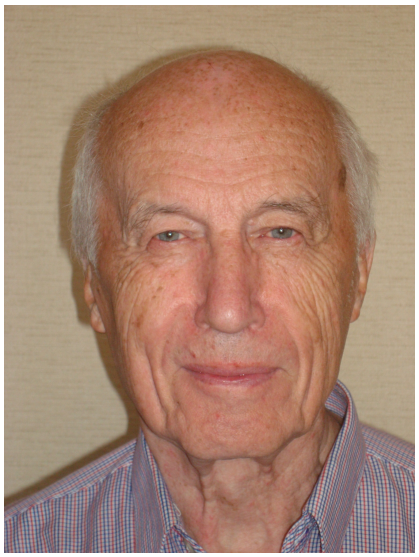
The journal was founded in 1995 by Professor V.A. Malyshev



This issue of MPRF publishes works
presented or discussed at the conference
"Perpetual Search: Mathematics, Physics, Life"
devoted to the 85th anniversary of
Vadim Aleksandrovich Malyshev (1938–2022)
a great mathematician and the founder of journal
"Markov Processes and Related Fields"

The conference has highlighted the recent developments in the areas of mathematics and mathematical physics where V.A. Malyshev has made major contributions. In particular, these areas include Random walks, Queueing theory, Gibbs random fields, Non-equilibrium thermodynamics, Random grammars and random graphs evolution.

The conference (http://malyshev85.org/) took place on June 26–30, 2023, at the Moscow State University, where Prof. Vadim Aleksandrovich Malyshev worked all his life. The diversity of subjects and themes largely discussed in collaboration with V.A. Malyshev himself, is reflected in the collection of papers by his colleagues and students presented here.

All conference talks are also available at
https://www.youtube.com/playlist?list=PL9mbuBZSefQVRTvtjgketT-M3eDT-GUeV

Vadim Aleksandrovich Malyshev is remembered as a remarkable man with endless energy, courage, inventions, who still inspires us through his works and also through his own web-page where he has posed new problems, ideas and projects: http://mech.math.msu.su/∼malyshev/.

On behalf of the organizing committee,

Tatyana Turova Schmeling,
Editor

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Markov Processes and **Related Fields**

Wick–Fourier–Hermite Series in the Theory of Linear and Nonlinear Transformations of Gaussian Distributions

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Abstract. This article provides information on Hermite polynomials and its application to some problems in risk theory and site percolation.

Keywords: Hermite polynomials, Wick exponent, Mehler formula, Gaussian mixture, transformations of Gaussian distributions, diagrams

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1. Introduction

The story of this paper is short but remarkable. All the authors of the present paper participated in the memorial conference dedicated to Dr. V. A. Malyshev on the occasion of his 85th birthday (Moscow, June 2023). After the talk of Stanislav Molchanov on applications of cluster estimates of Wick–Hermite polynomials (these estimates were developed in the well-known monograph by V. A. Malyshev and R. A. Minlos, [11]), the second coauthor, Albert Shiryaev, asked a question about the relation of this activity with the Mehler formula for the two-dimensional Gaussian densities and its possible generalizations (see Examples 9 and 10 below). The speaker has not heard about such a formula, though it was clear that this question is directly related to the topic of the

talk. The subsequent discussion with involvement of the third coauthor of the present paper had clarified the matter, and, in particular, the link between Mehler type formulas with quantum mechanics and perturbation theory for harmonic oscillator type models. The present paper is addressed to specialists in probability who are not acquainted with quantum mechanical and general theory of orthogonal polynomials.

2. General properties of Hermite polynomials

This section provides information on Hermite polynomials that can be found in any of the books on orthogonal polynomials. These general properties are given for the sake of completeness, and will be used in the subsequent proofs.

Being a representative of the broad and important class of orthogonal polynomials, the Hermite polynomials seem to be the most widely useful in various applications. For example, they found their applications in probability for asymptotic expansions in the limit theorems, in quantum mechanics in the model of harmonic oscillator, in theoretical physics in quantum field theory, etc. In the nonprobabilistic setting, Hermite polynomials are defined by orthogonalizing the monomials $\{1, x, x^2, x^3, \dots\}$ in the weighted Hilbert space $L^2(\mathbb{R}, p(x))$, $p(x) = \exp\{-x^2\}$ (the space of functions square integrable with the weight $\exp\{-x^2\}$). In probability, the corresponding weight function is slightly different: this function is defined as the density of the standard normal distribution $\phi(x) = \frac{1}{\sqrt{2\pi}} \exp\bigl(-\frac{x^2}{2}\bigr)$:

$$L^2(\mathbb{R}, p(x)) = \left\{ \varphi : \mathbb{R} \to \mathbb{R} : \int\limits_{\mathbb{R}} \varphi^2(x)\phi(x)\, dx < \infty \right\}.$$

A different approach involves the equivalent space of random variables representable as a function of the standard Gaussian random variable $X \sim \mathcal{N}(0,1)$ defined on some probability space $(\Omega, \mathcal{F}, P)$

$$\mathcal{L}^2(\Omega) = \left\{ Y = \varphi(X),\, \mathbb{E}Y^2 < \infty \right\}.$$

By $H_n(x)$, $n \geq 0$, we will denote the corresponding monic orthogonal polynomial in the space $L^2(\mathbb{R}, \phi(x))$ with the leading term x^n:

$$H_0(x) = 1, \quad H_1(x) = x, \quad H_2(x) = x^2 - 1, \dots H_n(x) = x^n + \dots$$

$$H_n(x) = (-1)^n \exp\bigl(\frac{x^2}{2}\bigr) \frac{d^n}{dx^n} \exp\bigl(-\frac{x^2}{2}\bigr) = (-1)^n \frac{\frac{d^n}{dx^n}\phi(x)}{\phi(x)}. \tag{2.1}$$

Formula (2.1) is known as the Rodrigues formula.

Applying the classical Taylor expansion, we obtain the generating function

$$\sum_{n=0}^{\infty} \frac{H_n(x)a^n}{n!} = \exp\big(-\frac{(x-a)^2}{2}\big)\exp\big(\frac{x^2}{2}\big) = \exp\big(ax - \frac{a^2}{2}\big). \tag{2.2}$$

Since the right-hand side of (2.2) is analytic, the variables a and x can be made to be complex, in particular, one can put $a = iz$, $z \in \mathbb{R}$. Now applying the Euler formula $e^{ixz} = \cos(xz) + i\sin(xz)$ and separating the real and imaginary parts, we get the generating functions for the even and odd Hermite polynomials:

$$\sum_{n=0}^{\infty}(-1)^n \frac{H_{2n}(x)z^{2n}}{(2n)!} = \exp\big(\frac{z^2}{2}\big)\cos(xz), \tag{2.3}$$

$$\sum_{n=0}^{\infty}(-1)^n \frac{H_{2n+1}(x)z^{2n+1}}{(2n+1)!} = \exp\big(\frac{z^2}{2}\big)\sin(xz). \tag{2.4}$$

Taking the derivative $\frac{\partial}{\partial x}$ of both sides of (2.2), we get

$$\begin{aligned}\sum_{n=0}^{\infty} \frac{H_n'(x)a^n}{n!} &= a\exp\big(ax - \frac{a^2}{2}\big)\\ &= \sum_{n=0}^{\infty} \frac{H_n(x)a^{n+1}}{n!},\end{aligned}$$

which gives

$$H_n'(x) = nH_{n-1}(x). \tag{2.5}$$

Another important relation can be obtained from the expression

$$\exp\big(-\frac{x^2}{2}\big)H_n(x) = (-1)^n \frac{d^n}{dx^n}\exp\big(-\frac{x^2}{2}\big).$$

Taking again the derivative $\frac{\partial}{\partial x}$, we get

$$-xH_n(x) + H_n'(x) = -H_{n+1}(x), \quad n \geq 1,$$

and hence

$$H_{n+1}(x) = xH_n(x) - H_n'(x), \quad n \geq 0. \tag{2.6}$$

or, in an equivalent form

$$\phi(x)H_{n+1}(x) = -\left(\phi(x)H_n(x)\right)', \quad n \geq 0. \tag{2.7}$$

Starting with $H_0(x) = 1$, we obtain recursively

$$H_1(x) = x, \quad H_2(x) = x^2 - 1, \quad H_3(x) = x^3 - 3x, \quad H_4(x) = x^4 - 6x^2 + 3.$$

In general, an induction argument shows that

$$\begin{aligned} H_n(x) &= x^n - \binom{n}{2} \cdot 1 \cdot x^{n-2} + \binom{n}{4} \cdot 1 \cdot 3 \cdot x^{n-4} + \dots \\ &\quad + \dots (-1)^k \binom{n}{2k} \cdot 1 \cdot 3 \cdot \dots \cdot (2k-1) \cdot x^{n-2k} + \dots \\ &= \sum_{k=0}^{[n/2]} (-1)^k \binom{n}{2k} (2k-1)!! x^{n-2k}, \end{aligned} \tag{2.8}$$

so that the constant term in (2.8) is 0 for odd n, and is

$$(-1)^k (2k-1)!! \quad \text{for} \quad n = 2k.$$

Note that $H_n(x)$ involves the powers of x with the same parity as n, i.e.,

$$H_n(-x) \equiv (-1)^n H_n(x).$$

This follows from the general theory of classical orthogonal polynomials (see, for example, Theorem 1.1.3 in [17]), since the weight function $\phi(x)$ is even, and since the orthogonality interval is symmetric about the origin.

It is also worth pointing out that all zeros of the Hermite polynomials are real and distinct (this follows, for example, from the general theory of orthogonal polynomials; see [17], Theorem 1.1.9); in addition, the zeros of the neighboring polynomials $H_n(x)$ and $H_{n+1}(x)$ interlace (see [17], Theorem 1.1.10).

The long expression for the nth polynomial (2.8) can be compactly written in the integral form

$$H_n(x) = \int_{-\infty}^{\infty} (x+it)^n \phi(t)\, dt = \int_{-\infty}^{\infty} (x+it)^n \frac{1}{\sqrt{2\pi}} \exp\bigl(-\frac{t^2}{2}\bigr)\, dt, \tag{2.9}$$

where we recall that

$$1 \cdot 3 \cdot \dots \cdot (2k-1) = (2k-1)!! = \int_{-\infty}^{\infty} t^{2k} \phi(t)\, dt.$$

Note that from (2.9), using binomial theorem, one can easily find that

$$H_n(x+y) = \sum_{k=0}^{n} \binom{n}{k} y^k H_{n-k}(x). \tag{2.10}$$

$$2^n H_n(x+y) = \sum_{k=0}^{n} \binom{n}{k} H_k(2x) H_{n-k}(2y). \tag{2.11}$$

It is also easily seen (see above) that the value of the Hermite polynomials at the origin is given by

$$H_n(0) = \begin{cases} (-1)^k (2k-1)!!, & n = 2k, \\ 0, & n = 2k+1. \end{cases} \tag{2.12}$$

Differentiating (2.9) with respect to x, we again arrive at (2.5). Integrating (2.9) with respect to x, we find that

$$\int_0^a H_n(x)\,dx = \frac{H_{n+1}(a) - H_{n+1}(0)}{n+1}. \tag{2.13}$$

In addition to the integral representation (2.9) one can derive some other ones (see for example, [17]); in particular, using the Cauchy theorem, or the representation for the coefficients of the Taylor series for the generating function (2.2), we have

$$H_n(x) = \frac{n!}{2\pi i} \int_\Gamma e^{zx - \frac{z^2}{2}} \frac{dz}{z^{n+1}}, \tag{2.14}$$

where Γ is an arbitrary contour encircling the origin.

Another integral representation will be obtained below (see (2.22), (2.23) and (2.21)).

Lemma 1. *The nth Hermite polynomial $H_n(x)$ is a solution of the differential equation*

$$y'' - xy' + ny = 0,$$

or, in other words,

$$H_n''(x) - xH_n'(x) + nH_n(x) = 0. \tag{2.15}$$

For a proof it suffices to differentiate $n+1$ times (using the Leibniz rule) the equality

$$\phi'(x) = -x\phi(x),$$

where $\phi(x) = \frac{1}{\sqrt{2\pi}} \exp\bigl(-\frac{x^2}{2}\bigr)$, use the substitution

$$\phi^{(n)}(x) = (-1)^n \phi(x) H_n(x)$$

(see (2.1)) and differentiate one more time.

It is worth pointing out that the differential equation from Lemma 1 is closely related to the one-dimensional Schrödinger equation from quantum mechanics: the solution of the Schrödinger equation in dimension 1 with quadratic potential (harmonic oscillator) can be expressed in terms of the Hermite polynomial (see, for example [17, Chap. V, § 6]).

The recurrent relation for the Hermite polynomials can be obtained by differentiating the generating function (2.2) and equating the corresponding coefficients:

$$H_{n+1}(x) - xH_n(x) + nH_{n-1}(x) = 0. \tag{2.16}$$

The orthogonality of the Hermite polynomials follows from the expression for the generating function (2.2)

$$\Big(\sum_{n=0}^{\infty} \frac{H_n(x)a^n}{n!}\Big)\Big(\sum_{m=0}^{\infty} \frac{H_m(x)b^m}{m!}\Big) = e^{(a+b)x-\frac{a^2+b^2}{2}}$$
$$= e^{(a+b)x-\frac{(a+b)^2}{2}} e^{ab}.$$

Integrating the left- and right-hand sides of the last expression with the weight function $\phi(x)$, we get

$$\sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{a^n}{n!}\frac{b^m}{m!} \int_{-\infty}^{\infty} H_n(x)H_m(x)\phi(x)\,dx = e^{ab},$$

which implies that

$$\int_{-\infty}^{\infty} H_n(x)H_m(x)\phi(x)\,dx = \big(H_n, H_m\big)_{\phi} = 0, \quad m \neq n,$$

$$\big(H_n, H_m\big)_{\phi} = n!\delta_{m,n}. \tag{2.17}$$

This means that the functions

$$\frac{H_n(x)}{\sqrt{n!}} = e_n(x), \quad n \geq 0 \tag{2.18}$$

form an orthonormal basis for the space $L^2(\mathbb{R}, \phi(x))$.

For any $f(x) \in L^2(\mathbb{R}, \phi(x))$, consider its Fourier–Hermite series expansion

$$f(x) = \sum_{n=0}^{\infty} e_n(x)\big(f, e_n\big)_{\phi} = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} \int_{-\infty}^{\infty} f(y)H_n(y)\phi(y)\,dy. \tag{2.19}$$

Here, direct evaluation of the coefficients

$$\big(f, e_n\big)_{\phi} = \int_{-\infty}^{\infty} f(y)H_n(y)\phi(y)\,dy$$

is not always convenient; sometimes, it is useful to apply the following tricks.

We recall the following integral representation (the inversion formula for the Fourier transform $\widehat{\phi}(k) = e^{-\frac{k^2}{2}}$):

$$\phi(y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-\frac{k^2}{2} - iyk} dk = \frac{1}{\pi} \int_{0}^{\infty} e^{-\frac{k^2}{2}} \cos(yk)\, dk. \tag{2.20}$$

Differentiating this relation n times and using $H_n(t)\phi(y) = (-1)^n \frac{d^n}{dy^n}\phi(y)$ (see (2.1)), we find that

$$H_n(y)\phi(y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} (ik)^n e^{-\frac{k^2}{2} - iyk} dk. \tag{2.21}$$

The last formula, when divided by $\phi(y)$, can be looked upon as an integral representation of Hermite polynomials, or, more precisely,

$$H_{2n}(y) = \frac{(-1)^n}{\sqrt{2\pi}} e^{\frac{y^2}{2}} \int_{0}^{\infty} k^{2n} e^{-\frac{k^2}{2}} \cos(ky) dk, \tag{2.22}$$

$$H_{2n+1}(y) = \frac{(-1)^n}{\sqrt{2\pi}} e^{\frac{y^2}{2}} \int_{0}^{\infty} k^{2n+1} e^{-\frac{k^2}{2}} \sin(ky) dk. \tag{2.23}$$

Using (2.21), changing the integration order, and assuming $f(x) \in L^1(\mathbb{R}, dx)$, we have

$$\big(f, e_n\big)_\phi = \int_{-\infty}^{\infty} f(y) H_n(y) \phi(y)\, dy = \frac{1}{2\pi} \int_{-\infty}^{\infty} \widehat{f}(k)(ik)^n \exp\left(-\frac{k^2}{2}\right) dk, \tag{2.24}$$

where $\widehat{f}(k) = \int_{-\infty}^{\infty} f(x) e^{ikx}\, dx$ is the Fourier transform of the function $f(x)$.

Formula (2.24) can also be obtained differently via the Parseval identity

$$\int_{-\infty}^{\infty} f(x) H_n(x) \phi(x)\, dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} \widehat{f}(k) \big(\widehat{H_n \phi}\big)(k)\, dk$$

under the additional assumption that $f(x) \in L^2(\mathbb{R}, dx)$, and with the help of the formula

$$\widehat{H_n \phi}(k) = (-1)^n \widehat{\phi^{(n)}}(k) = (ik)^n \widehat{\phi}(k) = (ik)^n \exp\left(-\frac{k^2}{2}\right), \tag{2.25}$$

which easily follows, for example, from (2.1) by integration by parts (see also [4, Ch. XVI, the end of § 1]).

As a result, we finally have

$$f(x) = \frac{1}{2\pi} \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} i^n \int_{-\infty}^{\infty} \widehat{f}(k) k^n \exp\left(-\frac{k^2}{2}\right) dk. \tag{2.26}$$

Another method of evaluation of $\big(f, e_n\big)_\phi = \int_{-\infty}^{\infty} f(y) H_n(y) \phi(y)\, dy$, under the assumption $f \in C^\infty(\mathbb{R})$, is based on (2.1) and integration by parts:

$$\begin{aligned} \int_{-\infty}^{\infty} f(y) H_n(y) \phi(y)\, dy &= (-1)^n \int_{-\infty}^{\infty} f(y) \frac{d^n}{dy^n} \phi(y)\, dy \\ &= \int_{-\infty}^{\infty} \phi(y) \frac{d^n}{dy^n} f(y)\, dy. \end{aligned}$$

We finally have

$$f(x) = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} \int_{-\infty}^{\infty} \phi(y) \frac{d^n}{dy^n} f(y)\, dy. \tag{2.27}$$

In some cases, it proves possible to obtain a Fourier series expansion in Hermite polynomials (2.19) without having recourse to formulas (2.26) and (2.27) (see Example 1 below).

Consider some examples.

Example 1. From (2.2), (2.3), (2.4) we have, respectively, the expansions

$$e^{ax} = e^{\frac{a^2}{2}} \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} a^n, \tag{2.28}$$

$$\cos x = \sum_{n=0}^{\infty} (-1)^n \frac{H_{2n}(x)}{(2n)!}, \tag{2.29}$$

$$\sin x = \sum_{n=0}^{\infty} (-1)^n \frac{H_{2n+1}(x)}{(2n+1)!}. \tag{2.30}$$

In view of (2.28) and since $\cosh x = \frac{e^x + e^{-x}}{2}$, $\sinh x = \frac{e^x - e^{-x}}{2}$, we have, respectively,

$$\cosh x = \sum_{n=0}^{\infty} \frac{H_{2n}(x)}{(2n)!}, \tag{2.31}$$

$$\sinh x = \sum_{n=0}^{\infty} \frac{H_{2n+1}(x)}{(2n+1)!}. \tag{2.32}$$

Example 2. $f(x) = \operatorname{sign} \mathrm{x}$.

$$\begin{aligned}\operatorname{sign} \mathrm{x} &= \sqrt{\frac{2}{\pi}} \sum_{n=0}^{\infty} (-1)^n \frac{H_{2n+1}(x)}{(2n+1)!} (2n-1)!! \\ &= \sqrt{\frac{2}{\pi}} \sum_{n=0}^{\infty} (-1)^n \frac{H_{2n+1}(x)}{(2n+1)(2n)!!}.\end{aligned} \tag{2.33}$$

Example 3. $f(x) = x^N$, $x \in \mathbb{R}$. Using (2.27), we separately evaluate

$$\begin{aligned}&\int_{-\infty}^{\infty} \phi(y) \frac{d^n}{dy^n} y^N \, dy \\ &\quad = \begin{cases} \frac{N!}{(N-n)!} (N-n-1)!!, & N-n = 2m,\ m = 0, 1, \ldots, [N/2]; \\ 0, & \text{otherwise.} \end{cases}\end{aligned}$$

As a result, we have

$$x^N = \sum_{m=0}^{[N/2]} H_{N-2m}(x) \binom{2m}{N} (2m-1)!! \tag{2.34}$$

The last formula can be looked upon as an inversion of (2.8).

3. The Wick exponent. One-dimensional Gaussian distribution

In this section we define the nth Wick power of a random variable X and show that if $X \sim \mathcal{N}(0,1)$ then the nth Wick power coincides the nth Hermite polynomial.

A different point of view on Hermite polynomials occurs in physics (see, for example, [11], [14], [5]). The expression $:X^n:$, known as the nth Wick power of a random variable X (not necessarily Gaussian), is defined inductively by

$$\begin{aligned}&: X^0 : = 1, \\ &\frac{d}{dX} : X^n : = n : X^{n-1} :,\ n = 1, 2, \ldots \\ &\mathbb{E} : X^n : = 0,\ n = 1, 2, \ldots\end{aligned} \tag{3.1}$$

Using the generating function (the Wick exponent)

$$: \exp(aX) : = \sum_{n=0}^{\infty} \frac{a^n}{n!} : X^n :,$$

we get

$$\frac{d}{dX} :\exp(aX): = a :\exp(aX):,$$
$$\mathbb{E} :\exp(aX): = 1.$$

From the point of view of formal powers series

$$:\exp(aX): = \frac{\exp(aX)}{\mathbb{E}\exp(aX)}.$$

In the case of a Gaussian random variable $X \sim \mathcal{N}(0, \sigma^2)$,

$$:\exp(aX): = \exp\left(aX - \frac{\sigma^2}{2}a^2\right).$$

Equating the coefficients of a^n, we obtain

$$:X^n: = \sum_{m=0}^{\left[\frac{n}{2}\right]} \frac{n!}{m!(n-2m)!} X^{n-2m} \left(-\frac{1}{2}\sigma^2\right)^m.$$

In the particular case $\sigma^2 = 1$, this formula was given above (see (2.8)).

Comparing the coefficients of a^n in the expression $\exp(aX) = :\exp(aX): \exp(\frac{\sigma^2}{2}a^2)$, we get

$$X^n = \sum_{m=0}^{\left[\frac{n}{2}\right]} \frac{n!}{m!(n-2m)!} :X^{n-2m}: \left(\frac{1}{2}\sigma^2\right)^m.$$

In the particular case $\sigma^2 = 1$, this formula was given above (see (2.34)).

In other words, if $X \sim \mathcal{N}(0, 1)$, then the Wick power is the Hermite polynomial,

$$H_n(X) = :X^n:.$$

Further, according to the above, $:X^n:$ is the perpendicular from $X^n \in \mathcal{L}^2(\Omega)$ onto the subspace of polynomials of X of degree $< n$. In what follows, we will use both notation for Hermite–Wick polynomials.

Let us consider examples of Fourier series expansions in Hermite–Wick polynomials of functions related to Gaussian distributions.

Example 4.

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right), \quad x \in \mathbb{R},$$

i.e., the density of the normal distribution with zero expectation and variance σ^2, $\mathcal{N}(0, \sigma^2)$.

Using $\widehat{f}(k) = \exp\left(-\frac{k^2\sigma^2}{2}\right)$ and (2.26), we have

$$f(x) = \frac{1}{2\pi}\sum_{n=0}^{\infty}\frac{H_n(x)}{n!}i^n\int\limits_{-\infty}^{\infty}k^n\exp\left(-\frac{k^2(1+\sigma^2)}{2}\right)dk$$
$$= \frac{1}{2\pi}\sum_{n=0}^{\infty}\frac{H_{2n}(x)}{(2n)!}(-1)^n\int\limits_{-\infty}^{\infty}k^{2n}\exp\left(-\frac{k^2(1+\sigma^2)}{2}\right)dk,$$

and now using the formula for even moments of the centered normal distribution

$$\frac{1}{\sqrt{2\pi\tau^2}}\int\limits_{-\infty}^{\infty}k^{2n}\exp\left(-\frac{k^2}{2\tau^2}\right)dk = (2n-1)!!\tau^{2n}$$

we obtain

$$\begin{aligned}\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{x^2}{2\sigma^2}\right) &= \frac{1}{\sqrt{2\pi(1+\sigma^2)}}\sum_{n=0}^{\infty}(-1)^n\frac{H_{2n}(x)}{(1+\sigma^2)^n}\frac{(2n-1)!!}{(2n)!}\\ &= \frac{1}{\sqrt{2\pi(1+\sigma^2)}}\sum_{n=0}^{\infty}(-1)^n\frac{H_{2n}(x)}{(1+\sigma^2)^n(2n)!!}\\ &= \frac{1}{\sqrt{2\pi(1+\sigma^2)}}\sum_{n=0}^{\infty}(-1)^n\frac{H_{2n}(x)}{[2(1+\sigma^2)]^n n!}\,. \end{aligned}\tag{3.2}$$

The coefficients of the Fourier series can be evaluated directly:

$$\int\limits_{-\infty}^{\infty}f(y)H_n(y)\phi(y)\,dy = \frac{1}{\sqrt{2\pi(1+\sigma^2)}}\int\limits_{-\infty}^{\infty}H_n(y)\phi_\tau(y)\,dy$$

where

$$\phi_\tau(y) = \frac{1}{\sqrt{2\pi}\tau}\exp\Big(-\frac{x^2}{2\tau^2}\Big)$$

is the density of the normal distribution $\mathcal{N}(0,\tau^2)$; $\tau^2 = \frac{\sigma^2}{1+\sigma^2}$.

To evaluate the last integral, we use the formula for the generating function of the Hermite polynomials (2.2), and integrate the right- and left-hand sides with the weight function $\phi_\tau(y)$. We have

$$\begin{aligned}\int\limits_{-\infty}^{\infty}H_n(y)\phi_\tau(y)\,dy &= \begin{cases}\frac{(2m)!}{m!}\left(\frac{\tau^2-1}{2}\right)^m, & n=2m;\\ 0, & n=2m+1;\end{cases}\\ &= \begin{cases}(2m-1)!!\left(\tau^2-1\right)^m, & n=2m;\\ 0, & n=2m+1;\end{cases}\end{aligned}\tag{3.3}$$

$$\int_{-\infty}^{\infty} f(y)H_n(y)\phi(y)\,dy = \begin{cases} (-1)^m \frac{(2m-1)!!}{\sqrt{2\pi}[1+\sigma^2]^{m+1/2}}, & n=2m; \\ 0, & n=2m+1. \end{cases}$$

Example 5. $f(x) = \int_0^x \phi(y)\,dy$, $x \geq 0$, i.e., $1/2 + f(x) = \Phi(x)$ is a distribution function of $\mathcal{N}(0,1)$ law.

Integrating (3.2) and using (2.13), we have

$$\int_0^x \phi(y)\,dy = \frac{1}{2\sqrt{\pi}} \sum_{n=0}^{\infty} (-1)^n \frac{H_{2n+1}(x)}{2^n} \frac{(2n-1)!!}{(2n+1)!}$$
$$= \frac{1}{\sqrt{\pi}} \sum_{n=0}^{\infty} (-1)^n \frac{H_{2n+1}(x)}{(2n+1)n!2^{2n+1}}.$$

In the following examples, we consider Gaussian mixtures.

Example 6.

$$f(x) = \int_0^{\infty} \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{x^2}{2\sigma^2}) g(\sigma)\,d\sigma, \quad x \in \mathbb{R},$$

$$g(\sigma) \geq 0, \quad \sigma \geq 0, \quad \int_0^{\infty} g(\sigma)\,d\sigma = 1,$$

i.e., the density of the mixture of the normal distribution with zero expectation and the mixing density function $g(\sigma)$.

Here, it is worth recalling the following interpretation of the random variable X with this density function $f(x)$ (see [16, Ch. VI, § 9]). On the one hand, we have (in distribution)

$$X = \xi\sqrt{\eta},$$

where ξ is the standard normal random variable, i.e., $\xi \sim \mathcal{N}(0,1)$, η is a nonnegative random variable with density function $g(\cdot)$. This result becomes transparent in the Fourier transform:

$$\widehat{f}(k) = \int_0^{\infty} e^{-\frac{k^2\sigma^2}{2}} g(\sigma)\,d\sigma = G(k^2/2);$$

here $G(\cdot)$ is the Laplace transform of the random variable $\sqrt{\eta}$.

On the other hand, we have the equality (in distribution)

$$X = W(\eta),$$

where $W(t)$, $t \geq 0$ is the standard Wiener process, η is a nonnegative random variable with density function $g(\cdot)$.

If η is an infinitely divisible random variable, then so is X (see [16, Ch. VI, § 9]).

In view of (3.2), we have

$$\begin{aligned} &\int_0^\infty \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right) g(\sigma)\, d\sigma \\ &\quad = \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{\infty} (-1)^n \frac{H_{2n}(x)}{2^n n!} \int_0^\infty \frac{g(\sigma)}{(1+\sigma^2)^{n+1/2}} d\sigma. \end{aligned} \tag{3.4}$$

Consider separately

$$\int_0^\infty \frac{g(\sigma)}{(1+\sigma^2)^{n+1/2}} d\sigma = \int_0^\infty \frac{g(\sqrt{t})}{2\sqrt{t}(1+t)^{n+1/2}} dt = \int_0^\infty \frac{\tilde{g}(t)}{(1+t)^{n+1/2}} dt.$$

Assume that $\tilde{g}(t)$ is the density function of a stable law with parameter $\beta/2$, $\beta \in (0,2)$, i.e.,

$$G(\lambda) = \int_0^\infty e^{-\lambda t} \tilde{g}(t)\, dt = e^{-c\lambda^{\beta/2}}$$

(for the canonical representation of the Laplace transform of stable distributions on the positive half-axis, see, for example, [16, V. Theorem 3.5]).

In this case, the corresponding Gaussian mixture is a symmetric stable law of distribution with parameter β:

$$\begin{aligned} \widehat{f}(k) &= \int_{-\infty}^\infty e^{ikx} f(x)\, dx = \int_0^\infty e^{-\frac{k^2\sigma^2}{2}} g(\sigma)\, d\sigma \\ &= \int_0^\infty e^{-\frac{k^2 t}{2}} \tilde{g}(t)\, dt = G\left(\frac{k^2}{2}\right) \\ &= e^{-c\left(\frac{k^2}{2}\right)^{\beta/2}} = e^{-c_1|k|^\beta}, \quad \beta \in (0,2), \end{aligned}$$

(for the canonical representation of characteristic functions of symmetric stable distributions, see, for example, [16, V. Theorem 3.5]). This result is well known (see, for example, [16, VI, Theorem 9.3]).

It is worth pointing out that symmetric stable distributions (with parameter β) are Gaussian mixtures (in variance, i.e., in the scaling parameter) with

mixing stable distribution (on the half-axis, with parameter $\beta/2$). In particular, the Cauchy distribution is a Gaussian mixture with mixing density $\frac{e^{-1/(2t)}}{\sqrt{2\pi}t^{3/2}}$ (Lévy distribution i.e. stable law with $\alpha = 1/2$, $\beta = 1$). This fact is well known in the literature (see, for example, [8]).

As an example of expansion into a Fourier series in Hermite polynomials, consider the above particular case of the standard Cauchy distribution:

$$f(x) = \frac{1}{\pi(1+x^2)} = \int_0^\infty \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{x^2}{2t}\right) \frac{e^{-1/(2t)}}{\sqrt{2\pi}t^{3/2}}\, dt, \quad x \in \mathbb{R}.$$

Let us evaluate the coefficients of the Fourier series (the function is even, and hence the coefficients of odd powers are zero) using (2.26). We have

$$\begin{aligned}\int_{-\infty}^\infty f(x)H_{2n}(x)\, dx &= \frac{(-1)^n}{2\pi} \int_{-\infty}^\infty \widehat{f}(k)k^{2n} \exp\left(-\frac{k^2}{2}\right) dk \\ &= \frac{(-1)^n}{2\pi} \int_{-\infty}^\infty e^{-|k|}k^{2n} \exp\left(-\frac{k^2}{2}\right) dk \\ &= \frac{(-1)^n}{\pi} \int_0^\infty k^{2n} \exp\left(-\frac{k^2}{2} - k\right) dk.\end{aligned}$$

Consider separately the integral

$$\begin{aligned}\int_0^\infty k^{2n} \exp\left(-\frac{k^2}{2} - k\right) dk &= \sqrt{e} \int_1^\infty (z-1)^{2n} \exp\left(-\frac{z^2}{2}\right) dz \\ &= \sqrt{e} \sum_{l=0}^n \binom{2n}{2l} \int_1^\infty z^{2l} \exp\left(-\frac{z^2}{2}\right) dz.\end{aligned}$$

Integrating by parts, the integral can be either evaluated recurrently as follows

$$\begin{aligned}&\int_1^\infty z^{2l} \exp\left(-\frac{z^2}{2}\right) dz \\ &\quad = -\int_1^\infty z^{2l-1}\, d\exp\left(-\frac{z^2}{2}\right) \\ &\quad = \frac{1}{\sqrt{e}} + (2l-1) \int_1^\infty z^{2l-2} \exp\left(-\frac{z^2}{2}\right) dz\end{aligned}$$

$$= \frac{1}{\sqrt{e}} + (2l-1)\left(\frac{1}{\sqrt{e}} + (2l-3)\int\limits_1^\infty z^{2l-4}\exp\left(-\frac{z^2}{2}\right)\,dz\right) = \dots$$

$$= \frac{(2l-1)!!}{\sqrt{e}}\sum_{j=1}^{l}\frac{1}{(2l-2j+1)!!} + (2l-1)!!\int\limits_1^\infty \exp\left(-\frac{z^2}{2}\right)\,dz,$$

or via formula 3.462(1) in [6], which gives an answer in terms of the value of the function of parabolic cylinder.

The following example is dual in a sense to the previous one: $f(x) = \frac{1}{\pi(1+x^2)} = x \in \mathbb{R}$, $\widehat{f}(k) = e^{-|k|}$, $k \in \mathbb{R}$ is the density distribution function and the characteristic function of the standard Cauchy distribution, respectively, and $f(x) = e^{-|x|}$, $x \in \mathbb{R}$, $\widehat{f}(k) = \frac{1}{1+k^2} = k \in \mathbb{R}$ is the density distribution function and the characteristic function of the standard Laplace distribution.

Example 7. Let $f(x) = e^{-|x|}$, $x \in \mathbb{R}$ be the density distribution function of the standard Laplace distribution, which can also be understood as a mixture of a Gaussian law (in terms on the accuracy value, i.e., the reciprocal variance):

$$f(x) = e^{-|x|} = \int\limits_0^\infty \frac{\sqrt{t}}{\sqrt{2\pi}}\exp\left(-\frac{x^2 t}{2}\right)\frac{e^{-1/(2t)}}{\sqrt{2\pi}t^{3/2}}\,dt, \quad x \in \mathbb{R}, \tag{3.5}$$

$$\widehat{f}(x) = \frac{1}{1+k^2} = \int\limits_0^\infty \exp\left(-\frac{k^2 t}{2}\right)\frac{e^{-1/(2t)}}{\sqrt{2\pi}t^{3/2}}\,dt, \quad k \in \mathbb{R}. \tag{3.6}$$

Let us evaluate the coefficients of the Fourier series (the function is even, and hence the coefficients of odd powers are zero) using (2.26). We have

$$\begin{aligned}
&\int\limits_{-\infty}^{\infty} f(x)H_{2n}(x)\,dx \\
&\quad = \frac{(-1)^n}{2\pi}\int\limits_{-\infty}^{\infty}\widehat{f}(k)k^{2n}\exp\left(-\frac{k^2}{2}\right)\,dk \\
&\quad = \frac{(-1)^n}{\pi}\int\limits_0^\infty \frac{k^{2n}}{1+k^2}\exp\left(-\frac{k^2}{2}\right)\,dk \\
&\quad = \frac{(-1)^n}{\pi}\int\limits_0^\infty \frac{x^{n-1/2}}{1+x}\exp\left(-\frac{x}{2}\right)\,dx \\
&\quad = \frac{(-1)^n}{\pi}I_n^{(1)}.
\end{aligned}$$

Consider separately the integral $I_n^{(1)} = \int_0^\infty \frac{x^n}{1+x} \frac{\exp\left(-\frac{x}{2}\right)}{\sqrt{x}}\, dx$:

$$\begin{aligned} I_0^{(1)} &= \int\limits_0^\infty \frac{\exp\left(-\frac{x}{2}\right)}{(1+x)\sqrt{x}}\, dx \\ &= \sqrt{2} \int\limits_0^\infty \frac{\exp\left(-y\right)}{(1+2y)\sqrt{y}}\, dy \\ &= \sqrt{\pi}(2e)^{1/4} \mathrm{W}_{-\frac{1}{4},-\frac{1}{4}}\left(\frac{1}{2}\right). \end{aligned} \tag{3.7}$$

The integral $I_0^{(1)}$ expresses in terms of the value of the special function Whittaker (3.383(8) in [6]).

$$I_n^{(1)} = \int\limits_0^\infty \frac{x^n}{1+x} \frac{\exp\left(-\frac{x}{2}\right)}{\sqrt{x}}\, dx = \int\limits_0^\infty \frac{x^n+1}{1+x} \frac{\exp\left(-\frac{x}{2}\right)}{\sqrt{x}}\, dx - I_0^{(1)}, \quad n \geq 1. \tag{3.8}$$

Let us evaluate the first term in (3.8)

$$\begin{aligned} &\int\limits_0^\infty \frac{x^n+1}{1+x} \frac{\exp\left(-\frac{x}{2}\right)}{\sqrt{x}}\, dx \\ &\quad = \int\limits_0^\infty \left(x^{n-1} - x^{n-2} + x^{n-3} + \ldots + (-1)^{n-1}\right) \frac{\exp\left(-\frac{x}{2}\right)}{\sqrt{x}}\, dx \\ &\quad = 2^{n-1/2}\Gamma(n-1/2) - 2^{n-3/2}\Gamma(n-3/2) + 2^{n-5/2}\Gamma(n-5/2) + \ldots \\ &\qquad + (-1)^{n-1} 2^{1/2}\Gamma(1/2) \\ &\quad = \sum_{k=0}^{n-1} (-1)^k 2^{n-\frac{1}{2}-k} \Gamma\left(n - \frac{1}{2} - k\right), \end{aligned}$$

here $\Gamma(z) = \int_0^\infty t^{z-1} e^{-t}\, dt$, $z \in \mathbb{C}$, $\mathrm{Re} z > 0$, – Gamma function.

Note that

$$2^{n-\frac{1}{2}-k}\Gamma\Big(n - \frac{1}{2} - k\Big) = \sqrt{2\pi}\frac{\big(2(n-k-1)\big)!}{(n-k-1)!2^{n-k-1}} = \sqrt{2\pi}\big(2(n-k)-3\big)!!$$

Thus

$$I_n^{(1)} = \sqrt{2\pi} \sum_{k=0}^{n-1} (-1)^k \big(2(n-k)-3\big)!! - I_0^{(1)}, \quad n \geq 1.$$

Note that asymptotically

$$I_n^{(1)} \sim \sqrt{2\pi}\big(2n-3\big)!!, \quad n \to \infty.$$

The following example is a mixture of a Gaussian distributions with the mixing density of the gamma distribution (with parameters $\alpha > 0$, $\beta > 0$). We again have the gamma distribution but which is symmetric (on the entire axis) with parameters α, $\sqrt{\beta}$ (see for example, [16, VI. Theorem 9.5]).

Example 8.

$$\begin{aligned} f(x) &= \int_0^\infty \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{x^2}{2t}\right) \frac{t^{\alpha-1}e^{-\beta t}\beta^\alpha}{\Gamma(\alpha)}\, dt,\ x \in \mathbb{R}, \\ \widehat{f}(k) &= \int_0^\infty \exp\left(-\frac{k^2 t}{2}\right) \frac{t^{\alpha-1}e^{-\beta t}\beta^\alpha}{\Gamma(\alpha)}\, dt = \left(\frac{\beta}{\beta + k^2/2}\right)^\alpha, \quad k \in \mathbb{R}. \end{aligned} \tag{3.9}$$

For $\alpha = 1$, $\beta = 1/2$ we have the particular case of the Laplace distribution (see the previous example).

Let us evaluate the coefficients of the Fourier series for the particular case $\alpha = 2$, $\beta = 1/2$:

$$\begin{aligned} f(x) &= \int_0^\infty \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{x^2}{2t}\right) \frac{te^{-t/2}}{4}\, dt,\ x \in \mathbb{R}, \\ \widehat{f}(k) &= \int_0^\infty \exp\left(-\frac{k^2 t}{2}\right) \frac{te^{-t/2}}{4}\, dt = \frac{1}{(1+k^2)^2}, \quad k \in \mathbb{R}. \end{aligned} \tag{3.10}$$

The function is even, and hence the coefficients of odd powers are zero by (2.26). We have

$$\begin{aligned} \int_{-\infty}^\infty f(x) H_{2n}(x)\phi(x)\, dx &= \frac{(-1)^n}{2\pi} \int_{-\infty}^\infty \widehat{f}(k) k^{2n} \exp\left(-\frac{k^2}{2}\right) dk \\ &= \frac{(-1)^n}{\pi} \int_0^\infty \frac{k^{2n}}{(1+k^2)^2} \exp\left(-\frac{k^2}{2}\right) dk \\ &= \frac{(-1)^n}{\pi} \int_0^\infty \frac{x^{n-1/2}}{(1+x)^2} \exp\left(-\frac{x}{2}\right) dx \\ &= \frac{(-1)^n}{\pi} I_n^{(2)}. \end{aligned}$$

Consider separately the integral $I_n^{(2)} = \int_0^\infty \frac{x^n}{(1+x)^2} \frac{\exp\left(-\frac{x}{2}\right)}{\sqrt{x}}\, dx$:

$$I_0^{(2)} = \int_0^\infty \frac{\exp\left(-\frac{x}{2}\right)}{(1+x)^2\sqrt{x}}\, dx = \sqrt{2} \int_0^\infty \frac{\exp\left(-y\right)}{(1+2y)^2\sqrt{y}}\, dy$$

$$= \sqrt{\pi}\left(\frac{e}{4}\right)^{1/4} \mathrm{W}_{-\frac{3}{4},-\frac{3}{4}}\left(\frac{1}{2}\right), \tag{3.11}$$

$$I_1^{(2)} = \int_0^\infty \frac{\sqrt{x}}{(1+x)^2}\exp\left(-\frac{x}{2}\right)dx = 2^{3/2}\int_0^\infty \frac{\sqrt{y}e^{-y}}{(1+2y)^2}\,dy$$

$$= \sqrt{\pi}\left(\frac{e}{8}\right)^{1/4} \mathrm{W}_{-\frac{1}{4},-\frac{5}{4}}\left(\frac{1}{2}\right). \tag{3.12}$$

The integrals $I_0^{(2)}$ and $I_1^{(2)}$ express in terms of the value of the special function Whittaker (3.383(8) in [6]).

$$I_n^{(2)} = \int_0^\infty \frac{x^n}{(1+x)^2}\frac{\exp\left(-\frac{x}{2}\right)}{\sqrt{x}}\,dx, \quad n \neq 0, 1. \tag{3.13}$$

Let us express $\frac{x^n}{(1+x)^2}$ as a sum of a polynomial of the $(n-2)$-degree and a irreducible fraction

$$\begin{aligned}
I_n^{(2)} &= \int_0^\infty \frac{x^n}{(1+x)^2}\frac{\exp\left(-\frac{x}{2}\right)}{\sqrt{x}}\,dx \\
&= \int_0^\infty \left(\sum_{k=1}^{n-1}(-1)^{k-1}kx^{n-1-k} + (-1)^{n-1}\frac{nx+(n-1)}{(x+1)^2}\right)\frac{\exp\left(-\frac{x}{2}\right)}{\sqrt{x}}\,dx \\
&= \sum_{k=1}^{n-1}(-1)^{k-1}k\int_0^\infty x^{n-k-3/2}\exp\left(-\frac{x}{2}\right)dx \\
&\quad + (-1)^{n-1}\int_0^\infty \left(\frac{n}{1+x} - \frac{1}{(1+x)^2}\right)\frac{\exp\left(-\frac{x}{2}\right)}{\sqrt{x}}\,dx \\
&= \sum_{k=1}^{n-1}(-1)^{k-1}k2^{n-k-\frac{1}{2}}\Gamma\left(n-\frac{1}{2}-k\right) \\
&\quad + (-1)^{n-1}nI_0^{(1)} + (-1)^n I_0^{(2)} \\
&= \sqrt{2\pi}\sum_{k=1}^{n-1}(-1)^{k-1}k\big(2(n-k)-3\big)!! \\
&\quad + (-1)^{n-1}nI_0^{(1)} + (-1)^n I_0^{(2)}, \quad n \neq 0.
\end{aligned}$$

The integral $I_0^{(1)}$ defined in the previous example in (3.7).

Note that asymptotically

$$I_n^{(2)} \sim \sqrt{2\pi}\big(2n-5\big)!!, \quad n \to \infty,$$

$$\frac{I_n^{(1)}}{I_n^{(2)}} \sim 2n, \quad n \to \infty.$$

Analogously we can consider more general case in (3.9) $\alpha = N \in \mathbb{N}$, $\beta = 1/2$:

$$I_n^{(N)} \sim 2^{n-N+\frac{1}{2}}\Gamma\Big(n - N + \frac{1}{2}\Big) = \sqrt{2\pi}\big(2(n-N)-1\big)!!, \quad n \to \infty.$$

Using integration by parts one could derive the following recurrence:

$$\begin{aligned} I_n^{(N+1)} &= \int\limits_0^\infty \frac{x^n}{(1+x)^{N+1}} \frac{\exp\left(-\frac{x}{2}\right)}{\sqrt{x}}\, dx \\ &= -\frac{1}{N}\int\limits_0^\infty x^{n-\frac{1}{2}} \exp\left(-\frac{x}{2}\right)\, d\frac{1}{(1+x)^N} \\ &= \frac{1}{N}\int\limits_0^\infty \frac{1}{(1+x)^N}\left(\left(n-\frac{1}{2}\right)x^{n-\frac{3}{2}} - \frac{1}{2}x^{n-\frac{1}{2}}\right)\exp\left(-\frac{x}{2}\right)\, dx \\ &= \frac{1}{N}\left[\left(n-\frac{1}{2}\right) I_{n-1}^{(N)} - \frac{1}{2} I_n^{(N)}\right] \end{aligned} \tag{3.14}$$

4. The multivariate case

Consider the d-dimensional nondegenerate Gaussian vector $\mathbf{X}' \in \mathbb{R}^d$. For applied problems, it is convenient to work with the standardized vector $\mathbf{X}$, where

$$X_i = \frac{X_i' - \mathbb{E}X_i'}{\sqrt{\mathrm{Var}X_i'}}.$$

In other words, we consider $\mathbf{X} = (X_1, \ldots, X_d)^T \sim \mathcal{N}(\mathbf{0}, \mathrm{P})$,

$$\mathrm{P} = \begin{pmatrix} 1 & \rho_{12} & \rho_{13} & \ldots & \rho_{1d} \\ \rho_{21} & 1 & \rho_{23} & \ldots & \rho_{2d} \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ \rho_{d1} & \rho_{d2} & \rho_{d3} & \ldots & 1 \end{pmatrix},$$

$\rho_{ij} < 1$, $i \neq j$, $|\mathrm{P}| \neq 0$. Here,

$$\frac{1}{(2\pi)^{d/2}\sqrt{|\mathrm{P}|}} \exp\left(-\frac{1}{2}\mathbf{x}^T\mathrm{P}^{-1}\mathbf{x}\right), \ \mathbf{x} = (x_1, \ldots, x_d)^T \in \mathbb{R}^d \tag{4.1}$$

is the density distribution function of the d-dimensional normal vector $\mathbf{X} \sim \mathcal{N}(\mathbf{0}, \mathrm{P})$.

Let $P(\mathbf{x})$ be an arbitrary homogeneous polynomial of variables $x_1, \dots, x_d$ of degree k. The *Wick polynomial* $:P(\mathbf{X}):$ is the perpendicular (in the space of random variables with finite second moment and which are representable as a function of a Gaussian vector $\mathbf{X}$ from $P(\mathbf{X})$) onto the closed subspace generated by the polynomials of $X_1, \dots, X_d$ of degree $< k$.

If $X_1^{k_1} \cdot \ldots \cdot X_d^{k_d}$ is a monomial, then the Wick monomial is defined by $:X_1^{k_1} \cdot \ldots \cdot X_d^{k_d}:$.

Similarly to the one-dimensional case, a Wick monomial can be defined recurrently as follows:

$$\begin{aligned} &: X_1^0 \cdot \ldots \cdot X_n^0 : = 1, \\ &\frac{\partial}{\partial X_i} : X_1^{k_1} \cdot \ldots \cdot X_d^{k_d} : = k_i : X_1^{k_1} \cdot \ldots X_i^{k_i - 1} \ldots \cdot X_d^{k_d} : \end{aligned} \tag{4.2}$$

The following multinomial formula holds:

$$: \left(\sum_{i=1}^{d} \alpha_i X_i \right)^N : = \sum_{k_1 + \ldots + k_d = N} \frac{N!}{k_1! \ldots k_d!} \alpha_1^{k_1} \cdot \ldots \cdot \alpha_d^{k_d} : X_1^{k_1} \cdot \ldots \cdot X_d^{k_d} : \tag{4.3}$$

We point out the important formula

$$\mathbb{E}[:X_i^k : :X_j^l :] = \delta_{kl} \rho_{ij}^k k!, \tag{4.4}$$

which can be obtained from

$$: \exp(a_1 X_i) : : \exp(a_2 X_j) : = : \exp(a_1 X_i + a_2 X_j) : e^{a_1 a_2 \rho_{ij}}$$

by taking expectation and comparing the coefficients in exponent expansions.

As a corollary of (4.3) and (4.4), we have

$$\mathbb{E}[:X_1^{k_1} \cdot \ldots \cdot X_d^{k_d} : :X_1^{m_1} \cdot \ldots \cdot X_d^{m_d} :] = \delta_{k_1 m_1} \ldots \delta_{k_d m_d} k_1! \ldots k_d! \tag{4.5}$$

In the important particular case, where $\mathrm{P} = \mathrm{I}$,

$$:X_1^{k_1} \cdot \ldots \cdot X_d^{k_d} : = :X_1^{k_1} : \cdot \ldots \cdot :X_d^{k_d} : \tag{4.6}$$

the normalized Wick monomials

$$\frac{:X_1^{k_1} \cdot \ldots \cdot X_d^{k_d} :}{\sqrt{k_1! \ldots k_d!}} = \frac{:X_1^{k_1} : \cdot \ldots \cdot :X_d^{k_d} :}{\sqrt{k_1! \ldots k_d!}}$$

form an orthonormal basis for the space L^2.

Evaluation of functionals of Gaussian vectors can be facilitated by using the machinery of diagrams, which, by geometric transparency, does not involve too many formulas.

Let us recall the definitions of the mixed joint moment and semi-invariant (cumulant) of a random vector $\mathbf{X}$ (see [10]). Formally, they are defined as the coefficients in the Maclaurin series expansion of the characteristic function and its logarithm, respectively:

$$\mathbb{E}e^{i\sum_{k=1}^{d}\alpha_k X_k} = \sum_{k_1+\ldots+k_d\le n}\frac{i^{k_1+\ldots+k_d}}{k_1!\ldots k_d!}\alpha_1^{k_1}\ldots\alpha_d^{k_d}m_{\mathbf{X}}^{(k_1,\ldots,k_d)} \tag{4.7}$$

$$+\,o\left((|\alpha_1|+\ldots+|\alpha_d|)^n\right).$$

$$m_{\mathbf{X}}^{(k_1,\ldots,k_d)} = \frac{\partial^{k_1+\ldots+k_d}}{\partial\alpha_1^{k_1}\ldots\partial\alpha_d^{k_d}}\mathbb{E}e^{i\sum_{k=1}^{d}\alpha_k X_k}|_{\alpha_1=0,\ldots\alpha_d=0}. \tag{4.8}$$

$$\ln\mathbb{E}e^{i\sum_{k=1}^{d}\alpha_k X_k} = \sum_{k_1+\ldots+k_d\le n}\frac{i^{k_1+\ldots+k_d}}{k_1!\ldots k_d!}\alpha_1^{k_1}\ldots\alpha_d^{k_d}s_{\mathbf{X}}^{(k_1,\ldots,k_d)} \tag{4.9}$$

$$+\,o\left((|\alpha_1|+\ldots+|\alpha_d|)^n\right).$$

$$s_{\mathbf{X}}^{(k_1,\ldots,k_d)} = \frac{\partial^{k_1+\ldots+k_d}}{\partial\alpha_1^{k_1}\ldots\partial\alpha_d^{k_d}}\ln\mathbb{E}e^{i\sum_{k=1}^{d}\alpha_k X_k}|_{\alpha_1=0,\ldots\alpha_d=0}. \tag{4.10}$$

In (4.7), (4.9), the sum $\sum_{k_1+\ldots+k_d\le n}$ is taken over all nonnegative integers $k_1,\ldots,k_d$ whose sum is majorized by n.

In the particular case $k_1 = 1,\ldots,k_d = 1$, the corresponding moments and semi-invariants are known as simple ones and are denoted as $m_{\mathbf{X}}$ and $s_{\mathbf{X}}$.

Given a subset $T \subset \{1,2,\ldots,d\}$, we define $X_T = \prod_{j\in T} X_j$.

To formulate the required theorem on diagrams (see [11, Chap. II, § 2.2]), we introduce the following notation. Let $\alpha = \{T_1, T_2, \ldots, T_k\}$ be a partition of the set $\{1,2,\ldots,d\}$. We define $\xi = (\xi_1,\ldots,\xi_k)^T \in \mathbb{R}^k$, where $\xi_j = X_{T_j}$, and $\eta = (\eta_1,\ldots,\eta_k)^T \in \mathbb{R}^k$, where $\eta_j = :X_{T_j}:$.

For odd d , the variables m_ξ, s_ξ, m_η, s_η are zero. To verify this, it suffices to consider the vector $\mathbf{X}' = -\mathbf{X}$, which has the same distribution, but for which the numerical characteristics differ by the factor $(-1)^d$.

For even $d = 2N$, consider some partition of the set $\{1,2,\ldots,2N\}$ into pairs $\beta = \{(i_1,j_1),(i_2,j_2),\ldots,(i_N,j_N)\}$. For each pair (α,β), $\alpha = \{T_1,T_2,\ldots,T_k\}$, $\beta = \{(i_1,j_1),(i_2,j_2),\ldots,(i_N,j_N)\}$, we define the *graph* (*diagram*) G with vertex set V (blocks of partition of α) and edge set E (blocks of partition of β) so that the edge (i,j) connects vertices $T_{i'}$ and $T_{j'}$ if $T_{i'}$, $T_{j'} \in \alpha$ and $i \in T_{i'}$, $j \in T_{j'}$. For each diagram G, consider the *contribution* of G defined by

$$I(G) = \prod_{(i,j)\in E}\rho_{ij}, \quad \rho_{ij} = \mathbb{E}X_iX_j, \tag{4.11}$$

where the product is taken over all blocks of partition of β.

Theorem 1. *In the above notation, the values of 1)* m_ξ, *2)* s_ξ, *3)* m_η, *4)* s_η *are given by the common formula*

$$\sum_G I(G) \tag{4.12}$$

where the sums are taken, respectively, over the set of diagrams with fixed partition α

1) *over all diagrams;*
2) *over all connected diagrams;*
3) *over all loop-free diagrams;*
4) *over all connected loop-free diagrams.*

An important particular case mentioned above is formula (4.4):

$$\mathbb{E}[:X_i^k::X_j^l:] = \begin{cases} k!\rho_{ij}^k, & k = l; \\ 0, & k \neq l. \end{cases}$$

We will also require the following estimate (a more accurate estimate was obtained in Chap. 2, §3, Theorem 4 of [11]).

Theorem 2. *For a Gaussian vector with zero expectation and the correlation matrix*

$$\mathrm{P} = \begin{pmatrix} 1 & \rho_{12} & \rho_{13} & \dots & \rho_{1d} \\ \rho_{21} & 1 & \rho_{23} & \dots & \rho_{2d} \\ \dots & \dots & \dots & \dots & \dots \\ \rho_{d1} & \rho_{d2} & \rho_{d3} & \dots & 1 \end{pmatrix},$$

we set

$$\alpha = \max_j \sum_{i:i\neq j} |\rho_{ij}|, \tag{4.13}$$

$$N = \sum_{j=1}^d k_j.$$

If N *is even, then*

$$\mathbb{E}[:X_1^{k_1}::X_2^{k_2}:\dots:X_d^{k_d}:] \leq \alpha^{N/2} \prod_{j=1}^d \sqrt{k_j!}(2\pi(k_j+1))^{1/4}. \tag{4.14}$$

Since

$$\prod_{i-1}^d :e^{a_i X_i}: = \frac{e^{\sum_{i=1}^d a_i X_i}}{\prod_{i-1}^d \mathbb{E}e^{a_i X_i}} = \sum_{k_1\geq 0,\dots,k_d\geq 0} \frac{a_1^{k_1}\dots a_d^{k_d}}{k_1!\dots k_d!} : X_1^{k_1}::X_2^{k_2}:\dots:X_d^{k_d}:$$

using the Cauchy formula, we have

$$\begin{aligned}
&\mathbb{E}[:X_1^{k_1}::X_2^{k_2}:\ldots:X_d^{k_d}:] \\
&\quad = k_1!\ldots k_d! \operatorname*{coeff}_{a_1^{k_1}\ldots a_d^{k_d}} \exp\left(\frac{1}{2}\sum_{i,j:\, i\neq j}\rho_{ij}a_ia_j\right) \\
&\quad = \frac{\prod_{j=1}^d k_j!}{(2\pi i)^d}\oint_{|z_1|=r_1}\ldots\oint_{|z_d|=r_d}\frac{\exp\left(\frac{1}{2}\sum_{i,j:\, i\neq j}\rho_{ij}z_iz_j\right)}{z_1^{k_1+1}\ldots z_d^{k_d+1}}\,dz_1\ldots dz_d,
\end{aligned}$$

Next, employing the estimate

$$|\sum_{i,j:\, i\neq j}\rho_{ij}z_iz_j| \le \alpha\sum_i |z_i|^2$$

we obtain

$$\left|\mathbb{E}[:X_1^{k_1}::X_2^{k_2}:\ldots:X_d^{k_d}:]\right| \le \prod_{j=1}^d \frac{k_j!}{r_j^{k_j}}\exp\left(\frac{\alpha}{2}\sum_i r_i^2\right).$$

Setting $r_j = k_j/\alpha$, and using the estimate $\sqrt{n!} < \left(\frac{n}{e}\right)^{n/2}(2\pi(n+1))^{1/4}$, we get the required inequality.

The next example is the Mehler formula that is mentioned in the introduction.

Example 9.

$$g(x,y) = \frac{1}{2\pi\sqrt{1-\rho^2}}\exp(-\frac{x^2+y^2-2\rho xy}{2(1-\rho^2)}), \quad x,y\in\mathbb{R},$$

is the probability density function of the two-dimensional normal vector

$$\mathcal{N}\left(\begin{pmatrix}0\\0\end{pmatrix},\begin{bmatrix}1 & \rho\\ \rho & 1\end{bmatrix}\right), \quad \rho| < 1,$$

$$f(x,y) = \frac{g(x,y)}{\phi(x)\phi(y)}.$$

The Fourier transform of the function $g(x,y)$ is given by

$$\exp\left(-\frac{k_1^2+k_2^2+2\rho k_1k_2}{2}\right) = \exp\left(-\frac{k_1^2+k_2^2}{2}\right)\sum_{n=0}^{\infty}(-1)^n\frac{\rho^n}{n!}(k_1k_2)^n.$$

Note that

$$\exp\Big(-\frac{k_1^2+k_2^2}{2}\Big)(-k_1k_2)^n$$

corresponds to the Fourier transform for $H_n(x)H_n(y)\phi(x)\phi(y)$, where $\phi(x) = \frac{1}{\sqrt{2\pi}}\exp(-\frac{x^2}{2})$ is the density of the standard normal distribution (see (2.25)).

So, we have

$$f(x,y) = \sum_{n=0}^{\infty} \frac{\rho^n}{n!} H_n(x)H_n(y)$$

or, what is the same,

$$\frac{1}{2\pi\sqrt{1-\rho^2}} \exp\left(-\frac{x^2+y^2-2\rho xy}{2(1-\rho^2)}\right) = \phi(x)\phi(y)\sum_{n=0}^{\infty}\frac{\rho^n}{n!}H_n(x)H_n(y). \quad (4.15)$$

Formula (4.15) is known as the Mehler formula, see [12].

The extension to the next dimensions is similar.

Example 10.

$$g(\mathbf{x}) = \frac{1}{(2\pi)^{d/2}\sqrt{|\mathrm{P}|}} \exp\left(-\frac{1}{2}\mathbf{x}^T\mathrm{P}^{-1}\mathbf{x}\right), \quad \mathbf{x} = (x_1,\dots,x_d)^T \in \mathbb{R}^d$$

is the density distribution function of the d-dimensional normal vector $\mathbf{X} = (X_1,\dots,X_d)^T \sim \mathcal{N}(\mathbf{0},\mathrm{P})$,

$$\mathrm{P} = \begin{pmatrix} 1 & \rho_{12} & \rho_{13} & \dots & \rho_{1d} \\ \rho_{21} & 1 & \rho_{23} & \dots & \rho_{2d} \\ \dots & \dots & \dots & \dots & \dots \\ \rho_{d1} & \rho_{d2} & \rho_{d3} & \dots & 1 \end{pmatrix},$$

$\rho_{ij} < 1$, $i \neq j$, $|\mathrm{P}| \neq 0$.

$$f(\mathbf{x}) = \frac{g(\mathbf{x})}{\prod_{j=1}^{d}\phi(x_j)}.$$

As in the two-dimensional case, the Fourier transform of the function $g(\mathbf{x})$ is given by

$$\begin{aligned} &\exp\left(-\frac{1}{2}\sum_{i=1}^{d}k_i^2 - \sum_{i<j}\rho_{ij}k_ik_j\right) \\ &\quad= \exp\Big(-\frac{1}{2}\sum_{i=1}^{d}k_i^2\Big)\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\Big(\sum_{i<j}\rho_{ij}k_ik_j\Big)^n \\ &\quad= \exp\Big(-\frac{1}{2}\sum_{i=1}^{d}k_i^2\Big)\sum_{\substack{m_{12}\geq 0\\ m_{13}\geq 0\\ \dots\\ m_{(d-1)d}\geq 0}} \frac{(-\rho_{12}k_1k_2)^{m_{12}}}{m_{12}!}\frac{(-\rho_{13}k_1k_3)^{m_{13}}}{m_{13}!}\dots \end{aligned}$$

$$\times \frac{\left(-\rho_{(d-1)d}k_dk_{d-1}\right)^{m_{(d-1)d}}}{m_{(d-1)d}!}.$$

Consider the separate term, i.e., for a fixed m_{ij}, $i<j$,

$$\exp\Big(-\frac{1}{2}\sum_{i=1}^{d}k_i^2\Big)\frac{\rho_{12}^{m_{12}}}{m_{12}!}\frac{\rho_{13}^{m_{13}}}{m_{13}!}\dots\frac{\rho_{d(d-1)}^{m_{(d-1)d}}}{m_{(d-1)d}!}(ik_1)^{s_1}(ik_2)^{s_2}\dots(ik_d)^{s_d},$$

where $s_j=\sum_{l:\,l<j}m_{lj}+\sum_{l:\,l>j}m_{jl}$, $j=1,\dots,d$. The factor multiplying

$$\frac{\rho_{12}^{m_{12}}}{m_{12}!}\frac{\rho_{13}^{m_{13}}}{m_{13}!}\dots\frac{\rho_{d(d-1)}^{m_{(d-1)d}}}{m_{(d-1)d}!}$$

is the Fourier transform of

$$\prod_{j=1}^{d}\phi(x_j)H_{s_j}(x_j),$$

where $\phi(x)=\frac{1}{\sqrt{2\pi}}\exp\left(-\frac{x^2}{2}\right)$ is the density of the standard normal distribution (see (2.25)).

So, we have

$$\frac{1}{(2\pi)^{d/2}\sqrt{|\mathrm{P}|}}\exp\Big(-\frac{1}{2}\mathbf{x}^T\mathrm{P}^{-1}\mathbf{x}\Big)$$

$$=\sum_{\substack{m_{12}\ge0\\ m_{13}\ge0\\ \dots\\ m_{(d-1)d}\ge0}}\frac{\rho_{12}^{m_{12}}}{m_{12}!}\frac{\rho_{13}^{m_{13}}}{m_{13}!}\dots\frac{\rho_{d(d-1)}^{m_{(d-1)d}}}{m_{(d-1)d}!}\prod_{j=1}^{d}\phi(x_j)H_{s_j}(x_j)\tag{4.16}$$

or, what is the same,

$$\frac{1}{(2\pi)^{d/2}\sqrt{|\mathrm{P}|}}\exp\left(-\frac{1}{2}\mathbf{x}^T(\mathrm{P}^{-1}-\mathrm{I})\mathbf{x}\right)$$

$$=\sum_{\substack{m_{12}\ge0\\ m_{13}\ge0\\ \dots\\ m_{(d-1)d}\ge0}}\frac{\rho_{12}^{m_{12}}}{m_{12}!}\frac{\rho_{13}^{m_{13}}}{m_{13}!}\dots\frac{\rho_{d(d-1)}^{m_{(d-1)d}}}{m_{(d-1)d}!}\prod_{j=1}^{d}H_{s_j}(x_j),\tag{4.17}$$

where $s_j=\sum_{l:\,l<j}m_{lj}+\sum_{l:\,l>j}m_{jl}$, $j=1,\dots,d$.

Formula (4.16) is known as the inversion of the two-dimensional Mehler formula (see [9], [15]).

Example 11. As in the previous Example 10, consider the d-dimensional normal vector $\mathbf{X} = (X_1, \dots, X_d)^T \sim \mathcal{N}(\mathbf{0}, \mathrm{P})$, and put

$$f(\mathbf{x}) = \int_{x_1}^{\infty} \dots \int_{x_d}^{\infty} \frac{1}{(2\pi)^{d/2}\sqrt{|\mathrm{P}|}} \exp\Big(-\frac{1}{2}\mathbf{u}^T \mathrm{P}^{-1}\mathbf{u}\Big)\, du_1 \dots du_d,$$

i.e., the tail of the distribution function of the d-dimensional normal vector $\mathbf{X}$.

We integrate (4.16), taking into account that in view of (2.7)

$$\begin{aligned}
&\int_x^{\infty} \phi(u) H_n(u)\, du = \phi(x) H_{n-1}(x), \quad n \ge 1,\\
&\int_{x_1}^{\infty} \dots \int_{x_d}^{\infty} \frac{1}{(2\pi)^{d/2}\sqrt{|\mathrm{P}|}} \exp\Big(-\frac{1}{2}\mathbf{u}^T \mathrm{P}^{-1}\mathbf{u}\Big)\, du_1 \dots du_d\\
&\quad = \sum_{\substack{m_{12}\ge 0\\ m_{13}\ge 0\\ \dots\\ m_{(d-1)d}\ge 0}} \frac{\rho_{12}^{m_{12}}}{m_{12}!}\frac{\rho_{13}^{m_{13}}}{m_{13}!} \dots \frac{\rho_{d(d-1)}^{m_{(d-1)d}}}{m_{(d-1)d}!} \times \qquad (4.18)\\
&\qquad \times \prod_{j=1}^{d} \Big[\mathbb{I}\{s_j \ge 1\} \phi(x_j) H_{s_j-1}(x_j) + \mathbb{I}\{s_j = 0\} \int_{x_j}^{\infty} \phi(u)\, du \Big],
\end{aligned}$$

where $s_j = \sum_{l:\, l<j} m_{lj} + \sum_{l:\, l>j} m_{jl}$, $j = 1, \dots, d$.

In particular, if all $x_i = h$, $i = 1, 2, \dots, d$, then

$$\begin{aligned}
&\mathbb{P}\{X_i > h,\ i = 1, 2, \dots, d\}\\
&\quad = \phi^d(h) \sum_{\substack{m_{12}\ge 0\\ m_{13}\ge 0\\ \dots\\ m_{(d-1)d}\ge 0}} \frac{\rho_{12}^{m_{12}}}{m_{12}!}\frac{\rho_{13}^{m_{13}}}{m_{13}!} \dots \frac{\rho_{d(d-1)}^{m_{(d-1)d}}}{m_{(d-1)d}!} \times \qquad (4.19)\\
&\qquad \times \prod_{j=1}^{d} \left[\mathbb{I}\{s_j \ge 1\} H_{s_j-1}(h) + \mathbb{I}\{s_j = 0\} \frac{\int_h^{\infty} \phi(u)\, du}{\phi(h)} \right],
\end{aligned}$$

where $s_j = \sum_{l:\, l<j} m_{lj} + \sum_{l:\, l>j} m_{jl}$, $j = 1, \dots, d$.

5. Applications of Wick–Hermite polynomials

5.1. Problems in risk theory

In financial applications, the components of a Gaussian vector can be interpreted as some fundamental quantitative indicators (risk factors, portfolio).

The values of these factors (like oil price per barrel, production volume of semiconductor materials, etc.) are measured in units (dollars, tons). This is why, as noted above, the vector should be standardized (the indexes should be dimensionless). As in the previous section, we will consider $\mathbf{X} = (X_1, \dots, X_d)^T \sim \mathcal{N}(\mathbf{0}, \mathrm{P})$, and

$$\mathrm{P} = \begin{pmatrix} 1 & \rho_{12} & \rho_{13} & \dots & \rho_{1d} \\ \rho_{21} & 1 & \rho_{23} & \dots & \rho_{2d} \\ \dots & \dots & \dots & \dots & \dots \\ \rho_{d1} & \rho_{d2} & \rho_{d3} & \dots & 1 \end{pmatrix},$$

$\rho_{ij} < 1$, $i \neq j$, $|\mathrm{P}| \neq 0$.

$$\mu_{\mathrm{P}}(\Gamma) = \int\limits_{\Gamma} \frac{1}{(2\pi)^{d/2}\sqrt{|\mathrm{P}|}} \exp\left(-\frac{1}{2}\mathbf{x}^T \mathrm{P}^{-1}\mathbf{x}\right) d\mathbf{x}, \quad \Gamma \in \mathcal{B}(\mathbb{R}^d). \tag{5.1}$$

Consider two Hilbert spaces associated with the vector $\mathbf{X} \sim \mathcal{N}(\mathbf{0}, \mathrm{P})$. The first space $\mathcal{L}^2(\Omega, \mathrm{P})$ is the space of centered (this requirement is not necessary, and is introduced for convenience) random variables Y with finite moment and which are representable as some (Borel) function $Y = g(\mathbf{X})$ of a Gaussian random variable $\mathbf{X} \sim \mathcal{N}(\mathbf{0}, \mathrm{P})$. The norm on this space is defined by $\|Y\|_{\mathrm{P}}^2 = \mathbb{E}|g(\mathbf{X})|^2 = \int_{\mathbb{R}^d} |g(x)|^2 \mu_{\mathrm{P}}(dx)$.

The following important result holds.

Theorem 3. *The spaces $\mathcal{L}^2(\Omega, \mathrm{P})$ and $\mathcal{L}^2(\Omega, \mathrm{I})$, $\mathrm{P} \neq \mathrm{I}$ are not topologically equivalent, i.e., there exist random sequences $Y_k^{\pm}$ such that*

$$\lim_{k\to\infty} \frac{\|Y_k^+\|_{\mathrm{I}}}{\|Y_k^+\|_{\mathrm{P}}} = \infty, \quad \lim_{k\to\infty} \frac{\|Y_k^-\|_{\mathrm{I}}}{\|Y_k^-\|_{\mathrm{P}}} = 0. \tag{5.2}$$

As the required sequences one can consider $Y_k^+ = |\sum_{i=1}^d \xi_i^+ X_i|^k$, $Y_k^- = |\sum_{i=1}^d \xi_i^- X_i|^k$, where $(\xi_1^+, \dots, \xi_d^+)$ is the eigenvector of the matrix P corresponding to the maximal eigenvalue $\lambda_{\mathrm{P}}^+ > 1$, $(\xi_1^-, \dots, \xi_d^-)$ is the eigenvector of the matrix P corresponding to the minimal eigenvalue $\lambda_{\mathrm{P}}^- < 1$. Now since $\|Y_k^{\pm}\|_{\mathrm{I}}^2 = (2k-1)!!$, $\|Y_k^{\pm}\|_{\mathrm{P}}^2 = (2k-1)!!(\lambda_{\mathrm{P}}^{\pm})^2$, we have (5.2).

The second space $\tilde{\mathcal{L}}^2(\Omega, \mathrm{P}) \subset \mathcal{L}^2(\Omega, \mathrm{P})$ is the space of random variables of the form $Y = \sum_{i=1}^d g_i(X_i)$, where Borel functions $g_i : \mathbb{R} \to \mathbb{R}$ satisfy $\mathbb{E}g_i(X_i) = 0$, $\mathbb{E}g_i^2(X_i) < \infty$ $(i = 1, \dots, d)$. The space $\tilde{\mathcal{L}}^2(\Omega, \mathrm{P})$ is the direct sum of the subspaces introduced in the first section. If $\mathrm{P} = \mathrm{I}$, then these spaces are orthogonal.

The following important result holds.

Theorem 4. *The spaces $\tilde{\mathcal{L}}^2(\Omega, \mathrm{P})$ and $\tilde{\mathcal{L}}^2(\Omega, \mathrm{I})$ are topologically equivalent, i.e.,*

$$c_-\|Y\|_{\mathrm{I}} \leq \|Y\|_{\mathrm{P}} \leq c_+\|Y\|_{\mathrm{I}}, \tag{5.3}$$

where the constants c_-, c_+ correspond to the minimal and maximal eigenvalue of the covariance matrix P (*see [7]*).

The scheme of the proof is as follows. We expand each function $g_i(X_i)$, $i = 1, 2, \dots, d$ in the orthonormal basis of Wick–Hermite polynomials:

$$g_i(X_i) = \sum_{k=1}^{\infty} a_{ik} \frac{:X_i^k:}{\sqrt{k!}},$$
$$\sum_{i=1}^{d} g_i(X_i) = \sum_{k=1}^{\infty} \sum_{i=1}^{d} a_{ik} \frac{:X_i^k:}{\sqrt{k!}},$$
$$\sum_{i=1}^{d} \|g_i(X_i)\|_{\mathrm{P}}^2 = \sum_{k=1}^{\infty} \sum_{i=1}^{d} a_{ik}^2.$$

Formula (4.4) shows that the spaces

$$\tilde{\mathcal{L}}_1^2 = \operatorname{span}\{:\mathrm{X_i}: \mathrm{i} = 1, \dots, \mathrm{d}\}, \quad \tilde{\mathcal{L}}_2^2 = \operatorname{span}\left\{:\mathrm{X_i^2}: \mathrm{i} = 1, \dots, \mathrm{d}\right\}, \\ \tilde{\mathcal{L}}_3^2 = \operatorname{span}\left\{:\mathrm{X_i^3}: \mathrm{i} = 1, \dots, \mathrm{d}\right\}, \dots \tag{5.4}$$

are orthogonal. So, it suffices to show that, for any $k = 1, 2, \dots$,

$$c_- \sum_{i=1}^{d} a_{ik}^2 \le \left\| \sum_{i=1}^{d} a_{ik} \frac{:X_i^k:}{\sqrt{k!}} \right\|_{\mathrm{P}}^2 \le c_+ \sum_{i=1}^{d} a_{ik}^2.$$

Another appeal to (4.4) shows that

$$\left\| \sum_{i=1}^{d} a_{ik} \frac{:X_i^k:}{\sqrt{k!}} \right\|_{\mathrm{P}}^2 = \sum_{i=1}^{d} \sum_{k=1}^{d} a_{ik} a_{jk} \rho_{ij}^k.$$

The last expression lies between the smallest and the largest eigenvalues of the matrix $R_k = (\rho_{ij}^k)_{ij}$ multiplied by $\sum_{i=1}^{d} a_{ik}^2$. All the eigenvalues of the matrix R_k, $k = 1, 2, \dots$, lie between the smallest and the largest eigenvalues of the matrix R_1 (see [7]).

We interpret this result as follows (see [2], [3]). Let X_i, $i = 1, 2, \dots . d$, be values of various risk factors. Our aim is to estimate the random variable X (the portfolio risk) from X_i, $i = 1, 2, \dots . d$. It is assumed that all variables are already standardized (dimensional-free). It is also assumed that there are functions (obtained by the nonlinear regression method)

$$g_i(X_i) = \mathbb{E}[X|X_i],\ i = 1, 2, \dots, d.$$

However, due to the insufficient amount of data, we cannot use multiple regression with X estimated as $\mathbb{E}[X|X_1, \dots, X_d] = \arg\min_{\varphi \in \mathcal{L}^2(\Omega, \mathrm{P})} \mathbb{E}\varphi^2(X_1, \dots, X_d)$. Instead, we replace the space $\mathcal{L}^2(\Omega, \mathrm{P})$ by the space $\tilde{\mathcal{L}}^2(\Omega, \mathrm{P})$.

Theorem 5. *Let* $\mathbf{X} = (X_1, \dots, X_d)^T \sim \mathcal{N}(\mathbf{0}, \mathrm{P})$,

$$\mathrm{P} = \begin{pmatrix} 1 & \rho_{12} & \rho_{13} & \dots & \rho_{1d} \\ \rho_{21} & 1 & \rho_{23} & \dots & \rho_{2d} \\ \dots & \dots & \dots & \dots & \dots \\ \rho_{d1} & \rho_{d2} & \rho_{d3} & \dots & 1 \end{pmatrix},$$

where $\rho_{ij} < 1$, $i \neq j$, $|\mathrm{P}| \neq 0$. *Then the unique solution of the constrained optimization problem*

$$\begin{cases} \min\limits_{\varphi \in \tilde{L}^2(\Omega, \mathrm{P})} \mathbb{E}\varphi^2(X_1, \dots, X_d) \\ \mathbb{E}[\varphi(X_1, \dots, X_d)|X_i] = g_i(X_i),\ i = 1, 2, \dots, d \end{cases} \tag{5.5}$$

is a random variable representable as the L_2*-convergent series*

$$\sum_{k=1}^{\infty} \sum_{i=1}^{d} b_{ik} \frac{:X_i^k:}{\sqrt{k!}}, \tag{5.6}$$

where the vectors $(b_{1,k}, \dots, b_{dk})$, $k = 1, 2, \dots$, *are found by solving the linear system of equations with matrix* $R_k = (\rho_{ij}^k)_{i,j=1^d}$ *and the free vector composed of the coefficients of the expansion of the functions* $g_i(X_i)$ *in Hermite–Wick polynomials:* $g_i(X_i) = \sum_{k=1}^{\infty} a_{ik} \frac{:X_i^k:}{\sqrt{k!}}$, *i.e.,*

$$(b_{1,k}, \dots, b_{dk}) = (a_{1k}, \dots, a_{dk}) R_k^{-1}.$$

In view of Theorem 4, estimate (5.6) is robust (stable) if the components of the risk factor depend weakly relative to the mean-square loss function.

5.2. Some site percolation problems

Originally, the term *percolation* was used in hydrology to mean water soak through the soil — this occurs only when the critical soil water capacity is exceeded.

Consider one of the most simple (but still baseline) model, see [13], which was introduced by Hammersley. This is a model of nodes on the two-dimensional integer lattice $\mathbb{Z}^2$. Let $\xi(x)$ be a random Bernoulli function on the lattice assuming the values $+1$ and -1 with probabilities p and $q = 1 - p$, respectively. This version is called *site* percolation in contrast to the other version which is called *bond* percolation (we do not consider here). The entire lattice is split into two disjoint sets

$$D^+ = \{x : \xi(x) = +1\},$$
$$D^- = \{x : \xi(x) = -1\},$$

each of which, in turn, is split into connected components relative to the standard (edge) connection

$$D^+ = \cup_i D_i^+, \quad D^- = \cup_i D_i^-.$$

One says that $+1$ percolates (takes place) at infinity if there is an infinite component among D_i^+. The definition for -1 is similar. By the Kolmogorov's "0–1 law", these events occur with probability 0 and 1. Since the two fields $\xi^{(1)}(x)$, $\xi^{(2)}(x)$, $x \in \mathbb{Z}^2$, corresponding to different values of the Bernoulli parameter $p_1 > p_2$ can be implemented on a common probability space so that $D^{(2)+} \subset D^{(1)+}$ and that the picture is statistically reproducible if $+1$ is replaced by -1 (or if q is substituted for p), it follows that on $[0,1]$ one can identify two points $p_{\rm cr}$ and $q_{\rm cr}$ such that, for $p > p_{\rm cr}$, $+1$ percolates a.s., there is no percolation for $p < p_{\rm cr}$ a.s.; for $q > q_{\rm cr}$, -1 percolate a.s., and for $q < q_{\rm cr}$ there is no percolation a.s.

Following Hammersley, we will demonstrate on this example that $0 < q_{\rm cr} < 1$ and $0 < q_{\rm cr} < 1$. So, a variation of p results, for $p_{\rm cr} = q_{\rm cr} = 1/2$, in one qualitative change in the levels sets of the field $\xi(x)$ (there are even two changes if $p_{\rm cr} \neq q_{\rm cr} = 1/2$). In physical applications, such changes are interpreted as phase transitions.

We claim that $p_{\rm cr} > 0$. Assume that $+1$ percolates to infinity. Since the model is homogeneous and the number of lattice nodes is countable, we have

$$\mathbb{P}(B) > 0,$$

where B is the event that the lattice point 0 belongs to the infinite class $+1$. Then there exists an infinite path (which can be assumed to be non-self-intersecting) consists in $+1$ which goes off from 0 to infinity. For each $n = 1, 2, \ldots$, let B_n be the event that there exists a connected non-self-intersecting path of length n from $+1$ which emanates from 0. However, we have

$$\mathbb{P}(B_n) \leq 4p^n 3^{n-1}.$$

From the Borel–Cantelli lemma it follows that, for $p < 1/3$, only a finite number of events B_n occur a.s., i.e., $\mathbb{P}(B) = 0$. So, $p_{\rm cr} \geq 1/3$.

We claim that $p_{\rm cr} < 1$. Assume that $+1$ does not percolate to infinity. Then there exists an infinite system of "locking" (i.e., consisting of -1's) hypersurfaces (which, in our simplest case of a two-dimensional lattices, are contours of $\sqrt{2}$-connections without self-intersections, i.e., they are formed by edges and diagonals of unit squares). Let C_n be the event that there exists a contour consists in -1 of length n which encircles the origin 0. It easily follows that

$$\mathbb{P}(C_n) \leq n8q^n 7^{n-1}$$

because each such "locking"contours (with $\sqrt{2}$-connections) of length n contains a point on the x-axis at a distance from the original less then n and the number of such contours is less then $8n7^{n-1}$.

According to the Borel–Cantelli lemma, for $q < 1/7$, only a finite number of events C_n occur a.s., i.e., $+1$ percolates to infinity. So, $p_{\rm cr} \le 6/7$.

Thus in this model of site percolation on the two-dimensional lattice

$$\frac{1}{3} \le p_{\rm cr} \le \frac{6}{7}.$$

Let us complicate the above model by assuming now that $\xi(x)$, $x \in \mathbb{Z}^2$, is a homogeneous Gaussian field with zero expectation and the correlation function $\mathbb{E}\xi(x)\xi(y) = B(x-y)$ normalized by $B(0) = 1$.

Given a fixed level h, we split, as above, the lattice into the random sets

$$D^+(h) = \{x : \xi(x) \ge h\}, \quad D^-(h) = \{x : \xi(x) < h\}.$$

Theorem 6. *Assume that $\alpha = \sum_{z \ne 0} |B(z)| < \infty$. Then there exists a critical level h_{cr} (depending on the correlation function, and, in general, on the dimension), so that, for $h > h_{cr}$, $D^-(h)$ percolates to infinity, and the set $D^+(h)$ has only finite connected components, and the size of a typical connected component (say, which contains the origin) has exponential moments.*

In order to follow the above scheme of the proof, it suffices to verify that, for any $d = 1, 2, \dots$ and for each set of points of the lattice $x_1, x_2, \dots, x_d$,

$$\mathbb{P}\{\xi(x_1) \ge h, \dots, \xi(x_d) \ge h\} \le c_1 f_1^d(h), \tag{5.7}$$

$$\mathbb{P}\{\xi(x_1) < h, \dots, \xi(x_d) < h\} \le c_2 f_2^d(h), \tag{5.8}$$

where $f_1(h)$, $f_2(h)$ are some functions satisfying

$$\lim_{h \to \infty} f_1(h) = 0, \tag{5.9}$$

$$\lim_{h \to -\infty} f_2(h) = 0, \tag{5.10}$$

and c_1, c_2 are positive constants. Next,

$$\begin{aligned}
&\mathbb{P}\{\xi(x_1) \ge h, \dots, \xi(x_d) \ge h\} \\
&\quad = \mathbb{E} \prod_{i=1}^{d} \mathbb{I}\{\xi(x_i) \ge h\} \\
&\quad = \mathbb{E} \prod_{j=1}^{d} \sum_{k_j \ge 0} \frac{a_{k_j}}{k_j!} :\xi(x_j)^{k_j}: \\
&\quad = \sum_{k_1 \ge 0, \dots, k_d \ge 0} \frac{a_{k_1} \dots a_{k_d}}{k_1! \dots k_d!} \mathbb{E} :\xi(x_1)^{k_1} : \dots : \xi(x_d)^{k_d}:,
\end{aligned}$$

where $a_{k_j} = a_{k_j}(h) = \mathbb{E}\left[\mathbb{I}\{\xi(x_j) \ge h\} :\xi(x_j)^{k_j}:\right]$.

An appeal to estimate (4.14) from Theorem 2 gives

$$\begin{aligned}
&\mathbb{P}\{\xi(x_1) \geq h, \dots, \xi(x_d) \geq h\} \\
&\quad \leq \sum_{k_1 \geq 0, \dots, k_d \geq 0} \frac{|a_{k_1}| \dots |a_{k_d}|}{k_1! \dots k_d!} \left| \mathbb{E} : \xi(x_1)^{k_1} : \dots : \xi(x_d)^{k_d} : \right| \\
&\quad \leq \sum_{k_1 \geq 0, \dots, k_d \geq 0} \frac{|a_{k_1}| \dots |a_{k_d}|}{k_1! \dots k_d!} \alpha^{\frac{1}{2} \sum_{j=1}^d k_j} \prod_{j=1}^d \sqrt{k_j!} (2\pi(k_j+1))^{1/4} \\
&\quad = \left(\sum_{k=0}^{\infty} \frac{|a_k|}{\sqrt{k!}} \alpha^{k/2} (2\pi(k+1))^{1/4} \right)^d .
\end{aligned}$$

In view of (2.7), we have

$$a_k = \int_h^{\infty} H_k(x) \phi(x)\, dx = \phi(h) H_{k-1}(h), \quad k \geq 1,$$

$$a_0 = \int_h^{\infty} \phi(x)\, dx \leq \phi(h)/h,$$

and

$$\begin{aligned}
&\sum_{k=0}^{\infty} \frac{|a_k|}{\sqrt{k!}} \alpha^{k/2} (2\pi(k+1))^{1/4} \\
&\quad = \phi(h)(2\pi)^{1/4} + \phi(h) \sum_{k=1}^{\infty} \frac{|H_{k-1}(h)|}{\sqrt{k!}} \alpha^{k/2} (2\pi(k+1))^{1/4} \\
&\quad \leq \phi(h)(2\pi)^{1/4} + \phi(h)\sqrt{\alpha}(4\pi)^{1/4} + \phi(h)\sqrt{\alpha}(2\pi)^{1/4} \sum_{k=0}^{\infty} \frac{|H_k(h)|}{\sqrt{k!}} \alpha^{k/2}.
\end{aligned}$$

The last sum is roughly estimated as follows:

$$\sum_{k=0}^{\infty} \frac{|H_k(h)|}{\sqrt{k!}} \alpha^{k/2} \leq \sum_{k=0}^{\infty} \frac{|H_k(h)|}{k!} \alpha^{k/2} = \exp(\sqrt{\alpha} h - \alpha/2).$$

$$\begin{aligned}
&\mathbb{P}\{\xi(x_1) \geq h, \dots, \xi(x_d) \geq h\} \\
&\quad \leq \left[\phi(h)(2\pi)^{1/4} \left(1 + \sqrt{\alpha\sqrt{2}} + \sqrt{\alpha} e^{\sqrt{\alpha} h - \alpha/2} \right) \right]^d . \qquad (5.11)
\end{aligned}$$

So, the function f_1 in inequality (5.7)

$$f_1(h) = \phi(h)(C_1 + C_2 e^{\sqrt{\alpha} h}) \qquad (5.12)$$

satisfies the required limit (5.9).

Note that all calculations take place for the function f_2 in inequality (5.8). Because of (2.7), in this case we have

$$a_k = \int_{-\infty}^{h} H_k(x)\phi(x)\,dx = -\phi(h)H_{k-1}(h),$$

The second method of the proof of this result depends on an application of the Mehler formula in the multidimensional case. Namely, using formula (4.19), we have

$$\begin{aligned}
&\mathbb{P}\{\xi(x_1) \ge h, \dots, \xi(x_d) \ge h\} \\
&\quad = \phi^d(h) \sum_{\substack{m_{12}\ge 0\\ m_{13}\ge 0\\ \dots\\ m_{(d-1)d}\ge 0}} \frac{B(x_1-x_2)^{m_{12}}}{m_{12}!}\frac{B(x_1-x_3)^{m_{13}}}{m_{13}!}\cdots\frac{B(x_d-x_{d-1})^{m_{(d-1)d}}}{m_{(d-1)d}!} \\
&\qquad \times \prod_{j=1}^{d}\left[\mathbb{I}\{s_j\ge 1\}H_{s_j-1}(h) + \mathbb{I}\{s_j=0\}\frac{\int_h^\infty \phi(u)\,du}{\phi(h)}\right],
\end{aligned} \tag{5.13}$$

where $s_j = \sum_{l:\,l<j} m_{lj} + \sum_{l:\,l>j} m_{jl}$, $j = 1, \dots, d$. Since $\lim_{h\to\infty} \frac{|H_n(h)|}{h^n} = 1$, we have, as $h \to \infty$,

$$\begin{aligned}
&\mathbb{P}\{\xi(x_1) \ge h, \dots, \xi(x_n) \ge h\} \\
&\quad \le \left(\frac{\phi(h)}{h}\right)^d \prod_{ij:i<j}\sum_{m_{ij}=0}^{\infty}\frac{(h|B(x_i-x_j|)^{m_{ij}}}{m_{ij}!} \\
&\quad = \left(\frac{\phi(h)}{h}\right)^d \exp\Big(h\sum_{i,j:i<j}|B(x_i-x_j)|\Big) \\
&\quad \le \left[\frac{\phi(h)}{h}\exp\Big(h\sum_{z\ne 0}|B(z)|\Big)\right]^d \\
&\quad = \Big[\frac{\phi(h)}{h}\exp(h\alpha)\Big]^d.
\end{aligned} \tag{5.14}$$

It is now clear that the required property (5.7), (5.9) holds.

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Markov Processes and **Related Fields**

On Malyshev's Method of Automorphic Functions in Diffraction by Wedges

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Dedicated to the memory of Vadim Malyshev

Abstract. We describe Malyshev's method of automorphic functions in application to boundary value problems in angles and to diffraction by wedges. We give a concise survey of related results of A. Sommerfeld, S.L. Sobolev, J.B. Keller, G.E. Shilov and others.

Keywords: elliptic equation; Helmholtz equation; boundary value problem; plane angle; Fourier transform; analytic function; Riemann surface; characteristics; covering map; automorphic function; Riemann–Hilbert problem; diffraction; wedge; limiting absorption principle; limiting amplitude principle; limiting amplitude: the Sommerfeld radiation condition

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Contents

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1. Introduction

Vadim Malyshev was a very talented and versatile mathematician. He owns significant results in the field of probability theory and Gibbs fields, Markov processes and Euclidean quantum field theory. He also possessed outstanding organizational skills, in particular, he founded the successful and respected mathematical journal "Markov Processes and Related Fields".

In 1970, V. Malyshev invented the method of automorphic functions [36], and applied to random walks on the lattice in the quarter of plane. Later on, he applied the method to queueing systems and analytic combinatorics [16]. In 1972–2022, the method was extended to boundary value problems for partial differential equations in angles [22, 32] and to diffraction by wedges [30]. The main steps of Malyshev's method are as follows:

I. Undetermined algebraic equation on the Riemann surface and analytic continuation.

II. Elimination of one unknown function using covering automorphisms.

III. The reduction to the Riemann–Hilbert problem.

Malyshev's method played the crucial role in the progress in the theory of diffraction by wedges with general boundary conditions since 1972. The problem was stated by M.I. Vishik in the Summer of 1967. In 1969–1971, one of the authors (AK) tried to solve this problem while preparing his PhD Thesis. As the result of these three-year efforts, the problem has been reduced to an undetermined algebraic equation on the Riemann surface [23], though next steps remained obscure. Fortunately, at the end of 1971, AK received the

impetus from his friend Alexander Shnirelman who noticed something similar in Malyshev's book [36], which he had recently reviewed by request of M.I. Vishik. AK did not understand this book completely, but discovered two pages which could have contained a creative idea. The book, opened on these pages, lied on his desk for about two or three months, when AK pinned down two lines with the key idea of automorphicity. The remaining work took about six months...

The extension of the research to diffraction problems was done in an intensive collaboration of both authors, and took about 50 years. The main results of the collaboration were the *limiting absorption principle* [44, 45], proof of the completeness of Ursell's trapping modes [31] , the extension to the nonconvex angles [25, 30], and the Sommerfeld representation [24]. Moreover, our general methods [30] allowed us to reproduce the formulas obtained by Sommerfeld, Sobolev and Keller [28, 29, 47]. The identifications justify these formulas as the *limiting amplitudes* in diffraction.

In the present, we give a concise survey of the development of Malyshev's method of automorphic functions since 1972 in the context of i) boundary value problems in angles for elliptic partial differential equations, and ii) theory of stationary and time-dependent diffraction by wedges. We focus on principal ideas omitting nonessential technical details. All the details can be found in [30].

2. Diffraction by wedges and radar/sonar detection

The radar or sonar emits the incident wave, which generates the reflected and diffracted waves (the latter in green color) as shown in Fig. 1. Here W denotes a conducting wedge (for example, the edge of an airplane wing), and $Q= \mathbb{R}^2 \setminus W$ is an angle of magnitude Φ. The incident wave reaches the wedge and generates the reflected and diffracted waves. The diffracted wave is defined as the total wave minus the incident and reflected waves.

The reflected wave is defined by geometric optics, and is absorbed by the ground. On the other hand, the diffracted wave spreads in all directions, and **only this part of radiation** returns to the radar which allows to detect the airplane location.

3. Stationary diffraction and boundary value problems in angles

The stationary diffraction by wedge is described by the boundary value problem for the Helmholz equation in an angle $Q \subset \mathbb{R}^2$ of magnitude $\Phi \in (0, 2\pi]$:

$$\left\{ \begin{array}{rcll} (\Delta + \omega^2)u(x) & = & 0, & x \in Q \\ B_l u(x) & = & f_l(x), & x \in \Gamma_l, \quad l = 1, 2 \end{array} \right|, \tag{3.1}$$

where Γ_1 and Γ_2 denote the sides of the angle, the functions f_l are defined by the incident wave, and $\omega \in \mathbb{R}$ is its frequency, see Fig. 1 and (7.9). The operators B_l

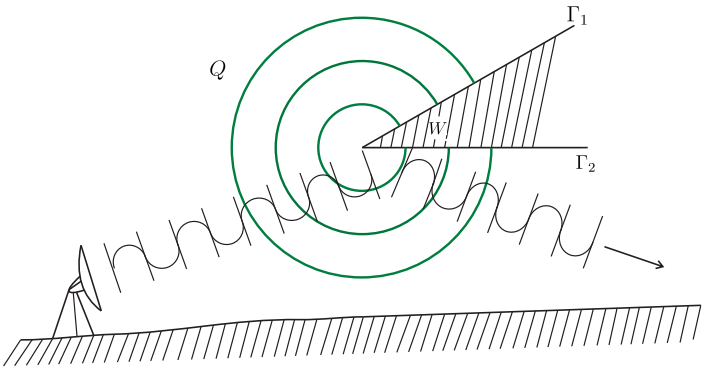

Figure 1. Incident, reflected, and diffracted waves (the latter in green color).

in the boundary conditions correspond to the material properties of the wedge (conductor, insulator, ferromagnetic, etc).

The relation of stationary problem (3.1) to time-dependent diffraction is highly nontrivial. The key issue is that for $\omega \in \mathbb{R}$, the problem admits an infinite number of linearly independent solutions. We discuss this issue in detail in Section 7.

The stationary diffraction problem (3.1) with the Dirichlet and Neumann boundary conditions ($B_l = 1$ or $B_l = \frac{\partial}{\partial n}$) was solved in 1896–1912 for $\Phi = 2\pi$, by A. Sommerfeld [61]– [66] (the detailed exposition and comments can be found in [49]). The extension to all $\Phi \in (0, 2\pi)$ was obtained in 1920 by H.S. Carslaw [8], in 1932–1937 by V.I. Smirnov and S.L. Sobolev [56–60], and in 1951 by J.B. Keller and A. Blank [21]. In 1958, G.D. Malujinetz solved the problem for all $\Phi \in (0, 2\pi)$ with the impedance (Leontovich) boundary condition $\frac{\partial u(x)}{\partial n} + ib_l u(x) = f_l(x),\ x \in \Gamma_l$; see [34,35]. The detailed exposition of all these results can be found in [2] and [30].

The *mixed boundary value problems* of type

$$\left\{ \begin{array}{rcll} Au(x) & = & 0, & x \in Q \\ B_l u(x) & = & f_l(x), & x \in \Gamma_l, \quad l = 1, 2 \end{array} \right| , \qquad (3.2)$$

$$A = \sum_{|\alpha| \le m} a_\alpha \partial^\alpha, \quad B_l = \sum_{|\alpha| \le n_l} b_{l\alpha} \partial^\alpha$$

were considered in 1958 by S.L. Sobolev [60] and in 1960–1961 by G.E. Shilov [54, 55] in the quadrant $x_1 > 0$, $x_2 > 0$ for the case of hyperbolic operator A in the variable x_2 and with the Cauchy initial conditions at $x_2 = 0$.

For strongly-elliptic second order operators A and general differential boundary operators B_l, the problem (3.2) was solved in 1972 in **convex angles** Q of magnitude $\Phi \in (0, \pi)$, see [22, 23]. Strong ellipticity means that

$$|\hat{A}(z)| \geq \varkappa(|z|^2 + 1), \qquad z \in \mathbb{R}^2, \tag{3.3}$$

where **the symbol**

$$\hat{A}(z) := \sum_{|\alpha| \leq 2} a_\alpha (-iz)^\alpha$$

and $\varkappa > 0$. In particular, the operator $A = -\Delta + 1$ with the symbol $\hat{A}(z) = z^2 + 1$ is strongly elliptic, and also the Helmholtz operator $H = \Delta + \omega^2$ from (3.1) is strongly elliptic for $\operatorname{Im} \omega \neq 0$. The method [22,23] relies on the Malyshev's ideas of automorphic functions [36] which is presented in the next section.

The extension of this result to nonconvex angles of magnitudes $\Phi \in (\pi, 2\pi)$, was done in 1992 by the authors [25].

Let us note that the Helmholtz operator

$$A = \Delta + \omega^2$$

is not strongly elliptic if $\omega \in \mathbb{R}$ since its symbol has the form

$$\hat{A}(z) = -z^2 + \omega^2.$$

Problem (3.2) for the Helmholtz operator in **convex angles** was solved in 1972–1977 by A.E. Merzon [44, 45], who proved that *for real* $\omega \in \mathbb{R}$, the problem admits only a finite number of solutions satisfying the **limiting absorption principle**:

$$u_\omega(x) = \lim_{\varepsilon \to 0+} u_{\omega + i\varepsilon}(x), \qquad x \in Q, \tag{3.4}$$

where $u_{\omega+i\varepsilon}$ denotes suitable solution to (3.1) with $\omega + i\varepsilon$ instead of ω.

The application of these results to time-dependent diffraction by wedges was done in 2006–2019 by the authors [26, 27, 30], where, in particular, the **limiting amplitude principle** (7.3) was established as well as (3.4).

Another approach to the construction of solutions to (3.2) has been suggested by Maz'ya and Plamenevskii [37, 38]. This approach is applicable only to equations with real coefficients that is not sufficient for application to the diffraction problems.

Many works published since 1980' concern a wide spectrum of properties of solutions to the boundary problems of type (3.2) in different regions with angles, see Grisvard [18], Costabel and Stephan [10], Dauge [12], Bernard [3,4], Nazarov and Plamenevskii [50], Bonnet-Ben Dhia and Joly [6], Bonnet-Ben Dhia, Dauge and Ramdani [5], Meister with collaborators [39]– [43], Penzel and Teixeira [51], Castro and Kapanadze [9], and others. The detailed survey can be found in [30].

Note that Malyshev's method plays an important role in the theory of Queueing Systems and Analytic Combinatorics [16].

Another important area of application of Malyshev's method is the linear theory of water waves. In particular, the method was applied in 1996–2002 by the authors together with P.N. Zhevandrov to trapped modes on a sloping beach. As the result, the long-standing problem of the completeness of the Ursell's modes has been solved [31, 46], (see also [48, 68] where this method was used). This progress is due to the fact that the method allows one to obtain *all* solutions of the boundary value problems in angles.

We expect that the method can give a valuable progress in diffraction by ferromagnetic wedges which is a challenging open problem of radar detection. In this case, the operators B_l in (3.2) are nonlocal pseudodifferential operators.

4. Malyshev's method of automorphic functions

In this section, we present basic steps of the method [22] which relies on Malyshev's ideas of automorphic functions [36].

Note that in the case of rational angles $\Phi = \pi/n$ and the Dirichlet and Neumann boundary conditions, the boundary value problem (3.1) can be easily solved by reflections in the sides of the angle. This method was well known at least since the Gauss theory of electrostatics [17]. For $\Phi \neq \pi/n$ the reflections do not give a solution, and for irrational Φ/π, the method suggested the reflections on a "Riemann surface" formed by the reflected angles. This was the original step of the Sommerfeld approach which leaded him to the famous "Sommerfeld integral representation" for solutions [61]. The reflection on the Riemann surface and the theory of branching solutions to the wave equation have been developed later by Sobolev [58] and [59, Chapter XII].

Very surprisingly, the method of automorphic functions [22, 36] also relies on the reflections on a suitable Riemann surface V. However, in this approach, V is the surface in the Fourier space, contrary to the original ideas of Sommerfeld. Namely, V is the Riemann surface of complex characteristics of the elliptic operator A:

$$V = \{z \in \mathbb{C}^2 : \hat{A}(z) = 0\}. \tag{4.1}$$

Remark 4.1. The main idea of the Malyshev approach is the invariance of the Cauchy data of solutions under covering maps of the Riemann surface V, see Remark 4.7.

In [22], the problem (3.2) with strongly–elliptic operators A in **convex angles** Q is solved in the following steps:

1. Reduction to an undetermined algebraic equation with two unknown functions on the Riemann surface V.

2. Elimination of one unknown function using its invariance with respect to the

covering map of the Riemann surface.

3. Reduction of the obtained equation with one unknown function to the Riemann–Hilbert problem on V.

Below in this section, we describe some details.

4.1. Reduction to undetermined algebraic equation on the Riemann surface

As an example, we consider the Dirichlet boundary value problem in the quadrant $Q = \mathbb{R}^+ \times \mathbb{R}^+$:

$$\left\{ \begin{array}{rcl} Au(x_1, x_2) & = & 0 \\ u(x_1, 0) & = & f_1(x_1),\ u(0, x_2) = f_2(x_2) \end{array} \right|, \quad x_1 > 0,\ x_2 > 0. \tag{4.2}$$

4.1.1. Fourier–Laplace transform

We assume that the solution $u(x) \in C^2(\overline{Q})$ and is bounded by a polynomial:

$$|u(x)| + |\nabla u(x)| \le C(1 + |x|)^p, \qquad x \in \mathbb{R}^2. \tag{4.3}$$

Denote $\mathbb{C}^+ = \{\zeta \in \mathbb{C} : \operatorname{Im} \zeta > 0\}$ and $Z^+ = \mathbb{C}^+ \times \mathbb{C}^+$, and consider the complex Fourier–Laplace transform of solution

$$\hat{u}(z) = \int_0^\infty \int_0^\infty e^{izx} u(x) dx_1 dx_2, \qquad z = (z_1, z_2) \in Z^+. \tag{4.4}$$

By (4.3), this integral is absolutely convergent and hence it is an analytic function of two complex variables (this is a particular case of the Paley–Wiener Theorem). Let us denote the Neumann data of the solution as

$$\varphi_1(x_1) = \partial_2 u(x_1, 0),\ \ x_1 \ge 0; \qquad \varphi_2(x_2) = \partial_1 u(0, x_2),\ \ x_2 \ge 0. \tag{4.5}$$

It is well known that the solution $u(x)$ can be expressed via the Dirichlet and Neumann data $f_1, f_2, \varphi_1, \varphi_2$ by the Green integral formula [11]. In our case, it is useful to obtain this formula in the Fourier transform. For this purpose, multiply the first equation in (3.2) by e^{izx} and integrate over Q. Integrating by parts, we immediately obtain

$$0 = \int_0^\infty \int_0^\infty e^{izx} Au(x) dx_1 dx_2 = \hat{A}(z)\hat{u}(z) + F(z), \qquad z \in Z^+, \tag{4.6}$$

where

$$F(z) = P_1(z)\hat{f}_1(z_1) + P_2(z)\hat{f}_2(z_2) + S_1(z)\hat{\varphi}_1(z_1) + S_2(z)\hat{\varphi}_2(z_2), \qquad z \in Z^+, \tag{4.7}$$

and the functions P_l and S_l are polynomials.

4.1.2. Undetermined algebraic equation on the Riemann surface

Rewrite (4.6) as

$$\hat{A}(z)\hat{u}(z) = -F(z), \qquad z \in Z^+. \tag{4.8}$$

Now (4.1) implies the identity

$$F(z) = 0, \qquad z \in V^+ := V \cap Z^+ \tag{4.9}$$

since all the functions $\hat{A}(z), \hat{u}(z), F(z)$ are **analytic** in the domain Z^+!

Remark 4.2. Note that the set of complex characteristics V is nonempty even for strongly elliptic operators (3.3), though its intersection with the real plane $\mathbb{R}^2$ is empty; see Example 4.5 below.

The identity (4.9) can be rewritten as **undetermined linear algebraic equation**

$$S_1(z)\varphi_1(z_1) + S_2(z)\varphi_2(z_2) = G(z), \qquad z \in V^+ \tag{4.10}$$

with **two unknown functions** $\varphi_1(z_1)$, $\varphi_2(z_2)$, and with known right-hand side:

$$G(z) := -P_1(z)\hat{f}_1(z_1) - P_2(z)\hat{f}_2(z_2), \qquad z \in V^+. \tag{4.11}$$

Remark 4.3. The identity (4.8) implies the formula for the solution

$$u(x) = -\Big[\mathcal{F}^{-1}\frac{F(z)}{\hat{A}(z)}\Big](x), \qquad x \in Q, \tag{4.12}$$

where $\mathcal{F}^{-1}$ denotes the inverse to the Fourier–Laplace transform (4.4), and the right hand side is well defined due to (3.3). The formula (4.12) can be transformed into the well known Green formula which expresses the solution $u(x)$ via its Cauchy data.

4.2. Method of automorphic functions

4.2.1. Covering maps

Denote

$$\psi_1(z) = \varphi_1(z_1), \ \ \psi_2(z) = \varphi_2(z_2), \quad \hat{g}_1(z) = \hat{f}_1(z_1), \ \ \hat{g}_2(z) = \hat{f}_2(z_2). \tag{4.13}$$

Now (4.10) becomes

$$S_1(z)\psi_1(z) + S_2(z)\psi_2(z) = G(z), \qquad z \in V^+, \tag{4.14}$$

where

$$G(z) := -P_1(z)\hat{g}_1(z) - P_2(z)\hat{g}_2(z). \tag{4.15}$$

Of course, this equation is not equivalent to (4.10). To keep the equivalence, we need an additional characterisation of the functions $\psi_l(z)$. This is the key observation of Malyshev that the functions are automorphic with respect to an appropriate groups of transformation of the Riemann surface V.

First, consider the coordinate projections $p_l : V \to \mathbb{C}$ defined by

$$p_1(z_1, z_2) = z_1, \qquad p_2(z_1, z_2) = z_2. \tag{4.16}$$

These projections are two-sheeted since, for example, $p_1(z_1, z_2) = z_1$ means that z_2 is the root of the quadratic equation $\hat{A}(z_1, z_2) = 0$. Accordingly, the inverse maps $p_l^{-1} : \mathbb{C} \to V$ are double-valued: for $z_1, z_2 \in \mathbb{C}$,

$$p_1^{-1}(z_1) = \{\zeta_1^-, \zeta_1^+\}, \qquad p_2^{-1}(z_2) = \{\zeta_2^-, \zeta_2^+\}, \tag{4.17}$$

and at the branching points of p_l^{-1}, the two points $\zeta_l^\pm \in V$ coincide.

Definition 4.4. ***Covering maps*** $h_1, h_2 : V \to V$ are defined as follows: for any $z_1, z_2 \in \mathbb{C}$,

$$h_1\zeta_1^\pm = \zeta_1^\mp, \qquad h_2\zeta_2^\pm = \zeta_2^\mp. \tag{4.18}$$

Example 4.5. For the strongly-elliptic operator $A = -\Delta + 1$, the corresponding Riemann surface V: $z_1^2 + z_2^2 + 1 = 0$ is shown in Fig. 2 in projection onto the plane $\operatorname{Im} z_1, \operatorname{Im} z_2$. It is easy to see that this projection does not cover the circle $|\operatorname{Im} z_1|^2 + |\operatorname{Im} z_2|^2 < 1$, and it covers twice each point with $|\operatorname{Im} z_1|^2 + |\operatorname{Im} z_2|^2 > 1$. The surface consists of two sheets shown in Fig. 2, and glued along the cuts.

Thus, h_1 permutes the points $\zeta_1^\pm \in V$ with the identical projections $z_1 = p_1\zeta_1^\pm$, and similarly, h_2 permutes the points $\zeta_2^\pm \in V$ with the identical projections $z_2 = p_2\zeta_2^\pm$ (see Fig. 2):

$$p_1 h_1 \zeta_1^\pm = p_1\zeta_1^\mp = z_1, \qquad p_2 h_2 \zeta_2^\pm = p_2\zeta_2^\mp = z_2. \tag{4.19}$$

The maps $h_l : V \to V$ with $l = 1, 2$ define the corresponding automorphisms of the ring of (meromorphic) functions $\psi(z)$ on the Riemann surface V:

$$\psi^{h_l}(z) := \psi(h_l z), \qquad z \in V. \tag{4.20}$$

Figure 2 shows that

$$p_1\zeta_1^+ = z_1 = p_1\zeta_1^-, \quad \text{so } \psi_1(\zeta_1^+) = \varphi_1(z_1) = \psi_1(\zeta_1^-),$$

$$p_2\zeta_2^+ = z_2 = p_2\zeta_2^-, \quad \text{so } \psi_2(\zeta_2^+) = \varphi_2(z_2) = \psi_2(\zeta_2^-).$$

Now it is clear that the functions $\psi_l(z) := \varphi_l(z_l)$ with $l = 1, 2$ are invariant with respect to the automorphisms h_l:

$$\psi_l^{h_l}(z) = \psi_l(z), \qquad z \in V^+. \tag{4.21}$$

In other words, the functions ψ_l are **automorphic**, and the automorphisms defined by h_l belong to the corresponding **Galois groups** of extensions of the ring of functions of z_l.

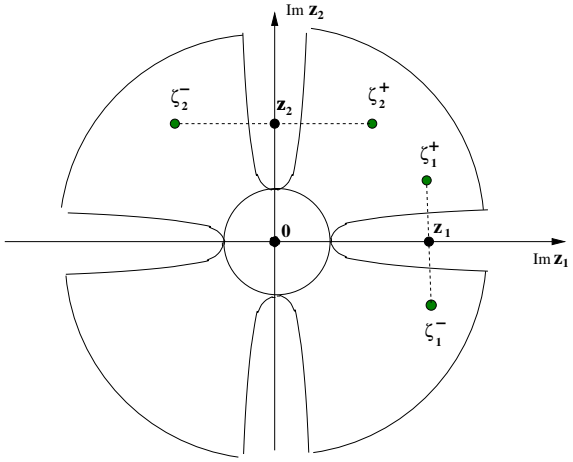

Figure 2. Riemann surface $V\colon z_1^2 + z_2^2 + 1 = 0$ in projection onto the plane $\operatorname{Im} z_1, \operatorname{Im} z_2$.

4.2.2. Shift equation

Applying **formally** h_1 to (4.14), and using (4.21) with $l = 1$, we get **a new equation** for the same unknown functions:

$$S_1^{h_1}(z)\psi_1(z) + S_2^{h_1}(z)\psi_2^{h_1}(z) = G^{h_1}(z). \tag{4.22}$$

The problem is that $\psi_2^{h_1}(z) = \psi_2(h_1 z)$ and $G^{h_1}(z) = G(h_1 z)$ are not defined generally for $z \in V^+$ since V^+ is not invariant with respect to the covering map h_1. In particular, we have by (4.15),

$$G^{h_1}(z) := -P_1^{h_1}(z)\hat{g}_1(z) - P_2^{h_1}(z)\hat{g}_2^{h_1}(z), \tag{4.23}$$

where $\hat{g}_2^{h_1}(z) = \hat{g}_2(h_1 z)$ is not defined generally for $z \in V^+$. To save the situation, consider the case $f_2 = 0$. Then $\hat{g}_2 = 0$, and now the right hand side of equation (4.22) is well defined for $z \in V^+$. It is important that in this case $\psi_2^{h_1}(z)$ is also well defined [30, Ch. 14]. The case $f_1 = 0$ can be considered similarly.

Remark 4.6. The function $\psi_2(z)$ admits an analytic continuation outside the region $V_l^+ := \{z \in V : \operatorname{Im} z_2 > 0\}$ *on the Riemann surface* V, see [30, Ch. 14]. Let us stress that this is analytic continuation *along the surface* V.

Now we can **eliminate** the function ψ_1 from (4.14) and (4.22). As a result, we obtain an algebraic equation with a shift for **one unknown function**

$$R_1(z)\psi_2^{h_1}(z) - R_2(z)\psi_2(z) = H(z), \quad z \in V^+. \tag{4.24}$$

Finally, using (4.21) ***with l=2***, we get

$$R_1(z)\psi_2^h(z) - R_2(z)\psi_2(z) = H(z), \quad z \in V^+; \qquad h = h_2h_1. \tag{4.25}$$

Remark 4.7. The elimination of unknown functions using their invariance with respect to suitable "reflections" is the main idea of Malyshev's method.

4.3. Reduction to the Riemann–Hilbert problem

Let us illustrate the reduction of equation (4.24) to the Riemann–Hilbert problem for a particular case of strongly-elliptic operator $A = -\Delta + 1$. Its symbol is $\hat{A}(z) = z^2 + 1$, so $V = \{(z_1, z_2) \in \mathbb{C}^2 : z_1^2 + z_2^2 = -1\}$ and the covering maps are

$$h_1(z_1, z_2) = (z_1, -z_2), \qquad h_2(z_1, z_2) = (-z_1, z_2). \tag{4.26}$$

Introduce the coordinate w on the universal covering $\hat{V} = \mathbb{C}$ of the surface V by

$$z_1 = i\cos w, \qquad z_2 = i\sin w. \tag{4.27}$$

The maps (4.26) can be lifted to $\hat{V}$ as

$$\hat{h}_1 w = -w, \qquad \hat{h}_2 w = -w + \pi. \tag{4.28}$$

Now $h = w + \pi$, so (4.25) becomes

$$\tilde{R}_1(w)\tilde{\psi}_2(w + \pi) - \tilde{R}_2(w)\tilde{\psi}_2(w) = \tilde{H}(w). \tag{4.29}$$

where $\tilde{R}_1$, etc, denote the liftings of the corresponding functions to the universal covering. The equation (4.29) holds for an appropriate region of $w \in \mathbb{C}$. Restricted to the strip $\operatorname{Re} w \in [0, \pi]$, this equation is the Riemann–Hilbert problem which can be solved in quadratures [30, Chs 17 and 18]. Let us recall some details.

The function $z = e^{2iw}$ analytically transforms the strip to the plane with the cut $[0, \infty)$. Denote the function $\check{\psi}_2(t) = \tilde{\psi}_2(w)$, $\check{H}(t) = \tilde{H}(w)$ and $\check{R}_k(t) = \tilde{R}_k(w)$ for $k = 1, 2$. Then relation (4.29) becomes

$$\check{R}_1(t)\check{\psi}_2(t - i0) - \check{R}_2(t)\check{\psi}_2(t + i0) = \check{H}(t), \qquad t > 0. \tag{4.30}$$

As the first step of the Riemann–Hilbert method, one must solve the corresponding homogeneous problem:

$$\check{R}_1(t)T(t - i0) - \check{R}_2(t)\check{T}(t + i0) = 0, \qquad t > 0. \tag{4.31}$$

Equivalently,

$$\frac{T(t + i0)}{T(t - i0)} = q(t) := \frac{\check{R}_1(t)}{\check{R}_2(t)}, \qquad t > 0. \tag{4.32}$$

The solution to this equation depends on zeros of the functions $\check{R}_1(t)$ and $\check{R}_2(t)$ for $t > 0$. Let us consider the simplest case when such zeros do not exist, and moreover,

$$q(0) = q(\infty) = 1. \tag{4.33}$$

Then the equation is equivalent to

$$\log T(t + i0) - \log T(t - i0) = \log q(t), \qquad t > 0. \tag{4.34}$$

The solution is given by the Cauchy-type integral

$$\log T(t) = \frac{1}{2\pi i} \int_0^\infty \frac{\log q(s)}{t - s} ds, \qquad t \in \mathbb{C} \setminus [0, \infty). \tag{4.35}$$

It is important that $T(t)$ is analytic and nonvanishing in the region $\mathbb{C} \setminus [0, \infty)$. Now the nonhomogeneous problem (4.30) can be solved as follows. First, (4.30) and (4.31) imply

$$\frac{\check{\psi}_2(t - i0)}{T(t - i0)} - \frac{\check{\psi}_2(t + i0)}{T(t + i0)} = \frac{\check{H}(t)}{\check{R}_1(t) T(t - i0)}, \qquad t > 0. \tag{4.36}$$

Therefore, similarly to (4.34),

$$\frac{\check{\psi}_2(t)}{T(t)} = -\frac{1}{2\pi i} \int_0^\infty \frac{\check{H}(s)}{\check{R}_1(s) T(s - i0)(t - s)} ds, \qquad t \in \mathbb{C} \setminus [0, \infty) \tag{4.37}$$

since the function $\frac{\check{\psi}_2(t)}{T(t)}$ is analytic in $\mathbb{C} \setminus [0, \infty)$.

Thus, we have calculated the function $\check{\psi}_2(t)$. Now $\psi_2(z)$ can be obtained from the relation (4.22). Hence, the functions $\hat{\varphi}_1(z_1)$ and $\hat{\varphi}_2(z_2)$ are known. It remains to substitute the obtained functions into the formula (4.7) for the function F. Then the solution to (3.2) is expressed by (4.12), which can be reduced to the integral of Sommerfeld type [24].

Remark 4.8. Equation (4.24) is obtained using the invariance (4.21) with $l = 1$, while (4.25) uses also $l = 2$. Note that the equation (4.24) reads now

$$\tilde{T}_1(w) \tilde{\psi}_2(-w) - \tilde{T}_2(w) \tilde{\psi}_2(w) = \tilde{H}(w), \tag{4.38}$$

which provisionally cannot be reduced to a nonsingular Riemann–Hilbert problem, see [33]. Thus, both invariance conditions (4.21) are necessary for the reduction.

Remark 4.9. For the random walks studied in [16, 36], the corresponding Riemann surface and the covering maps h_l can be more complicated than for 2-nd order elliptic operators which requires more sophisticated methods of the Galois theory.

5. Nonconvex angles of magnitude $\Phi > \pi$

The extension of the theory outlined above to the case of nonconvex angle Q differs drastically from the convex one. As an example, consider the Dirichlet boundary value problem in the angle $Q = \mathbb{R}^2 \setminus \mathbb{R}^+ \times \mathbb{R}^+$:

$$\left\{ \begin{array}{rcl} Au(x) & = & 0, \qquad x \in Q \\ u(x_1, 0) & = & f_1(x_1),\ x_1 > 0; \quad u(0, x_2) = f_2(x_2),\ x_2 > 0. \end{array} \right| . \tag{5.1}$$

Note that the relations (4.6) and (4.8), (4.12) remain true in this case, but now the function (4.7) is changed to its negative:

$$F(z) = -P_1(z)\hat{f}_1(z_1) - P_2(z)\hat{f}_2(z_2) - S_1(z)\hat{\varphi}_1(z_1) - S_2(z)\hat{\varphi}_2(z_2), \quad z \in \mathbb{R}^2. \tag{5.2}$$

On the other hand, the key relation (4.9) is not well defined in contrast to the case when the support of u belongs to a convex angle. This is due to the fact that the Fourier–Laplace transform (4.4) of the function u with the support in a nonconvex angle generally does not admit an analytical continuation to a region of $\mathbb{C}^2$. Nevertheless, the function (5.2) in this case is analytic in the same region $Z^+ = \mathbb{C}^+ \times \mathbb{C}^+$ as the function (4.7).

The answer to this riddle was found in [25]. First, the function (5.2) admits the splitting

$$\begin{aligned} F(z) &= \gamma_1(z) + \gamma_2(z), \\ \gamma_1(z) &= -P_1(z)\hat{f}_1(z_1) - S_1(z)\hat{\varphi}_1(z_1), \\ \gamma_2(z) &= -P_2(z)\hat{f}_2(z_2) - S_2(z)\hat{\varphi}_2(z_2), \end{aligned} \tag{5.3}$$

where the functions $\gamma_l(z)$ are analytic in the regions

$$V_l^+ = \{z \in V : \operatorname{Im} z_l > 0\}, \qquad l = 1, 2. \tag{5.4}$$

Second, as shown in [25] (see also [30, Theorem 20.1]), each function γ_l admits an analytic continuation from V_l^+ to the region $V^- := \{z \in V : \operatorname{Im} z_1 < 0, \operatorname{Im} z_2 < 0\}$, and the following identity holds:

$$\gamma_1(z) + \gamma_2(z) = 0, \qquad z \in V^-. \tag{5.5}$$

This identity formally coincides with the undetermined equation (4.10), and it allows us to calculate both unknown functions $\hat{\varphi}_l$ by methods of Sections 4.2 and 4.3.

6. Time-dependent diffraction by wedge

The time-dependent diffraction by a wedge W is described by the solution of the wave equation in the plane angle $Q = \mathbb{R}^2 \setminus W$ with appropriate boundary

conditions. For example, consider the Dirichlet boundary conditions

$$\left\{\begin{array}{rcl} \ddot{u}(x,t) &=& \Delta u(x,t), \quad x \in Q \\ u(x,t) &=& 0, \quad x \in \Gamma_1 \cup \Gamma_2 \end{array}\right|, \quad t \in \mathbb{R}. \tag{6.1}$$

The incident wave is defined by the initial condition

$$u(x,t) = u^{in}(x,t), \qquad u^{in}(x,t) := f(kx - \omega_0 t)e^{i(kx-\omega_0 t)}, \qquad t < 0, \tag{6.2}$$

where the frequency $\omega_0 \in \mathbb{R}$ and $k \in \mathbb{R}^2$ is the **wave vector**. The incident wave $u^{in}(x,t)$ must be a solution to (6.1) for $t < 0$:

$$\left\{\begin{array}{rcl} \ddot{u}^{in}(x,t) &=& \Delta u^{in}(x,t), \quad x \in Q \\ u^{in}(x,t) &=& 0, \quad x \in \Gamma_1 \cup \Gamma_2 \end{array}\right|, \quad t < 0. \tag{6.3}$$

The wave equation in (6.3) holds for any function $f(s)$ **for all** $t \in \mathbb{R}$ if $|k| = |\omega_0|$. The boundary condition in (6.3) can be satisfied only in the case of nonconvex angle Q of magnitude $\Phi > \pi$ and the wave vector k satisfying the inequalities $k \cdot x \geq 0$ for $x \in W = \mathbb{R}^2 \setminus Q$. Then for $\omega_0 > 0$ the boundary condition holds if

$$f(s) = 0, \qquad s > 0. \tag{6.4}$$

7. Limiting amplitude principle

Let us assume that there exists the limit

$$f(-\infty) := \lim_{s \to -\infty} f(s), \tag{7.1}$$

and the convergence is sufficiently fast, for example, $f(s) = \theta(-s)$. Then the incident wave (6.2) admits the long-time asymptotics

$$u^{in}(x,t) \sim f(-\infty)e^{ikx}e^{-i\omega_0 t}, \qquad t \to \infty \tag{7.2}$$

which suggests similar asymptotics of solution

$$u(x,t) \sim a_{\omega_0}(x)e^{-i\omega_0 t}, \qquad t \to \infty. \tag{7.3}$$

Such asymptotics are called as **limiting amplitude principle**.

Determination of the **limiting amplitudes** $a_{\omega_0}(x)$ for different diffraction processes is the main goal of the theory of diffraction [7, 66] (see also [30]). The proof of the asymptotics is the main goal of the mathematical theory of diffraction. For diffraction by wedges, this asymptotics has been established for the first time in [26]. Formal substitution of the asymptotics (7.3) into (6.1) gives a problem of type (3.1):

$$\left\{\begin{array}{rcl} -\omega_0^2 a_{\omega_0}(x) &=& \Delta a_{\omega_0}(x), \quad x \in Q \\ a_{\omega_0}(x) &=& 0, \quad x \in \Gamma_1 \cup \Gamma_2 \end{array}\right|. \tag{7.4}$$

However, this boundary problem is **ill-posed** since it admits an infinite number of linearly independent solutions for real $\omega_0 \in \mathbb{R}$. Thus, this problem does not allow us to find the limiting amplitude. This fact is the main peculiarity of the diffraction theory. This can be easily checked in the case $\Phi = \pi$ when the angle Q is the half-plane, so all solutions can be calculated by the Fourier transform along the boundary $\partial\Omega$. For the problems of type (7.4) in **convex angles** of magnitude $\Phi < \pi$, this nonuniqueness was discovered in 1973 by one of the authors [45].

Let us recall how to prove the asymptotics (7.3) and how to calculate the limiting amplitudes $a_{\omega_0}(x)$. First, note that for the incident wave $u^{in}(x,t)$ the asymptotics of type (7.3) holds by (7.1):

$$u^{in}(x,t) \sim f(-\infty)e^{ikx}e^{-i\omega_0 t}, \qquad t \to \infty. \tag{7.5}$$

The reflected wave is defined by geometric optics, and its main properties are as follows:

$$u^r(x,t) = -u^{in}(x,t), \quad x \in \partial Q; \qquad u^r(x,t) \sim a^r(x)e^{-i\omega_0 t}, \qquad t \to \infty. \tag{7.6}$$

The diffracted wave $u^d(x,t)$ is defined by the splitting the total solution as

$$u(x,t) = u^{in}(x,t) + u^r(x,t) + u^d(x,t). \tag{7.7}$$

Hence, it remains to calculate the corresponding asymptotics for the diffracted wave

$$u^d(x,t) \sim a^d_{\omega_0}(x)e^{-i\omega_0 t}, \qquad t \to \infty, \tag{7.8}$$

Substituting (7.7) into (6.1), using (7.6) and the fact that the wave equation in (6.3) holds for all $t \in \mathbb{R}$, we get the boundary problem for the diffracted wave

$$\left.\begin{cases} \ddot{u}^d(x,t) &= \Delta u^d(x,t) + F(x,t), \quad x \in Q \\ u^d(x,t) &= 0, \quad x \in \Gamma_1 \cup \Gamma_2 \end{cases}\right|,$$
$$F(x,t) := (\partial_t^2 - \Delta)u^r(x,t) \sim b(x)e^{-i\omega_0 t}, \ t \to \infty. \tag{7.9}$$

Formal substitution of the asymptotics (7.8) into (7.9), gives the boundary problem

$$\left.\begin{cases} -\omega_0^2 a^d_{\omega_0}(x,t) &= \Delta a^d_{\omega_0}(x) + b(x), \quad x \in Q \\ a^d(x) &= 0, \quad x \in \Gamma_1 \cup \Gamma_2 \end{cases}\right|. \tag{7.10}$$

For $\omega_0 \in \mathbb{R}$, this system also admits an infinite number of linearly independent solutions, as well as (7.4). Similar problem of nonuniqueness arises in every diffraction problem in unbounded regions. The problem of nonuniqeness was resolved by the discovery of additional features of the limiting amplitude $a^d_{\omega_0}(x)$.

The key discovery was the **limiting absorption principle** (3.4) for the limiting amplitude of the diffracted wave. In application to problem (7.10), we have

$$a^d_{\omega_0}(x) = \lim_{\varepsilon\to 0+} a^d_{\omega_0+i\varepsilon}(x), \qquad x \in Q, \tag{7.11}$$

where $a^d_{\omega_0+i\varepsilon}$ denotes a solution to (7.10) with $\omega_0 + i\varepsilon$ instead of ω_0.

Remark 7.1. The convergence (7.11) holds for the limiting amplitude $a^d_{\omega_0}(x)$ of the diffracted wave $u^d_{\omega_0}(x,t)$ (formal proof can be found in [30, Section 4.1]). However, it does not hold for the limiting amplitude $a(x)$ of the total solution $u(x,t)$ although these amplitudes satisfy quite similar equations (7.10) and (7.4). The difference is that the initial state of the diffracted wave $u^d_{\omega_0}(x,0)$ is of finite energy (in our case zero), while for the total solution the initial state $(u(x,0), \dot u(x,0))$ is the plane wave (6.2) and its derivative in time at $t = 0$.

The limiting absorption principle has been introduced for the first time in 1905 by W. Ignatovsky [19]. Rigorous proofs of this principle for limiting amplitudes of solutions with finite energy initial states were achieved much later. The results for the wave and Schrödinger equations in the entire space and for diffraction problems with smooth boundaries were obtained by Agmon [1], Eidus [13–15], Jensen and Kato [20], A.Ya. Povzner [52], B.R. Vainberg [67] and others.

The convergence (7.11) for **stationary diffraction problems** has been established for the first time in 1977 by one of the authors [45]: it was proven that stationary problem (7.10) and problems (3.2) with $A = \Delta + \omega^2$ and general boundary conditions in **convex angles** of magnitude $\Phi < \pi$,

i) for complex $\omega \notin \mathbb{R}$ admit only a finite number of linearly independent solutions in appropriate class of functions;

ii) for real $\omega \in \mathbb{R}$ admit an infinite number of linearly independent solutions,

iii) for real $\omega \in \mathbb{R}$ admit only a **finite number** of linearly independent solutions satisfying (7.11).

For the **time-dependent** diffraction problem (6.1), (6.2), the limiting absorption principle (7.11) and the limiting amplitude principle (7.3) were justified in 2006 by the authors [26]. The proofs rely on the analysis of the Fourier-Laplace transform in time:

$$\tilde u(x,\omega) = \int_0^\infty e^{i\omega t} u(x,t)dt, \qquad \omega \in \mathbb{C}^+. \tag{7.12}$$

The function $\tilde u(x,\omega)$ satisfies a boundary value problem of type (7.10) with complex $\omega \notin \mathbb{R}$. In this case the Helmholtz operator $A = \Delta + \omega^2$ is strongly elliptic. Hence, $\tilde u(x,\omega)$ can be calculated and analysed by the methods described in previous sections. The limiting amplitude is calculated in [26] using the limit (7.11).

Remark 7.2. In 1912, A. Sommerfeld discovered the **Sommerfeld radiation condition** [63] (see also [53]), which provides the uniqueness of solution to the boundary problem of type (7.10) in the case when Q is the exterior of a bounded region in $\mathbb{R}^3$. This condition is more practical for numerical calculation of the limiting amplitudes than (7.11).

8. The Sommerfeld diffraction theory and related results

For the angle $\Phi = 2\pi$, A. Sommerfeld constructed in 1896 a solution $a(x)$ to **stationary diffraction problem** of type (7.4) with Dirichlet and Neumann boundary conditions. In this case the wedge is the half-plane, which is represented by the semi-axis $[0, \infty)$ in the corresponding 2D problem. The main ideas were i) to treat the semi-axis as the cut on an appropriate Riemann surface, and ii) to extend the known method of reflections to Riemann surfaces. As a result, A. Sommerfeld constructed a universal integral representation of a class of **branching solutions** of the Helmholtz equation on the Riemann surface in the form of the **Sommerfeld integral** with a fixed integral kernel and a with a suitable density function. Further, A. Sommerfeld chose an appropriate densities to satisfy the boundary conditions.

Sommerfeld's strategy of constructing the solution remains a mysterious riddle to this day. This approach is reproduced with some comments in [30, Ch. 5], see also [49]. However, the Sommerfeld integral representation turned out to be extremely fruitful, and in particular, was used by G.D. Malujinetz to solve the problem with the Leontovich boundary condition [34, 35], see also [2].

For any angles $\Phi \in (0, 2\pi)$ the **stationary diffraction problem** (7.4) for the Dirichlet and Neumannn boundary conditions in the angles of this magnitude was solved by other methods in 1920 by H.S. Carslaw [8], in 1932–1937 by V.I. Smirnov and S.L. Sobolev [56–60], and in 1951 by J.B. Keller and A. Blank [21].

Remark 8.1.

i) In all the works, cited above, the limiting amplitude principle was not established, and the choice of suitable solution of the **ill-posed problem** (7.4) was not rigorously clarified. Nevertheless, as shown in [28, 29, 47], all the obtained solutions coincide with the **limiting amplitudes** calculated in [26] and admit the Sommerfeld representation.

ii) S.L. Sobolev mentions, in the articles cited above, that the functions of type (6.2) must be solutions to the wave equation even if the amplitude $a(s)$ is a discontinuous function. These remarks later inspired the theory of weak derivatives of S.L. Sobolev and the theory of distributions of L. Schwartz.

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Markov Processes Relat. Fields **29**, 515–532 (2023)

Markov Processes and **Related Fields**

Minimal Action Principle for Gravity and Electrodynamics, Einstein Lambda, and Lagrange Points

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Abstract. The relativistic equations of gravitation and electromagnetism in the form of Vlasov – Einstein – Maxwell equations are proposed and analyzed. For weakly relativistic equations we get an analog of Mealn – McCree solution. We also study Lagrange points in non-relativistic case with Einstein lambda-term.

Keywords: Minimal action principle, Vlasov equation, Einstein Lambda,Lagrange points, Vlasov – Einstein equations, Vlasov – Maxwell equations

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Introduction

Usually equations for gravitational and electromagnetic fields are proposed without deriving the functions on the right-hand sides (see [1–4]). This can be done within the Vlasov equations [5–11]. The accelerated expansion of the Universe, which is awarded the Nobel Prize in Physics in 2011 is in focus of contemporary research. The generally accepted explanation of this phenomenon is the addition of the Einstein lambda-term to the relativistic action, which in turn corresponds to adding a repulsive quadratic potential in non-relativistic theory

[41–43]. Here we propose a derivation and an investigation of the corresponding relativistic and weakly relativistic equations in the general case and for the Lorentz metric. We also study the Lagrange points in the non-relativistic case with Einstein lambda-term.

1. Action in general relativity and equations for fields and particles

Let us consider the classical action for electrodynamics and gravitation [1–4].

$$S = -cm \int \sqrt{g_{\mu\nu}(x,t)u^\mu u^\nu}\, dt - \frac{e}{c}\int A_\mu(x,t)u^\mu dt + k_1 \int (R+\Lambda)\sqrt{-g}\, d^4x + k_2 \int (F_{\mu\nu}F^{\mu\nu})\sqrt{-g}\, d^4x. \tag{1.1}$$

Here c is the speed of light, $u^0 = c$ and $u^i = \nu^i\,(i = 1,2,3)$ is three-dimensional speed, t is time, $x^0 = ct, x^i,\quad i = 1,2,3$, are coordinates, $g_{\mu\nu}(\chi,t)$ is a metric, $(\mu,\nu = 0,1,2,3)$, $A_\mu(\chi,t)$ [1–4] is the electromagnetic field potential, $F_{\mu\nu}(\chi,t) = \partial A_\mu(\chi,t)/\partial x^\nu - \partial A_\nu(\chi,t)/\partial x^\mu$ are electromagnetic fields, R is the total curvature, Λ is the Einstein lambda-term, $k_1 = -c^3/16\pi\gamma$ and $k_2 = -1/16\pi c$ are constants [1–4], g is the metric determinant $g_{\mu\nu}$, γ is the gravitational constant, the repeated indices are summed up. Action (1.1) is classical and fundamental, the 2-nd and 4-th terms belong to Maxwell, 1-st – to Einstein, when he introduced geometry into the theory of gravitation in general relativity, 3-rd – to Hilbert, all together was collected by Poincare, Born, Schwarzschild, Pauli and others (see [1–4]). Equations for particles and fields are derived from this action, but equations without right-hand parts are derived for fields [1–4]. This gap is covered in papers [5–11] by the following rather natural and simple method. To derive the equations for gravitational and electromagnetic fields, let us first rewrite action (1.1) by introducing a distribution function, Then we passing from the Lagrangian coordinates in the first two terms of action (1.1) to the Eulerian ones. Let $f\,(t,x,v,m,e)$ be the distribution function of particles in space $\mathbf{x} \in \mathbb{R}^3$, velocities $v \in \mathbb{R}^3$, masses $m \in \mathbb{R}^+$ and charge $e \in \mathbb{R}$ at the time $t \in \mathbb{R}$. This means that the number of particles in the volume $dxdvdmde$ is equal to $f\,(t,x,v,m,e)\,dx\,dv\,dm\,de$. We obtain the following action:

$$S = -c\int mf(t,\mathbf{x},\mathbf{v},m,e)\sqrt{g_{\mu\nu}u^\mu u^\nu}d^3x\,d^3\nu\,dm\,de\,dt - \frac{1}{c}\int ef(t,\mathbf{x},\mathbf{v},m,e)A_\mu u^\mu d^3x\,d^3\nu\,dm\,de\,dt + k_1\int (R+\Lambda)\sqrt{-g}d^4x + k_2\int F_{\mu\nu}F^{\mu\nu}\sqrt{-g}d^4x. \tag{1.2}$$

The type of action (1.2) is already suitable for deriving the Einstein and Maxwell equations when varying by fields $g_{\mu\nu}$ and A_μ. This way of deriving the Vlasov–

Maxwell and Vlasov – Einstein equations was used in [5–11]. When varying (1.1) by $g_{\mu\nu}$ we obtain the Einstein equation:

$$k_1\left(R^{\mu\nu}-\frac{1}{2}g^{\mu\nu}(R+\Lambda)\right)\sqrt{-g} = \int m\frac{f(t,x,\nu,m,e)}{2\sqrt{g_{\mu\nu}u^\mu u^\nu}}u^\mu u^\nu d^3\nu\, dm\, de - k_2(-2F^{\mu\nu}F^{\nu\beta}g_{\alpha\beta}+\frac{1}{2}F_{\alpha\beta}F^{\alpha\beta}g^{\mu\nu})\sqrt{-g}. \tag{1.3}$$

The first term of the right-hand side of this equation is the energy-momentum tensor by Hilbert's definition. It was first presented in [9–11] but in a less general form without the distribution of masses and charges. Attempts to write down the energy-momentum tensor via the distribution function were made, as far as we know, only in the relativistic kinetic theory in the framework of the Vlasov – Einstein equation [5–15]. However, the major difficulties were not resolved, as we will show below. The equation of electromagnetic fields is obtained by varying (1.1) by A_μ, it leads to the Maxwell equation:

$$k_2\frac{\partial\sqrt{-g}F^{\mu\nu}}{\partial x_\nu}=\frac{1}{c^2}\int eu^\mu f(t,x,\nu,m,e)d^3\nu\, dm\, de. \tag{1.4}$$

Let us show that the action form (1.1) is more general than (1) in [1–4]. To obtain the standard action form, let us take the distribution function as a δ-function for one particle.

$$f(x,\nu,m,e,t)=\delta\left(x-x'(t)\right)\delta(\nu-\nu'(t))\delta\left(m-m'\right)\delta(e-e'). \tag{1.5}$$

Substituting (1.4) into action (1.2) and omitting the sign of ($'$), we obtain action (1) in [1–4].

Electrons and ions in plasma, planets in galaxies, galaxies in supergalaxies, cluster of galaxies in the universe can play the role of particles. In equality (1.4) we can take the sum of delta functions and obtain usual action [1–4] for finite system of particles. This justifies the action (1.2) and the meaning of Eulerian and Lagrangian coordinate relations in kinetic theory. Thus we have obtained the equations for fields, and we need to derive the equations for particles for the distribution function. This is Vlasov's approach. The derivation of equations for particles has been done in [5–11], where the equations for the distribution function in velocities were derived. Next we will derive equation in momenta using the Hamiltonian approach, having in mind the aim to obtain the Hamilton-Jacobi equations for the case of the Vlasov – Maxwell – Einstein equation.

A historical remark should be made here. The equation appears under different names, as Vlasov – Poisson, Vlasov – Maxwell, Vlasov – Einstein, and even Vlasov – Yang – Mills, see particular the work of Choquet – Bruhat [13]. The

name Vlasov – Poisson equations is used for for gravity and plasma, Vlasov – Maxwell equations for electrodynamics and Vlasov– Einstein equations for relativistic gravity. In the case of Vlasov – Einstein equation, however, (mostly European) scientists worked in velocities [12–14], and correct corresponding equations were proved difficult to obtain.

The only author who set the task of deriving the Vlasov – Einstein equations from the principle of least action was Philip Morrison [15–17]. He worked in momentum, and using Hamiltonian dynamics he obtained correct equations for particles and the Liouville equation [16]. The equations for fields he got, however, by other (more difficult) methods [15–17].

Morrison's approach appear to be most natural: it is necessary to pass to momenta in equations for fields (1.2)–(1.3), but at first it is necessary to write down a relation of velocities and momenta according to the standard scheme of Hamiltonian mechanics. Hence, to obtain the equation of motion of a single particle in the given fields we begin to consider the first two terms of the action (1.1)

$$S = -cm \int \sqrt{g_{\mu\nu} u^\mu u^\nu} dt - \frac{e}{c} \int A_\mu u^\mu dt,$$

$$L = -cm\sqrt{g_{\mu\nu} u^\mu u^\nu} - \frac{e}{c} A_\mu u^\mu, \quad S = \int L dt$$

and introduce the momenta

$$p_\mu = \frac{\partial L}{\partial u^\mu} = -mc \frac{g_{\mu\alpha} u^\alpha}{\sqrt{g_{\eta\xi} u^\eta u^\xi}} - \frac{e}{c} A_\mu. \tag{1.6}$$

Here the expression for p_0 is obtained formally by differentiating by $u_0 = c$, $u_0 = c, u = (c, \nu)$. The equation of motion for particles we obtain already in the Hamiltonian form, where the Hamiltonian function is the zero-point component of the momentum expressed in terms of the mass relations. This is based on the fact that the Lagrangian is a first degree function on the four velocity components and the Euler formula: $u_\mu \frac{\partial L}{\partial u^\mu} - L = 0$, where $H = \nu^i \frac{\partial L}{\partial \nu^i} - L$ or $c\frac{\partial L}{\partial u^0} + H = 0$. Here the summation over i is three-dimensional, and over μ is four-dimensional. Thus, we obtain a simple formula for the Hamiltonian where the zero-point component of the momentum $p_0(x, p, t)$ should be expressed as the solution of the quadratic mass ratio equation through the three-dimensional momenta

$$\left(p_\alpha - \frac{e}{c} A_\alpha\right)\left(p_\beta - \frac{e}{c} A_\beta\right) g^{\alpha\beta} = (mc)^2, \tag{1.7}$$

and then

$$H = -u^0 \frac{\partial L}{\partial u^0} = -cp_0(x, p, t). \tag{1.8}$$

This gives us an expression for both the velocities, $\nu^i = \frac{\partial H}{\partial p_i} = \nu^i(p) = -c\frac{\partial p_0}{\partial p_i}$, and the forces $-c\frac{\partial p_0}{\partial x_i}$. We can write down now the Liouville equations in the

usual form

$$\frac{\partial f}{\partial t} + \{f, H\} = 0, \tag{1.9}$$

where $\{f, H\} = \frac{\partial H}{\partial p_i}\frac{\partial f}{\partial x^i} - \frac{\partial H}{\partial x^i}\frac{\partial f}{\partial p_i}$ is the Poisson bracket. We have to rewrite Einstein's equations (1.2) using the distribution function in momentum to close the equations for gravitation and electrodynamics in momentum. We shall take advantage of the fact that the invariant is the number of particles

$$f(t, x, \nu, m, e)dxd\nu dmde = f(t, x, p, m, e)dxdpdmde,$$

and we shall express velocities through impulses. This leads to

$$\begin{aligned} k_1 &\left(R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}(R + \Lambda)\right)\sqrt{-g} \\ &= c\int m\frac{f(t, \chi, p, m, e)}{2}\frac{(p_\mu - \frac{e}{c}A_\mu)(p_\nu - \frac{e}{c}A_\nu)}{(p^0 - \frac{e}{c}A^0)(mc)^2}d^3p\,dm\,de \\ &\quad - k_2(-2F^{\mu\alpha}F^{\nu\beta}g_{\alpha\beta} + \frac{1}{2}F_{\alpha\beta}F^{\alpha\beta}g^{\mu\nu})\sqrt{-g}, \end{aligned} \tag{1.10}$$

and Maxwell's equation (1.3)

$$k_2\frac{\partial F_\mu{}^\nu}{\partial x^\nu}\sqrt{-g} = \frac{1}{c^2}\int e(p_\mu - \frac{e}{c}A_\mu)f(t, \chi, p, m, e)d^3p\,dm\,de. \tag{1.11}$$

The system of equations (1.9)–(1.11) with the Hamiltonian (1.8) is the system of the Vlasov – Maxwell – Einstein equations.

Let us derive some other forms of the equations of gravitation and electrodynamics, namely the hydrodynamic and Hamilton – Jacobi equation. The hydrodynamic form is obtained by means of the hydrodynamic substitution $f(t, x, p, m) = \rho(t, \chi, m, e)\ \delta(p - Q(t, x, m, e))$, which is a limiting case of the Maxwell distribution at temperature tending to zero. Following the general scheme [5–11,22–26] we get the straightforward consequence of equations (1.9)–(1.11):

$$\frac{\partial p}{\partial t} - \frac{\left(pc\frac{\partial p_0}{\partial p_i}(x, Q)\right)}{\partial x^i} = 0, \tag{1.12}$$

$$p\left(\frac{\partial Q_k}{\partial t} - (c\frac{\partial p_0}{\partial p_i}(x, Q))\frac{\partial Q_k}{\partial x^i} + c\frac{\partial p_0}{\partial x^k}(x, Q)\right) = 0, \tag{1.13}$$

$$\begin{aligned} k_1 &\left(R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}(R + \Lambda)\right)\sqrt{-g} \\ &= c\int m\frac{\rho(t, \chi, m, e)}{2}\frac{(Q_\mu - \frac{e}{c}A_\mu)(Q_\nu - \frac{e}{c}A_\nu)}{g^{0\alpha}(Q_\alpha - \frac{e}{c}A_\alpha)(mc)^2}dm\,de \end{aligned}$$

$$-\frac{1}{2}k_2 F_{\alpha\beta}F^{\alpha\beta}g_{\mu\nu}\sqrt{-g}, \tag{1.14}$$

$$k_2\frac{\partial F_\mu{}^\nu}{\partial x^\nu}\sqrt{-g} = \frac{1}{c^2}\int e\left(Q_\mu - \frac{e}{c}A_\mu\right)\rho(t,\chi,m,e)dm\,de. \tag{1.15}$$

Here (1.12) is the continuity equation, and the system (1.12)–(1.15) describes the gas dynamics of a self-gravitating charged gas. To obtain the Hamilton – Jacobi consequence, we must, according to the general scheme for Hamiltonian systems [18–26] by E. Madelung, V.V. Kozlov and ours, substitute $Q = \nabla W$ in equation (1.12)–(1.15). This substitution suits exactly the Hamiltonian systems [18–26], allowing us to obtain one Hamilton – Jacobi equation instead of three equations (1.13)

$$\left(\frac{\partial W}{\partial x^\alpha} - \frac{e}{c}A_\alpha\right)\left(\frac{\partial W}{\partial x^\beta} - \frac{e}{c}A_\beta\right)g^{\alpha\beta} = (mc)^2\,. \tag{1.16}$$

Combining equations (1.12), (1.14), (1.15), where we also have to replace Q_μ with $\frac{\partial W}{\partial x^\mu}$, together with equation (1.16), we get the Hamilton-Jacobi consequence of the Vlasov – Maxwell – Einstein equations.

Hence, we have obtained three forms of the Maxwell – Einstein – Vlasov equations. Using momentum, we avoided the appearance of Christopher symbols. The meaning of Vlasov-type equations becomes clear: this is the only form of equations that provides a closed system of equations of gravitation and electrodynamics. Furthermore, this is derived solely from the principle of least action – a cherished dream of Euler, Lagrange, Newton, Maxwell and Einstein. Thus, gravity and electrodynamics became rigorous mathematics. Other consequences we will discuss elsewhere, but here we shall provide a few examples.

2. Lorentz metric and Einstein's lambda

Let us consider the following action

$$\begin{aligned} S = -c\int m\Big[\sqrt{g_{\mu\nu}u^\mu u^\nu} + \frac{\mathrm{U}}{c}\Big]f\,(t,x,\mathrm{v},m)\,dx\,d\mathrm{v}\,dm\,dt \\ -\frac{1}{8\pi\gamma}\int(\nabla\mathrm{U})^2\,dx\,dt + \frac{c^2\Lambda}{8\pi\gamma}\int \mathrm{U}dx\,dt, \end{aligned} \tag{2.1}$$

where $g_{\mu\nu} = diag(1,-1,-1,-1)$ is the Lorentz metric. Here $f\,(t,x,v,m)$ is the distribution function of particles (galaxies, super-galaxies) in space x, velocities v, masses m at time t, U is a gravitational field potential, γ is the gravitational constant, Λ is the Einstein lambda-term. Varying by U, we obtain the following equations for fields:

$$\Delta\mathrm{U} = 4\pi\gamma\int mf\,(t,x,\mathrm{v},m)\,d\mathrm{v}dm - \frac{1}{2}c^2\Lambda. \tag{2.2}$$

Let us pass to the action for one particle. As it is usually done in the derivation of equation for particles in given fields [1–15], we substitute $f(t, X, V, M) = \delta(x - X)\delta(v - V)\delta(m - M)$,

$$S = -cm \int \left[\sqrt{c^2 - u^2} + \frac{U}{c} \right] dt. \tag{2.3}$$

For this action, the Lagrangian and the Hamiltonian are given by

$$L(x, v) = -mc\sqrt{c^2 - u^2} - mU, \tag{2.4}$$

$$H(x, p) = mc^2 \sqrt{1 + \frac{p^2}{(mc)^2}} + mU. \tag{2.5}$$

Thus, we can obtain the equation of motion and the Liouville equation for the Hamiltonian system

$$\frac{\partial f}{\partial t} + \left(\frac{\partial H}{\partial p}, \frac{\partial f}{\partial x} \right) - \left(\frac{\partial H}{\partial x}, \frac{\partial f}{\partial p} \right) = 0,$$

or in our case

$$\frac{\partial f}{\partial t} + \frac{1}{\sqrt{1 + \frac{p^2}{(mc)^2}}} \left(\frac{p}{m}, \frac{\partial f}{\partial x} \right) - m \left(\frac{\partial U}{\partial x}, \frac{\partial f}{\partial p} \right) = 0. \tag{2.6}$$

The system of the following equations is the Vlasov – Poisson system for our action with the Lorentz metric

$$\frac{\partial f}{\partial t} + \frac{1}{\sqrt{1 + \frac{p^2}{(mc)^2}}} \left(\frac{p}{m}, \frac{\partial f}{\partial x} \right) - m \left(\frac{\partial U}{\partial x}, \frac{\partial f}{\partial p} \right) = 0,$$

$$\Delta U = 4\pi\gamma \int m f(t, \mathbf{x}, \mathbf{p}, m)\, d\mathbf{p} dm - \frac{1}{2} c^2 \Lambda.$$

Let us proceed to the hydrodynamic consequences of this system. For this purpose we substitute $f(t, x, p, m) = \delta(p - Q(t, x))$, where Q is the macroscopic momentum. For an arbitrary system $\frac{dx}{dt} = v(x, t)$, $\frac{dp}{dt} = g(x, p)$ we obtain the following consequence of the Liouville equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho \nu_i(x, Q)}{\partial x^i} = 0,$$

$$\rho \left(\frac{\partial Q_k}{\partial t} + \nu_i(x, Q) \frac{\partial Q_k}{\partial x^i} - g_k(x, Q) \right) = 0.$$

Also, if we consider a Hamiltonian system, a further substitution takes place $Q = \nabla W$ [16-26], and we obtain the following relations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho \nu_i \left(x, \Delta W\right)}{\partial x^i} = 0,$$

$$\rho \frac{\partial}{\partial x_k} \left(\frac{\partial W}{\partial t} + H\left(x, \Delta W\right) \right) = 0.$$

Substituting the Hamiltonian of our system

$$H\left(x,p\right) = mc^2 \sqrt{1 + \frac{p^2}{\left(mc\right)^2}} + mU$$

we obtain a hydrodynamic-Hamilton – Jacobian consequence of our weakly relativistic system of Vlasov – Poisson equations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho \nu_i \left(x, \nabla W\right)}{\partial x^i} = 0,$$

$$\frac{\partial W}{\partial t} + c\sqrt{\left(mc\right)^2 + \left(\nabla W\right)^2} + mU(x) = 0, \tag{2.7}$$

$$\Delta U = 4\pi\gamma \int m\rho dm - \frac{1}{2}c^2\Lambda,$$

where

$$\nu\left(x,p\right) = \frac{p}{m\sqrt{1 + \frac{p^2}{\left(mc\right)^2}}}.$$

Let us now consider the equations in the isotropic case, i.e. when $U = U\left(r,t\right)$, $W = W\left(t,r,m\right)$, $r = \sqrt{x_1^2 + x_2^2 + x_3^2}$.

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x^i} \left(\frac{\rho c W' x_i}{r\sqrt{\left(mc\right)^2 + \left(W'\right)^2}} \right) = 0,$$

$$\frac{\partial W}{\partial t} + c\sqrt{\left(mc\right)^2 + \left(W'\right)^2} + mU\left(x\right) = 0,$$

$$3\left(\frac{U'}{r}\right) + r\left(\frac{U'}{r}\right)' = 4\pi\gamma \int m\rho\, dm - \frac{1}{2}c^2\Lambda.$$

We denote by $W', U' \ldots$ the differentiation over r. From the third equation in the cosmological case, i.e. when the density does not depend on the coordinate $\rho\left(x,m,t\right) = \rho\left(m,t\right)$ the following form of the potential follows:

$$U = \frac{r^2 B\left(t\right)}{6} - \frac{D\left(t\right)}{r},$$

where $B(t) = 4\pi\gamma \int m\rho dm - \frac{1}{2}c^2\Lambda$. Considering the cosmological case, one can also transform the first two equations:

$$\frac{\partial\rho}{\partial t} + \rho\frac{\partial}{\partial x^i}\left(\frac{cW'x_i}{r\sqrt{(mc)^2 + (W')^2}}\right) = \frac{\partial\rho}{\partial t} + 3H\rho = 0,$$

H is Hubble constant, from the definition of which it follows that

$$H = \varphi + \frac{r}{3}\varphi',$$

where φ satisfies

$$\varphi = \frac{cW'}{r\sqrt{(mc)^2 + (W')^2}}.$$

The solution to the last equation is the function $\varphi = H + \frac{A(t)}{r^3}$. Thus we have obtained a system of equations for cosmological solution of Vlasov–Poisson system with Lorentz metric:

$$\begin{gathered}
\frac{\partial\rho}{\partial t} + 3H\rho = 0, \\
\frac{\partial\rho}{\partial t} + \frac{\partial\rho\nu_i(x, \nabla W)}{\partial x^i} = 0, \\
\frac{W'}{\sqrt{(mc)^2 + (W')^2}} = \frac{1}{c}\left(rH + \frac{A(t)}{r^2}\right), \\
\frac{\partial W}{\partial t} + c\sqrt{(mc)^2 + (W')^2} + mU(x) = 0.
\end{gathered} \tag{2.8}$$

Let us denote $\alpha(r,t) = \frac{1}{c}(rH + A(t)/r^2)$, $S = W'$. Then from the second equation we obtain

$$S = \frac{mc\alpha}{\sqrt{1-\alpha^2}}, \quad \dot{S} = \frac{mc\dot{\alpha}}{(1-\alpha^2)^{3/2}}, \quad S' = \frac{mc\alpha'}{(1-\alpha^2)^{3/2}}.$$

We denote by $\dot{S}$ the differentiation with respect to t. Let us differentiate the last equation (2.8) with respect to r:

$$\frac{\partial S}{\partial t} + c\frac{SS'}{\sqrt{(mc)^2 + S^2}} + mU'(x) = 0, \quad \frac{mc\dot{\alpha}}{(1-\alpha^2)^{\frac{3}{2}}} + c\frac{mc\alpha'\alpha}{(1-\alpha^2)^{\frac{3}{2}}} + mU'(x) = 0,$$

or

$$\left(c\dot{\alpha} + c^2\alpha'\alpha\right)^2 - \left(U'(x)\right)^2\left(1-\alpha^2\right)^3 = 0.$$

Thus, if we substitute

$$\alpha(r,t) = \frac{1}{c}\Big(rH(m,t) + \frac{A(t)}{r^2}\Big),$$
$$\dot{\alpha}(r,t) = \frac{1}{c}\Big(rH(\dot{m},t) + \frac{\dot{A}(t)}{r^2}\Big),$$
$$\alpha'(r,t) = \frac{1}{c}\Big(H(m,t) - \frac{2A(t)}{r^3}\Big)$$

into this equation, we obtain the following expression

$$\Big(r\dot{H} + \frac{\dot{A}}{r^2} + \Big(rH + \frac{A}{r^2}\Big)\Big(H - \frac{2A}{r^3}\Big)\Big)^2 - \Big(\frac{rB}{3} + \frac{D}{r^2}\Big)^2\Big(1 - \Big(rH + \frac{A}{r^2}\Big)^2\Big)^3 = 0.$$

Opening the brackets in this equation, on the left we get an expression which is rational in r. Therefore, the coefficients for all degrees of r in this expression have to be zero. Let us consider the coefficient at r^8. After opening the first term, the degree of r is not greater than 2, when opening the second, we get the only term with the degree $\frac{r^8H^6B^2}{3}$, and therefore, $H^6B^6 = 0$. Assuming that $B(t) = 4\pi\gamma\int m\rho(m,t)\,dm - \frac{1}{2}c^2\Lambda \neq 0$, we obtain $H = 0$.

$$\Big(\frac{\dot{A}}{r^2} - \frac{2A^2}{r^5}\Big)^2 - \Big(\frac{rB}{3} + \frac{D}{r^2}\Big)^2\Big(1 - \Big(\frac{A}{r^2}\Big)^2\Big)^3 = 0.$$

We conclude that $B = 0$ considering the coefficient atr^2. Assuming now that $B(t) = 4\pi\gamma\int m\rho(m,t)\,dm - \frac{1}{2}c^2\Lambda = 0$, we have the following

$$\Big(r\dot{H} + \frac{\dot{A}}{r^2} + \Big(rH + \frac{A}{r^2}\Big)\Big(H - \frac{2A}{r^3}\Big)\Big)^2 - \Big(\frac{D}{r^2}\Big)^2\Big(1 - \Big(rH + \frac{A}{r^2}\Big)^2\Big)^3 = 0.$$

Then the coefficient $atr^(-16)$ is equal to $A^6D^2/3$. Therefore, either $D = 0$, $U(x) = 0$, or $A = 0$, $\big(r\dot{H} + rH^2\big)^2 - \big(\frac{D}{r^2}\big)^2\big(1 - (rH)^2\big)^3 = 0$ which still implies that $D = 0$, $U(x) = 0$. Thus, a cosmological solution for a relativistic action in the Lorentz metric exists only when $U(x) = 0$. We also obtained the equation for H:

$$\dot{H} + H^2 = 0 \tag{2.9}$$

Let us collect our results in the following theorem.

Theorem. For the action (2.1) the equation for fields (2.2) and the equation of motion with Lagrangian (2.3) and Hamiltonian (2.5) hold. The equation of motion yields the proper Liouville equation (2.6) and a system of Vlasov–Poisson equations (2.2), (2.6) for Minkowski metric. The latter system implies Hamilton–Jacobi consequence (2.7), from which one gets its cosmological version (2.8). System of equations (2.8) have the only non-trivial solution (2.9) for Hubble constant with exact expressions for W and U.

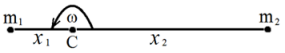

Figure 1.

We obtained in [38,39] a non-relativistic analogue of the Friedman equations generalizing the Milne – McCree solution [33,34] in various directions. In particular, we introduced the lambda term, we introduced the repulsion of substance by analogy with Coulomb, and moved to the Hamilton – Jacobi equation. We also raised the question of the dependence of the Hubble constant on the mass and charge of the substance. Here we have obtained an analogue of such solutions for Lorentz metric.

2.1. Lagrange points in the potential $U(r) = -\frac{\gamma}{r} - \frac{c^2\Lambda}{12}r^2$ and features of motion

Let us consider the features of Lagrange points in the potential that takes into account the lambda term [35–43].

Triangular libration point in the interaction of masses under the action of an central force Let us consider the circular problem of two bodies (Fig. 1). Two masses m_1 and m_2 are located at the distance $a = r_1 + r_2$ from each other, they are attracted by the central force according to the law $F = m_1 m_2 f(a)$, and rotate with angular velocity ω relative to the point C. From the balance equation of gravitational and centrifugal forces

$$m_1\omega^2 r_1 = m_1 m_2 f(a), \quad m_2\omega^2 r_2 = m_1 m_2 f(a), \quad a = r_1 + r_2. \tag{2.10}$$

We find that $m_1 r_1 = m_2 r_2$ that is, the point is the center of mass. Thus, when rotating around its center of mass the masses m_1, m_2 will be stationary. A small mass which is stationary in this coordinate system, is called a libration point.

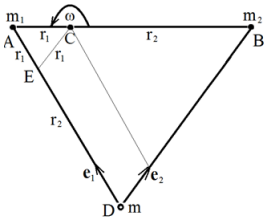

Figure 2.

Lagrange [44] in 1772 showed that a small mass m located at the vertex of an equilateral triangle is a libration point (Fig. 2). This libration point is called

triangular. The most general result in the problem under consideration was obtained by Lyapunov [45,46]. For a function $f(r)$ inversely proportional to the n degree of distance, the triangular libration point is also a libration point, and it is stable in linear approximation at

$$\frac{(m_0+m_1+m_2)^2}{m_0m_1+m_0m_2+m_1m_2} > 3\Big(\frac{1+n}{3-n}\Big)^2.$$

For $n=2, m_0=0$ the classical Gasho stability condition, obtained in 1843, follows from this

$$0<27\mu\,(1-\mu)<1, \quad \mu=\frac{m_2}{m_1+m_2} \Rightarrow 0<\mu<0.03852. \tag{2.11}$$

To solve the problem of the influence of linear force on the stability of equilibrium positions of triangular libration points, we prove the following general result.

Theorem. A triangular point is a libration point at any central force $F = m_1m_2f\,(r)$.

Proof. From the balance equation for the attraction forces and centrifugal forces (2.10) it follows

$$m_2f\,(a)=\omega^2r_1, \quad m_1f\,(a)=\omega^2r_2. \tag{2.12}$$

Now consider an equilateral triangle ABD. The masses m_1 and m_2 are located at the points A, B and the small mass is located at the point D (Fig. 2). The forces of attraction $mm_1f(a)$ and $mm_2f(a)$, directed along the unit vectors e_1 and e_2, act on the small mass m from the side of the masses m_1 and m_2. The total force of attraction using (2.1) is reduced to the following

$$\begin{aligned} F_1+F_2 &= m\,(m_1f\,(a)\,\mathbf{e}_1+m_2f\,(a)\,\mathbf{e}_2) \\ &= m\left(\omega^2r_2\mathbf{e}_1+\omega^2r_1\mathbf{e}_2\right)=m\omega^2\,(r_2\mathbf{e}_1+r_1\mathbf{e}_2)\,. \end{aligned}$$

From the parallelogram rule in Fig. 2 we get $r_2\mathbf{e}_1+r_1\mathbf{e}_2=\overrightarrow{DC} \Rightarrow F_1+F_2=m\omega^2\overrightarrow{DC}$. Thus, the sum of the forces of attraction acting on the mass is directed opposite to the vector of centrifugal force, with the same magnitude. The sum of the centrifugal force and the forces of attraction is zero. Hence, the mass m located at the vertex D of the right triangle is in equilibrium, and thus is the libration point.

2.2. Interactions according to Newton's law of gravitation with the addition of a linear force

Let us consider the case of masses interaction, in which the interaction force has the following form

$$F=m_1m_2f\,(r)\,, \quad f\,(r)=-\frac{dU}{dr}=-\frac{\gamma}{r^2}+\frac{c^2\Lambda}{6}r.$$

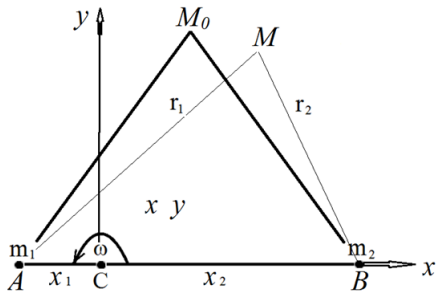

Figure 3.

This law differs from the classical one in the presence of a linear repulsive force. According to the theorem proved above, the point D in Fig. 2 and the symmetric point M_0 in Fig. 3 are libration points. Let us construct a Lagrange function for the perturbed motion of a mass m located at a point M in Fig. 3. An equilateral triangle AM_0B has sides of a length. At the apex of the equilateral triangle AM_0B, the small mass is in equilibrium at the apex of M_0. In the vicinity of equilibrium at the M point, the motion of the small mass is described by the Lagrange equations, with the Lagrange function

$$L = \frac{1}{2}\left(\dot{x}^2 + \dot{y}^2\right) + \omega\left(x\dot{y} - y\dot{x}\right) + \frac{\omega^2}{2}\left(x^2 + y^2\right) - V,$$

$$\omega^2 = \frac{m_1 + m_2}{a}\Big(\frac{\gamma}{a^2} - \frac{c^2\Lambda}{6}a\Big), \quad V = -m_1\Big(\frac{\gamma}{r_1} - \frac{c^2\Lambda}{12}r_1^2\Big) - m_2\Big(\frac{\gamma}{r_2} - \frac{c^2\Lambda}{12}r_2^2\Big).$$

For $\Lambda = 0$ we obtain the classical case. The dimensionless form of the equations is obtained by the following substitution:

$$x = aX, \quad y = aY, \quad \dot{x} = a\dot{X}\omega, \quad \dot{y} = a\dot{Y}\omega,$$
$$\frac{c^2\Lambda}{6} = \frac{\gamma}{a^3}\lambda, \quad r_1 = aR_1, \quad r_2 = aR_2.$$

This transforms the equilateral triangle AM_0B into a triangle with unit sides. The dimensionless Lagrange function has the following form

$$\frac{1}{2}\left(\dot{X}^2 + \dot{Y}^2\right) + \left(X\dot{Y} - Y\dot{X}\right) + \frac{1}{2}\left(X^2 + Y^2\right) - V_1,$$

$$V_1 = -\Big(\frac{1-\mu}{R_1} + \frac{\mu}{R_2}\Big) - K\Big[\Big(\frac{1-\mu}{R_1} + \frac{\mu}{R_2}\Big) + (1-\mu)\,R_1 + \mu R_2\Big],$$

$$K = \frac{\lambda}{1-\lambda}, \quad \mu = \frac{m_2}{m_1 + m_2}.$$

The coordinates of the apex of an equilateral triangle $X = \frac{1}{2} - \mu, Y = \frac{\sqrt{3}}{2}$ determine the equilibrium point of the system. We make the substitution as follows $X = \frac{1}{2} - \mu + q_1$, $Y = \frac{\sqrt{3}}{2} + q_2$ and find the Hamiltonian of motion of the system in the vicinity of the equilibrium point. The Hamiltonian function of the linear approximation is

$$H = \frac{1}{8}\left(4{p_1}^2 + 8p_1q_2 + 4{p_2}^2 - 8p_2q_1 + {q_1}^2 + 6\sqrt{3}(2\mu - 1)q_1q_2 - 5{q_2}^2\right) + \frac{1}{8}K\left(-3{q_1}^2 + 6\sqrt{3}(2\mu - 1)q_1q_2 - 9{q_2}^2\right). \tag{2.13}$$

Hamilton's linear equations

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}$$

have two pairs of eigenvalues $l_2 = -l_1$, $l_4 = -l_3$, differing in sign. Their squares can be reduced to the following form, convenient for analysis:

$$\begin{aligned} {l_1}^2 &= \frac{1}{2}\left(-\sqrt{(1-3K)^2 - 27M(1+K)^2} - (1-3K)\right), \\ {l_3}^2 &= \frac{1}{2}\left(\sqrt{(1-3K)^2 - 27M(1+K)^2} - (1-3K)\right), \\ K &= \frac{\lambda}{1-\lambda}, \quad M = \mu - \mu^2, \quad \lambda = \frac{c^2\Lambda a^3}{6\gamma}, \end{aligned}$$

where λ is dimensionless lambda term. Under the condition

$$M < M_*(K) = \frac{1}{27}\left(\frac{1-3K}{1+K}\right)^2, \quad K < \frac{1}{3},$$

the eigenvalues are purely imaginary and the equilibrium is stable in the linear approximation. At $K = 0 \Rightarrow \lambda = 0$ we obtain the classical result (2.11) of Gascheau G. – 1843, (see [46]) on the stability of the libration point in the linear approximation. The stability conditions are given in terms of initial parameters as follows

$$\begin{aligned} \mu < \mu_*(\lambda) &= \left(9 - \sqrt{-192\lambda^2 + 96\lambda + 69}\right) \\ &= \frac{2(1-4\lambda)^2}{3\left(\sqrt{-192\lambda^2 + 96\lambda + 69} + 9\right)}, \quad \lambda < \frac{1}{4}. \end{aligned} \tag{2.14}$$

The $\mu_*(\lambda)$ relationship is shown in the graph.

If this condition is not met, then one of the eigenvalues has a positive real part, whence follows the exponential instability. From the instability in linear approximation by Lyapunov theorem follows the instability of the exact nonlinear problem. Under condition (2.13) the stability of the nonlinear problem

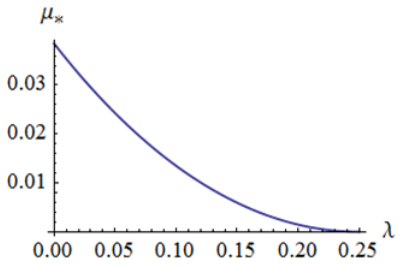

Figure 4.

is possible and, as studies of the classical case show, the stability of nonlinear problem follows, except for a finite number of values of parameters μ, λ.

We summarize our results in the following theorem.

Theorem. For any potential dependent only on distance the Lagrangian points are the same as in classical case. For Lagrange points in the potential $U(r) = -\frac{y}{r} - \frac{c^2\Lambda}{12}r^2$ all deviations are ruled by Hamiltonian (2.12). The conditions of stability of those points have the form (2.13). For $\Lambda = 0$ we obtain the classical result of Gascheau G. 1843 [46] on the stability of libration point in the linear approximation.

Conclusion

We have demonstrated a way to obtain the equations of gravitation from the principle of least action in the closed form, and this is the form of Vlasov's equation (cf. [5–15]). This tells us the Vlasov type equations is the only way to obtain both the gravitation equation and the equations of electrodynamics from the principle of least action. It is also the only way so far to close the system of equations of gravitation and electrodynamics using the principle of least action, using the distribution function of objects (as e.g., electrons, ions, stars in galaxies, galaxies in supergalaxies or in the universe) by velocity and space. The corresponding hydrodynamic level equations (e.g. magnetic hydrodynamics equations) are also naturally obtained from the Vlasov-type equations by hydrodynamic substitution (so far the only way to relate the latter equations to the classical action).

It is of considerable interest to investigate different classes of solutions to the equations obtained, as was done in [27–31]. Of particular interest should be the asymptotic behavior of the solutions to the Vlasov equations, and its analogy with the Liouville equation [30–32] might help. We have also shown that the obtained Vlasov-type equations should be applied to explain the evolution of the Universe, because it is from the Vlasov – Poisson equation that the nonrelativistic analogues of Friedmann solutions, the Milne – McCree solutions [33,34]

follow. Moreover, they are an exact consequence of the Vlasov – Poisson equation, so they are obtained without the heuristic assumptions of the papers [33,34] and justify and generalize them. These solutions made it possible to clarify the role of the Lambda term, its equivalence to the potential $U(r) = -\frac{y}{r} - \frac{c^2\Lambda}{12}r^2$ and the equivalence of this to any homogeneous substance associated with the solution of the Poisson equation [38–39]. The right-hand side of the Einstein equation gives hope for an explanation of the accelerated expansion of the Universe without these additional assumptions.

Finally, the dependence of the boundary of stable equilibrium positions of a small mass at the triangular point of libration is obtained. The parameter for the stable positions varies within certain limits. It would be useful to extend the results about libration points to the relativistic case.

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Markov Processes and **Related Fields**

Persistence in Perturbed Contact Models in Continuum

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Abstract. Can a local disaster lead to extinction? We answer this question in this work. In the paper [19] we considered contact processes on locally compact metric spaces with state dependent birth and death rates and formulated sufficient conditions on the rates that ensure the existence of invariant measures. One of the crucial conditions in [19] was the critical regime condition, which meant the existence of a balance between birth and death rates in average. In the present work, we reject the criticality condition and suppose that the balance condition is violated. This implies that the evolution of the correlation functions of the contact model under consideration is determined by a nonlocal convolution type operator perturbed by a (negative) potential. We show that local peaks in mortality do not typically lead to extinction. We prove that a family of invariant measures exists even without the criticality condition and these measures can be described using the Feynman-Kac formula.

Keywords: inhomogeneous contact model, stationary measure, correlation functions, Feynman-Kac formula, persistence and extinction

AMS Subject Classification: 82B21, 82C22, 60K35

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1. Introduction

The contact processes on the lattice have been introduced in the pioneer papers of Harris [4], Holley and Liggett [5], see also the monograph of Liggett [14]. In recent years, the study of contact processes running in continuous spaces has attracted great interest, see e.g. [6, 7, 10]. This class of processes is a particular case of continuous time birth and death processes, and particle configurations

in continuum appeared to be more adapted to modeling evolutions in various biological systems and models of population dynamics.

Taking into account applications of the contact processes as models describing a spread of epidemic diseases or a population growth, one of the main problem under consideration is to determine the parameters of the model providing stationary regime and to prove the existence of invariant measures. The appearance of limiting invariant states was proved only in the so-called critical regime, see e.g. [18, 19], that is, when there is a certain stochastic balance between birth and death. As was shown in [6], there exists a continuum of invariant measures for the contact processes in $\mathbb{R}^d,\ d \geq 3$, in the critical regime with a constant death rates. In small dimensions $d = 1, 2$, the existence of the stationary regime depends on the behavior of the dispersal kernel at infinity. It was proved in [7] that for the contact processes in $\mathbb{R}^d,\ d = 1, 2$, invariant measures exist only if the dispersal kernel has a heavy tail at infinity. In the case of light tails the pair correlation function grows to infinity as $t \to \infty$, and hence invariant measures do not exist. Thus heavy tails of dispersal kernels appear to make the critical regime more stable contrary to light tails.

The existence of invariant measures in the marked contact model in $\mathbb{R}^d,\ d \geq 3$, with a compact spin space and for constant death rates was proved in [9]. Such models are used, in particular, to describe evolution in quasi-species populations with mutations, see [15].

A more general framework has been investigated in [18], where we have formulated conditions providing the existence of a one-parameter family of invariant measures in contact processes on general locally compact separable metric spaces. One of the conditions, the so-called transience condition, was formulated in terms of the associated Markov jump process. It means that any pair of independent trajectories of this jump process run away from each other. The transience condition is not needed for a special class of contact processes - the contact processes with immigration. For such processes a unique invariant measure exists in any dimension, see [3], [17].

In the present work, we consider contact processes without the assumption of criticality. We will show that local violation of criticality due to excess mortality does not destroy invariant measures, but only perturbs them. A similar phenomenon exists in the theory of Schrödinger operators, when local positive potentials do not change a spectrum of Laplacian, see e.g. [20, Chapter 13]. In our study of the contact model, we need not only to solve the equation for the first correlation function specified by a Schrödinger type operator, but also to explore an infinite chain of hierarchical equations for all correlation functions of the model. Thus, the first step of our research is to construct the first correlation function of the stationary system using the Feynman-Kac formula, and then we find the solution of the whole chain by the inductive procedure.

The case studied here is unlike to the case from [1], [2], [8], where local negative fluctuations of the mortality can lead to an exponential popultion growth in any compact region.

In proving the main results of this work, we adapt the arguments from [6, 9, 18] developed for contact models in the critical regime to the analysis of contact models in the absence of the critical regime condition. The remainder of this paper is organised as follows. In Section 2, we introduce the model and formulate assumptions on the model. We formulate the main result in Section 3. In Section 4, we give the proof of the main theorem.

2. The model

Let $\mathfrak{X}$ be a locally compact separable metric space, $\mathcal{B}(\mathfrak{X})$ be its Borel σ-algebra, and m will denote a locally finite Borel measure on $\mathcal{B}(\mathfrak{X})$, i.e. m is finite on compact sets. Denote by $\mathcal{M}(\mathfrak{X})$ the space of locally finite Borel measures on $\mathcal{B}(\mathfrak{X})$ and by $\mathcal{B}_{\mathrm{b}}(\mathfrak{X})$ the system of all compact sets from $\mathcal{B}(\mathfrak{X})$.

A configuration $\gamma \in \Gamma(\mathfrak{X})$ on $\mathfrak{X}$ is a finite or countably infinite locally finite unordered set of points in $\mathfrak{X}$, and some of them can be multiple, i.e. repetitions are permitted. If the measure $m \in \mathcal{M}(\mathfrak{X})$ is atomic then $\Gamma(\mathfrak{X})$ contains configurations with multiple points. This case is realized on graphs with a counting measure m. For the continuous contact models, when m is non-atomic (see e.g. [6, 7, 10]), as the phase space Γ one can take the set of locally finite configurations in $\mathfrak{X}$ with distinct elements:

$$\Gamma_c = \Gamma_c(\mathfrak{X}) := \Big\{\gamma \subset \mathfrak{X} \;\Big|\; |\gamma \cap \Lambda| < \infty, \text{ for all } \Lambda \in \mathcal{B}_{\mathrm{b}}(\mathfrak{X})\Big\}, \tag{2.1}$$

where $|\cdot|$ denotes the number of elements of a set.

We can identify each $\gamma \in \Gamma$ with an integer-valued measure $\sum_{x\in\gamma} \delta_x \in \mathcal{M}(\mathfrak{X})$, where δ_x is the Dirac measure with unit mass, and the sum is taken considering the multiplicity of elements in the configuration γ. For any $\Lambda \in \mathcal{B}_{\mathrm{b}}(\mathfrak{X})$ we denote by $|\gamma \cap \Lambda|$ the value $\gamma(\Lambda)$ of the measure γ on Λ.

The contact model is a continuous time Markov process on $\Gamma(\mathfrak{X})$ which is a particular case of a general birth-and-death process. The model is given by a heuristic generator defined on a proper class of functions $F : \Gamma \to \mathbb{R}$ as follows:

$$\begin{aligned}(LF)(\gamma) = &\sum_{x\in\gamma} U(x)\,(F(\gamma\backslash x) - F(\gamma)) \\ &+ \int_{\mathfrak{X}} \sum_{x\in\gamma} a(y,x)(F(\gamma \cup y) - F(\gamma))m(dy).\end{aligned} \tag{2.2}$$

Notations $\gamma\backslash x$ and $\gamma \cup x$ in (2.2) stand for removing and adding one particle at position $x \in \mathfrak{X}$. Similarly, $x \in \gamma$ refers to any particle in the configuration

γ. The first term in (2.2) corresponds to the death of a particle at position x: each element $x \in \gamma$ of the configuration $\gamma \in \Gamma$ can die with the death rate

$$U(x) = V(x) + W(x),$$

where the critical regime condition (see (2.6) below) is valid for $V(x) > 0$, and $W(x) \geq 0$ is a non-negative local perturbation of $V(x)$, see condition (2.11) below. The second term of (2.2) describes the birth of a new particle in a neighborhood dy of the point y with the birth density $A(y,\gamma) := \sum_{x\in\gamma} a(y,x)$. It worth noting that this form of the birth rates suggests that it is not known who is the parent of the new particle, since the birth of a new particle at position y has a cumulative rate $\sum_{x\in\gamma} a(y,x)$. Function $a(x,y)$ is also called the dispersal kernel.

We formulate now assumptions on the birth and death rates that provide the existence of invariant measures.

1. *Measurability* condition. Let $a : \mathfrak{X} \times \mathfrak{X} \to [0,\infty)$, $W : \mathfrak{X} \to [0,\infty)$ be non-negative bounded measurable functions, and $V : \mathfrak{X} \to (0,\infty)$ is a strictly positive bounded measurable function:

$$0 \;<\; V_{\min} = \inf_{\mathfrak{X}} V(x) \;\leq\; V(x) \;\leq\; \sup_{\mathfrak{X}} V(x) = V_{\max} \;<\; \infty; \tag{2.3}$$

$$0 \;\leq\; W_{\min} = \inf_{\mathfrak{X}} W(x) \;\leq\; W(x) \;\leq\; \sup_{\mathfrak{X}} W(x) = W_{\max} \;<\; \infty. \tag{2.4}$$

2. *Regularity* condition. There exists a constant $C > 0$, such that

$$\sup_{x\in\mathfrak{X}} \int_{\mathfrak{X}} a(y,x)\, m(dy) \;<\; C. \tag{2.5}$$

3. *Critical regime* condition for V. There exists a strictly positive bounded measurable function $\Psi(x)$, $\Psi(x) \geq p_0 > 0$ such that

$$\int_{\mathfrak{X}} a(x,y)\, \Psi(y)\, m(dy) \;=\; V(x)\, \Psi(x) \quad \text{for all } x \in \mathfrak{X}. \tag{2.6}$$

Critical regime condition is a balance condition between birth and death rates for the unperturbed system if particles are distributed according the measure $\Psi(y)\, m(dy)$. Define the new measure $\bar{\mathfrak{m}}$ and the new intensity of birth $b(x,y)$ as follows

$$\bar{\mathfrak{m}}(dy) = \Psi(y) m(dy), \qquad b(x,y) = \frac{a(x,y)}{\Psi(x)}, \tag{2.7}$$

then relation (2.6) is rewritten as

$$\int_{\mathfrak{X}} b(x,y) \bar{\mathfrak{m}}(dy) \;=\; V(x) \quad \text{for all } x \in \mathfrak{X}. \tag{2.8}$$

4. *Transience* condition. Let us consider the continuous time jump Markov process with generator

$$\mathcal{L}f(x) = \int\limits_{\mathfrak{X}} b(x,y)\big(f(y) - f(x)\big)\bar{\mathfrak{m}}(dy). \tag{2.9}$$

Then we assume that for two independent copies $X(t)$ and $Y(t)$ of this process starting with $X(0) = x$ and $Y(0) = y$ the following condition holds

$$\sup_{x,y} \int_0^\infty \mathbb{E}_{x,y} b(X(t), Y(t))dt < H \tag{2.10}$$

with a constant $H > 0$. Moreover, we assume that the integral in (2.10) converges uniformly in x, y.

5. *W-integrability* condition. The perturbation $W(x)$ is non-negative, bounded and satisfies estimate

$$\sup_{x} \int_0^\infty \mathbb{E}_x W(X(t))dt < L \tag{2.11}$$

with some $L > 0$, and the integral converges uniformly in x. Here as above $X(t)$ is the trajectory of the process with generator (2.9) starting at x.

Remark 2.1. It worth noting that the form of the generator in (2.9) as well as the transience condition (2.10) do not depend on the function $W(x)$.

Remark 2.2. The sufficient condition for (2.10) together with required uniform convergence reads

$$\int\limits_0^\infty \sup_{x,y} \mathbb{E}_x b(X(t), y)dt < H \tag{2.12}$$

Proof. Denote by $p(x, dy, t)$ the transition function of the Markov jump process with generator (2.9) at time t. Then we get

$$\begin{aligned}
&\sup_{x,y} \int\limits_0^\infty \mathbb{E}_{x,y} b(X(t), Y(t))dt \\
&\quad = \sup_{x,y} \int\limits_0^\infty \int\limits_{\mathfrak{X}} \int\limits_{\mathfrak{X}} b(x', y')p(x, dx', t)p(y, dy', t)dt \\
&\quad \le \sup_{y} \int\limits_0^\infty \int\limits_{\mathfrak{X}} \Big(\sup_{x} \int\limits_{\mathfrak{X}} b(x', y')p(x, dx', t)\Big)p(y, dy', t)dt \\
&\quad = \sup_{y} \int\limits_0^\infty \int\limits_{\mathfrak{X}} \Big(\sup_{x} \mathbb{E}_x b(X(t), y')\Big)p(y, dy', t)dt
\end{aligned}$$

$$\leq \int_0^\infty \sup_y \int_{\mathfrak{X}} \Big(\sup_{y'} \sup_x \ \mathbb{E}_x b(X(t), y') \Big) p(y, dy', t) dt$$
$$= \int_0^\infty \sup_{x,y'} \ \mathbb{E}_x b(X(t), y') dt.$$

Therefore, condition (2.12) implies the uniform convergence in (2.10). □

Remark 2.3. The sufficient condition for (2.11) reads

$$\int_0^\infty \sup_x \ \mathbb{E}_x W(X(t)) dt < L. \tag{2.13}$$

It is easy to see that both estimates (2.12) and (2.13) are valid if $\mathfrak{X} = \mathbb{R}^d$, $d \geq 3$, $a(x, y) = a(x - y)$ is a bounded probability density, $V(x) \equiv 1$, $\Psi(x) \equiv 1$, and $W(x) \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$. The proof of this fact follows from the standard (Polya-type) arguments on the transience of non-degenerate homogeneous random walks in $\mathbb{R}^d$, $d \geq 3$, see e.g. [11], [16], [19]. In the case of small dimensions $d = 1, 2$, estimates (2.12) and (2.13) hold if the density $a(x, y) = a(x - y)$ has heavy enough tails, see [7].

3. Time evolution of correlation functions. Main results

Denote by $\mathcal{M}_{fm}(\Gamma)$ the set of all probability measures μ which have finite local moments of all orders, i.e.

$$\int_\Gamma |\gamma \cap \Lambda|^n \ \mu(d\gamma) \ < \ \infty$$

for all $\Lambda \in \mathcal{B}_b(\mathfrak{X})$ and $n \in N$.

Together with the configuration space Γ we define the space Γ_0 of finite configurations, and let $\Gamma_{0,\Lambda}^{(n)} = \{\eta \subset \Lambda : \ |\eta| = n\}$ be the set of n-point configurations in $\Lambda \in \mathcal{B}_b(\mathfrak{X})$. If a measure $\mu \in \mathcal{M}_{fm}(\Gamma)$ is locally absolutely continuous with respect to the Lebesque-Poisson measure

$$\lambda_{z,\,\bar{\mathfrak{m}}} \ = \ \sum_{n=0}^\infty \frac{z^n}{n!} \bar{\mathfrak{m}}^{\otimes n}, \quad \text{i.e.} \ \ \lambda_{z,\,\bar{\mathfrak{m}}}(\Gamma_{0,\Lambda}^{(n)}) \ = \ \frac{z^n \, (\bar{\mathfrak{m}}(\Lambda))^n}{n!}, \ n = 0, 1, \ldots,$$

where $\bar{\mathfrak{m}}(\Lambda) = \int_\Lambda \bar{\mathfrak{m}}(dx)$, then there exists the corresponding system of the correlation functions, i.e. densities of the correlation measure with respect to the Lebesque-Poisson measure. The terminology originates in statistical mechanics, see, for instance, [21, Ch. 4]. Denote by $\mathcal{M}_{\rm corr}(\Gamma)$ the subclass of the class

$\mathcal{M}_{fm}(\Gamma)$ consisting of probability measures on Γ for which correlation functions exists.

The evolution equation for the system of n-point correlation functions corresponding to the continuous contact model in $\mathfrak{X}$ has the following recurrent forms, see e.g. [6, 18]:

$$\frac{\partial k_t^{(n)}}{\partial t} \;=\; \hat{L}_n^* k_t^{(n)} - W_n k_t^{(n)} + f_t^{(n)}, \quad n \geq 1; \qquad k_t^{(0)} \equiv 1, \tag{3.1}$$

where

$$\begin{aligned} \hat{L}_n^* k_t^{(n)}(x_1, \ldots, x_n) = &-\Big(\sum_{i=1}^n V(x_i)\Big) k_t^{(n)}(x_1, \ldots, x_n) \\ &+ \sum_{i=1}^n \int_{\mathfrak{X}} b(x_i, y) k_t^{(n)}(x_1, \ldots, x_{i-1}, y, x_{i+1}, \ldots, x_n) \bar{\mathfrak{m}}(dy), \end{aligned} \tag{3.2}$$

and W_n is the operator of multiplication

$$W_n k_t^{(n)}(x_1, \ldots, x_n) \;=\; \Big(\sum_{i=1}^n W(x_i)\Big) k_t^{(n)}(x_1, \ldots, x_n). \tag{3.3}$$

Denote

$$S_n = \hat{L}_n^* - W_n. \tag{3.4}$$

Then (3.1) is rewritten as

$$\frac{\partial k_t^{(n)}}{\partial t} \;=\; S_n k_t^{(n)} + f_t^{(n)}, \quad n \geq 1. \tag{3.5}$$

Here $f_t^{(n)}$ are functions on $\mathfrak{X}^n$ defined for $n \geq 2$ by

$$f_t^{(n)}(x_1, \ldots, x_n) \;=\; \sum_{i=1}^n k_t^{(n-1)}(x_1, \ldots, \check{x}_i, \ldots, x_n) \sum_{j \neq i} b(x_i, x_j), \tag{3.6}$$

and $f_t^{(1)} \equiv 0$. The notation $\check{x}_i$ means that this coordinate is excluded.

Note that the operator $S_n = \hat{L}_n^* - W_n$ is similar to the n-particle Schrödinger operator with the potential W_n taken with a minus sign.

Let $\mathbb{X}_n = \mathbb{B}(\mathfrak{X}^n)$ be the Banach space of all measurable real-valued bounded functions on $\mathfrak{X}^n$ with the sup-norm. Consider the operator S_n as an operator on the Banach space $\mathbb{X}_n$ for any $n \geq 1$. Then it is a bounded linear operator in $\mathbb{X}_n$, and the arguments based on the variation of parameters formula yields that

$$k_t^{(n)} \;=\; e^{tS_n} k_0^{(n)} \;+\; \int_0^t e^{(t-s)S_n} f_s^{(n)} \, ds, \tag{3.7}$$

where $f_s^{(n)}$ is expressed through $k_s^{(n-1)}$ by (3.6). Thus, the solution to the Cauchy problem (3.1) in $\mathbb{X}_n$ with arbitrary initial values $k_0^{(n)} \in \mathbb{X}_n$ exists and is unique provided $f_t^{(n)}$ is constructed recurrently via the solution to the same Cauchy problem (3.1) for $n-1$.

The goal of this paper is to prove the existence of a family of invariant measures for the contact processes that are out of critical regime. These measures are described in terms of the corresponding correlation functions $\{k^{(n)}\}_{n\geq 0}$ as solutions to the following system:

$$S_n k^{(n)} + f^{(n)} = 0, \quad n \geq 1, \quad k^{(0)} \equiv 1, \tag{3.8}$$

where S_n, $f^{(n)}$ were defined by (3.2)–(3.6). In the sequel, we say that $k : \Gamma_0 \to \mathbb{R}$ solves the system (3.8) in the Banach spaces $(\mathbb{X}_n)_{n\geq 1}$ if the corresponding $k^{(n)} \in \mathbb{X}_n$, $n \geq 1$ solve (3.8).

The main result of the paper is the following theorem.

Theorem 3.1. *Assume that all the above conditions* (2.3)–(2.11) *are fulfilled. Then the following assertions hold.*

(*i*) *There exists a one-parameter set of probability measures $\mu^\varrho \in \mathcal{M}_{\rm corr}(\Gamma)$ on Γ depending on the parameter $\varrho > 0$ such that the correlation functions $k_\varrho : \Gamma_0 \to \mathbb{R}_+$ solve* (3.8) *in the Banach spaces $(\mathbb{X}_n)_{n\geq 1}$. Moreover, the following bounds hold for all $(x_1, \dots, x_n) \in \mathfrak{X}^n$*

$$k_\varrho^{(n)}(x_1, \dots, x_n) \ \leq DH^n (n!)^2 \qquad \textit{with} \ \ D = \sum_{n=1}^{\infty} \frac{(\varrho/H)^n}{(n!)^2} \tag{3.9}$$

where H is the same constant as in (2.10).

(*ii*) *Let $\{k_t^{(n)}\}_{n\geq 1}$ be the solution to the Cauchy problem* (3.1) *with initial data $k_0 = \{k_0^{(n)}\}$ corresponding to the Poisson measure π_ϱ with intensity ϱ:*

$$k_0^{(0)} = 1, \quad k_0^{(n)}(x_1, \dots, x_n) = \varrho^n, \ n \geq 1. \tag{3.10}$$

Then

$$\|k_t^{(n)} \ - \ k_\varrho^{(n)}\|_{\mathbb{X}_n} \ \to \ 0, \quad t \to \infty, \quad \forall n \geq 1. \tag{3.11}$$

The main strategy of the proof follows the same line as in [18]. However, in the present paper we should modify the previous proof, considering the operator S_n for any n as a sum of the "unperturbed" generator $\hat{L}_n^*$ corresponding to the contact process in the critical regime and the "perturbation" W_n.

Theorem 3.1 states that even in the "perturbed case", when $U(x) = V(x) + W(x)$, the invariant measures exist, and consequently local positive fluctuations $W(x)$ of mortality (with respect to the level of mortality $V(x)$ corresponding to the critical regime) does not lead to the extinction.

4. The proof of Theorem 3.1

The proof of the first statement of Theorem 3.1 we start with construction of the first correlation function $k^{(1)}$ and then using the induction in $n \in \mathbb{N}$ we obtain the solution $\{k^{(n)}\}_{n\geq 1}$ of the full system (3.8) recurrently.

For the first correlation function $k^{(1)}$ we get from (3.2), (3.4) and (3.8) the following equation

$$-U(x)k^{(1)}(x) + \int\limits_{\mathfrak{X}} b(x,y)k^{(1)}(y)\bar{\mathfrak{m}}(dy) = 0, \tag{4.1}$$

that can be written using the critical regime condition (2.8) as

$$\int\limits_{\mathfrak{X}} b(x,y)\big(k^{(1)}(y) - k^{(1)}(x)\big)\bar{\mathfrak{m}}(dy) - W(x)k^{(1)}(x) = 0. \tag{4.2}$$

To find a solution of (4.2) we first study the corresponding evolution problem:

$$\frac{\partial\, u}{\partial\, t} = \mathcal{L}u - Wu, \qquad u(x,0) = \varrho, \quad \varrho > 0, \tag{4.3}$$

where $\mathcal{L}$ is the generator (2.9) of the Markov jump process in $\mathfrak{X}$. Equation (4.3) is a variant of a non-local heat equation with absorption. The solution of (4.3) at time t is given by the Feynman-Kac formula

$$u_\varrho(x,t) \;=\; \varrho\,\mathbb{E}_x\big[\exp\big(-\int\limits_0^t W(X(s))ds\big)\big], \tag{4.4}$$

see e.g. [22, Chapter III], [23, Chapter II]. Here $X(t)$ is the trajectory of the process with generator (2.9) starting at x.

It worth noting that the solution $u_\varrho(x,t)$ to (4.3) is the same as the solution $k_t^{(1)}(x)$ of (3.1).

We define the stationary solution $k^{(1)} = k_\varrho^{(1)}$ as the limit

$$k_\varrho^{(1)}(x) \;=\; \lim_{t\to\infty} u_\varrho(x,t) \;=\; \varrho\,\mathbb{E}_x\big[\exp\big(-\int\limits_0^\infty W(X(s))ds\big)\big]. \tag{4.5}$$

We use the notation $k_\varrho^{(1)}$ to emphasize the dependence of the stationary solution on the parameter $\varrho > 0$. It follows from condition (2.11) and the Jensen inequality that the limit (4.5) exists and strictly positive:

$$\varrho\, e^{-L} \leq \varrho\,\mathbb{E}_x\big[\exp\big(-\int\limits_0^\infty W(X(t))dt\big)\big] \leq \varrho. \tag{4.6}$$

We denote this limit by

$$\Phi_\varrho(x) = \varrho\,\mathbb{E}_x\big[\exp\big(-\int_0^\infty W(X(t))dt\big)\big]. \tag{4.7}$$

Thus formula (4.5) defines a positive bounded function $k_\varrho^{(1)}(x) = \Phi_\varrho(x)$, and

$$S_1\Phi_\varrho(x) = (\hat{L}_1^* - W_1)\Phi_\varrho(x) = 0.$$

Clearly $k_\varrho^{(1)}(x)$ is an element of $\mathbb{X}_1$ and it solves (4.2) (and (4.1)). We notice that this function can be interpreted as the spatial density of particles of the stationary distribution, and formulas (4.4)–(4.5) mean that

$$k_t^{(1)}(x) = e^{tS_1}k_0^{(1)}(x) = e^{tS_1}\varrho \;\to\; \Phi_\varrho(x) = k_\varrho^{(1)}(x).$$

Example. If $\mathfrak{X} = \mathbb{R}^d$, $d \geq 3$, and $W \in C_0(\mathbb{R}^d)$, i.e. W has a compact support, then formula (4.5) implies that $k^{(1)}(x) \to \varrho$ as $|x| \to \infty$.

Next we will construct a solution to the system (3.8) satisfying estimates (3.9). Further we need the following lemma.

Lemma 4.1. *The operators $e^{t\hat{L}_n^*}$ and e^{tS_n}, where $\hat{L}_n^*$ and S_n were defined in* (3.2) *and* (3.4) *correspondingly, are positive, i.e. it maps non-negative functions to non-negative functions, and*

$$e^{tS_n}f \;\leq\; e^{t\hat{L}_n^*}f \tag{4.8}$$

for all $f \geq 0$.

Proof. For the operator $e^{t\hat{L}_n^*}$ see the proof in Lemma 4.1, [19]. We will prove the lemma for e^{tS_n}. The operator

$$A^i k^{(n)}(x_1,\dots,x_n) \;:=\; \int_{\mathfrak{X}} b(x_i,y)k^{(n)}(x_1,\dots,x_{i-1},y,x_{i+1},\dots,x_n)\bar{\mathfrak{m}}(dy)$$

is positive and bounded on $\mathbb{X}_n$ for any $1 \leq i \leq n$. Set

$$\begin{aligned} S^i k^{(n)}(x_1,\dots,x_n) \;&= \int_{\mathfrak{X}} b(x_i,y)k^{(n)}(x_1,\dots,x_{i-1},y,x_{i+1},\dots,x_n)\bar{\mathfrak{m}}(dy) \\ &\quad - U(x_i)k^{(n)}(x_1,\dots,x_n). \end{aligned} \tag{4.9}$$

Using the Trotter formula for the sum $A + B$ of two bounded operators:

$$e^{t(A+B)} = \lim_{n\to\infty}\Big(e^{\frac{tA}{n}}e^{\frac{tB}{n}}\Big)^n$$

we conclude that

$$e^{t\,S^i} f = \lim_{n\to\infty} \left(e^{t\,\frac{A^i}{n}} e^{-t\,\frac{U}{n}} \right)^n f \geq e^{-t\,U_{\max}}\, e^{t\,A^i} f \geq 0 \tag{4.10}$$

for any non-negative function f. Here U is the operator of multiplication on the positive bounded function $U(x)$, and $U_{\max} = \sup_{x\in\mathfrak{X}}(V(x) + W(x))$.

Representations (3.2), (3.3)–(3.4) yield

$$e^{tS_n} \;=\; \otimes_{i=1}^n\, e^{t\,S^i}.$$

Then taking into account that

$$\otimes_{i=1}^n\, e^{-t\,U_{\max}}\, e^{t\,A^i} \tag{4.11}$$

is a positive operator, we get the desired conclusion.

Relation $\hat{L}_n^* = S_n + W_n$ with $W_n \geq 0$ immediately implies estimate (4.8). □

As follows from (3.6), the function $f^{(n)}$ is the sum of functions of the form

$$f_{i,j}(x_1,\dots,x_n) = k^{(n-1)}(x_1,\dots,\check{x}_i,\dots,x_n) b(x_i,x_j), \quad i\neq j. \tag{4.12}$$

We suppose by induction that

$$k^{(n-1)}(x_1,\dots,x_{n-1}) \;\leq\; K_{n-1}, \quad \text{for all } \; (x_1,\dots,x_{n-1}) \in \mathfrak{X}^{n-1}, \quad n\geq 2,$$

where $K_n = DC^n(n!)^2$, and D, C are some constants. Consequently,

$$f_{i,j}(x_1,\dots,x_n) \;\leq\; K_{n-1} b(x_i,x_j), \quad (x_1,\dots,x_n)\in\mathfrak{X}^n. \tag{4.13}$$

Using (4.13), the positivity of the operator e^{tS_n} and estimate (4.8) we have

$$\begin{aligned} \left(e^{tS_n} f_{i,j}\right)(x_1,\dots,x_n) \;&\leq K_{n-1} \left(e^{tS_n} b(\cdot_i,\cdot_j)\right)(x_1,\dots,x_n) \\ &\leq K_{n-1} \left(e^{t\hat{L}_n^*} b(\cdot_i,\cdot_j)\right)(x_1,\dots,x_n). \end{aligned} \tag{4.14}$$

Denote

$$\begin{aligned} \mathcal{L}^i k^{(n)}(x_1,\dots,x_n) \;&= \int_{\mathfrak{X}} b(x_i,y) k^{(n)}(x_1,\dots,x_{i-1},y,x_{i+1},\dots,x_n)\bar{\mathfrak{m}}(dy) \\ &\quad - V(x_i) k^{(n)}(x_1,\dots,x_n). \end{aligned} \tag{4.15}$$

Using the critical regime condition (2.8) we conclude that $e^{t\mathcal{L}^i}\mathbb{1} = \mathbb{1}$, $\forall i = 1,\dots,n$, where $\mathbb{1}(x)\equiv 1$. Thus we get

$$\left(e^{t\hat{L}_n^*} b(\cdot_i,\cdot_j)\right)(x_1,\dots,x_n) \;=\; \left(e^{t(\mathcal{L}^i+\mathcal{L}^j)} b(\cdot_i,\cdot_j)\right)(x_1,\dots,x_n). \tag{4.16}$$

Note that the latter function depends only on variables x_i and x_j.

Notice that $e^{t\hat{L}_n^*} f_{i,j}$ is integrable with respect to t on $\mathbb{R}_+$. Indeed, estimate (4.12), condition (2.10) and the identity

$$e^{t\hat{L}_n^*} b(x,y) = \mathbb{E}_{x,y} b(X(t), Y(t)) \tag{4.17}$$

imply that

$$\int_0^\infty e^{t\hat{L}_n^*} f_{i,j}(x_1, \dots, x_n)\, dt \ \le K_{n-1}\, H, \tag{4.18}$$

where H is the same constant as in (2.10). Define

$$v_{i,j}^{(n)} \ = \ \int_0^\infty e^{tS_n} f_{i,j}\, dt, \tag{4.19}$$

then (4.14) and (4.18) yield

$$v_{i,j}^{(n)} \ \le \ K_{n-1}\, H. \tag{4.20}$$

Starting from now, the proof of the main result completely repeats the reasoning given in the proof of Theorem 3.1 from [18]. We briefly present next steps of the proof here for the reader's convenience. Denote

$$v^{(n)} = \sum_{i \neq j} v_{i,j}^{(n)} = \int_0^\infty e^{tS_n} f^{(n)} dt, \qquad f^{(n)} = \sum_{i \neq j} f_{i,j}, \tag{4.21}$$

where $f_{i,j}$ was defined by (4.12). Next we prove that function $v^{(n)}$ is a solution to (3.8) in $\mathbb{X}_n$. It is easily seen from (4.19) and induction procedure that $v^{(n)} \in \mathbb{X}_n$. Since e^{tS_n} is a strongly continuous semigroup we have

$$e^{tS_n} f^{(n)} = f^{(n)} + S_n \int_0^t e^{sS_n} f^{(n)} ds. \tag{4.22}$$

It was proved, see e.g. [18], that the following limit holds in $\mathbb{X}_n$:

$$e^{t\hat{L}_n^*} f^{(n)} \to 0, \quad t \to \infty. \tag{4.23}$$

Consequently, using (4.8) we conclude that

$$e^{tS_n} f^{(n)} \to 0, \quad t \to \infty. \tag{4.24}$$

A passage to the limit in (4.22) as $t \to \infty$ together with (4.24) shows that $v^{(n)}$ defined in (4.21) can be taken as a solution $k^{(n)}$ to (3.8).

Since the function $f^{(n)}$ is the sum of functions $f_{i,j}$, $i \neq j$ we deduce from (4.19) that $v^{(n)}$ is bounded by $n^2 K_{n-1} H$. Thus we get the recurrence inequality

$$K_n \ \leq \ n^2 K_{n-1} H, \tag{4.25}$$

and by induction it follows that

$$K_n \ \leq \ H^n \, (n!)^2 \, k^{(1)}. \tag{4.26}$$

Thus this solution $k^{(n)} = v^{(n)}$ with $v^{(n)}$ defined in (4.21) satisfies estimate

$$v^{(n)}(x_1, \ldots, x_n) \ \leq \ H^n \, (n!)^2 \, k^{(1)}. \tag{4.27}$$

Moreover for (4.7) being a solution to the system (3.8), any family of function of the form

$$k_\varrho^{(1)} = \Phi_\varrho, \quad k_\varrho^{(n)} = \int_0^\infty e^{tS_n} f^{(n)} \, dt + \Upsilon_\varrho^{(n)}, \quad n \geq 2,$$

is a solution to the system (3.8), if $\Upsilon_\varrho^{(n)}(x_1, \ldots, x_n)$ is an arbitrary function such that $S_n \Upsilon_\varrho^{(n)} = 0$. Taking

$$\Upsilon_\varrho^{(n)}(x_1, \ldots, x_n) \ = \ \prod_1^n \Phi_\varrho(x_i)$$

we conclude that

$$\begin{aligned} &k_\varrho^{(1)} = \Phi_\varrho, \\ &k_\varrho^{(n)} = \int_0^\infty e^{tS_n} f^{(n)} dt + \prod_1^n \Phi_\varrho(x_i) = v^{(n)} + \prod_1^n \Phi_\varrho(x_i), \quad n \geq 2, \end{aligned} \tag{4.28}$$

is the desired solution to the stationary problem (3.8) in the Banach spaces $(\mathbb{X}_n)_{n \geq 1}$. To emphasize the dependence of $f^{(n)}$ on ϱ (see (4.12)), we will use further notation $f_\varrho^{(n)}$ for $f^{(n)}$.

It follows from estimate (4.6) and formula (4.28) that for $\{k_\varrho^{(n)}\}_{n \geq 1}$ the following recurrence inequality holds

$$K_n \ \leq \ n^2 K_{n-1} H \ + \ \varrho^n. \tag{4.29}$$

Taking $L_n = \frac{K_n}{H^n (n!)^2}$ we get from (4.29)

$$L_n \leq L_{n-1} + \frac{\varrho^n}{H^n (n!)^2} \leq D \quad \forall \, n = 1, 2, \ldots; \qquad L_0 = 0.$$

This yields

$$K_n \ \leq \ DH^n(n!)^2 \qquad \text{with } D = \sum_{n=1}^{\infty} \frac{(\varrho/H)^n}{(n!)^2}. \tag{4.30}$$

To be certain that the constructed system $\{k_\varrho^{(n)}\}_{n\geq 1}$ is a system of correlation functions, i.e. it corresponds to a probability measure μ^ϱ on the configuration space Γ, we will prove below that $\{k_\varrho^{(n)}\}_{n\geq 1}$ can be constructed as the limit when $t \to \infty$ of the system of correlation functions $\{k_t^{(n)}\}_{n\geq 1}$ associated with the solution to the Cauchy problem (3.1) with the initial data (3.10).

We recall that by the variation of parameters formula we have relation (3.7) for the solution to the Cauchy problem (3.1). On the other hand, we proved above the existence of the solution $\{k_\varrho^{(n)}\}_{n\geq 1}$ of the stationary problem:

$$S_n k_\varrho^{(n)} \ = \ -f_\varrho^{(n)}, \tag{4.31}$$

with

$$f_\varrho^{(n)}(x_1,\dots,x_n) \ = \ \sum_{i,j:\ i\neq j} k_\varrho^{(n-1)}(x_1,\dots,\check{x}_i,\dots,x_n)\ b(x_i,x_j).$$

This solution is given by formula (4.28), and (4.31) implies the following relation

$$\left(e^{tS_n}-1\right) k_\varrho^{(n)} \ = \ -\int_0^t \frac{d}{ds} e^{(t-s)S_n} k_\varrho^{(n)} ds \ = \ -\int_0^t e^{(t-s)S_n} f_\varrho^{(n)}\ ds. \tag{4.32}$$

Therefore from (3.7) and (4.32) we obtain

$$k_t^{(n)} - k_\varrho^{(n)} \ = \ e^{tS_n}(k_0^{(n)} - k_\varrho^{(n)}) \ + \ \int_0^t e^{(t-s)S_n}(f_s^{(n)} - f_\varrho^{(n)})\ ds. \tag{4.33}$$

We will prove now that both terms in the right-hand side of (4.33) converge to 0 in the norm of $\mathbb{X}_n$ as $t \to \infty$.

Formula (4.28) and equality $S_n \prod_1^n \Phi_\varrho(x_i) = 0$ yield

$$e^{tS_n}\left(k_0^{(n)} - k_\varrho^{(n)}\right) \ = \ -e^{tS_n} v^{(n)} + \left(e^{tS_n} k_0^{(n)} - \prod_1^n \Phi_\varrho(x_i)\right). \tag{4.34}$$

The second term in (4.34) tends to 0 as $t \to \infty$ because by (4.7) we get

$$e^{tS_1} k_0^{(1)}(x) = e^{tS_1}\varrho \to \Phi_\varrho(x),$$

and $k_0^{(n)}(x_1,\dots,x_n)=\prod_1^n k_0^{(1)}(x_i)=\varrho^n$ (see (3.10)). According (4.21) the first term in the r.h.s. of (4.34) can be rewritten as

$$e^{tS_n}\ v^{(n)}=\int_0^\infty e^{(t+s)S_n}f_\varrho^{(n)}\,ds=\int_t^\infty e^{rS_n}f_\varrho^{(n)}\,dr\le\int_t^\infty e^{r\hat{L}_n^*}f_\varrho^{(n)}\,dr.$$

Due to the structure (4.12) of the function $f_\varrho^{(n)}$ and the uniform convergence of the integral in (2.10) we conclude that

$$||e^{tS_n}\ v^{(n)}||_{\mathbb{X}_n}\to 0,\quad t\to\infty. \tag{4.35}$$

The second term in the r.h.s. of (4.33) also tends to 0, and it can be proved in the same way as in our previous works, see e.g. [9].

Thus we proved the strong convergence (3.11), and the proof of the second part of Theorem 3.1 is completed.

Now we go back to the first part of the Theorem 3.1, and the final step of the proof is to show that the system of correlation functions $\{k_\varrho^{(n)}\}_{n\ge1}$ corresponds to a probability measure μ^ϱ on the configuration space Γ. For this we have constructed above $k_\varrho^{(n)}$ as the limit when $t\to\infty$ of solution $k_t^{(n)}$ of the Cauchy problem (3.1) with initial data (3.10):

$$k_\varrho^{(n)}\ =\ \lim_{t\to\infty}k_t^{(n)}. \tag{4.36}$$

Then one can prove that solution $k_t^{(n)}$ of the Cauchy problem satisfies the Lenard positivity and the moment growth conditions, see [12]- [13]. The detailed proof of this fact can be found in [7]. Finally, these conditions imply that for any $\varrho>0$ there exists a unique probability measure $\mu^\varrho\in\mathcal{M}_{\rm corr}(\Gamma)$, whose correlation functions are $\{k_\varrho^{(n)}\}_{n\ge1}$. This complets the proof of Theorem 3.1.

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Markov Processes and **Related Fields**

Uniform Anderson Localization and Non-local Minami-type Estimates in Limit-periodic Media

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Abstract. We prove a uniform exponential localization of eigenfunctions and simplicity of spectrum for a class of limit-periodic lattice Schrödinger operators. An important ingredient of the proof is a generalized variant of the well-known Minami estimates (correlation inequalities for the eigenvalues) to the case where the spectral intervals can be arbitrarily placed in the real line. The new correlation inequalities allow us to substantially simplify and make more transparent the application of the KAM (Kolmogorov-Arnold-Moser) techniques.

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1. Introduction. The model

We study a particular class of finite-difference operators $H_\varepsilon = \varepsilon\Delta + V$, usually called lattice Schrödinger operators, acting in the Hilbert space $\mathscr{H} = \ell^2(\mathbb{Z})$:

$$\begin{aligned} \big(H_\varepsilon(\theta)f\big)(x) &= \big(\varepsilon\Delta f\big)(x) + V(x,\theta)f(x),\ x\in\mathbb{Z},\ \varepsilon>0,\\ \big(\Delta f\big)(x) &= \sum_{y:\,|y-x|=1} f(y)\,. \end{aligned} \tag{1.1}$$

Here, θ is an element of an auxiliary parameter space Θ endowed with the structure of a probability space $(\Theta, \mathfrak{B}^\Theta, \mathbb{P}^\Theta)$ where

$$\Theta = \bigtimes_{n\geq 1} \bigtimes_{k=0}^{T_n-1} [0,1]\,, \quad T_n = 2^n\,, \tag{1.2}$$

$\mathfrak{B}^\Theta$ is the cylinder sigma-algebra, and $\mathbb{P}^\Theta$ is the product measure generated by the Lebesgue measures on the Cartesian factors $[0,1]$. We restrict our analysis to the dimension $d = 1$ only to make some notations and arguments shorter, but as the reader will see, our techniques apply to the lattice $\mathbb{Z}^d$ of any dimension $d \geq 1$.

Below we often use a fairly standard notation $[\![a,b]\!] := [a,b] \cap \mathbb{Z}$.

The potentials $V(x,\theta)$ have the form

$$\begin{aligned} V(x,\theta) &= \sum_{n\geq 1} a_n \sum_{k\in[\![0,T_n-1]\!]} \theta_{n,k}\,\chi_{n,k}(x)\,, \quad a_n = \mathrm{e}^{-n^2}, \\ \chi_{n,k}(x) &:= \sum_{l\in\mathbb{Z}} \mathbf{1}_{k+lT_n}(x) = \chi_{n,k}(x+T_n)\,. \end{aligned} \tag{1.3}$$

Equivalently, we can write

$$V(x,\theta) = \sum_{n\geq 1} a_n\,\theta_{n,\,[x]_n}\,, \qquad [x]_n := x \mod T_n. \tag{1.4}$$

It is to be stressed that, as in our earlier works [3–5], using the parameter space Θ, equipped with the structure of a probability space for convenience, does not change the nature of the potential which remains **limit-periodic**. Moreover, if the introduction of the space $(\Theta, \mathfrak{B}^\Theta, \mathbb{P}^\Theta)$ ever rendered the potential V more stochastic, so that the standard techniques of "random" operators could apply and prove localization with no difficulty, the resulting localization could never be uniform.

Our analysis is perturbative, and it requires the amplitude $\varepsilon > 0$ of the kinetic energy operator Δ to be small.

Historically, the linear variant of the Kolmogorov–Arnold–Moser (KAM) approach to the Anderson localization pre-dates the multi-scale analysis (MSA) and the fractional-moments method (FMM) which became quite popular in the spectral theory of random operators; see [2] where the eigenbasis of a quasi-periodic Hamiltonian was constructed recursively, by **unitary** transformations.

A direct application of the MSA and FMM techniques, efficiently used for the ergodic potentials with a fully developed randomness, to almost-periodic operators where the randomness is severely restricted, stumbles on the problem of assessing the regularity of the probability distribution of the random eigenvalues. The KAM-type approach alone does not completely solve this hard

technical problem, which explains why KAM analysis presented in [5] was substantially more elaborate than in [2]. Exploiting an idea proposed originally in [11], we worked in [5] with a sequence of approximate eigenbases which are only **approximately** orthogonal, with accuracy rapidly improving in the course of the inductive procedure.

In the present paper, we assess the regularity of the random approximate eigenvalues (AEV) appearing in the KAM inductive scheme in a new way, with the help of the correlation inequalities generalizing the well-known Minami estimate [10]. This results in a considerable simplification of the KAM inductive procedure as compared to the one used in [5].

Specifically, we address the problem of regularity of joint probability measures of a finite family of eigenvalues $\lambda_1(\omega), \ldots \quad \lambda_K(\omega)$, $K \geq 1$, numbered in some measurable way. The original Minami estimate [10] for $K = 2$ eigenvalues was extended to any $K \geq 2$ in [1, 8] and refined in several subsequent works. A particularity of the aforementioned works consists in the fact that the regularity of the the two-point correlation measure, depending of course upon the regularity of the IID random potential, was proved for the squares $I \times I \subset \mathbb{R}$ and not for arbitrary rectangles $I_1 \times I_2$. It is to be noted that a weaker result was proved in [7] for rectangles $I_1 \times I_2$, assuming the random potential is IID with continuity modulus $\mathfrak{g}(\cdot)$ of the common marginal measure:

$$\mathbb{E}\left[\left(\mathrm{tr}\ P^{\Lambda}_{I_1}(H(\omega))\right) \mathrm{tr}\ P^{\Lambda}_{I_2}(H(\omega)) - \min\left[\mathrm{tr}\ P^{\Lambda}_{I_1}(H(\omega))\ , \mathrm{tr}\ P^{\Lambda}_{I_2}(H(\omega))\right] \right] \leq 2\,|\Lambda|^2 \mathfrak{g}_\Lambda(|I_1|)\,\mathfrak{g}_\Lambda(|I_2|)\,, \tag{1.5}$$

while a more efficient estimate

$$\mathbb{E}\left[\left(\mathrm{tr}\ P^{\Lambda}_{I_1}(H(\omega))\right) \mathrm{tr}\ P^{\Lambda}_{I_2}(H(\omega)) \right] \leq |\Lambda|^2 \mathfrak{g}_\Lambda(|I_1|)\,\mathfrak{g}_\Lambda(|I_2|) \tag{1.6}$$

was proved only in the case where $I_1 \subset I_2$. See further references in [7].

A different situation was studied in [9] where I_1 and I_2 were assumed to be disjoint. Nevertheless, the general case where the positions of the intervals I_1 and I_2 can be arbitrary is known to be more difficult.

In this, relatively short paper we do not discuss prior papers on the uniform localization of eigenfunctions nor on limit-periodic Schrödinger operators.

1.1. Main results

The results on localization in our model are as follows.

Theorem 1. *Consider the parametric family of limit-periodic lattice Schrödinger operators defined in* (1.1). *There exists* $\varepsilon_* \in (0, +\infty)$ *such that, for any* $\varepsilon \in (0, \varepsilon_*)$, *there exists a subset* $\Theta^\infty(\varepsilon) \subset \Theta$ *with* $\mathbb{P}^\Theta\{\Theta^\infty(\varepsilon)\} \uparrow 1$ *as* $\varepsilon \downarrow 0$ *such that, for all* $\theta \in \Theta^\infty(\varepsilon)$, *the following holds true.*

(A) $H_\varepsilon(\theta)$ *has pure point spectrum.*

(B) *For every $x \in \mathbb{Z}$, there is exactly one eigenfunction $y \mapsto \varphi_x(y,\theta)$ such that*

$$|\varphi_x(x,\theta)|^2 > \frac{1}{2}\,,$$

i.e., φ_x is unimodal with the "localization center" x, and so there is a natural bijection between the elements of the eigenbasis $\{\varphi_x(\cdot\,,\theta)\}$ and the lattice $\mathbb{Z}$.

(C) *φ_x feature a uniform exponential decay away from their localization centers:*

$$\forall\, y \in \mathbb{Z} \qquad |\varphi_x(y,\theta)| \le \mathrm{e}^{-m|y-x|}, \quad m = m(\varepsilon) \underset{\varepsilon\to 0}{\longrightarrow} +\infty. \tag{1.7}$$

(D) *The spectrum of $H_\varepsilon(\theta)$ is simple.*

In Section 7, we prove explicit lower bounds (2.16) on the spacings $|\lambda_x(\theta) - \lambda_y(\theta)|$.

Theorem 2. *Let $K \in \mathbb{N} \setminus \{0\}$ and $\mathscr{X} = \{x_1, \dots, x_K\} \subset \mathbb{Z}^K$ with $x_1 < x_2 \cdots < x_K$. Under the assumptions and with notations of Theorem 1, for any bounded intervals $I_1, \dots, I_K \subset \mathbb{R}$, the following bound holds for some $c \in (0, +\infty)$:*

$$\mathbb{P}^\Theta\{\,\forall\, k \in [\![1, K]\!] \;\; \lambda_{x_k}(\theta) \in I_k\,\} \le \mathrm{e}^{cK\ln^2(\mathrm{diam}(\mathscr{X}))} \prod_{1\le k\le K} |I_k|\,. \tag{1.8}$$

2. The inductive hypotheses

For each $N \ge 1$, consider an approximant of the potential $x \mapsto V(x,\theta)$,

$$V_N(x,\theta) = \sum_{1\le n\le N} a_n \sum_{1\le k\le K_n} \theta_{n,k}\,\chi_{n,k}(\omega),$$

and the truncated Hamiltonian $H_\varepsilon^{(N)} := \varepsilon\Delta + V_N$. Observe that

$$\begin{aligned} \|V - V_N\|_\infty &\le \sum_{n\ge N+1} \mathrm{e}^{-n^2} \\ &< \frac{1}{2}\mathrm{e}^{-N} a_N\,. \end{aligned} \tag{2.1}$$

It is important that the right-hand side of (2.1) is much smaller than the amplitude a_N of the distribution of random coefficients $a_N\theta_{N,k}$, $0 \le k < T_N$. This is why a_n have to decay faster that exponentially.

Consider a formal parameter vector $\mathbf{t} = (t_z)_{z\in\mathbb{Z}}$ and introduce a parametric family of the potentials

$$x \mapsto \widetilde{V}(x,\,\cdot\,;\mathbf{t}) := V(x,\,\cdot\,) + \sum_{z\in\mathbb{Z}} t_z\,\mathbf{1}_z(x) \tag{2.2}$$

To prove the crucial measure-theoretic bounds on the small denominators appearing in the KAM induction, we shall establish derivability of various objects appearing in our inductive scheme, starting with the spacings $\mathfrak{s}^j_{xy} = \lambda^j_x - \lambda^j_y$ between the approximate eigenvalues (AEV) $\lambda^j_\bullet$ constructed on each induction step j. Moreover, we shall prove some explicit bounds on the respective derivatives $\partial_{t_z}(\cdot) = \partial(\cdot)/\partial t_z$.

As in [5], it is convenient to use the norms defined for the functions on $\mathbb{Z}$ and for the matrices $A_{x,y}$ with entries indexed by $x, y \in \mathbb{Z}$ (cf. [2]): with $m > 0$ fixed, let

$$\|\!| f |\!\|_x = \sum_{y\in\mathbb{Z}} \mathrm{e}^{m|y-x|} \big|f(y)\big|, \quad x \in \mathbb{Z}, \tag{2.3}$$

$$\|\!| A |\!\| = \sup_{x\in\mathbb{Z}} \sum_{y\in\mathbb{Z}} \mathrm{e}^{m|y-x|} \big|A_{xy}\big|. \tag{2.4}$$

Note that with $m = 0$, $\|\!| \cdot |\!\|_x$ is the conventional norm in $\ell^2(\mathbb{Z})$, but for any $m > 0$, $\|\!| f |\!\|_x < +\infty$ implies an exponential decay of f.

Introduce an integer sequence $(\mathrm{L}_j)_{j\in\mathbb{N}}$ (the length scales) given by

$$\mathrm{L}_j := \mathrm{L}_0 q^j \quad q = \frac{3}{2}\,, \tag{2.5}$$

and let

$$\tilde{n}_i := \left\lceil \frac{5\ln \mathrm{L}_i}{\ln 2} \right\rceil = \left\lceil \frac{5i\ln q}{\ln 2} \right\rceil, \quad i \geq 0, \quad \text{hence} \quad 2^{\tilde{n}_i} \geq \mathrm{L}_i^5\,. \tag{2.6}$$

Introduce also the sequences $(\epsilon_j)_{j\in\mathbb{N}}$, $(\delta_j)_{j\in\mathbb{N}}$, $(\beta_j)_{j\in\mathbb{N}}$ of the form

$$\epsilon_j = (\epsilon_0)^{q^j}\,, \qquad \epsilon_0(\varepsilon) := \varepsilon^{1/4}\,, \tag{2.7}$$

$$\delta_j = a_{\tilde{n}_j}\beta_j\,, \quad \beta_j = \mathrm{e}^{-\tilde{n}_j}\,. \tag{2.8}$$

Below we often use for brevity the notations like "$\epsilon_i^{b^\pm}$" as shortcuts for "$\epsilon_i^{b\pm c}$ *with* $c > 0$ *that can be chosen* (*before the induction starts*) *as small as necessary or convenient*".

It is readily seen that, for any fixed $A > 0$,

$$\delta_j^A = \mathrm{e}^{-A\,\tilde{n}_j^2(1+\tilde{n}_j^{-1})} = \mathrm{e}^{-A\,C(1+\mathrm{o}(1))\ln^2(\mathrm{L}_j)} = \big(\epsilon_0^{L_j/L_0}\big)^{0^+} = \epsilon_j^{0^+}\,,$$

where $\mathrm{o}\,(1)$ is relative to $j \to +\infty$. In particular, for $k = 1, 2$, one has

$$\delta_j^{-k}\epsilon_j^{1^+} \leq \epsilon_j^{1^+}. \tag{2.9}$$

The relation (2.9) will be used on a number of occasions. One can take $1 \le k \le K$ with any $K \in \mathbb{N}$, but then ε would have to be chosen smaller than some $\varepsilon_*(K)$.

In some situations where $b > 0$ can be arbitrarily large, e.g., $b = k =$ the induction step number, we write "$b\,1^-$" to distinguish between an additive "loss" in the value b, viz. $b \rightsquigarrow b - c$ with $0 < c \ll 1$, and a multiplicative one, $b \rightsquigarrow b(1-c) = b - bc$, where bc may or might be large despite a small value of c.

Inductive hypothesis $\mathbf{K(L_j)}$: For all $0 \le i \le j$, there exists a measurable subset $\widetilde{\Theta}^i \subset \Theta$ with $\mathbb{P}^\Theta\{\widetilde{\Theta}^i\} \ge 1 - \beta_i^{1/2}$ such that for all $\theta \in \Theta^j := \cap_{i=0}^j \widetilde{\Theta}^i$ the following objects are well-defined:

(K1) The matrices $\mathrm{H}^i(\theta)$, $\Lambda^i(\theta)$, $\mathrm{K}^i(\theta)$ with entries indexed by $(x, y) \in \mathbb{Z}^2$ and such that $\mathrm{H}^i(\theta) = \Lambda^i(\theta) + \mathrm{K}^i(\theta)$. Here $\Lambda^i(\theta)$ is diagonal,

$$\Lambda^i_{yx}(\theta) = \lambda^0_x(\theta)\,\delta_{yx}\,, \tag{2.10}$$

and $\mathrm{K}^i(\theta)$ is off-diagonal: for all $x \in \mathbb{Z}$, $\mathrm{K}^i_{xx}(\theta) = 0$.

Uniformly in $\theta \in \Theta^i$, the following conditions are fulfilled:

(K2) The matrices $\mathrm{M}^i = \mathrm{M}^i(\theta), \mathscr{M}^i = \mathscr{M}^i(\theta)$ satisfying the identities

$$\begin{aligned} \mathscr{M}^i &= \prod_{l=1}^{i} \mathrm{e}^{\mathrm{M}^l} := \mathrm{e}^{\mathrm{M}^i} \,\cdots\, \mathrm{e}^{\mathrm{M}^1}\,, \\ \mathrm{H}^i &= \mathrm{Ad}_{\mathscr{M}^i}[H_\varepsilon] = (\mathscr{M}^i)^{-1} H_\varepsilon \mathscr{M}^i = \Lambda^i + \mathrm{K}^i\,, \end{aligned} \tag{2.11}$$

admit the norm bounds

$$\|\mathrm{K}^i(\theta)\|_x \le \epsilon_i^{1^+}\,, \quad \|\mathrm{M}^i(\theta)\|_x \le \epsilon_i^{1^+}\,, \tag{2.12}$$

$$\|\mathscr{M}^i - \mathbf{1}\| \le \mathrm{e}^{\sum_{l=1}^i \epsilon_l} \sum_{1 \le l \le i} \epsilon_l\,. \tag{2.13}$$

(K3) For $i = 0$, one has

$$\begin{aligned} \lambda^0_x(\theta) &= V(x, \theta)\,, \\ \mathrm{K}^0_{yx}(\theta) &= \varepsilon \sum_{y:\,|y-x|=1} \mathbf{1}_{\{y\}}\,. \end{aligned} \tag{2.14}$$

(K4) There exist $C > 0$ and a function $\hat{\mathrm{j}} : \mathbb{Z} \times \mathbb{Z} \to \mathbb{N}$ such that, for all $x, y \in \mathbb{Z}$ with $1 \le |y - x| \le \mathrm{L}_i^2$

$$\mathfrak{s}_i(x, y; \theta) := |\lambda^i_x(\theta) - \lambda^i_y(\theta)| \ge 4\delta_i\,. \tag{2.15}$$

Moreover, there exist some $C, C_1 \in (0, +\infty)$ such that

$$\forall\, j \ge C_1 \ln|x - y| \qquad \left|\mathfrak{s}^j(x, y; \theta)\right| \ge \mathrm{e}^{-C \ln^4|x-y|}\,. \tag{2.16}$$

(K5) For all $0 \le i \le j-1$, one has

$$\sup_x |\lambda_x^{i+1}(\theta) - \lambda_x^i(\theta)| \le \epsilon_i^{2^+} . \tag{2.17}$$

(K6) For all $0 \le i \le j-1$, one has:

$$\sup_z \sup_x \left|\partial_{t_z} \lambda_x^j(\theta)\right| \le 1 + \sum_{0 \le i \le j} \epsilon_j \,, \tag{2.18}$$

$$\sup_z \sup_{x \ne y} \left|\partial_{t_z} \mathrm{K}_{xy}^j(\theta)\right| \le \epsilon_j^{1^+} . \tag{2.19}$$

For brevity, the θ-dependence of various objects, e.g., K^i, M^i, $\mathfrak{s}_{yx}^i$, will often be dropped from notation.

3. The base of induction

The Hamiltonian H_ε is a second-order lattice Schrödinger operator on $\mathbb{Z}$, so its matrix in the standard delta-basis has the structure $H_\varepsilon = \mathrm{K}^0 + \Lambda^0$, with K^0 and Λ^0 described above (cf. (2.14)).

From this point on, we assume that $0 < \varepsilon \le \frac{1}{4}$, and set

$$m(\varepsilon) := \ln \varepsilon^{-1/C} \underset{\varepsilon \to 0}{\longrightarrow} +\infty \,,$$

Recall that we have introduced in (2.7) the sequence $\epsilon_i = \epsilon_0^{q^i}$, $q = 3/2$, $i \ge 0$.

Further, recalling $\mathrm{L}_j = \mathrm{L}_0 q^j$, let

$$\tilde{n}_{j+1} := \left\lceil \frac{5 \ln \mathrm{L}_{j+1}}{\ln 2} \right\rceil \tag{3.1}$$

so that $2^{\tilde{n}_{j+1}} \ge \mathrm{L}_{j+1}^5$.

Among the implicit exponents, like in $\epsilon_j^{b^+}$ etc., the one figuring in (2.15) is quite important, so we denote it by υ to make explicit some preliminary calculations. Assume that

$$\varepsilon \le \mathrm{e}^{-8\upsilon^{-1}\tilde{n}^2} = \mathrm{e}^{-8\upsilon^{-1}\ln^4(L_0)} \,,$$

then (cf. (2.8))

$$\delta_0(\varepsilon) = \mathrm{e}^{-\tilde{n}^2(L_0) - \tilde{n}(L_0)} \ge \frac{1}{5}\mathrm{e}^{-2\tilde{n}^2} \ge \frac{1}{5}\varepsilon^{\upsilon/4} = \frac{1}{5}\epsilon_0^{\upsilon}(\varepsilon) \,.$$

We have

$$\|\!|\mathrm{K}^0|\!\| = \varepsilon \sum_{y:\,|y|=1} \mathrm{e}^{m|y|} = 2\mathrm{e}^m \,\varepsilon = 2d\varepsilon^{1/2} \cdot \mathrm{e}^m \varepsilon^{1/2} \le 1 \cdot \epsilon^{-1/4+1/2} = \epsilon^{1/4}. \tag{3.2}$$

Taking $\varepsilon > 0$ small enough, one can have both an arbitrary small $\epsilon_0 > 0$ and an arbitrarily large decay exponent $m > 0$.

To perform the first induction step (cf. (4.1) in Section 4), we need some bounds on the spectral spacings

$$\mathfrak{s}^0_{yx} := \lambda^0_x - \lambda^0_y \,. \tag{3.3}$$

We defer this task to Section 4.3, assuming the bound (2.15), and focus now on the functional analytic arguments.

4. The first induction step

4.1. Norm estimates

Assuming that $|\lambda^0_x(\omega,\theta) - \lambda^0_{x-1}(\omega,\theta)| \geq \delta_0$, for any $\theta \in \Theta^0$ with Θ^0 yet to be constructed, the matrix $\mathrm{M}^1(\theta)$ with the only nonzero entries

$$\mathrm{M}^1_{x-1,x}(\omega,\theta) = \frac{\mathrm{K}^0_{x-1,x}(\omega,\theta)}{\lambda^0_x(\omega,\theta) - \lambda^0_{x-1}(\omega,\theta)} \tag{4.1}$$

is well-defined and admits the norm-bound

$$\|\!|\mathrm{M}^1|\!\| \leq \delta_0^{-1} \|\!|\mathrm{K}^0|\!\| \leq \delta_0^{-1} \epsilon_0^{1^+} \leq \epsilon_0^{1^+} . \tag{4.2}$$

Let $\mathscr{K}^1 := \mathrm{Ad}_{\mathrm{M}^1}\left[\Lambda^0\right] + \mathrm{Ad}_{\mathrm{M}^1}\left[\mathrm{K}^0\right] - \Lambda^0$. Since $\left[\Lambda^0, \mathrm{M}^1\right] = -\mathrm{K}^0$, we get

$$\begin{aligned} \mathscr{K}^1 &= \sum_{k\geq 1} \frac{1}{k!} \,\mathrm{ad}^k_{\mathrm{M}^1}\left[\Lambda^0\right] + \sum_{k\geq 0} \frac{1}{k!} \,\mathrm{ad}^k_{\mathrm{M}^1_N}\left[\mathrm{K}^0\right] \\ &= \sum_{k\geq 1} \frac{1}{k!} \,\mathrm{ad}^{k-1}_{\mathrm{M}^1}\left[\left[\Lambda^0, \mathrm{M}^1\right]\right] + \sum_{l\geq 1} \frac{1}{(l-1)!} \,\mathrm{ad}^{l-1}_{\mathrm{M}^1}\left[\mathrm{K}^0\right] \\ &= \sum_{k\geq 1} \mathfrak{k}_k \,\mathrm{ad}^k_{\mathrm{M}^1}\left[\mathrm{K}^0\right] , \quad \mathfrak{k}_k := (k-1)/k! \leq \frac{1}{(k-1)!} \,. \end{aligned} \tag{4.3}$$

Now, define the operators Λ^1 and K^1 by their matrix elements:

$$\begin{aligned} \Lambda^1_{yx} &:= \Lambda^0_{yx} + \delta_{yx} \mathscr{K}^1_{xx} \,, \\ \mathrm{K}^1_{yx} &:= (1-\delta_{yx}) \mathscr{K}^1_{yx} \,, \end{aligned} \tag{4.4}$$

so that

$$\begin{aligned} \mathrm{Ad}_{\mathrm{M}^1}[H_\varepsilon] &= \Lambda^1 + \mathrm{K}^1 \,, \\ \max\left[\|\Lambda^1 - \Lambda^0\| \,, \|\!|\mathrm{K}^1|\!\|\right] &\leq \|\!|\mathscr{K}^1|\!\| \,, \end{aligned} \tag{4.5}$$

where

$$\begin{aligned} \|\!|\mathscr{K}^1|\!\| &\leq \sum_{k\geq 1} \mathfrak{k}_k \|\!| \,\mathrm{ad}_{\mathrm{M}^1}[\mathrm{K}^0]|\!\| \leq \|\!|\mathrm{K}^0|\!\| \sum_{k\geq 1} 2^k \mathfrak{k}_k \|\!|\mathrm{M}^1|\!\|^k \\ &= 2\|\!|\mathrm{K}^0|\!\| \,\|\!|\mathrm{M}^1|\!\| \,\mathrm{e}^{2\|\!|\mathrm{M}^1|\!\|} \leq 4\|\!|\mathrm{K}^0|\!\| \,\|\!|\mathrm{M}^1|\!\| \,. \end{aligned} \tag{4.6}$$

Since $\|\!|\mathrm{M}^1|\!\| \leq \epsilon_0^{1^+}$ (cf. (4.1)), we have

$$\|\!|\mathscr{K}^1|\!\| \leq 4\delta_0^{-1}\|\!|\mathrm{K}^0|\!\|^2 \leq \epsilon_0^{2^+}\,, \tag{4.7}$$

whence

$$\sup_x \|\!|\mathrm{K}^1(\theta)|\!\| \leq \epsilon_0^{2^+} \tag{4.8}$$

$$\sup_x \left|\lambda_x^1(\theta) - \lambda_x^0(\theta)\right| \leq \|\Lambda^0 - \Lambda^1\| \leq \epsilon_0^{2^+}. \tag{4.9}$$

In particular, that, for any $y \neq x$, one has

$$\left|\lambda_x^1(,\theta) - \lambda_y^1(\theta)\right| \geq \left|\lambda_x^0(\theta) - \lambda_y^0(\theta)\right| - \epsilon_0^{2^-}\,, \tag{4.10}$$

so for all pairs (x, y) obeying $\left|\lambda_x^0(\theta) - \lambda_y^0(\theta)\right| \geq 4\delta_0$,

$$\left|\lambda_x^1(\theta) - \lambda_y^1(\theta)\right| \geq 4\delta_0 - \epsilon_0^{2^-} \geq 4\delta_0\big(1 - \epsilon_0^{2^-}\big)\,. \tag{4.11}$$

The matrix with column-vectors $\varphi_x^j(\theta)$ given by those of the transformed basis is

$$\Phi^1 = \mathrm{e}^{\mathrm{M}^1} = \mathbf{1} + \sum_{k\geq 1} \frac{1}{k!}(\mathrm{M}^1)^k\,, \tag{4.12}$$

thus letting $\Phi^0 = \mathbf{1}$, one has

$$\|\!|\Phi^1 - \Phi^0|\!\| \leq \sum_{k\geq 1} \frac{1}{k!}\|\!|\mathrm{M}^1|\!\|^k \leq \|\!|\mathrm{M}^1|\!\|\mathrm{e}^{\|\!|\mathrm{M}^1|\!\|} \leq 2\|\!|\mathrm{M}^1|\!\| \leq 2\delta_0^{-1}\epsilon_0^{1^+} \leq \epsilon_0^{1^+}\,, \tag{4.13}$$

yielding the perturbation bounds on the basis vectors

$$\sup_x \|\!|\varphi_x^j(\theta) - \varphi_x^0(\theta)|\!\|_x \leq \epsilon_0^{1^+}\,. \tag{4.14}$$

4.2. Parametric smoothness estimates

Consider a formal parameter vector $\mathbf{t} = (t_z)_{z\in\mathbb{Z}}$ and introduce a parametric family of the potentials

$$x \mapsto \widetilde{V}(x, \cdot; \mathbf{t}) := V(x, \cdot) + \sum_{z\in\mathbb{Z}} t_z\, \mathbf{1}_z(x) \tag{4.15}$$

Now we shall establish derivability of various objects appearing in our inductive scheme and prove uniform bounds on their derivatives $\partial_{t_z}(\cdot) = \partial(\cdot)/\partial t_z$. We start with the AEV $\lambda_x^0(\cdot)$; it is readily seen that

$$\partial_{t_z}\lambda_x^0(\cdot) = \partial_{t_z}\widetilde{V}(x, \cdot; \mathbf{t}) = \delta_{xz}\,. \tag{4.16}$$

Recalling $\mathfrak{s}^0_{yx} = \big(\lambda^0_x - \lambda^0_y\big)^{-1}$, we have $\mathrm{M}^1_{yx} = \mathrm{K}^0_{yx}\,\mathfrak{s}_{yx}$, thus

$$\partial_{t_z}\mathrm{K}^0 = \partial_{t_z}(\varepsilon\Delta) = 0, \tag{4.17}$$

$$\begin{aligned}\partial_{t_z}\mathrm{M}^1_{yx} &= \partial_{t_z}\left(\varepsilon\mathrm{K}^0_{yx}\mathfrak{s}_{yx}\right)\\ &= \varepsilon\mathrm{K}^0_{yx}\ \mathbf{1}_{z\in\{\,x,y\,\}}\left(\partial_{t_z}\lambda^0_x - \partial_{t_z}\lambda^0_y\right)\ (\mathfrak{s}^0_{yx})^2.\end{aligned} \tag{4.18}$$

Using the recursion in $k \geq 1$,

$$\partial_{t_z}\,\mathrm{ad}^k_{\mathrm{M}^1}[\mathrm{K}^0] = \partial_{t_z}(\mathrm{ad}^{k-1}_{\mathrm{M}^1}[\mathrm{K}^0]\mathrm{M}^1) - \partial_{t_z}(\mathrm{M}^1\,\mathrm{ad}^{k-1}_{\mathrm{M}^1}[\mathrm{K}^0])\,, \tag{4.19}$$

the iterated commutator $\mathrm{ad}^k_{\mathrm{M}^1}[\mathrm{K}^0]$ is expanded in the sum of 2^k products of the form $\mathbf{Y}^{(k)} = Y_1\cdots Y_{k+1}$ where one of the factors Y_i is K^0, with $\partial_{t_z}\mathrm{K}^0 = 0$, and k factors are equal to M^1. For example,

$$\begin{aligned}\mathrm{ad}^2_{\mathrm{M}^1}[\mathrm{K}^0] &= [\mathrm{K}^0,\mathrm{M}^1]\mathrm{M}^1 - \mathrm{M}^1[\mathrm{K}^0,\mathrm{M}^1]\\ &= \mathrm{K}^0\mathrm{M}^1\mathrm{M}^1 - \mathrm{M}^1\mathrm{K}^0\mathrm{M}^1 - \mathrm{M}^1\mathrm{K}^0\mathrm{M}^1 + \mathrm{M}^1\mathrm{M}^1\mathrm{K}^0\,.\end{aligned}$$

Expanding by Leibniz rule the derivative $\partial_{t_z}\mathbf{Y}^{(k)}$ of one of these products $\mathbf{Y}^{(k)}$, we get $k+1$ new products; each of them differs from $\mathbf{Y}^{(k)}$ in exactly one position $i \in \{\,1,2,\ldots,k+1\,\}$ where Y_i is replaced with $\partial_{t_z}Y_i$. The product with $\partial_{t_z}\mathrm{K}^0$ vanishes, so we have k (possibly) nonzero products of the form $\mathbf{Z}^{(k)} = Z_1\cdots Z_{k+1}$ where exactly one factor $Z_i = \partial_{t_z}Y_i$, and for all the other positions $l \neq i$, $Z_l = Y_l$. Since $\delta_0 = (\epsilon_0)^{0^+}$, we have:

$$\|\!|Z_l|\!\| \leq \begin{cases} \delta_0^{-1}\epsilon_0^{1^+} \leq \epsilon_0^{1^+}, & \text{if } Z_l = Y_l\,,\\ \delta_0^{-2}\epsilon_0^{1^+} \leq \epsilon_0^{1^+}, & \text{if } Z_l = \partial_{t_z}Y_l\,.\end{cases} \tag{4.20}$$

Since $\partial_{t_z}\,\mathrm{ad}^k_{\mathrm{M}^1}[\mathrm{K}^0]$ is the sum of $k\,2^k$ products of the form $\mathbf{Z}^{(k)}$, we conclude that

$$\|\!|\partial_{t_z}\,\mathrm{ad}^k_{\mathrm{M}^1}[\mathrm{K}^0]|\!\| \leq \epsilon_0^{1^+}\cdot(\epsilon_0^{1^+})^k \leq \epsilon_0^{(k+1)\,1^+}\,. \tag{4.21}$$

By convergence of the series

$$\sum_{k\geq 1}\mathfrak{k}_k\,\|\!|\partial_{t_z}\,\mathrm{ad}^k_{\mathrm{M}^1}[\mathrm{K}^0]|\!\| \leq \sum_{k\geq 1}\frac{1}{(k-1)!}\,k2^k\epsilon_0^{(k+1)\,1^+} \leq \epsilon_0^{2^+}\,, \tag{4.22}$$

the derivative $\partial_{t_z}\mathscr{K}^1$ exists, and one has

$$\|\!|\partial_{t_z}\mathscr{K}^1|\!\| \leq \epsilon_0^{2^+}\,. \tag{4.23}$$

This implies the ∂_{t_z}-derivability of $\Lambda^1 = \Lambda^0 + \big(\Lambda^1 - \Lambda^0\big)$, with

$$\sup_z\ \|\!|\partial_{t_z}\big(\Lambda^1(\cdot\,,\cdot\,) - \Lambda^0(\cdot\,,\cdot\,)\big)|\!\| \leq \epsilon_0^{2^+}\,. \tag{4.24}$$

Hence, by $\big|\partial_{t_z}\lambda_x^1\big| \le \big|\lambda_x^0\big| + \big|\partial_{t_z}(\lambda_x^1 - \lambda_x^0)\big|$,

$$\begin{aligned} \sup_z \ \big|\partial_{t_z}\lambda_z^1(\,\cdot\,,\,\cdot\,)\big| &\le 1 + \epsilon_0^{2^+}\,, \\ \sup_z \ \sup_{x\neq z} \ \big|\partial_{t_z}\lambda_x^1(\,\cdot\,,\,\cdot\,)\big| &\le 0 + \epsilon_0^{2^+} = \epsilon_0^{2^+}. \end{aligned} \tag{4.25}$$

It is readily seen that the bound (4.24), efficient for $x = z$, can be substantially improved for $|x - z| \ge 1$, particularly when $r := |x - z| \gg 1$.

First, assume that $r = |x - z| \ge 2$; the remaining case $r = 1$ is simpler and will be treated a bit later. Consider the diagonal matrix elements $(\mathrm{ad}^k_{\mathrm{M}^1}[\mathrm{K}^0])_{xx}$ contributing to $\lambda_x^1 - \lambda_x^0$. Fix some $x \in \mathbb{Z}$, pick a product $\mathbf{Z}^{(k)} = Z_1 \cdots Z_{k+1}$ and expand the derivatives of its diagonal matrix elements as follows:

$$\partial_{t_z}\mathbf{Z}^{(k)}_{xx} = \sum_{\gamma=(x_0,\,x_1,\,\ldots,\,x_{k+1})} \widetilde{\mathbf{Z}}(\gamma)\,, \quad \widetilde{\mathbf{Z}}(\gamma) = \widetilde{Z}_1(\gamma)\cdots\widetilde{Z}_{k+1}(\gamma), \tag{4.26}$$

$$\widetilde{Z}_i(\gamma) \in \{\mathrm{K}^0_{x_{i-1},\,x_i}\,, \partial_{t_z}\mathrm{M}^1_{x_{i-1},\,x_i}\} \quad (\text{recall } \partial_{t_z}\mathrm{K}^0 = 0)\ , \tag{4.27}$$

$$\Big|\widetilde{Z}_i(\gamma)\Big| \le \max\Big[\sup_{y\neq x}\big|\mathrm{K}^0_{yx}\big|\ ,\ \ \big|\partial_{t_z}\mathrm{M}^1_{yx}\big|\Big] \tag{4.28}$$

$$\le 2\sup_u \big|\partial_{t_z}\lambda_u^0\big|\,\delta_0^{-2}\epsilon_0^{1^+} \le \epsilon_0^{1^+}\,, \quad (\text{cf. (4.18)}) \tag{4.29}$$

where $\gamma = (x_0\,, x_1\,, \ldots\,, x_{k+1})$, with $x_0 = x_{k+1} = x$, is a path over the edges of the graph $\mathbb{Z}$, because $(Z_i)_{x_{i-1},\,x_i} = 0$ unless $|x_i - x_{i-1}| = 1$. Clearly, any product $\widetilde{\mathbf{Z}}(\gamma)$ containing a factor of the form (cf. (4.18))

$$\partial_{t_z}\mathrm{M}^1_{x_{i-1},\,x_i} = \mathbf{1}_{z\in\{\,x_{i-1},\,x_i\,\}}\cdot\varepsilon\mathrm{K}^0_{x_{i-1},\,x_i}\,\Big(\partial_{t_z}\lambda^0_{x_i} - \partial_{t_z}\lambda^0_{x_{i-1}}\Big)\,(\mathfrak{s}^0_{x_ix_{i-1}})^2 \tag{4.30}$$

vanishes, if $z \notin \{\,x_{i-1}, x_i\,\}$. Therefore, if $\gamma \not\ni z$, then $\widetilde{\mathbf{Z}}(\gamma) = 0$. We conclude that, for any x with $r = |x - z| \ge 2$, the nonzero contributions to $\partial_{t_z}\lambda_x^1 = \partial_{t_z}(\lambda_x^1 - \lambda_x^0)$ are made only by the paths $\gamma \ni z$, thus containing at least two sub-paths of length at least r each: the one starting at x and arriving at z for the first time, and another one leaving z for the last time and coming back to x. Let $|\gamma| := k + 1 =$ the path's length (the number of steps). Then any path γ providing a nonzero contribution has length $|\gamma| \ge 2r = 2\,|x - z|$, and so by (4.28), one has $\Big|\widetilde{Z}_1\cdots\widetilde{Z}_{k+1}\Big| \le \epsilon_0^{2r\,1^+}$. The convergence of the series

$$\sum_{k=2r\ge 2} k\big((k-1)!\big)^{-1}\cdot k2^k\big(\epsilon_0^{1^+}\big)^k \le \epsilon_0^{2r\,1^+}$$

implies that, for x such that $|x - z| \ge 2$, one has

$$\big|\partial_{t_z}\lambda_x^1\big| = \big|\partial_{t_z}\big(\,\mathrm{ad}^k_{\mathrm{M}^1}[\mathrm{K}^0]\big)_{xx}\big| \le \epsilon_0^{2|x-z|\,1^+}, \tag{4.31}$$

Now let $|x-z|=1$. Here, the main contribution to $\partial_{t_z}\left(\lambda^1_x-\lambda^0_x\right)$ is due to

$$\begin{aligned}\partial_{t_z}(\mathrm{ad}_{\mathrm{M}^1}[\mathrm{K}^0])_{xx} &= \left(\partial_{t_z}(\mathrm{K}^0\mathrm{M}^1)-\partial_{t_z}(\mathrm{M}^1\mathrm{K}^0)\right)_{xx}\\ &= (\mathrm{K}^0\partial_{t_z}\mathrm{M}^1))_{xx}-\left((\partial_{t_z}\mathrm{M}^1)\mathrm{K}^0\right)_{xx}\\ &= \mathrm{K}^0_{xz}\,\partial_{t_z}\mathrm{M}^1_{zx}-(\partial_{t_z}\mathrm{M}^1_{xz})\,\mathrm{K}^0_{zx}\end{aligned}$$

and the bounds on $\left|\mathrm{K}^0_{xz}\right|$ and $\left|\partial_{t_z}\mathrm{M}^1_{xz}\right|$ used above show that, in the case $r=|x-z|=1$, the bound of the form (4.31) still applies: $\left|\partial_{t_z}\lambda^1_x\right|\le\epsilon_0^{2|x-z|\,1^+}$, thus

$$\begin{gathered}\forall\, z\in\mathbb{Z}\quad \forall\, x\neq z\quad \left|\partial_{t_z}\lambda^1_x\right|\le\epsilon_0^{2r\,1^+}\equiv\epsilon_0^{2|x-z|\,1^+}\le \mathrm{e}^{-2^+\hat m|x-z|}\,,\\ \hat m=\hat m(\epsilon_0):=4\ln^{1/2}\epsilon_0^{-1}.\end{gathered}\tag{4.32}$$

For any $0<a<\hat a(\epsilon_0):=2\ln(\epsilon_0^{-1})$,

$$\sum_{x\neq z}\mathrm{e}^{a\,|x-z|}\,\left|\partial_{t_z}\lambda^1_x\right|\le 2\sum_{r\ge1}\mathrm{e}^{-(\hat a(\epsilon_0)-a)\,|x-z|}\le\frac{2\mathrm{e}^{-(\hat a(\epsilon_0)-a)}}{1-\mathrm{e}^{-(\hat a(\epsilon_0)-a)}}\,.\tag{4.33}$$

Assuming, for example, that $a\in(0,\hat a(\epsilon_0)]$, one obtains a simpler bound

$$\sum_{x\neq z}\mathrm{e}^{a\,|x-z|}\,\left|\partial_{t_z}\lambda^1_x\right|\le 4\mathrm{e}^{-\frac12\hat a(\epsilon_0)}=4\mathrm{e}^{-\frac12\ln(\epsilon_0^{-1})}=4\epsilon_0^{1/2}\,.\tag{4.34}$$

The roles of z and x can be exchanged, since the above bounds depend only on $|z-x|=|x-z|$, thus

$$\begin{aligned}\sup_{z\in\mathbb{Z}}\sum_{x\neq z}\mathrm{e}^{a\,|x-z|}\,\left|\partial_{t_z}\left(\lambda^1_x-\lambda^0_x\right)\right|\le 4\epsilon_0^{1/2}\,,\\ \sup_{x\in\mathbb{Z}}\sum_{z\neq x}\mathrm{e}^{a\,|x-z|}\,\left|\partial_{t_z}\left(\lambda^1_x-\lambda^0_x\right)\right|\le 4\epsilon_0^{1/2}\,.\end{aligned}\tag{4.35}$$

It is to be stressed that the above estimates hold under the condition

$$\inf_x\,\left|\mathfrak{s}^0_{x,x-1}\right|=\inf_x\,\left|\lambda^0_x-\lambda^0_{x-1}\right|=\inf_x\,|V(x,\theta)-V(x-1,\theta)|\ge\delta_0\,,\tag{4.36}$$

so we turn now to assessing the probability of the subset of Θ on which the above condition holds true.

4.3. Measure-theoretic estimates for the spacings $\mathfrak{s}^0_\bullet$

Recalling that the integer $\tilde n_0$ was defined in (2.6), decompose $\mathfrak{s}^0_x(\theta)$ as follows:

$$\begin{aligned}\mathfrak{s}^0_x(\theta)&=\lambda^0_x(\theta)-\lambda^0_{x-1}(\theta)=V(x,\theta)-V(x-1,\theta)\\ &=v_{\tilde n_0}(x,\theta)-v_{\tilde n_0}(x-1,\theta)+r_{\tilde n_0}(\theta)\,,\\ r_{\tilde n_0}(\theta)&=\sum_{n>\tilde n_0}a_n\left(\left(\theta_n([x]_n)-\theta_n([x-1]_n)\right)\right)\,.\end{aligned}\tag{4.37}$$

Note that

$$|r_{\tilde{n}_0}(\theta)| \leq 2 \sum_{n>\tilde{n}_0} a_n \leq \mathrm{e}^{-\tilde{n}_0}\, a_{\tilde{n}_0}\,, \tag{4.38}$$

and focus now on $V_{\tilde{n}_0}(x,\theta)$ and $V_{\tilde{n}_0}(x-1,\theta)$. Let $\mathfrak{B}^{\Theta}_{<\tilde{n}_0}(x) \subset \mathfrak{B}^{\Theta}$ be the sigma-algebra generated by

$$\{\, \theta_n([x]_n),\, n \in [\![1, \tilde{n}_0 - 1]\!]\,;\, \theta_n([y]_n),\, y \in [\![0, 2^n - 1]\!] \setminus \{\, x \,\}, n \in [\![1, \tilde{n}_0]\!] \,\}\,, \tag{4.39}$$

so that we have a decomposition

$$\begin{aligned} v_{\tilde{n}_0}(x,\theta) - v_{\tilde{n}_0}(x-1,\theta) &= \xi_{\tilde{n}_0} + \zeta_{\tilde{n}_0}(\theta)\,, \\ \xi_{\tilde{n}_0}(\theta) &:= a_{\tilde{n}_0}\theta_{\tilde{n}_0}([x]_{\tilde{n}_0}). \end{aligned} \tag{4.40}$$

Here, $\zeta_{\tilde{n}_0}$ is $\mathfrak{B}^{\Theta}_{<\tilde{n}_0}$-measurable, and $\xi_{\tilde{n}_0}(\theta)$ has the uniform distribution Unif($[0, a_{\tilde{n}_0}]$). Consider the event

$$\Theta^0_x := \{\, |\xi_{\tilde{n}_0} + \zeta_{\tilde{n}_0}| \leq 5\delta_0 \,\} \subset \Theta \tag{4.41}$$

and assess its probability using conditioning on $\mathfrak{B}^{\Theta}_{<\tilde{n}_0}(x)$:

$$\mathbb{P}^{\Theta}\left\{\, \Theta^0_x \,\right\} = \mathbb{E}^{\Theta}\left[\, \mathbb{P}^{\Theta}\left\{\, |\zeta_{\tilde{n}_0} + \zeta_{\tilde{n}_0}| \leq 5\delta_0 \,\middle|\, \mathfrak{B}^{\Theta}_{<\tilde{n}_0} \,\right\}\right] \tag{4.42}$$

Conditional on $\mathfrak{B}^{\Theta}_{<\tilde{n}_0}$, the sum $\xi_{\tilde{n}_0} + \zeta_{\tilde{n}_0}$ has the probability density admitting the same bound as $\xi_{\tilde{n}_0} \sim \mathrm{Unif}([0, a_{\tilde{n}_0}])$, thus

$$\mathbb{P}^{\Theta}\left\{\, \Theta^0_x \,\right\} \leq 5a^{-1}_{\tilde{n}_0}\delta_0 = 10a^{-1}_{\tilde{n}_0} \cdot \beta_{\tilde{n}_0} a_{\tilde{n}_0} = 10\,\beta_{\tilde{n}_0} \tag{4.43}$$

$\mathbb{P}^{\Theta}$ is translation-invariant and $x \mapsto v_{\tilde{n}_0}(x,\theta)$is $2^{\tilde{n}_0}$-periodic, thus, setting

$$\Theta^0 = \Theta \setminus \bigcup_{x \in \mathbb{Z}} \Theta^0_x \tag{4.44}$$

we get an upper bound

$$1 - \mathbb{P}^{\Theta}\left\{\, \Theta^0 \,\right\} \leq \bigcup_{x \in [\![0, 2^{\tilde{n}_0} - 1]\!]} \Theta^0_x \leq 10\mathrm{e}^{-\tilde{n}_0} = \mathrm{e}^{-\frac{1}{2}\tilde{n}_0} \leq \beta_0^{1/2}\,. \tag{4.45}$$

The above bounds have been proved for the AEV relative to the truncated potential V_N, but making use to (4.37) and (4.38), we infer for the full, non-truncated potential V a slightly weaker but satisfactory bound:

$$\forall\, \theta \in \Theta^0 \quad \forall\, x \in \mathbb{Z} \qquad \left|\mathfrak{s}^0_{x,x-1}\right| \geq 5\delta_0 - \mathrm{o}\,(\delta_0) \geq 4\delta_0\,. \tag{4.46}$$

Finally, note that, since $\zeta_{\tilde{n}_0}$ and $\xi_{\tilde{n}_0}$ are $\mathfrak{B}^{\Theta}_{\leq\tilde{n}_0}$-measurable, so is Θ^0.

4.4. Conclusion

We have shown that there exists a set $\Theta^0 \in \mathfrak{B}^{\Theta}_{\leq \tilde{n}_0}$ such that

$$\begin{aligned} &\mathbb{P}^{\Theta}\left\{\,\Theta^0\,\right\} \geq 1-\beta_0^{1/2}\,, \\ \forall\,\theta\in\Theta^0 \quad \forall\, x\in\mathbb{Z} \quad &\left|\mathfrak{s}^0_{x,x-1}(\theta)\right| \geq 4\delta_0\,. \end{aligned} \tag{4.47}$$

5. General induction step

Assume the inductive hypotheses K1 – K5 of a step $j \geq 1$.

5.1. The orthogonal rotation generator M^{j+1}

By the hypothesis K4,

$$\inf_{\theta\in\Theta^j} \inf_{1\leq|x-y|\leq \mathrm{L}_{j+1}^2} \left|\lambda_x^j(\theta)-\lambda_y^j(\theta)\right| \geq 4\delta_j \tag{5.1}$$

and $\|\!|\mathrm{K}^j|\!\| \leq \epsilon_j^{1^+}$. Thus, for all $\theta\in\Theta^{(j)}$, the operator $\mathrm{M}^{j+1}(\theta)$ with the matrix

$$\mathrm{M}^{j+1}_{yx}(\theta) = \begin{cases} \frac{\mathrm{K}^j_{yx}(\theta)}{\lambda_x^j(\theta)-\lambda_y^j(\theta)}, & \text{if } 1\leq|x-y|\leq \mathrm{L}_j \text{ and } \mathrm{K}^j_{yx}\neq 0; \\ 0, & \text{otherwise,} \end{cases} \tag{5.2}$$

is well-defined and admits the bound

$$\|\!|\mathrm{M}^{j+1}(\theta)|\!\| \leq \delta_j^{-1}\|\!|\mathrm{K}^j(\theta)|\!\| \leq \delta_j^{-1}\,\epsilon_j^{1^+} \leq \epsilon_j^{1^+}, \tag{5.3}$$

so the operators $\mathrm{e}^{\pm\mathrm{M}^{j+1}}$ are well-defined and unitary, as M^{j+1} is anti-symmetric.

5.2. Transformation of the basis. The new AEV

Let $\mathscr{K}^{j+1} := \mathrm{Ad}_{\mathrm{M}^{j+1}}\left[\Lambda^j\right] + \mathrm{Ad}_{\mathrm{M}^{j+1}}\left[\mathrm{K}^j\right] - \Lambda^j$. By $\left[\Lambda^j, \mathrm{M}^{j+1}\right] = -\mathrm{K}^j$, we get

$$\begin{aligned} \mathscr{K}^{j+1} &= \sum_{k\geq 1}\frac{1}{k!}\,\mathrm{ad}^k_{\mathrm{M}^{j+1}}\left[\Lambda^j\right] + \sum_{k\geq 0}\frac{1}{k!}\,\mathrm{ad}^k_{\mathrm{M}_N^{j+1}}\left[\mathrm{K}^j\right] \\ &= \sum_{k\geq 1}\frac{1}{k!}\,\mathrm{ad}^{k-1}_{\mathrm{M}^{j+1}}\left[\left[\Lambda^j,\mathrm{M}^j\right]\right] + \sum_{l\geq 1}\frac{1}{(l-1)!}\,\mathrm{ad}^{l-1}_{\mathrm{M}^{j+1}}\left[\mathrm{K}^j\right] \\ &= \sum_{k\geq 1}\mathfrak{k}_k\,\mathrm{ad}^k_{\mathrm{M}^{j+1}}\left[\mathrm{K}^j\right], \\ \mathfrak{k}_k &:= \frac{k-1}{k!} \leq \frac{1}{(k-1)!}\,. \end{aligned} \tag{5.4}$$

Therefore, we come to a new decomposition of the Hamiltonian:

$$\begin{aligned}
\mathrm{Ad}_{\mathrm{M}^{j+1}}[\mathrm{H}^j] &= \Lambda^{i+1} + \mathrm{K}^{j+1} =: \mathrm{H}^{j+1}\,,\\
\Lambda^{i+1}_{yx} &:= \delta_{yx}\lambda^{j+1}_x\,,\\
\lambda^{j+1}_x &:= \lambda^j_x + \mathscr{K}^{j+1}_{xx}\,,\\
\mathrm{K}^{j+1}_{yx} &:= (1-\delta_{yx})\mathscr{K}^{j+1}_{yx}\,.
\end{aligned} \tag{5.5}$$

A direct analog of (4.5) is

$$\begin{aligned}
&\max\left[\|\Lambda^{i+1}-\Lambda^j\|\,,\|\!|\mathrm{K}^{j+1}|\!|\right]\\
&\le |\!|\!|\mathscr{K}^{j+1}|\!|\!|\\
&\le \sum_{k\ge 1}\mathfrak{k}_k|\!|\!|\,\mathrm{ad}_{\mathrm{M}^{j+1}}[\mathrm{K}^j]|\!|\!|\\
&\le |\!|\!|\mathrm{K}^j|\!|\!|\ \sum_{k\ge 1}2^k\mathfrak{k}_k|\!|\!|\mathrm{M}^{j+1}|\!|\!|^k\\
&= 2|\!|\!|\mathrm{K}^j|\!|\!|\ |\!|\!|\mathrm{M}^j|\!|\!|\ \mathrm{e}^{2|\!|\!|\mathrm{M}^{j+1}|\!|\!|}\\
&\le 4|\!|\!|\mathrm{K}^j|\!|\!|\ |\!|\!|\mathrm{M}^{j+1}|\!|\!|\,.
\end{aligned} \tag{5.6}$$

By (5.3), $|\!|\!|\mathrm{M}^{j+1}|\!|\!| \le \epsilon_j^{1^+}$, whence

$$|\!|\!|\mathscr{K}^{j+1}|\!|\!| \le 4\delta_j^{-1}\epsilon_j^{2^-} \le \epsilon_j^{2^+} < \epsilon_j^{q\,1^+} \le \epsilon_{j+1}^{1^+}\,, \tag{5.7}$$

and so the perturbations of the AEV can be uniformly bounded as follows:

$$\sup_x\ \left|\lambda^{j+1}_x(\theta)-\lambda^j_x(\theta)\right| \le \|\Lambda^j-\Lambda^{i+1}\| \le \epsilon_j^{2^+} \le \epsilon_{j+1}^{1^+}\,. \tag{5.8}$$

Furthermore,

$$|\!|\!|\mathrm{e}^{\pm\mathrm{M}^{j+1}}-\mathbf{1}\,|\!|\!| \le \sum_{k\ge 1}2^k\mathfrak{k}\left(\delta_j^{-1}|\!|\!|\mathrm{K}^j|\!|\!|\right)^k \le \epsilon_j^{1^+}\,. \tag{5.9}$$

For the unitary transformation of the initial, canonical basis,

$$\mathscr{M}^{j+1} = \prod_{i=1}^{j+1}\mathrm{e}^{\mathrm{M}^i} = \mathrm{e}^{\mathrm{M}^{j+1}}\ \cdots\ \mathrm{e}^{\mathrm{M}^1}, \tag{5.10}$$

we thus have both the inductive and a global (uniform in j) upper bound

$$|\!|\!|\mathscr{M}^{j+1}-\mathbf{1}\,|\!|\!| \le \mathrm{e}^{\sum_{i=1}^{j+1}\epsilon_i^{1^+}}\ \sum_{i=1}^{j+1}\epsilon_i^{1^+} \le \epsilon_0^{1/2}\,. \tag{5.11}$$

5.3. Parametric smoothness estimates

As in Section 4.2, consider the parameters $\mathbf{t} = (t_z)_{z\in\mathbb{Z}}$ and the parametric family of potentials

$$x \mapsto \widetilde{V}(x,\,\cdot\,,\cdot\,;\mathbf{t}) := V(x,\,\cdot\,,\cdot\,) + \sum_{z\in\mathbb{Z}} t_z\,\mathbf{1}_z(x).$$

We have $\mathrm{M}^{j+1}_{yx} = \mathrm{K}^j_{yx}\,\mathfrak{s}^j_{yx}$ where K^j fulfills (2.19) and $\mathfrak{s}^j := \left(\lambda^j_x - \lambda^j_y\right)^{-1}$ with $\lambda^j_\bullet$ satisfying (2.18). Therefore, there exists the derivative

$$\partial_{t_z}\mathrm{M}^{j+1}_{yx} = \partial_{t_z}\left(\mathrm{K}^j_{yx}\mathfrak{s}^j_{yx}\right) = \left(\partial_{t_z}\mathrm{K}^j_{yx}\right)\mathfrak{s}^j_{yx} + \mathrm{K}^j_{yx}\,\left(\partial_{t_z}\lambda^j_x - \partial_{t_z}\lambda^j_y\right)\,(\mathfrak{s}^j_{yx})^2\,. \quad (5.12)$$

Using the recursion

$$\partial_{t_z}\,\mathrm{ad}^k_{\mathrm{M}^{j+1}}[\mathrm{K}^j] = \partial_{t_z}(\mathrm{ad}^{k-1}_{\mathrm{M}^{j+1}}[\mathrm{K}^j]\mathrm{M}^{j+1}) - \partial_{t_z}(\mathrm{M}^{j+1}\,\mathrm{ad}^{k-1}_{\mathrm{M}^{j+1}}[\mathrm{K}^j])\,, \quad (5.13)$$

the iterated commutator $\mathrm{ad}^k_{\mathrm{M}^{j+1}}[\mathrm{K}^j]$ is expanded in the sum of 2^k products of the form $\mathbf{Y}^{(k)} = Y_1\cdots Y_{k+1}$ where one of the factors Y_i is K^j, and k factors are equal to M^{j+1}.

Expanding by the Leibniz rule the derivative $\partial_{t_z}\mathbf{Y}^{(k)}$, we get $k+1$ new products; each of them differs from $\mathbf{Y}^{(k)}$ in exactly one position $i \in \{\,1,2,\ldots,k+1\,\}$ where Y_i is replaced with $Z_i := \partial_{t_z}Y_i$. Therefore, $\partial_{t_z}\,\mathrm{ad}^k_{\mathrm{M}^{j+1}}[\mathrm{K}^j]$ is expanded in the sum of $k\,2^k$ products of the form $\mathbf{Z}^{(k)}$, where

$$\|\!|Z_l|\!\| \le \begin{cases} \delta_j^{-1}\epsilon_j^{1^+} \le \epsilon_j^{1^+}, & \text{if } Z_l = Y_l; \\ \delta_j^{-2}\epsilon_j^{1^+} \le \epsilon_j^{1^+}, & \text{if } Z_l = \partial_{t_z}Y_l\,. \end{cases} \quad (5.14)$$

Thus $\|\!|\mathbf{Z}^{(k)}|\!\| \le \epsilon_j^{(k+1)\,1^+}$, and so by convergence of the series

$$\sum_{k\ge1}\mathfrak{k}_k\,\|\!|\partial_{t_z}\,\mathrm{ad}^k_{\mathrm{M}^{j+1}}[\mathrm{K}^j]|\!\| \le \sum_{k\ge1}\frac{1}{(k-1)!}\,k2^k\epsilon_j^{(k+1)\,1^+} \le \epsilon_j^{2^+}, \quad (5.15)$$

the derivative $\partial_{t_z}\mathscr{K}^{j+1}$ exists, and one has

$$\|\!|\partial_{t_z}\mathscr{K}^{j+1}|\!\| \le \epsilon_j^{2^+}. \quad (5.16)$$

This implies the ∂_{t_z}-derivability of $\Lambda^{i+1} = \Lambda^j + \left(\Lambda^{i+1} - \Lambda^j\right)$, and we have

$$\sup_z\,\|\!|\partial_{t_z}\left(\Lambda^{i+1}(\,\cdot\,,\,\cdot\,) - \Lambda^j(\,\cdot\,,\,\cdot\,)\right)|\!\| \le \epsilon_j^{2^+}. \quad (5.17)$$

Hence, by $\left|\partial_{t_z}\lambda^{j+1}_x\right| \le \left|\lambda^j_x\right| + \left|\partial_{t_z}(\lambda^{j+1}_x - \lambda^j_x)\right|$,

$$\sup_z\,\left|\partial_{t_z}\lambda^{j+1}_z(\,\cdot\,,\,\cdot\,)\right| \le 1 + \sum_{0\le i\le j}\epsilon_i^{2^+} + \epsilon_{j+1}^{2^+} \le 1 + \sum_{0\le i\le j+1}\epsilon_i^{2^+}. \quad (5.18)$$

Further, recall that

$$\forall\, z \in \mathbb{Z} \quad \forall\, x \neq z \quad \left|\partial_{t_z} \lambda_x^j\right| \leq \mathrm{e}^{-2^+ \hat{m}|x-z|}\,, \tag{5.19}$$

hence

$$\sup_z \sup_{x \neq z} \left|\partial_{t_z} \lambda_x^{j+1}(\cdot\,,\cdot)\right| \leq \mathrm{e}^{-2^+ \hat{m}|x-z|} + \epsilon_{j+1}^{1^-}. \tag{5.20}$$

To improve the above general bound for $|x-z|$, we need a more accurate estimate. Arguing as in Section (4.2), we obtain first

$$\widetilde{\mathbf{Z}}(\gamma) \leq \mathrm{e}^{-2\hat{m}|z-x_i|} \cdot \delta_j^{-2} \epsilon_j^{(k+1)\,1^+}\,, \quad k+1 \geq 2. \tag{5.21}$$

Further, recall that, by (5.2), $\mathrm{M}_{yx}^{j+1} = 0$ whenever $|y-x| > \mathrm{L}_j$, and fix any $x \in \mathbb{Z}$.

Assume first that $\boldsymbol{k+1 < |x-z|\,/\mathrm{L}_j}$, and consider the matrix elements $(\mathrm{ad}^k_{\mathrm{M}^{j+1}}[\mathrm{K}^j])_{xx}$ contributing to $\lambda_x^{j+1} - \lambda_x^j$. Fix some $x \in \mathbb{Z}$, pick a product $\mathbf{Z}^{(k)} = Z_1 \cdots Z_{k+1}$ and expand the derivatives of its diagonal matrix elements as follows:

$$\partial_{t_z} \mathbf{Z}_{xx}^{(k)} = \sum_{\gamma=(x_0\,,x_1\,,\dots\,,x_{k+1})} \widetilde{\mathbf{Z}}(\gamma)\,, \quad \widetilde{\mathbf{Z}}(\gamma) = \widetilde{Z}_1(\gamma) \cdots \widetilde{Z}_{k+1}(\gamma), \tag{5.22}$$

$$\widetilde{Z}_i(\gamma) \in \{\mathrm{K}^j_{x_{i-1},\,x_i}\,, \partial_{t_z}\mathrm{K}^j_{x_{i-1},\,x_i}\,, \mathrm{M}^{j+1}_{x_{i-1},\,x_i}\,, \partial_{t_z}\mathrm{M}^{j+1}_{x_{i-1},\,x_i}\}\,, \tag{5.23}$$

$$\left|\widetilde{Z}_i(\gamma)\right| \leq \sup_{y \neq x} \|\!|\partial_{t_z} \mathrm{M}_{yx}^{j+1}|\!\| \leq 2 \sup_u \left|\partial_{t_z} \lambda_u^j\right| \delta_j^{-2} \varepsilon \leq \epsilon_j^{1^-}\,, \quad \text{(cf. (5.12))} \tag{5.24}$$

where $\gamma = (x_0\,, x_1\,, \dots\,, x_{k+1})$, $x_0 = x_{k+1} = x$, is a path with step lengths $\ell_i := |x_i - x_{i-1}| \leq \mathrm{L}_j$. By the triangle inequality and the assumption $k+1 < \frac{|x-z|}{\mathrm{L}_j}$,

$$|x_i - z| \geq |z-x| - |z-x_i| \geq |z-x| - \frac{k+1}{2}\mathrm{L}_j > \frac{|x-z|}{2} \tag{5.25}$$

for all $0 \leq i \leq k+1$, thus $\left|\partial_{t_z} \lambda_{x_i}^j\right| \leq \mathrm{e}^{-2^-\hat{m}|z-x_i|}$. Therefore, by (5.24)

$$\begin{aligned}
\widetilde{\mathbf{Z}}(\gamma) &\leq \mathrm{e}^{-2\hat{m}|z-x_i|} \cdot \delta_j^{-2} \epsilon_j^k = \mathrm{e}^{-2\hat{m}|z-x_i|} \cdot \delta_j^{-2} \epsilon_j^{k/2} \cdot \epsilon_j^{k/2} \\
&\leq \epsilon_j^{k/2}\, \mathrm{e}^{-2\hat{m}|z-x_i| - \frac{1^-|x-x_i|}{\mathrm{L}_j} q^j \ln \epsilon_0^{-1}} \\
&\leq \epsilon_j^{k/2}\, \mathrm{e}^{-2\hat{m}|z-x_i| - \frac{1^-|x-x_i|}{\mathrm{L}_0 q^j} q^j \ln \epsilon_0^{-1}} \\
&\leq \epsilon_j^{k/2}\, \exp\left(-2\hat{m}\left(|z-x_i| + |x-x_i|\,\frac{1^-\ln \epsilon_0^{-1}}{2\mathrm{L}_0 \hat{m}}\right)\right).
\end{aligned} \tag{5.26}$$

On the other hand, we have by (4.32)

$$\frac{\ln \epsilon_0^{-1}}{2\,\mathrm{L}_0\,\hat{m}} = \frac{\ln \epsilon_0^{-1}}{2\,\mathrm{L}_0 \ln^{1/2} \epsilon_0} = \frac{\ln^{1/2} \epsilon_0^{-1}}{2\,\mathrm{L}_0} > 2\,, \tag{5.27}$$

hence

$$\widetilde{\mathbf{Z}}(\gamma) \le \epsilon_j^{k/2}\, \mathrm{e}^{-2\hat{m}(|z-x_i|+|x-x_i|)} \le \mathrm{e}^{-2\hat{m}|z-x|}\, \epsilon_j^{k/2} \tag{5.28}$$

Next, assume that $k+1 \ge |z-x|\,/\mathbf{L}_j$. Then we obtain a similar bound:

$$\widetilde{\mathbf{Z}}(\gamma) \le \delta_j^{-2}\epsilon_j^k \le \epsilon_j^{k/2}\, \mathrm{e}^{-1^-\frac{r}{\mathrm{L}_j} q^j \ln \epsilon_0^{-1}} \le \epsilon_j^{k/2}\, \mathrm{e}^{-2^-\hat{m}r\frac{\ln \epsilon_0^{-1}}{2\,\mathrm{L}_0\,\hat{m}}} < \mathrm{e}^{-2\hat{m}r}\epsilon_j^{k/2}\,, \tag{5.29}$$

where the last right-hand side inequality is due to (5.27). By convergence of the series

$$\sum_{k\ge 2} k\big((k-1)!\big)^{-1} \cdot k2^k \cdot \mathrm{e}^{-2\hat{m}r}\epsilon_j^{k/2}\,,$$

for all x such that $|x-z| \ge 2$, we have

$$\big|\partial_{t_z}\lambda_x^{j+1} - \partial_{t_z}\lambda_x^j\big| = \big|\partial_{t_z}\big(\,\mathrm{ad}^k_{\mathrm{M}^1}[\mathrm{K}^0]\big)_{xx}\big| \le \mathrm{e}^{-2\hat{m}|x-z|}\epsilon_j^{2/4}, \tag{5.30}$$

On account of $\big|\partial_{t_z}\lambda_x^{j+1}\big| \le \big|\partial_{t_z}\lambda_x^j\big| + \big|\partial_{t_z}(\lambda_x^{j+1}-\lambda_x^j)\big|$, we thus get:

$$\sup_z\ \big|\partial_{t_z}\lambda_x^{j+1}\big| \le \Big(1+\mathrm{O}\big(\epsilon_0^{1/2}\big)\Big)\,\mathrm{e}^{-2\hat{m}|x-z|}. \tag{5.31}$$

5.4. From t-dependence to θ-dependence

Now we are going to apply rather abstract parametric regularity estimates of the approximate eigenvalues (AEV) to the analysis $\theta_{n,k}$-dependence of the AEV.

By the construction of the potential $V(\cdot,\theta)$ (cf. (1.3) and (1.4)),

$$\begin{aligned} V(x,\theta) &= \sum_{n\ge 1} a_n \sum_{k\in[\![0,T_n-1]\!]} \theta_{n,k}\chi_{n,k}(x) \\ &= \sum_{n\ge 1} a_n \sum_{1\le k\le T_n} \theta_{n,k} \sum_{l\in\mathbb{Z}} \mathbf{1}_0\big(x-(k+lT_n)\big). \end{aligned} \tag{5.32}$$

For all $x \in [\![0, 2T_n-1]\!]$, the last sum over l is reduced to the term with $l=0$, and, for each $n\ge 1$, the sum over $k\in[\![0,T_n-1]\!]$ is reduced to the term with $k=x$:

$$V(z,\theta) = \sum_{n\ge 1} a_n\theta_n([x]_n). \tag{5.33}$$

Representing $\theta\in\Theta$ as an infinite word $(\overline{\theta}_1\,,\overline{\theta}_2\,,\ldots\,,\overline{\theta}_n\,,\ldots)$ where, for each $n\ge 1$, $\overline{\theta}_n := (\theta_{n,k}\,, k\in[\![0,T_n-1]\!])$, we shall use the notations like

$$\theta_{\le n} := \big(\overline{\theta}_1\,,\ldots\,,\overline{\theta}_n\big)\,,\quad \theta_{>n} := \big(\overline{\theta}_{n+1}\,,\overline{\theta}_{n+2}\,,\ldots\big)\,, \tag{5.34}$$

to work with sub-words of θ where only $\overline{\theta}_l$ with l in a subset of $\mathbb{N}\setminus\{\,0\,\}$, clearly specified by the relations like "$l\le n$" etc., are kept while the others are removed.

Note that, equivalently, one can set the "unwanted" components $\overline{\theta}_l$ to the sub-words with zero values, e.g., setting $\overline{\theta}_1 = (0,0)$ in $\overline{\theta}_{>1} = \big((0,0), \overline{\theta}_2, \overline{\theta}_3, \dots\big)$ where $\theta_{n,k}$ remain unchanged.

We shall focus first on the AEV

$$\hat{\lambda}_x^{j+1}(\theta) := \lambda_x^{j+1}(\theta_{\le \tilde{n}_{j+1}}) \tag{5.35}$$

and assess the modified spectral spacings $\hat{\mathfrak{s}}_{x,y}^{j+1}(\theta) := \hat{\lambda}_x^{j+1} - \hat{\lambda}_y^{j+1}$ for $\theta_{\le \tilde{n}_{j+1}} \in \Theta^{j+1}$ where Θ^{j+1} is a suitably chosen subset of Θ. In the next subsection 5.4.1, the lower bounds on $\hat{\mathfrak{s}}_{x,y}^{j+1}(\theta)$ will be extended to all θ of the form $(\theta_{\le \tilde{n}_{j+1}}, \theta_{>\tilde{n}_{j+1}}$ with $\theta_{\le \tilde{n}_{j+1}} \in \Theta^{j+1}$ and ***any*** $\theta_{>\tilde{n}_{j+1}}$.

Next, given any $\theta \in \Theta^{(j)}$, truncate it to $\theta_{\le \tilde{n}_{j+1}}$. Pick any $x \in [\![0, \mathrm{L}_{j+1}^2 - 1]\!]$, and let $\mathfrak{B}^{\Theta}_{<\tilde{n}_{j+1}}(x) \subset \mathfrak{B}^{\Theta}$ be the sigma-algebra generated by

$$\Big\{ \theta_n([x]_n),\, n \in [\![1, \tilde{n}_j]\!] \Big\} \bigcup \Big\{ \theta_n([y]_n),\; y \in [\![0, 2^n - 1]\!] \setminus \{\, x \,\},\; n \in [\![1, \tilde{n}_{j+1}]\!] \Big\} \tag{5.36}$$

Conditional on $\mathfrak{B}^{\Theta}_{<\tilde{n}_{j+1}}(x)$, $\hat{\lambda}^{j+1}(\theta)$ is a function of exactly one Θ-random variable $a_{\tilde{n}_{j+1}} \theta_{\tilde{n}_{j+1}}[x]_{\tilde{n}_{j+1}}$, so we can identify the latter with the parameter t_x. Set temporarily for brevity $\hat{\theta}_x := \theta_{\tilde{n}_{j+1}}[x]_{\tilde{n}_{j+1}}$, then by the previously obtained bounds on $\partial_{t_z} \lambda_y^{j+1}$, $y, z \in \mathbb{Z}$, we get:

$$\frac{\partial\, \hat{\mathfrak{s}}_{x,y}^{j+1}}{\partial \hat{\theta}_x} = \frac{\partial \left(\hat{\lambda}_x^{j+1} - \hat{\lambda}_y^{j+1} \right)}{\partial \big(a_{\tilde{n}_{j+1}}^{-1} t_x \big)} = a_{\tilde{n}_{j+1}} \left(1 + \mathrm{O}\left(\epsilon_0^2\right) - \mathrm{O}\big(\epsilon_0\big) \right) \ge a_{\tilde{n}_{j+1}}/2\,. \tag{5.37}$$

Therefore, there exists a differentiable function $F_{x,y}^{[j+1]}$ such that

$$\hat{\mathfrak{s}}_{x,y}^{j+1} = F_{x,y}^{[j+1]}(\hat{\theta}_x)\,, \quad \mathrm{d}F_{x,y}^{[j+1]}/\mathrm{d}t \ge a_{\tilde{n}_{j+1}}/2\,. \tag{5.38}$$

Since $\hat{\theta}_x = \theta_{\tilde{n}_{j+1}}[x]_{\tilde{n}_{j+1}} \sim \mathrm{Unif}([0,1])$, the probability measure of $\hat{\mathfrak{s}}_{x,y}^{j+1}(\hat{\theta}_x)$ has a density ρ with respect to the Lebesgue measure on $[0,1]$ with $\|\rho\|_\infty \le 2 a_{\tilde{n}_{j+1}}^{-1}$. Let

$$\overline{\Theta}_{xy}^{j+1} := \big\{\, \theta :\, \big|\hat{\mathfrak{s}}_{yx}^{j+1}\big| \le 5\delta_{j+1} \,\big\}\,. \tag{5.39}$$

Then, recalling that $\delta_{\tilde{n}_{j+1}} = a_{\tilde{n}_{j+1}} \beta_{\tilde{n}_{j+1}}$, we get:

$$\mathbb{P}^{\Theta} \left\{ \overline{\Theta}_{xy}^{j+1} \right\} \le 2 a_{\tilde{n}_{j+1}}^{-1}\, 8\delta_{j+1} \le 16\, \beta_{\tilde{n}_{j+1}}\,. \tag{5.40}$$

Let

$$\overline{\Theta}^{j+1} := \bigcup_{\substack{x \ne y \\ 0 \le x, y < \mathrm{L}_{j+1}^2}} \overline{\Theta}_{xy}^{j+1}\,, \quad \widetilde{\Theta}^{j+1} := \Theta \setminus \overline{\Theta}^{j+1}\,. \tag{5.41}$$

Then we have

$$\begin{aligned}\mathbb{P}^{\Theta}\left\{\,\overline{\Theta}^{j+1}\,\right\} &\le 16\,\mathrm{L}_{j+1}^{2}\,\beta_{\tilde{n}_{j+1}} \le 16\mathrm{e}^{-\tilde{n}_{j+1}+2\ln \mathrm{L}_{j+1}} \\ &\le 16\mathrm{e}^{-5\ln \mathrm{L}_{j+1}+2\ln \mathrm{L}_{j+1}} \le \beta_{\tilde{n}_{j+1}}^{1/2} \quad \text{(cf. (2.6))}.\end{aligned} \tag{5.42}$$

Therefore,

$$\begin{aligned}\forall\,\theta\in\Theta^{j}\cap\widetilde{\Theta}^{j+1} \quad \left|\hat{\mathfrak{s}}_{xy}^{j+1}\right| &\ge 5\delta_{j+1}\,, \\ \mathbb{P}^{\Theta}\left\{\,\widetilde{\Theta}^{j+1}\,\right\} &\ge 1-\beta_{j+1}^{1/2}\,.\end{aligned} \tag{5.43}$$

5.4.1. Non-truncated AEV

To assess the approximation error

$$\left|\lambda_{x}^{j+1}(\theta)-\hat{\lambda}_{x}^{j+1}(\theta)\right| = \left|\lambda_{x}^{j+1}(\theta)-\lambda_{x}^{j+1}(\theta_{\le\tilde{n}_{j+1}})\right| \tag{5.44}$$

we start with the identity (1.4) and apply it to the sample $\theta_{>\tilde{n}_{j+1}}$ considered as a sample θ in which all the components $\theta_{n',k}$ with $1\le n'\le\tilde{n}_{j+1}$ and any k are replaced by 0:

$$V(y,\theta_{>\tilde{n}_{j+1}}) = \sum_{n>\tilde{n}_{j+1}} a_{n}\,\theta_{n,\,[y]_{n}} \tag{5.45}$$

whence

$$\sup_{y}\left|V(y,\theta_{<\tilde{n}_{j+1}})-V(y,\theta_{<\tilde{n}_{j+1}})\right| \le \sum_{n\ge\tilde{n}_{j+1}} a_{n}\,\theta_{n,\,[y]_{n}} \le 2\mathrm{e}^{-(\tilde{n}_{j+1}+1)^{2}}\,. \tag{5.46}$$

Now it follows from the smoothness bounds established in the previous subsection (see in particular (5.37)) and $\delta_{j+1}=a_{\tilde{n}_{j+1}}\mathrm{e}^{-\tilde{n}_{j+1}}$

$$\left|\lambda_{x}^{j+1}(\theta)-\lambda_{x}^{j+1}(\theta_{<\tilde{n}_{j+1}})\right| \le 4\mathrm{e}^{-(\tilde{n}_{j+1}+1)^{2}} = \mathrm{o}\,(\delta_{j+1})\,. \tag{5.47}$$

Summarizing, we have constructed the set $\widetilde{\Theta}^{j+1}$ figuring in the inductive hypothesis (K4) on the next step $j+1$: for all $\theta\in\Theta^{j}\cap\widetilde{\Theta}^{j+1}$,

$$\begin{aligned}\left|\lambda_{x}^{j+1}(\theta)-\lambda_{y}^{j+1}(\theta)\right| &\ge \left|\hat{\lambda}_{x}^{j+1}(\theta)-\hat{\lambda}_{y}^{j+1}(\theta)\right| - 4\mathrm{e}^{-(\tilde{n}_{j+1}+1)^{2}} \\ &\ge 5\delta_{j+1}-4\mathrm{e}^{-(\tilde{n}_{j+1}+1)^{2}} \ge 4\delta_{j+1}\,.\end{aligned} \tag{5.48}$$

To prove the inductive bound (2.16), viz.

$$\mathfrak{s}^{i}(x,y;\theta) \ge \mathrm{e}^{-C\ln^{4}|x-y|}\,. \tag{5.49}$$

observe that the spacing between the AEV labeled by (x,y), with $x\ne y$, is never treated before the step

$$\hat{\mathrm{j}}(|x-y|) = \min\{\,j\ge 0:\ \mathrm{L}_{j}\le|x-y|<\mathrm{L}_{j+1}\,\}\,,$$

and on the step $\hat{\jmath} \equiv \hat{\jmath}(|x-y|)$, it is proved that $\mathfrak{s}^{\hat{\jmath}}(x,y;\theta) \geq 4\delta_{\hat{\jmath}} = \mathrm{e}^{-\tilde{n}_{\hat{\jmath}}^2 - \tilde{n}_{\hat{\jmath}}}$. Since $\tilde{n}_i \sim C \ln L_i$, $i \geq 1$, we get

$$\delta_{\hat{\jmath}} \geq \mathrm{e}^{-\tilde{n}_{\hat{\jmath}}^2 - \tilde{n}_{\hat{\jmath}}} \geq \mathrm{e}^{-C' \ln^4 \mathrm{L}_{\hat{\jmath}} - C'' \ln^2 \mathrm{L}_{\hat{\jmath}}} \geq \mathrm{e}^{-2C' \ln^4 \mathrm{L}_{\hat{\jmath}}} \geq \mathrm{e}^{-C \ln^4 |x-y|} \tag{5.50}$$

with suitable constants $C', C'', C > 0$. Therefore, $|\mathfrak{s}^{\hat{\jmath}}(x,y;\theta)| \geq 4\mathrm{e}^{-C \ln^4 |x-y|}$.

Finally, the uniform perturbation estimates $\left|\lambda_z^{j+1} - \lambda_z^j\right| \leq \epsilon_i^2$ show that, on all steps $j \geq \hat{\jmath} + 1$, a similar but slightly weaker uniform lower bound is guaranteed: uniformly in $j \geq \hat{\jmath} + 1$, $|\mathfrak{s}^{\hat{\jmath}}(x,y;\theta)| \geq 2\mathrm{e}^{-C \ln^4 |x-y|}$.

6. Proof of Theorem 1

By construction, we have $\mathscr{M}^{j+1} = \mathrm{e}^{\mathrm{M}^{j+1}}\, \mathscr{M}^j$ (cf. (5.10)), we have $\mathscr{M}^0 = \mathbf{1}$ and the recursion, for all $j \geq 1$,

$$\|\!|\mathscr{M}^{j+1} - \mathscr{M}^j|\!\| \leq \|\!|\mathrm{e}^{\mathrm{M}^{j+1}} - 1|\!\|\, \|\!|\mathscr{M}^j|\!\| \leq 2\, \|\!|\mathrm{M}^{j+1}|\!\|\, \|\!|\mathscr{M}^j|\!\| \leq \epsilon_{j+1}^{1^+}\, \|\!|\mathscr{M}^j|\!\| \tag{6.1}$$

whence the bound uniform in $j \geq 0$ (cf. (5.11)) $\|\!|\mathscr{M}^j|\!\| \leq 1 + \epsilon_0^{1^+} \leq 2$, yielding

$$\|\!|\mathscr{M}^{j+1} - \mathscr{M}^j|\!\| \leq \epsilon_{j+1}^{1^+}\,. \tag{6.2}$$

By convergence of the series $\sum_{j \geq 0} \epsilon_{j+1}^{1^+} \leq \epsilon_0^{1^+}$, the unitary transformations $\mathscr{M}^j$ converge in norm to a unitary transformation $\mathscr{M}$ such that

$$\|\!|\mathscr{M}|\!\| \leq 1 + \epsilon_{j+1}^{1^+} \quad \|\!|\mathscr{M} - \mathbf{1}|\!\| \leq \epsilon_{j+1}^{1^+}\,. \tag{6.3}$$

Furthermore, the diagonal entries λ_x^j of the diagonal matrices Λ^j obey (cf. (5.8))

$$\sup_{\theta \in \Theta^\infty} \sup_{x \in \mathbb{Z}} \left|\lambda_x^{j+1} - \lambda_x^j\right| \leq \epsilon_j^{2^+}\,, \tag{6.4}$$

hence, for all $\theta \in \Theta^\infty$ and $x \in \mathbb{Z}$, there exist the limits

$$\lambda_x(\theta) := \lim_{j \to +\infty} \lambda_x^j(\theta)\,.$$

Conclusions.

• Taking the norm-limit in the equation $(\mathscr{M}^j)^{-1} H_\varepsilon \mathscr{M}^j = \Lambda^j + \mathrm{K}^j$ and using $\|\!|\mathrm{K}^j|\!\| \leq \epsilon_j \to 0$ as $j \to +\infty$, we see that

$$\forall\, \theta \in \Theta^\infty \quad \mathscr{M}^{-1}(\theta) H_\varepsilon(\theta) \mathscr{M}(\theta) = \Lambda(\theta)\,, \quad \Lambda_{yx}(\theta) = \delta_{yx} \lambda_x(\theta)\,. \tag{6.5}$$

Since $\mathscr{M}(\theta)$ is unitary, its column-vectors $\varphi_x(\theta)$ form an orthonormal eigenbasis of $H_\varepsilon(\theta)$ with the associated eigenvalues $\lambda_x(\theta)$. This proves the assertion (A): for any $\theta \in \Theta^\infty$, $H_\varepsilon(\theta)$ has pure point spectrum.

• The assertion (B), viz. unimodality of each eigenfunction $\varphi_x(\cdot,\theta)$, follows from the norm bound $\|\varphi_x - \mathbf{1}_x\| \le \|\!|\mathscr{M} - \mathbf{1}|\!\| \le \epsilon_0 < 1/2$.

• The assertion (C) (uniform exponential decay of all eigenfunctions φ_x) is a direct consequence of the $\|\!|\cdot|\!\|$-bounds of the transformation operators $\mathscr{M}^j$. In fact, this is exactly why these norms have been used, as in [2], instead of the conventional Hilbert norm.

• The assertion (D), stating the minimal guaranteed spacings $|\lambda_x - \lambda_y|$ in terms of $[x-y|$, follow directly from the estimates on $\left|\lambda_x^j - \lambda_y^j\right|$ for all $j \ge 0$ combined with the perturbation estimates (6.4).

Theorem 1 is proved.

7. Non-local Minami-type estimates. Proof of Theorem 2

We need the following variant of the inverse function theorem (cf. [6]).

Proposition 1. *Consider finite-dimensional real normed spaces* $(\mathbb{X}, \|\cdot\|_{\mathbb{X}})$ *and* $(\mathbb{Y}, \|\cdot\|_{\mathbb{Y}})$, *and a mapping* $\mathfrak{f} : \mathbb{X} \to \mathbb{Y}$ *differentiable in a ball* $\mathscr{B}_\ell(0) \subset \mathbb{X}$, $\ell > 0$. *Assume that there is an invertible linear mapping* $\mathscr{A} : \mathbb{X} \to \mathbb{Y}$ *such that*

$$\sup_{\mathrm{x}\in\mathscr{B}_\ell(0)} \|\mathfrak{f}'(\mathrm{x}) - \mathscr{A}\| \le \eta \le \frac{\kappa}{\|\mathscr{A}^{-1}\|}\,, \quad \kappa \in (0, \tfrac{1}{2})\,.$$

Denote $\mathscr{B}_R^{\mathscr{A}}(0) := \big\{\, \mathrm{y} \in \mathbb{Y} :\ \|\mathscr{A}^{-1}\mathrm{y}\|_{\mathbb{X}} \le R \,\big\}$, $R \ge 0$. *Then* $\mathfrak{f}$ *admits a differentiable inverse* $\mathfrak{f}^{-1} : \mathscr{B}_{\kappa\ell}^{\mathscr{A}}(0) \to \mathscr{B}_\ell(0)$, *and for all* $\mathrm{y} \in \mathscr{B}_{\kappa\ell}^{\mathscr{A}}(0)$ *one has*

$$\mathfrak{f}^{-1}(\mathrm{y}) = \mathscr{A}^{-1}\mathrm{y} + \delta(\mathrm{y}), \qquad \|\delta(\mathrm{y})\|_{\mathbb{X}} \le 2\,\eta\,\|\mathscr{A}^{-1}\|\;\|\mathscr{A}^{-1}\mathrm{y}\|_{\mathbb{X}}\,. \tag{7.1}$$

Furthermore, for any rectangle of the form $\mathbf{\Lambda}(\boldsymbol{\alpha}, \boldsymbol{\epsilon}) = I_1 \times \cdots \times I_K \subset \mathrm{B}_{\ell/4}(0)$, *with* $I_k = [\alpha_k - \epsilon_k\,,\, \alpha_k + \epsilon_k]$, $0 < \epsilon_k \le \frac{1}{4}\ell$, *one has*

$$\mathfrak{f}^{-1}\left(\mathbf{\Lambda}(\boldsymbol{\alpha}, \boldsymbol{\epsilon})\right) \subset \bigtimes_{1\le k\le K} \Big[\alpha_k' - (1 + \mathrm{O}\,(\epsilon_k))\epsilon_k\,,\, \alpha_k' + (1 + \mathrm{O}\,(\epsilon_k))\epsilon_k\Big].$$

Proof of Theorem 2. It suffices to consider a set $\mathscr{X} = (x_1, \dots, x_N) \in \mathbb{N}^N$ with $0 = x_1 < x_2 \cdots < x_N =: R = \operatorname{diam}\mathscr{X}$, Let $\hat{\mathrm{n}} = \left\lceil \frac{\ln(R+1)}{\ln 2} \right\rceil$, so that $\mathscr{X} \subset [\![0, 2^{\hat{\mathrm{n}}} - 1]\!]$. Conditional on the sigma-algebra

$$\mathfrak{B}_{\neq\hat{\mathrm{n}}} = \{\, \theta_{n,l},\, n \ne \hat{\mathrm{n}}\,, l \in [\![0, 2^n - 1]\!] \,\} \tag{7.2}$$

the mappings $\theta \mapsto \lambda_{x_k}(\theta)$, $k = 1 \dots N$, are Borel functions of $\theta_{\hat{\mathrm{n}},l_k}$, $l_k = [x_k]_n$. We also "freeze" all $\theta_{\hat{\mathrm{n}},l}$ with $l \notin \{\, l_1, \dots, l_N \,\}$, i.e. condition on an even larger sigma-algebra $\mathfrak{B}'_{\hat{\mathrm{n}}}$. Further, identify $(a_{\hat{\mathrm{n}}}\theta_{\hat{\mathrm{n}},l_1}\,,\, \dots\,,\, a_{\hat{\mathrm{n}}}\theta_{\hat{\mathrm{n}},l_N})$ with the formal real parameters $(t_1, \dots, t_N) = \mathbf{t}$ considered as the standard coordinates

in $\mathbb{R}^N$ endowed with the scaled Lebesgue measure $a_{\hat{\mathfrak{n}}}^{-N}\,\mathbf{1}_{[0,a_{\hat{\mathfrak{n}}}]^N}(\mathbf{t})\,d\mathbf{t}$ on the cube $[0,a_{\hat{\mathfrak{n}}}]^N$. It follows from the results of Section 5.3 that the mapping $\mathfrak{f}:\ \mathbf{t}\mapsto(\lambda_{x_1}(\mathbf{t}),\dots,\lambda_{x_N}(\mathbf{t}))$ is differentiable, and its derivative can be represented as follows:

$$\mathfrak{f}'(\mathbf{t})=\mathbf{1}+\mathfrak{D}(\mathbf{t}),\ \ \|\mathfrak{D}(\mathbf{t})\|\le\eta:=\epsilon_0\,.$$

For all $\epsilon_0(\varepsilon)$ small enough, $\mathfrak{f}'(\mathbf{t})$ is invertible, and $\|(\mathfrak{f}'(\mathbf{t}))^{-1}\|\le 1+\mathrm{O}\,(\epsilon_0)\le\frac{3}{2}$. Now we can apply Proposition 1 with $\mathscr{A}=\mathfrak{f}'(0)$ and

$$\|\mathfrak{f}'(\mathbf{t})-\mathbf{1}\|\le\eta\le\varkappa/\|\mathscr{A}^{-1}\|,\quad \varkappa=\tfrac{1}{4}\,.$$

With $\eta<1/16$, we thus have $\|\mathfrak{f}^{-1}(\mathbf{t})-\mathscr{A}^{-1}\mathbf{t}\|\le\frac{1}{2}\|\mathbf{t}\|$, and so the inverse image $\mathfrak{f}^{-1}(I_1'\times\dots\times I_N')$ is covered by a rectangle $I_1''\times\dots\times I_N''$ with $|I_k''|\le 2|I_k'|\le 4|I_k|$, $k\in[\![1,N]\!]$. Concluding,

$$\mathbb{P}^{\Theta}\,\{\,\forall\,k\in[\![1,N]\!]\ \ \lambda_{x_k}\in I_k'\,\}\lesssim a_{\hat{\mathfrak{n}}(R)}^{-N}\,|I_1|\cdots|I_N|$$

with $a_{\hat{\mathfrak{n}}(R)}\ge\mathrm{e}^{-C\ln^2(R)}$, so the claim follows. □

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Markov Processes and **Related Fields**

Probabilistic Models Motivated by Cooperative Sequential Adsorption

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Abstract. This survey concerns probabilistic models motivated by cooperative sequential adsorption (CSA) models. CSA models are widely used in physics and chemistry for modelling adsorption processes in which adsorption rates depend on the spatial configuration of already adsorbed particles. Corresponding probabilistic models describe random sequential allocation of particles either in a subset of Euclidean space, or at vertices of a graph (e.g. sites of the lattice). Depending on a technical setup these probabilistic models are stated in terms of spatial or integer-valued interacting birth-and-death processes.

In this survey we consider several such models that have been studied in recent years.

Keywords: cooperative sequential adsorption, maximum likelihood estimation, interacting urn model, interacting spin model, Markov chain, reversibility, electric networks, positive recurrence, transience, explosion

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Contents

1. Introduction

This survey is concerned with probabilistic models motivated by cooperative sequential adsorption (CSA) models. Adsorption is a real life phenomenon which can be thought of as follows. Consider particles (e.g. molecules) diffusing around a surface of a material. When a particle hits the surface, it can be retained (adsorbed) by the latter. CSA describes adsorption process in which adsorption rates depend on the spatial configuration of existing particles. In other words, particles adsorb to a surface subject to interaction with previously adsorbed particles. For example, adsorbed particles can either attract, or repel subsequent arrivals. These types of interactions are common for many physical, chemical and biological processes.

In physics and chemistry cooperative effects in adsorption are usually studied by experiments and by computer simulations of an appropriate CSA model. CSA model is a probabilistic model for random sequential deposition of particles (e.g. points or objects of various shape) either in a bounded region of a continuous space, or at vertices (sites) of a graph (e.g. lattice). In such a model a particle is placed at location x with the probability that is proportional to a specified function of the current configuration of existing particles in a neighbourhood of x. Such a construction is technically flexible for modelling both attractive and repulsive interaction between a new particle and previously adsorbed particles, and can be used in modelling CSA like processes in many real-life applications.

The paper is organised as follows. In Section 2 we introduce a model for random sequential deposition of particles (points) in a bounded subset of Euclidean space. This continuous model can be naturally interpreted as a model for time series of spatial locations. Fitting the model to data requires estimation of model parameters. We show that statistical inference for the model parameters can be based on maximum likelihood estimation. In particular, we describe the corresponding estimation procedure and discuss asymptotic properties of maximum likelihood estimators. In Section 3 we consider a discrete model random sequential deposition of particles at vertices of a graph (a growth process with graph based interaction). A probabilistic model obtained from the growth process by allowing deposited particles to depart is considered in Section 4. This model is motivated by adsorption processes in which adsorbed particles can be released from the adsorbing substrate. The model is described in terms of a reversible Markov chain and can be regarded as an interacting spin model and closely related to such well known models of statistical physics and interacting particle systems as the contact process and the Ising model. Finally, in Section 5 we consider a point process motivated by the CSA model. The point process is a probability measure given by a density with respect to Poisson point process (in finite dimensional Euclidean space) and belongs to a class of point processes used in spatial statistics for modelling point patterns.

2. Continuous CSA model

In this section we consider a probabilistic model for sequential deposition of points in a bounded domain of Euclidean space. This model is a continuous analogue of the lattice CSA known as monomer filling with nearest neighbour cooperative effects (see [2] and references therein). This lattice model describes a random sequential deposition of particles on the lattice, where only one particle can be allocated at a site. The probability of allocating a particle at an empty site is proportional to the allocation rate, which depends on the number of existing particles in a neighbourhood of the site. For example, the model on the one-dimensional lattice is specified by parameters c_i, $i = 1, 2, 3$. Namely, a particle is placed at an empty site k with the rate c_i, if the total number of existing particles at its nearest neighbours $k - 1$ and $k + 1$ is equal to i. In the continuous analogue of the lattice CSA model particles (points) are placed sequentially at random into a bounded region of $\mathbb{R}^d$ as follows. Given the current configuration of points, the probability of the event that a particle is placed at location x is proportional to a parameter $\beta_k \geq 0$ (called the growth rate), where k is the number of existing points within a given distance R of x. This continuous CSA model was proposed in [21] and was further studied as a model for time series of spatial locations in [18] and [19].

In the rest of this section we formally define the model and discuss statistical inference for the model parameters.

2.1. The model definition

Start with some notations. Let $\mathbb{N}$ be the set of all positive integers and $\mathbb{Z}_+ = \mathbb{N} \cup \{0\}$. Let $\mathbb{R} = (-\infty, \infty)$ and $\mathbb{R}_+ = [0, \infty)$. By $\mathbf{1}_A$ we denote the indicator function of a set or an event A. We assume that all random variables under consideration are defined on a certain probability space with the probability measure P. The expectation with respect to P will be denoted by E.

Given points $x, y \in \mathbb{R}^d$ we denote by $\|x-y\|$ the Euclidean distance between x and y. Given a positive number R points $x, y \in \mathbb{R}^d$ are called neighbours, if $\|x - y\| \le R$, in which case we write $x \sim y$. Given a finite set (ordered or unordered) $\mathcal{X}$ of points in $\mathbb{R}^d$, define

$$\nu(x, \mathcal{X}) = \sum_{y \in \mathcal{X}} \mathbf{1}_{\{\|x-y\| \le R\}} \quad \text{for} \quad x \in \mathbb{R}^d, \tag{2.1}$$

in other words, $\nu(x, \mathcal{X})$ is the number of neighbours of x in the set $\mathcal{X}$. By definition $\nu(x, \emptyset) = 0$.

The continuous CSA model with the interaction radius $R > 0$ and parameters ($\beta_k \ge 0$, $k \in \mathbb{Z}_+$) is the probabilistic model for random sequential deposition of points in $\mathbb{R}^d$ defined as follows. Consider a compact convex set $D \subset \mathbb{R}^d$ (called the target region, or the observation window). Let $X(k) = (X_1, \dots, X_k)$, $k \ge 0$, be the sequence of locations of first k points allocated in D according to the model. By definition, $X(0) = \emptyset$. Given that $X(k) = x(k) = (x_1, \dots, x_k)$ for $k \ge 0$ the conditional probability density function of the next point X_{k+1} is

$$\psi_{k+1}(x|x(k)) = \frac{\beta_{\nu(x,x(k))}}{\int_D \beta_{\nu(y,x(k))} dy}, \ x \in D. \tag{2.2}$$

The joint density of $(X_1, \dots, X_\ell)$, $\ell \ge 1$ is given by

$$\begin{aligned} p_{\ell,\beta,D}(x_1, \dots, x_\ell) &= \prod_{k=1}^{\ell} \psi_k(x_k|x(k-1)) \\ &= \prod_{k=1}^{\ell} \frac{\beta_{\nu(x_k,x(k-1))}}{\int_D \beta_{\nu(u,x(k-1))} du}, \quad x_i \in D, \, i = 1, \dots, \ell. \end{aligned} \tag{2.3}$$

The described CSA can be regarded as a discrete time spatial birth process with birth rates $\beta_{\nu(x,x(k))}$, $x \in D$, provided that the state of the process at time k is $x(k) = (x_1, \dots, x_k)$.

Alternatively, the model can be described as the acceptance-rejection sampling described below. Namely, let $(Y_i,\, i \ge 1)$ be a sequence of independent random points uniformly distributed in D, and construct another sequence of random points by accepting each point of the original sequence with a certain probability to be described below, otherwise rejecting that point. Let

$X(k) = (X_1, \ldots, X_k)$ be the sequence of $k = k_n$ accepted points from the finite sequence Y_i, $i = 1, \ldots, n$. By definition $X(0) = \emptyset$. The point Y_{n+1} is accepted with probability $\beta_{\nu(Y_{n+1}, X(k))}/C$, where C is an arbitrary constant such that $\max_{0 \le i \le k} \beta_i \le C$. Regardless of the particular choice of C, the next accepted point X_{k+1} has the probability density $\psi_{k+1}(x|X(k))$ given by (2.2) In other words, given the sequence $X(\ell)$ of the first ℓ accepted points, the next accepted point $X_{\ell+1}$ is sampled from a distribution which is specified by the probability density proportional to the function $\beta_{\nu(x, X(\ell))}$, $x \in D$ (the value of C influences only the number of discarded points Y_i until the next acceptance).

Remark 2.1. The defined above continuous CSA model was introduced in [21]. In that paper the asymptotic structure of the model point pattern was studied under the assumption that the sequence $(\beta_n > 0,\, n \ge 0)$ converges to a positive limit as $n \to \infty$. This assumption can be interpreted as if "adsorption rates stabilize at saturation".

Remark 2.2. A special case of the model, when $\beta_i = 0$ for $i \ge 1$, is called random sequential adsorption (RSA) model. RSA is also known as the car parking model. In the latter cars are modelled by balls of radius R. Cars sequentially arrive to the target region D and choose a location to park at random. A new arrival is discarded with probability 1, if it overlaps any of previously parked cars. Otherwise it is parked (accepted) with probability 1.

2.2. CSA as a model for time series of spatial locations

It has been noted by physicists (e.g. [2]) that CSA model can be used for modelling sequential point patterns in disciplines such as geophysics, biology and ecology in situations, where a data set is presented by a sequential point pattern, i.e., a collection of spatial events which appear sequentially. In other words, CSA can be used as an approximation of spatial spread dynamics in various applications. This idea was explored in [18] and [19], where the continuous CSA was regarded as a model for time series of spatial locations, which is flexible for modelling both regular and clustered point patterns (e.g. see Figure 1). Note that models for clustered point patterns are of a particular interest in spatial statistics.

Fitting a parametric statistical model to real-life data requires estimation of the model parameters. Statistical inference based on maximum likelihood estimation was developed in [18] and [19] for CSA with a finite number of parameters β', which means that there exists a fixed positive integer N such that

$$\beta_k > 0 \quad \text{for} \quad 0 \le k \le N \quad \text{and} \quad \beta_k = 0 \quad \text{for} \quad k \ge N + 1. \tag{2.4}$$

It is easy to see that the density (2.2) (and hence (2.3)) is unaffected by multiplication of all parameters β_k by a constant. Therefore, for identifiability of

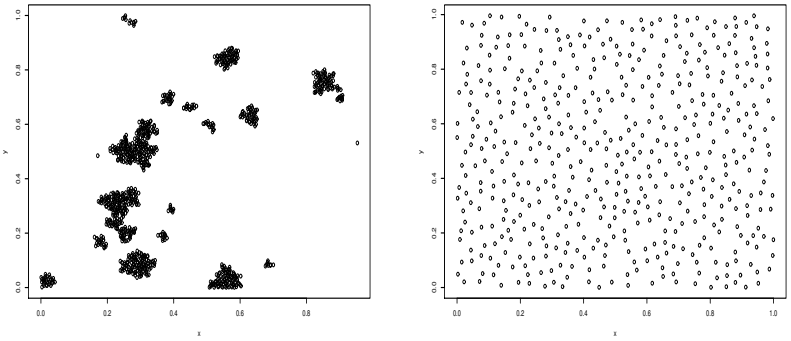

Figure 1. CSA simulations in $D = [0,1]^2$. Left: 1000 points, $R = 0.01$, $(\beta_i)_{i\geq 0} = (1, 1000, 10000, 0, 0, \ldots)$ Right: 500 points, $R = 0.03$, $(\beta_i)_{i\geq 0} = (1, 0, 0, \ldots)$, i.e. this is RSA model.

the model we also assume that $\beta_0 = 1$, so that the model is parameterised by parameters $\beta = (\beta_1, \ldots, \beta_N)$.

In general, both number N and the interaction radius R are also regarded as the model parameters and have to be estimated. The parameter N can be easily estimated by the maximal number of neighbours that a point has in an observed pattern (formal definition is given below). In contrast, estimation of the interaction radius in the general case is an open problem. If $N = 0$, i.e. in the case of RSA model, the natural estimator of the interaction radius is the minimal distance between an observed point and those points in the pattern that arrived earlier. In what follows, we assume that the interaction radius R is assumed to be a fixed and known constant.

2.3. MLE for CSA

In this section we explain how to develop statistical inference for parameters of the CSA model by using the method of maximum likelihood estimation (MLE).

Start with considering the model likelihood. Recall that $\mathbf{1}_A$ stands for the indicator of a set A. Given an observation $x(\ell) = (x_1, \ldots, x_\ell) \in D^\ell$, where $\ell \geq 2$, define

$$\Gamma_{j,k} = \int_D \mathbf{1}_{\{u:\nu(u,x(k))=j\}} du \quad \text{for} \quad 0 \leq j \leq k \leq \ell - 1,\ j = 0, \ldots, N, \tag{2.5}$$

$$\Gamma_{j,k} = 0 \quad \text{for} \quad k < j,\ j = 1, \ldots, N, \quad \text{and} \quad \Gamma_{0,0} = |D|. \tag{2.6}$$

Observe that

$$\int_D \beta_{\nu(u,x(k))} du = \sum_{j=0}^{k} \beta_j \Gamma_{j,k} = \Gamma_{0,k} + \sum_{j=1}^{N} \beta_j \Gamma_{j,k}.$$

Further, define

$$t_{k,\ell} = t_k(x(\ell)) := \sum_{i=1}^{\ell} \mathbf{1}_{\{\nu(x_i,x(i-1))=k\}} \quad \text{for} \quad k = 0, \ldots, N. \tag{2.7}$$

In terms of statistics (2.5) and (2.7) we have the following equation for the model likelihood

$$\begin{aligned} p_{\ell,\beta,D}(x_1, \ldots, x_\ell) &= \frac{\prod_{j=1}^{N} \beta_j^{t_j(x(\ell))}}{\prod_{k=1}^{\ell} \int_D \beta_{\nu(u,x(k-1))} du} \\ &= \frac{\prod_{j=1}^{N} \beta_j^{t_{j,\ell}}}{\prod_{k=1}^{\ell} \left(\Gamma_{0,k-1} + \sum_{j=1}^{N} \beta_j \Gamma_{j,k-1} \right)}. \end{aligned} \tag{2.8}$$

The log likelihood function is therefore given by

$$\begin{aligned} L_D(x(\ell), \beta) &:= \log(p_{\ell,\beta,D}(x_1, \ldots, x_\ell)) \\ &= \sum_{j=1}^{N} t_{j,\ell} \log(\beta_j) - \sum_{k=1}^{\ell} \log\Big(\Gamma_{0,k-1} + \sum_{j=1}^{N} \beta_j \Gamma_{j,k-1} \Big). \end{aligned} \tag{2.9}$$

Remark 2.3. Note that since $X(0) = \emptyset$ the first point X_1 is uniformly distributed in D, and, also, the first term in the sum $\sum_{k=1}^{\ell} \ldots$ in the preceding display is just a constant $\log(|D|)$.

Maximum likelihood estimators (MLEs) are defined as usual, i.e. as maximizers of the model likelihood and can be found by solving MLE equations obtained by equating to zero the log-likelihood derivatives.

If N is unknown, then it has to be estimated before estimating β's. Given $X(\ell) = (X_1, \ldots X_\ell)$, where, as before, we assume that $\ell \geq 2$, we estimate N by

$$\widehat{N} = \widehat{N}(X(\ell)) := \max_{X_i \in X(\ell)} \nu(X_i, X(i-1)) = \max\{j : t_{j,\ell} > 0\}. \tag{2.10}$$

It is easy to see $\widehat{N}$ is the maximum likelihood estimator of the parameter N.

Having estimated N by $\widehat{N}$ we have that

$$L_D(X(\ell), \beta) = \sum_{j=1}^{\widehat{N}} t_{j,\ell} \log(\beta_j) - \sum_{k=2}^{\ell} \log\Big(\Gamma_{0,k-1} + \sum_{j=1}^{\widehat{N}} \beta_j \Gamma_{j,k-1} \Big).$$

The maximum likelihood estimator $\widehat{\beta}(X(\ell)) = (\widehat{\beta}_1, \ldots, \widehat{\beta}_{\widehat{N}}, 0, 0, \ldots)$ of the true parameter vector $(\beta_1^{(0)}, \ldots, \beta_N^{(0)})$ is defined as the maximizer of the log likelihood $L_D(X(\ell), \beta)$ over vectors of the form $(\beta_1, \ldots, \beta_{\widehat{N}}, 0, 0 \ldots)$. Since $L_D(X(\ell), \beta)$ depends smoothly on $(\beta_1, \ldots, \beta_{\widehat{N}})$; the $(\widehat{\beta}_1, \ldots, \widehat{\beta}_{\widehat{N}})$ is a solution to the system of MLE equations

$$\frac{\partial L_D(X(\ell), \beta)}{\partial \beta_j} = 0, \quad j = 1, \ldots, \widehat{N}, \tag{2.11}$$

or, equivalently,

$$t_{j,\ell} - \sum_{k=2}^{\ell} \frac{\beta_j \Gamma_{j,k-1}}{\Gamma_{0,k-1} + \sum_{i=1}^{\widehat{N}} \beta_i \Gamma_{i,k-1}} = 0, \quad j = 1, \ldots, \widehat{N}, \tag{2.12}$$

where note that the sum $\sum_{k=2}$ in the right hand side starts from $k = 2$ because of Remark 2.3. It is obvious that $\widehat{N} \leq N$ almost surely. If $\widehat{N} < N$, then $t_{j,\ell} = 0$ for $N' + 1 \leq j \leq N$. It is also possible that $t_{j,\ell} = 0$ for some $j < \widehat{N}$. Therefore, if an observed point pattern is not a "typical" model pattern, then we might not have sufficient information to estimate the full set of parameters. However, if $\widehat{N} = N$ and all t-statistics are positive, then there exists a unique positive solution $(\widehat{\beta}_1, \ldots, \widehat{\beta}_N)$ of the likelihood equations. It turns out that these conditions hold with probability tending to 1, as the amount of observed information increases in a certain natural sense (to be explained).

Example 2.1. Suppose that $N = 1$, i.e., there is one unknown parameter $\beta = \beta_1$. Assume that an observed sequence of points $x(\ell) = (x_1, \ldots, x_\ell)$, $\ell \geq 2$ is such that $\widehat{N} = 1$ and the statistic $t_{1,\ell} > 0$ (the number of points having 1 neighbour). There is a a single MLE equation in this case,that is

$$t_{1,\ell} - \sum_{k=2}^{\ell} \frac{\beta \Gamma_{1,k}}{\Gamma_{0,k} + \beta \Gamma_{1,k}} = 0. \tag{2.13}$$

If $0 < t_{1,\ell} < \ell - 1$, then existence and uniqueness of the solution of the MLE equation follows from the fact that the left hand side of equation (2.13) is a strictly monotonic function of β. If $t_{1,\ell} = \ell - 1$, then this suggests that the observed pattern is generated by the model obtained by setting formally $\widehat{\beta} = \infty$. In the corresponding limit model a new point is allocated with probability one in the neighbourhood of existing points subject to the constraint that it cannot have more than one neighbour among those points.

Remark 2.4. It should be noted that the model log-likelihood, and, hence, MLEs for the CSA model, can be effectively computed numerically by the classical Monte-Carlo (required to compute Γ-statistics that are given by integrals). We refer to [18] for numerical examples.

2.4. Asymptotic properties of MLE estimators

In this section we briefly discuss asymptotic properties of MLE estimators for CSA in the situation, when the amount of observed information increases. In the classic case of i.i.d. observations this limit regime means that the number of observations tends to infinity. The analogue of this in spatial statistics is known as the increasing domain asymptotic framework, which means the number of observed points tends to infinity, as the target region (observation window) expands to the whole space. We describe below this limit regime in relation to CSA model with a finite number of non-zero parameters β, where there are natural restrictions on the number of observed points in a given target region.

Let D_1 denote the unit cube centred at the origin (or any compact convex set $D_1 \subset \mathbb{R}^d$). Consider a sequence of rescaled domains $D_m = m^{1/d} D_1$, $m \in \mathbb{Z}_+$. Given m, consider the CSA process as the acceptance/rejection sampling with target region $D = D_m$. Denote by $A_m(n)$ the (random) number of points accepted out of the first n incoming points. If $N < \infty$, then no particle can be placed at any location x with more than N existing particles within distance R of x. Therefore, the limit $\theta_m = \lim_{n\to\infty} A_m(n)$ exists almost surely, and is a finite random variable. Further, there exists a finite limit $\lim_{m\to\infty} \theta_m =: \theta_\infty$, known as the jamming density (see [18] for more details of this quantity).

The increasing domain asymptotic framework in the case of the CSA model can be now defined as follows.

Assumption 2.1. The number ℓ_m of observed points in the domain D_m is asymptotically linear in m with coefficient below the jamming density $\theta_\infty = \theta_\infty(R, \beta_1, \dots, \beta_N)$, that is

$$\lim_{m\to\infty} \left(\frac{\ell_m}{m} \right) = \mu \in (0, \theta_\infty).$$

Note that the above limit is known as the *thermodynamic limit* in the statistical physics literature.

Assume in the rest of the section that Assumption 2.1 *holds.* It turns out that under this assumption the log-likelihood derivatives in the case of CSA model behave asymptotically very similar to those in the i.i.d. case. This fact allows to combine methods of the classic MLE theory for i.i.d. observations (e.g., see [11]) with the modern theory for sums of locally determined functionals (to be explained) to establish consistency and asymptotic normality of MLE estimators for CSA model under assumption 2.1.

Given parameters N and $\beta = (\beta_1, \dots, \beta_N)$ consider the probability measure $\mathsf{P}_{m,\beta}$ on finite point sequences of length ℓ_m in D_m specified by the probability density $p_{\ell,\beta,D}$ with $\ell = \ell_m$ and $D = D_m$. Denote $\beta^{(0)} = \left(\beta_1^{(0)}, \dots, \beta_N^{(0)}\right)$ the true parameter and let $\mathsf{P}_m^{(0)} := \mathsf{P}_{m,\beta^{(0)}}$. Given observation $X(\ell_m) \in D_m$ define

the maximum likelihood estimators

$$\widehat{\beta}(m) = \widehat{\beta}(X(\ell_m)) = (\widehat{\beta}_{1,m}, \ldots, \widehat{\beta}_{N,m})$$

of parameters $\beta^{(0)} = (\beta_1^{(0)}, \ldots, \beta_N^{(0)})$ as those values that maximize the log likelihood function $L_m(\beta) := L_{D_m}(X(\ell_m), \beta)$, as explained in Section 2.3.

It was shown in [18, Corollary 2.1] that

$$\mathsf{P}_m^{(0)} \left\{ \frac{p_{\ell_m,\beta^{(0)},D_m}(X_1, \ldots, X_{\ell_m})}{p_{\ell_m,\beta,D_m}(X_1, \ldots, X_{\ell_m})} > 1 \right\} \to 1, \quad \text{as } m \to \infty,$$

for $\beta = (\beta_1, \ldots, \beta_N) \neq \beta^{(0)} = (\beta_1^{(0)}, \ldots, \beta_N^{(0)})$. This result is analogous to the well known result for the case of i.i.d. observations (e.g., see [11, Chapter, Theorem 2.1]) and justifies why statistical inference for the CSA model can be based on MLE. Furthermore, it was shown in [18, Theorem 2.2 and Lemma 5.2] that with $\mathsf{P}_m^{(0)}$-probability tending to 1, as $m \to \infty$, the estimator $\widehat{N}$ is equal to N and there exists a unique positive solution $(\widehat{\beta}_{1,m}, \ldots, \widehat{\beta}_{N,m})$ of the system of MLEs, such that $\widehat{\beta}_{i,m} \to \beta_i^{(0)}$ for $i = 1, \ldots, N$, in $\mathsf{P}_m^{(0)}$-probability, as $m \to \infty$.

Asymptotic normality of MLE estimator $\widehat{\beta}$ was established in [19]. Specifically, it was shown that $\sqrt{m}(\widehat{\beta}(m) - \beta^{(0)}) \to \xi(\mu)$ in $\mathsf{P}_m^{(0)}$-distribution, as $m \to \infty$, where $\xi(\mu)$ is the Gaussian vector with zero mean and covariance matrix given by the inverse matrix of the model limit information matrix. The latter is defined as the limit (in $\mathsf{P}_m^{(0)}$-probability, as $m \to \infty$) of the observed information matrix $-\frac{1}{m}\left(\frac{\partial^2 L_m(\beta)}{\partial\beta_i \partial\beta_j}\right)_{i,j=1}^{N}$ evaluated at the true parameter $\beta^{(0)}$. A detailed study of the structure of the information matrix can be found [19] to which we refer for further details.

Usefulness of showing asymptotic normality of a parameter estimator provides asymptotic justification for creating confidence intervals based on the normal distribution, when a sufficiently large number of points is observed in a sufficiently large region relative to the interaction radius R (see [19] for examples of creation of confidence intervals).

2.5. MLE for CSA and the theory of locally determined functionals

The asymptotic analysis of MLEs is based on the fact that the model statistics have special structure. Namely, these statistics are sums of so called locally determined functionals over a finite set of points. Below we briefly explain the idea.

Start with some definitions. A set of points $\mathcal{X} \subset \mathbb{R}^d$ is called locally finite, if its intersection with any ball of a finite radius consists of a finite number of points. A locally determined functional with a given range $r > 0$ is a measurable real-valued function $\xi(Y, \mathcal{X})$ defined for all pairs $(Y, \mathcal{X})$, where $Y \in \mathbb{R}^d$ and

$\mathcal{X} \subset \mathbb{R}^d$ is locally finite, with the property that $\xi(Y, \mathcal{X})$ is determined only by those points of $\mathcal{X}$ that are within distance r of Y. A locally determined functional $\xi(Y, \mathcal{X})$ is translation invariant if $\xi(Y, \mathcal{X}) = \xi(Y + a, \mathcal{X} + a)$ for any $a \in \mathbb{R}^d$. For example, the functional

$$\xi(x, \mathcal{X}) := \mathbf{1}_{\{\nu(x,\mathcal{X})=j\}}, \tag{2.14}$$

where the quantity $\nu(x, \mathcal{X})$ is defined by (2.1), is a bounded, translation-invariant, locally determined functional with the range equal to the interaction radius R.

Given a locally determined functional ξ, the corresponding additive functional H^ξ on finite sequences $X(\ell) = (X_1, \ldots, X_\ell) \in (\mathbb{R}^d)^\ell$ is defined as follows

$$H^\xi(X(\ell)) = \sum_{i=1}^{\ell} \xi(X_i, X(i-1)). \tag{2.15}$$

Observe now that both Γ-statistics (2.5) and t-statistics (2.7) are sums of locally determined functionals. Indeed, in the case of t-statistics

$$t_{j,\ell} = \sum_{i=1}^{\ell} \mathbf{1}_{\{\nu(X_i,X(i-1))=j\}}, \quad 0 \le j \le N, \tag{2.16}$$

we have that the statistic $t_{j,\ell}$ is the additive functional corresponding to the locally determined functional (2.14). Representation of Γ-statistics as sums of locally determined functionals is more technically involved and we refer to [18] for further details.

The general limit theory developed in [17]) for additive functionals (2.15) implies that, under Assumption 2.1, there exist strictly positive and continuous in μ functions $(\rho_j(\mu, \beta), 1 \le j \le N$ and $\gamma_j(\mu, \beta), 1 \le j \le N$, such that

$$\frac{t_{j,\ell_m}}{m} \to \rho_j(\mu, \beta) \quad \text{and} \quad \frac{\Gamma_{j,\ell_m}}{m} \to \gamma_j(\mu, \beta), \quad j = 0, \ldots, N, \tag{2.17}$$

in P_m-probability, as $m \to \infty$, and that are related by the system of equations

$$\rho_j(\mu, \beta) = \int_0^\mu \frac{\beta_j \gamma_j(\lambda, \beta)}{\gamma_0(\lambda, \beta) + \sum_{i=1}^N \beta_i \gamma_i(\lambda, \beta)} d\lambda, \quad j = 1, \ldots, N.$$

Further, let $\gamma_j^{(0)}(\lambda) := \gamma_j(\lambda, \beta^{(0)})$ and $\rho_j^{(0)}(\mu) := \rho_j(\mu, \beta^{(0)})$ for $j = 1, \ldots, N$. Given $\mu \in (0, \theta^{(0)})$, where $\theta^{(0)} = \theta_\infty(R, \beta_1^{(0)}, \ldots, \beta_N^{(0)})$, the vector of true parameters $\beta^{(0)} = (\beta_1^{(0)}, \ldots, \beta_N^{(0)})$ is a solution of the system of equations

$$\rho_j^{(0)}(\mu) - \int_0^\mu \frac{\beta_j \gamma_j^{(0)}(\lambda)}{\gamma_0^{(0)}(\lambda) + \sum_{i=1}^N \beta_i \gamma_i^{(0)}(\lambda)} d\lambda = 0, \quad j = 1, \ldots, N, \tag{2.18}$$

which is the infinite-volume limit of the MLE (2.12).

Example 2.2. Assume, as in Example 2.1, that $N = 1$. In this case the true single parameter $\beta^{(0)} = \beta_1^{(0)}$ is the unique solution of the limit equation

$$\rho_1^{(0)}(\mu) - \int_0^{\mu} \frac{\beta\gamma_1^{(0)}(\lambda)}{\gamma_0^{(0)}(\lambda) + \beta\gamma_1^{(0)}(\lambda)} d\lambda = 0.$$

Existence and uniqueness of the solution of this equation follows, similarly to the case of MLE equation in Example 2.1, from monotonicity of the integrand in the parameter β.

3. CSA growth model on graphs

In this section we consider a probabilistic model for random sequential deposition of particles at vertices of a graph. The model can be regarded as a discrete version of the continuous CSA model considered in the previous section. Recall that in the continuous model the probability of the event that a particle is placed at location x is proportional to the growth rate $\beta_k \geq 0$, where k is the number of existing points in the neighbourhood of x. In the discrete model we assume that the growth rate at a vertex v is equal to $e^{\alpha k+\beta m}$, where k is the number of existing particles at the vertex v, m is the total number of existing particles in vertices adjacent to v, and α, β are given constants. Thus, in general, we distinguish particles at the vertex itself and in its neighbours.

This growth model can be interpreted as an interacting urn model with a graph based log-linear interaction. Similarly to urn models, we are interested in the long term behaviour of the growth process. In particular, we would like to establish in which cases all vertices receive infinitely many particles and in which cases all but finitely particles are allocated at a certain subset of vertices (e.g. at a single vertex).

3.1. The model definition

The model set up is as follows. Consider an arbitrary finite graph $G = (V, E)$ with the set of vertices V and the set of edge E. If vertices $v, u \in V$ are adjacent, we call them *neighbours* and write $v \sim u$. If vertices v and u are not adjacent, then we write $v \nsim u$. By definition, vertex is not a neighbour of itself, i.e. $v \nsim v$.

The growth process with parameters $(\alpha, \beta) \in \mathbb{R}^2$ on the graph $G = (V, E)$ is a discrete time Markov chain $X(n) = (X_v(n),\, v \in V) \in \mathbb{Z}_+^V$ with the following transition probabilities

$$\mathsf{P}(X(n+1) = X(n)+\mathbf{e}_v | X(n) = \mathbf{x}) = \frac{e^{\alpha x_v + \beta \sum_{u\sim v} x_u}}{\Gamma(\mathbf{x})}, \quad \mathbf{x} = (x_w,\, w \in V) \in \mathbb{Z}_+^V, \tag{3.1}$$

where $\Gamma(\mathbf{x}) = \sum_{v \in V} e^{\alpha x_v + \beta \sum_{u \sim v} x_u}$ and $\mathbf{e}_v \in \mathbb{R}^V$ is the v-th unit vector, i.e. the vector, the v-th coordinate of which is equal to 1, and all other coordinates are zero.

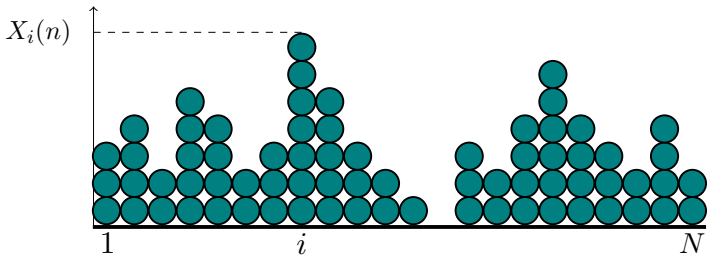

Figure 2. Deposition model on a linear graph $\{1 \sim \ldots \sim N\}$.

The growth process $X(n) = (X_v(n),\, v \in V)$ describes a random sequential allocation of particles on the graph, where $X_v(n)$ is interpreted as the number of particles at vertex v at time n. If $\beta = 0$, then the structure of the underlying graph is irrelevant, and the growth process is a special case of the generalised Pólya urn (GPU) model. Recall that GPU model is a model for random sequential allocation of particles at a finite number of urns, in which a particle is allocated at an urn v with x_v existing particles with probability proportional to the growth rate $f(x_v)$, where f is a given positive function. The growth process with parameter $\beta = 0$ is the GPU model with the exponential growth rate $f(k) = e^{\alpha k}$. If $\beta \neq 0$, then the growth process can be regarded as an interacting urn model obtained by adding graph based interaction. Observe that the growth rate $e^{\alpha x_v + \beta \sum_{u \sim v} x_u}$ (i.e. the function determining the allocation probability (3.1)) is a monotonically increasing function of the parameter β. Therefore, if $\beta > 0$, then interaction between components of the growth process is cooperative in the sense that particles in a neighbourhood of a vertex accelerate the growth rate at the vertex. In contrast, if $\beta < 0$, then the interaction between process's components is competitive in the sense that particles in a neighbourhood of a vertex the growth rate slow down the growth at the vertex.

Remark 3.1. The growth process on arbitrary graph was introduced in [14]. The growth process a single parameter $\lambda := \alpha = \beta \in \mathbb{R}$ on a cycle graph was introduced and studied in [22] (Recall that a cycle graph with $N \geq 2$ vertices is the graph $G = \{1 \sim 2 \sim \ldots \sim N-1 \sim N \sim 1\}$). The limit cases of the growth process on a cycle graph obtained by setting $\lambda = \infty$ and $\lambda = -\infty$ (with convention $\infty \cdot 0 = 0$) were studied in [23] (see an open problem at the end of

Section 3.2 for more details). A version of the growth process on a cycle graph, where the parameter λ depends on a vertex (i.e. $\alpha_v = \beta_v = \lambda_v > 0$, $v \in V$), was studied in [1].

3.2. Localisation in the growth model with attractive interaction

Recall some known results for GPU models. Consider a GPU model with the growth rate determined by a function f, as described in the preceding section. Assume that f is such that $\sum_{k=1}^{\infty} \frac{1}{f(k)} < \infty$. It is known that in this case, with probability one, all but a finite number of particles are allocated at a single random urn. In other words, the allocation process *localises* at a single urn. This result immediately implies the eventual localisation at a single vertex for the growth process with parameters $\alpha > 0$ and $\beta = 0$ (as it is just a special case of the aforementioned GPU model).

It was shown in [14] that a similar localisation effect occurs in the growth process with attractive interaction introduced by a positive parameter β. It turns out that in this case the growth process localises at special subsets of vertices rather than at a single vertex.

Recall some definitions from graph theory necessary to state the result. Let $G = (V, E)$ be a finite graph. Then, given a subset of vertices $V' \subseteq V$ the corresponding induced subgraph is a graph $G' = (V', E')$ whose edge set E' consists of all of the edges in E that have both endpoints in V'. The induced subgraph G' is also known as a subgraph induced by the set of vertices V'. A complete induced subgraph is called a clique, and a maximal clique is a clique that is not an induced subgraph of another clique.

The localisation result in [14, Theorem 1] is as follows. Consider the growth process $X(n) = (X_v(n),\, v \in V) \in \mathbb{Z}_+^V$ with parameters (α, β) on a finite connected graph $G = (V, E)$, and let $0 < \alpha \le \beta$. Then for every initial state $X(0) \in \mathbb{Z}_+^V$ with probability one there exists a random maximal clique with a vertex set $U \subseteq V$ such that

$$\lim_{n\to\infty} X_v(n) = \infty \text{ if and only if } v \in U, \text{ and } \lim_{n\to\infty} \frac{X_v(n)}{X_u(n)} = e^{C_{vu}}, \text{ for } v, u \in U,$$

where

$$C_{vu} = \lambda \lim_{n\to\infty} \sum_{w\in V} X_w(n)[\mathbf{1}_{\{w\sim v, w\not\sim u\}} - \mathbf{1}_{\{w\sim u, w\not\sim v\}}], \text{ if } 0 < \lambda := \alpha = \beta,$$

and $C_{vu} = 0$, if $0 < \alpha < \beta$.

The above localisation effect was first shown in [22, Theorem 3] (see also [1, Theorem 1]) in the case when $\alpha = \beta > 0$ and the underlying graph is a cyclic graph. In the special case of the cyclic graph any clique is just a pair of neighbouring vertices (assuming that the graph consists of at least three vertices).

The proof is based on the following key fact. Namely, given an *arbitrary* initial configuration the process localises at one of the graph's clique with probability that is *bounded away from zero*. This implies that with probability one the process eventually localises at one of the graph's cliques (the final clique).

Conditioned that particles are allocated only at vertices of a given clique, the numbers of allocated particles at these vertices grow according to a multinomial model in the case when $\alpha = \beta$. The allocation probabilities of this multinomial model are determined by the configuration of existing particles in the neighbourhood of the clique which remains unchanged since the start of the localisation. In other words, the multinomial model is determined by the limit quantities C_{vu} that depend on the state of the process at the time moment, when localisation starts at the final clique. In the case $\alpha < \beta$ these quantities irrelevant, and the numbers of particles at vertices of the final clique grow in the same way as in the case of the complete graph described in the example below.

Example 3.1 (Complete graph). Consider the growth process $X(n)=(X_1(n), \ldots, X_m(n))$ with parameters $0 < \alpha < \beta$ on a complete graph with $m \geq 2$ vertices labeled by $1, \ldots, m$. Let $Z_i(n) = X_i(n) - X_m(n)$, $i = 1, \ldots, m-1$. By [14, Lemma 3.3] the process of differences $Z(n) = (Z_1(n), \ldots, Z_{m-1}(n)) \in \mathbb{Z}^{m-1}$ is an irreducible positive recurrent Markov chain. Positive recurrence was shown by applying Foster's criterion (e.g. see [12, Theorem 2.6.4]) with the Lyapunov function given by

$$g(\mathbf{z}) = \sum_{i=1}^{m-1} z_i^2, \, \mathbf{z} = (z_1, \ldots, z_{m-1}) \in \mathbb{Z}^{m-1}.$$

It should be noted that exactly the same fact (see [22,]) is true for the process of differences in the GPU model with the growth rate $f(k) = e^{-\lambda k}$, $k \in \mathbb{Z}_+$, where $\lambda > 0$.

Remark 3.2. Localisation also occurs if $0 < \beta < \alpha$. In this case with probability one the growth process localises at a single vertex, which is similar to the GPU model with the growth rate give by the function $f(k) = e^{\alpha k}$.

Open problem: repulsive interaction The long term behaviour of the growth process in the case when $\lambda := \alpha = \beta < 0$ is largely unknown. In this case the interaction between the process's components is repulsive, which greatly complicates the study of the process's behaviour. Below we briefly describe some known results and state an open problem.

Consider the growth process on a cycle graph $G = \{1 \sim 2 \sim \ldots \sim m \sim 1\}$ (i.e. with m vertices labelled by $1, \ldots, m$) with parameters $\lambda := \alpha = \beta < 0$. Start with a special semi-deterministic case of the process obtained by formally setting $\lambda = -\infty$. Namely, in this case given the process's state $\mathbf{x} = (x_1, \ldots, x_m)$

(where x_i denotes, as before, the number of particles at vertex i) a next particle is allocated to a vertex x_i for which the quantity $u_i = x_{i-1} + x_i + x_{i+1}$ (with convention $1 - 1 = m$ and $m + 1 = 1$) is minimal. If there is more than one such vertex, then one of them is chosen at random. In this semi-deterministic model if the number of vertices of the graph is $m = 4$, then, given any initial configuration particles will be placed with probability one only at a pair of non-adjacent vertices (i.e. either at vertices $\{1, 3\}$, or at vertices $\{2, 4\}$). Moreover, after a finite number of steps the numbers of particles at the vertices of the final pair differ by no more than 1 and equal to each other every other step. Similar but much more complicated limit behaviour is observed in the case of the cycle graph with arbitrary number of vertices. We refer to [23] for further details, where complete classification of the long term behaviour of the model with $\lambda = -\infty$ on the cycle graph is given.

In the case $-\infty < \lambda < 0$ only a partial result is known in the case of the cycle graph with even number of vertices. Namely, it is shown in [22] that if initially there are no particles, then with a positive probability particles can be allocated either only at even, or only at odd vertices. The complete classification of the limit behaviour of the model in the case $-\infty < \lambda < 0$ is an open problem.

4. The reversible model

4.1. The model definition

In this section we consider a probabilistic model which is a version of the growth process (defined in Section 3.1) obtained by allowing deposited particles to depart from the graph.

It is convenient to define the model in terms of a continuous time Markov chain (CTMC). The model set up is as follows. Let, as before, $G = (V, E)$ be a finite graph with the set of vertices V and the set of edges E. Recall that $\mathbf{e}_v \in \mathbb{R}^V$ is the vector, the v-th coordinate of which is equal to 1, and all other coordinates are zero. Consider a CTMC $X(t) = (X_v(t),\, v \in V) \in \mathbb{Z}_+^V$ and the transition rates $r_{\alpha,\beta}(\mathbf{x}, \mathbf{y})$, $\mathbf{x}, \mathbf{y} \in \mathbb{Z}_+^V$ given by

$$r_{\alpha,\beta}(\mathbf{x}, \mathbf{y}) = \begin{cases} e^{\alpha x_v + \beta \sum_{u \sim v} x_u}, & \text{for } \mathbf{y} = \mathbf{x} + \mathbf{e}_v \text{ and } \mathbf{x} = (x_v,\, v \in V), \\ 1, & \text{for } \mathbf{y} = \mathbf{x} - \mathbf{e}_v \text{ and } \mathbf{x} = (x_v,\, v \in V) : x_v > 0, \\ 0, & \text{otherwise.} \end{cases} \tag{4.1}$$

where $\alpha, \beta \in \mathbb{R}$ are given constants.

Note that if the death rate was zero, then the CTMC $X(t)$ would be a continuous time version of the growth process. If $\beta = 0$, then CTMC $X(t)$ is a collection of independent processes labelled by the vertices of graph G. In this case a component of the Markov chain is a continuous time birth-and-death process on $\mathbb{Z}_+$ (or, equivalently, a nearest neighbour random walk on $\mathbb{Z}_+$) that

evolves as follows. Given state $k \in \mathbb{Z}_+$ it jumps to $k+1$ with the rate $e^{\alpha k}$ and jumps to $k-1$ (if $k > 0$) with the unit rate. Such a process is a special case of the birth-and-death (BD) process on the set on non-negative integers. The long term behaviour of an integer valued BD process is well known. Namely, given a set of transition characteristics one can, in principle, determine whether the corresponding Markov chain MC is (positive) recurrent or (explosive, if the time is continuous) transient, and compute various other characteristics of the process. In particular, the general theory implies the following long term behaviour of the CTMC $X(t)$ in the independent case (i.e. when $\beta = 0$).

- If $\alpha < 0$, then each component of $X(t)$ is positive recurrent, and, hence, $X(t)$ is positive recurrent.
- If $\alpha = 0$, then each component of $X(t)$ is a reflected symmetric simple random walk on $\mathbb{Z}_+$, which is null recurrent. The CTMC $X(t)$ is null recurrent if the number of components is either 1, or 2, and it is transient if the number of components is 3 or more.
- If $\alpha > 0$, then each component of $X(t)$ is explosive transient, and, hence, the CTMC $X(t)$ is explosive transient.

If $\beta \neq 0$, then the CTMC $X(t)$ can be regarded as a system of interacting birth-and-death processes that are labelled by vertices of the graph and evolve subject to interaction determined by the parameter β. Note that the presence of interaction can significantly affect the collective behaviour of a system and produce effects that might be of interest in modelling the evolution of multi-component random systems. The model provides a flexible and mathematically tractable choice for modelling various types of interaction. For example, if $\beta > 0$, then the interaction between components is cooperative meaning that a positive component accelerates growth of its neighbours. In the case $\beta < 0$ the interaction is competitive, since components suppress growth of each other.

The CTMC $\xi(t)$ was introduced in [24], where its long term behaviour was studied in some special cases. In full generality the long term behaviour of process was studied in [10]. Main results and research methods of these works are explained below.

4.2. Long term behaviour of the model

In this section we review the main results of [10] concerning the long term behaviour of the countable CTMC $X(t)$. Recall countable CTMCs can be non-explosive transient, explosive transient, null recurrent and positive recurrent. It turns out that all these limit behaviours are realised in the case of the CTMC $X(t)$ depending on parameters α, β and on the structure of the underlying graph. In addition, the long term behaviour of the Markov chain is largely determined

by a relationship between parameters α, β and the largest eigenvalue of the graph.

Let us give some definitions. Let $\mathcal{A} = (a_{vu},\, v, u \in V)$ be the adjacency matrix of the graph $G = (V, E)$, i.e. $\mathcal{A}$ is a symmetric matrix such that $a_{vu} = a_{uv} = 0$ for $u \nsim v$ and $a_{vu} = a_{uv} = 1$ for $u \sim v$. Since $\mathcal{A}$ is symmetric, its eigenvalues are real. Denote them by $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$, so that $\lambda_1 := \lambda_1(G)$ is the largest eigenvalue (Perron-Frobenius eigenvalue). It is well known that $\lambda_1(G) > 0$ (except the case when the graph has no edges). Not that in terms of the adjacency matrix $\mathcal{A}$ the birth rate in (4.9) can be written as follows

$$e^{\alpha x_v + \beta \sum\limits_{u \sim v} x_u} = e^{\alpha x_v + \beta (\mathcal{A}\mathbf{x})_v}. \tag{4.2}$$

Further, an *independent set* of vertices in a graph G is a set of the vertices such that no two vertices in the set are adjacent. The *independence number* $\kappa = \kappa(G)$ of a graph G is the cardinality of the largest independent set of vertices.

Theorem 4.1 below is an extract of [10, Theorem 2.3] that distinguishes between recurrence and transience.

Theorem 4.1. *Suppose that the graph G is connected and $\beta \neq 0$.*

1. *The CTMC $X(t)$ is recurrent in the following two cases*
   (a) *$\alpha < 0$ and $\alpha + \beta\lambda_1(G) < 0$;*
   (b) *$\alpha = 0$, $\beta < 0$ and $\kappa(G) \leq 2$.*
2. *The CTMC $X(t)$ is transient in all the cases below*
   (a) *$\alpha > 0$;*
   (b) *$\alpha = 0$ and $\beta > 0$;*
   (c) *$\alpha = 0$, $\beta < 0$ and $\kappa(G) \geq 3$;*
   (d) *$\alpha < 0$ and $\alpha + \beta\lambda_1(G) \geq 0$.*

The proof of the above result is greatly facilitated by the fact that the CTMC $X(t)$ is reversible, which in turn, allows to apply the method of electric networks. This is explained in the next section.

4.3. Reversibility of the model

Let $\mathbf{I}$ be the unit $V \times V$ matrix, let $\mathbf{e} \in \mathbb{R}^V$ be the vector all components of which are equal to 1, and let $(\cdot, \cdot)$ denote the Euclidean scalar product. Define the following functions

$$Q(\mathbf{x}) = -\frac{1}{2}((\alpha\mathbf{I} + \beta\mathcal{A})\mathbf{x}, \mathbf{x}) = -\frac{\alpha}{2}\sum_v x_v^2 - \beta \sum_{v \sim u} x_v x_u,\ \mathbf{x} = (x_v,\, v \in V) \in \mathbb{R}^V \tag{4.3}$$

$$S(\mathbf{x}) = (\mathbf{x}, \mathbf{e}) = \sum_v x_v, \quad \mathbf{x} = (x_v,\, v \in V) \in \mathbb{R}^V, \tag{4.4}$$

$$W(\mathbf{x}) = -Q(\mathbf{x}) - \frac{\alpha}{2} S(\mathbf{x}), \quad \mathbf{x} = (x_v,\, v \in V) \in \mathbb{R}^V. \tag{4.5}$$

We claim that the CTMC $X(t)$ is reversible with respect to the invariant measure

$$\begin{aligned} e^{W(\mathbf{x})} &= \exp\Big\{-Q(\mathbf{x}) - \frac{\alpha}{2} S(\mathbf{x})\Big\} \\ &= \exp\Big\{\frac{\alpha}{2} \sum_u x_u(x_u - 1) + \beta \sum_{w \sim u} x_w x_u\Big\}, \quad \mathbf{x} \in \mathbb{Z}_+^V, \end{aligned} \tag{4.6}$$

Indeed, given $v \in V$ and $\mathbf{x} \in \mathbb{Z}_+^V$ we have that

$$-Q(\mathbf{x}) - \frac{\alpha}{2} S(\mathbf{x}) + \alpha x_v + \beta(\mathcal{A}\mathbf{x})_v = -Q(\mathbf{x} + \mathbf{e}_v) - \frac{\alpha}{2} S(\mathbf{x} + \mathbf{e}_v).$$

Therefore,

$$\begin{aligned} e^{W(\mathbf{x})} \exp\Big\{\alpha x_v + \beta \sum_{u \sim v} x_u\Big\} &= \exp\Big\{-Q(\mathbf{x}) - \frac{\alpha}{2} S(\mathbf{x})\Big\} \exp\{\alpha x_v + \beta(\mathcal{A}\mathbf{x})_v\} \\ &= \exp\Big\{-Q(\mathbf{x} + \mathbf{e}_v) - \frac{\alpha}{2} S(\mathbf{x} + \mathbf{e}_v)\Big\} \\ &= \exp\big\{W(\mathbf{x} + \mathbf{e}_v)\big\} \end{aligned}$$

which, recalling (4.1), means that the detailed balance equation

$$e^{W(\mathbf{x})} r_{\alpha,\beta}(\mathbf{x}, \mathbf{y}) = e^{W(\mathbf{y})} r_{\alpha,\beta}(\mathbf{y}, \mathbf{x}) \quad \text{for} \quad \mathbf{x}, \mathbf{y} \in \mathbb{Z}_+^V, \tag{4.7}$$

holds for CTMC $X(t)$ and the invariant measure (4.6).

Remark 4.1. It should be noted that rewriting equation (4.8) as follows

$$e^{\alpha x_v} e^{W(\mathbf{x})} = e^{-\beta \sum_{u \sim v} x_u} e^{W(\mathbf{x} + \mathbf{e}_v)}, \tag{4.8}$$

shows that the measure $e^{W(\mathbf{x})}$, $\mathbf{x} \in \mathbb{Z}_+^V$ is also invariant for the CTMC $Y(t) = (Y_v(t),\, v \in V)$ with the transition rates $\hat{r}_{\alpha,\beta}(\mathbf{x}, \mathbf{y})$, $\mathbf{x}, \mathbf{y} \in \mathbb{Z}_+^V$ given by

$$\hat{r}_{\alpha,\beta}(\mathbf{x}, \mathbf{y}) = \begin{cases} e^{\alpha x_v}, & \text{for } \mathbf{y} = \mathbf{x} + \mathbf{e}_v, \text{ and } \mathbf{x} = (x_v,\, v \in V), \\ e^{-\beta \sum_{u \sim v} x_u}, & \text{for } \mathbf{y} = \mathbf{x} - \mathbf{e}_v \text{ and } \mathbf{x} = (x_v,\, v \in V) : x_v > 0, \\ 0, & \text{otherwise.} \end{cases} \tag{4.9}$$

It is shown in [10] that the long term behaviour of CTMC $\widehat{Y}(t)$ is largely the same as the long term behaviour of the CTMC $X(t)$.

Reversibility of a Markov chain allows to apply the method of electric networks for determining whether the Markov chain is recurrent or transient. The idea is that recurrence/transience of the reversible Markov chain can be established by analysing the so called effective resistance of a certain electric network. In the case of the CTMC $X(t)$ the corresponding electric network is defined as follows.

The CTMC $X(t)$ can be interpreted as a nearest neighbour random walk on the lattice graph $\mathbb{Z}_+^V$, i.e. the graph with vertices $\mathbf{x} = (x_v,\, v \in V : x_v \in \mathbb{Z}_+)$, where vertices $\mathbf{x}, \mathbf{y} \in \mathbb{Z}_+^V$ are connected by an edge if the Euclidean distance $\|\mathbf{x} - \mathbf{y}\| = 1$ (i.e. $\mathbf{x}$ and $\mathbf{y}$ are nearest neighbours on the lattice).

The electric network on this graph is obtained by assigning conductance (resistance^{-1}) to each edge, which is done as follows. Given $\mathbf{x} \in \mathbb{Z}_+^V$ and $v \in V$ assign the conductance $e^{W(\mathbf{x})}$, where the function U is defined in (4.5) for each edge $(\mathbf{x} - \mathbf{e}_v, \mathbf{x})$ with $\mathbf{x}_v \geq 1$. In other words, the edge conductance is equal to the value of the invariant measure of the CTMC $X(t)$ at the state $\mathbf{x}$. The edge $(\mathbf{0}, \mathbf{e}_v)\, v \in V$, where $\mathbf{0}$ is the origin, is assigned the unit conductance. Resistance of an edge is defined the reciprocal of conductance.

By the general method, the CTMC $X(t)$ is recurrent (transient), if the so called effective resistance of the described electric network on the graph $\mathbb{Z}_+^V$ is infinite (finite). The effective resistance in this case if defined, loosely speaking, as the resistance between the origin $\mathbf{0}$ and "infinite" vertex (see [9] for details). It turns out that in the case of the CTMC $X(t)$ the effective resistance of the electric network is relatively easy to estimate (see [10] for further details).

Further, the detailed balance equation can be solved for the model providing analytically tractable equation for the invariant measure. This allows to distinguish between null and positive recurrence.

4.4. Recurrent cases

The fact that the invariant measure of the Markov chain is known allows to distinguish between the null and positive recurrence in the recurrent cases of Theorem 4.1. This is done by analysing whether the invariant measure can be normalised to define the stationary distribution. A direct computation gives that in the case 1(a) of the theorem, i.e. when $\alpha < 0$ and $\alpha + \beta\lambda_1(G) < 0$, the invariant measure is summable, that is

$$Z_{\alpha,\beta,G} := \sum_{\mathbf{x} \in \mathbb{Z}_+^V} e^{W(\mathbf{x})} < \infty. \tag{4.10}$$

Recalling that an irreducible CTMC is positive recurrent if and only if it has a stationary distribution and is non-explosive. Since a recurrent CTMC is non-explosive we immediately obtain that if $\alpha < 0$ and $\alpha + \beta\lambda_1(G) < 0$, then $X(t)$

is positive recurrent with the stationary distribution given by

$$\mu_{\alpha,\beta,G}(\mathbf{x}) = \frac{1}{Z_{\alpha,\beta,G}} e^{W(\mathbf{x})} \quad \text{for} \quad \mathbf{x} = (x_v,\, v \in V) \in \mathbb{Z}_+^V. \tag{4.11}$$

In contrast, the Markov chain is null recurrent in the case 1(b) of the theorem. Indeed, if $\alpha = 0$, then

$$Z_{\alpha,\beta,G} = \sum_{\mathbf{x}\in\mathbb{Z}_+^V} e^{W(\mathbf{x})} \geq \sum_{k=0}^{\infty} e^{W(k\mathbf{e}_v)} = \sum_{k=0}^{\infty} 1 = \infty,$$

where $v \in V$ is any given vertex, i.e. the stationary distribution does not exist in this case (regardless of other characteristics of the model). Therefore, in the case $\alpha = 0$ the Markov chain cannot be positive recurrent, and, hence, in the recurrent case when $\beta < 0$ and $\kappa(G) \leq 2$ the Markov chain is just null recurrent.

Remark 4.2. In addition, note in [24] positive recurrence of the CTMC $X(t)$ was shown by using the Foster's criterion for positive recurrence in the case when $\alpha < 0, \beta > 0$ and $\alpha + \beta \max_{v\in V} d_v(G) < 0$, where $d_v(G)$ is the number of neighbours of the vertex $v \in V$, i.e. the number of vertices that are adjacent to v (the degree of the vertex v). The criterion was applied with the Lyapunov function $f(\mathbf{x}) = (Q(\mathbf{x}), \mathbf{x})$, where Q is the quadratic function defined in (4.3).

4.5. Transient cases

In the case of a transient CTMC it is natural to ask whether the CTMC is explosive. Note first that in the transient case 2(c) of Theorem 4.1 (i.e. when $\alpha = 0, \beta < 0$ and $\kappa(G) \geq 3$) the CTMC $X(t)$ is non-explosive. Indeed, it is easy to see that if $\alpha = 0, \beta < 0$, then the transition rates are uniformly bounded by 1, and, hence, the process cannot be explosive. In addition, note that in general there are only two possible long term behaviours of the Markov chain if $\alpha = 0$ and $\beta < 0$. Namely, by the results above CTMC $\xi(t)$ is either non-explosive transient or null recurrent, and this depends only on the independence number of the graph G.

Further, it was shown in [10, Lemma 6.3] that in the transient case $\alpha < 0$ and $\beta = \frac{-\alpha}{\lambda_1(G)}$ the CTMC $X(t)$ is not explosive. Although the transition rates are unbounded in this transient case, the process tends to infinity by staying in a domain where the rates are bounded, which prevents the explosion. This effect is rather easy to understand in the case when the graph consists of just two adjacent vertices (see [24, Theorems 1 and 4]), when the process is a special case of non-homogeneous random walks in the quarter plane. In this case, if $\alpha < 0$ and $\beta = -\alpha$, then the process is pushed away from the boundaries (where the rates can be arbitrarily large) towards the diagonal of the quarter plane, where the rates are bounded (see Figure 3). The same effect of non-explosion

takes place in the general case, although its proof is not straightforward (see [10, Lemma 6.3]). It should be noted that the diagonal here is the line determined by the vector $(1,1)^T$, which is the eigenvector of the adjacency matrix $\mathcal{A} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ of the graph $G = \{1 \sim 2\}$, that corresponds to the principle eigenvalue 1. If $\alpha < 0$ and $\beta = -\alpha$, then the rates around the diagonal are unbounded and the process becomes explosive (see an open problem below concerning explosion in the general case).

Further, recall that $d_v(G)$ denotes the number of neighbours of a vertex v. It was shown in [24, Theorems 1 and 2] that the Markov chain is explosive in the following cases:

(i) $\alpha > 0$, $\beta < 0$;

(ii) $\alpha + \beta \min\limits_{v \in V} d_v(G) > 0$ including subcases

- $\alpha > 0$ and $\beta \geq 0$;
- $\alpha = 0$ and $\beta > 0$;
- $\alpha < 0$ and $\beta > \frac{|\alpha|}{\min_{v \in V} d_v(G)}$.

In particular, in the cases 2(a), 2(b) of Theorem 4.1 the CTMC $X(t)$ is explosive.

Open problem: explosion Recall that in general $\min_{v \in V} d_v(G) \leq \lambda_1(G)$, i.e. the maximal eigenvalue of a graph G is not less than the minimal vertex degree of the graph. The above results concerning explosions do not include the transient case when

$$\alpha < 0 \quad \text{and} \quad -\frac{\alpha}{\lambda_1(G)} < \beta \leq -\frac{\alpha}{\min_{v \in V} d_v(G)},$$

which remains unsolved. It was conjectured in [10] that in this case the CTMC $X(t)$ is explosive. The conjecture is based on the intuition explained in the two-dimensional case above. Namely, that in this transient case the process escapes to infinity by "following" the line $\{s\mathbf{v}_1 : s \in R\}$, where $\mathbf{v}_1$ is the eigenvector corresponding to the largest eigenvalue $\lambda_1(G)$, and the transition rates grow exponentially along this line.

4.6. Phase transition

There is a phase transition phenomenon in the long term behaviour of CTMC $X(t)$ in the case $\alpha < 0$. Indeed, in this case we have the following classification of the process's behaviour

- Let $\alpha < 0$.

(i) If $\beta < -\frac{\alpha}{\lambda_1(G)}$, then $X(t)$ is positive recurrent. This includes the case when $\beta = 0$, i.e. when $X(t)$ is formed by a collection of independent positive recurrent reflected random walks on $\mathbb{Z}_+$, and is thus positive recurrent.

(ii) If $\beta = -\frac{\alpha}{\lambda_1(G)}$, then $X(t)$ is non-explosive transient.

(iii) If $-\frac{\alpha}{\lambda_1(G)} < \beta < -\frac{\alpha}{\min_{v\in V} d_v(G)}$, then $X(t)$ is transient. It is conjectured that $X(t)$ is explosive transient (see the open problem in the preceding section).

(iv) If $\beta > -\frac{\alpha}{\min_{v\in V} d_v(G)}$, then $X(t)$ is explosive transient.

If $\beta < 0$, then interaction in this case is competitive, as neighbours obstruct the growth of each other. The competition implies positive recurrence of the process (which is positive recurrent even without interaction). Suppose now that β is positive. One could intuitively expect that if β is not large, i.e. the cooperative interaction is not strong, so that the Markov chain is still positive recurrent. On the other hand, if $\beta > 0$ is sufficiently large, then the intuition suggests that the Markov chain might become transient. It turns out, that $\beta_{cr} = \frac{|\alpha|}{\lambda_1(G)}$ is the critical value at which the phase transition occurs. Precisely at this value of β the Markov chain is non-explosive transient. Moreover, it is conjectured that given $\alpha < 0$ the corresponding critical value β_{cr} is the only value of the parameter β when the Markov chain is non-explosive transient.

4.7. Examples

The largest eigenvalue of the adjacent matrix of the underlying graph plays essential role is determining the long term behaviour of the CTMC $X(t)$. Estimation of this eigenvalue, and more generally, graph eigenvalues, is a very important problem in many applications. There are well known bounds for the largest eigenvalue λ_1, although its explicit value is known only in some special cases. Below we give several simple examples where the largest eigenvalue λ_1 can be computed explicitly, which allows to rewrite the conditions of Theorem 4.1 in the case $\alpha < 0$ in more explicit form.

Example 4.1. If $G = (V, E)$ is with constant vertex degrees d, then $\lambda_1(G) = \min_{v\in V} d_v(G) = d$. For example, $d = 1$ for a graph consisting of two adjacent vertices, and $d = 2$ in for a cycle graph with at least three vertices. In this case the Markov chain is positive recurrent if and only if $\alpha < 0$ and $\alpha+\beta d < 0$. If $\alpha < 0$ and $\alpha + \beta d = 0$, then the Markov chain is non-explosive transient, and if $\alpha +$

$\beta d > 0$, then it is explosive transient. Figures 3 and 4 sketch directions of mean jumps of the process in the simplest case of just two interacting components.

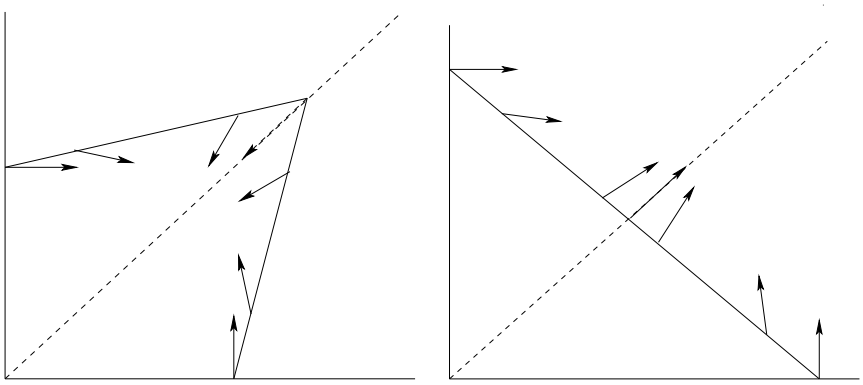

Figure 3. $G = \{1 \sim 2\}$, $\alpha < 0,\ \beta > 0$. Left: $\alpha + \beta < 0$; Right: $\alpha + \beta \geq 0$.

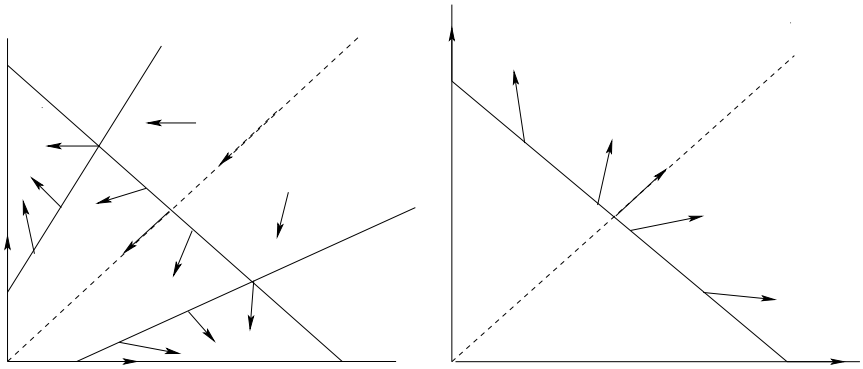

Figure 4. $G = \{1 \sim 2\}$, $\alpha > 0,\ \beta < 0$. Left: $\alpha + \beta < 0$; Right: $\alpha + \beta > 0$.

Example 4.2. Assume that the graph G is a star $\mathsf{K}_{1,m}$ with $m = n - 1$ non-central vertices, where $m \geq 1$. A direct computation gives that $\lambda_1 = \sqrt{m}$. Hence, the Markov chain is positive recurrent if and only if $\alpha < 0$ and $\alpha + \beta\sqrt{m} < 0$. If $\alpha < 0$ and $\alpha + \beta\sqrt{m} \geq 0$, then the Markov chain is transient.

Example 4.3. Consider a linear graph with $n+2$ vertices, where $n \in \mathbb{Z}_+$, that is a graph whose vertices can be enumerated by natural numbers $1, \ldots, n+2$, and such that $1 \sim 2 \sim \cdots \sim n+1 \sim n+2$. If $n = 0$, then this is the simplest

case of a constant degree graph, and if $n = 1$, then this is the simplest case of a star graph. If $n \geq 2$, then the adjacency matrix $\mathcal{A}$ of this graph is the tridiagonal matrix given below

$$\mathcal{A} = \begin{bmatrix} 0 & 1 & & & & & O \\ 1 & 0 & 1 & & & & \\ & 1 & \cdot & \cdot & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & \cdot & \cdot & 1 \\ O & & & & & 1 & 0 \end{bmatrix}_{(n+2)\times(n+2)}$$

This is the tridiagonal symmetric Toeplitz matrix which eigenvalues are given by

$$\lambda_k = 2\cos\left(\frac{k\pi}{n+3}\right),\ k = 1, \ldots, n+2.$$

The maximal eigenvalue is $\lambda_1 = 2\cos\left(\frac{\pi}{n+3}\right)$. Thus, the CTMC $X(t)$ is positive recurrent if and only if $\alpha < 0$ and $\alpha + 2\beta\cos\left(\frac{\pi}{n+3}\right) < 0$. If $\alpha < 0$ and $\alpha + 2\beta\cos\left(\frac{\pi}{n+3}\right) \geq 0$, then the Markov chain is transient.

Two next examples (from [10]) are the cases when the process is null recurrent, and this essentially is determined by the independence number $\kappa(G)$.

Example 4.4. Let, as in Example 4.2, G be a star $\mathsf{K}_{1,m}$, where $m \geq 1$. Then $\kappa(G) = m = n - 1$. Assume that $\alpha = 0$ and $\beta < 0$. Then, the Markov chain is null recurrent if $n \leq 3$, and transient if $n \geq 4$.

Example 4.5. Let G be a cycle C_n, where $n \geq 3$. Then $\kappa(G) = \lfloor n/2 \rfloor$. Assume that $\alpha = 0$ and $\beta < 0$. Then, the Markov chain is null recurrent if $n \leq 5$, and transient if $n \geq 6$.

4.8. The model with finite components

In this section we consider a version of the reversible model obtained by limiting the maximum number of particles at a vertex.

As before, let $G = (V, E)$ be a finite connected graph with the adjacency matrix $\mathcal{A}$. Let $\Lambda_N = \{0, \ldots, N\}^V$, where $N \geq 1$ is a given natural number. Consider a CTMC $\hat{X}(t) = (\hat{X}_v(t),\, v \in V) \in \Lambda_N$ with transition rates $\hat{r}_{\alpha,\beta}(\mathbf{x}, \mathbf{y})$, $\mathbf{x}, \mathbf{y} \in \mathbb{Z}_+^V$ given by

$$\hat{r}_{\alpha,\beta}(\mathbf{x}, \mathbf{y}) = \begin{cases} e^{\alpha x_v + \beta \sum_{u\sim v} x_u}, & \text{for } \mathbf{y} = \mathbf{x} + \mathbf{e}_v \text{ and } \mathbf{x} = (x_v,\, v \in V) : x_v < N, \\ 1, & \text{for } \mathbf{y} = \mathbf{x} - \mathbf{e}_v \text{ and } \mathbf{x} = (x_v,\, v \in V) : x_v > 0, \\ 0, & \text{otherwise.} \end{cases} \tag{4.12}$$

where $\alpha, \beta \in \mathbb{R}$ are given constants. In other words, the CTMC $\hat{X}(t)$ evolves precisely as the CTMC $X(t)$ transition rates (4.1) subject to the constraint that at most N particles can be placed at a vertex.

Similarly to the CTMC $X(t)$, the finite CTMC $\hat{X}(t)$ is irreducible and reversible with the stationary distribution $\mu^{(N)}_{\alpha,\beta,N}(\mathbf{x})$, $\mathbf{x} \in \Lambda_N$, given by

$$\mu^{(N)}_{\alpha,\beta,G}(\mathbf{x}) = \frac{1}{Z_{\alpha,\beta,G,N}} e^{W(\mathbf{x})} \quad \text{for} \quad \mathbf{x} = (x_v,\, v \in V) \in \Lambda_N^V, \tag{4.13}$$

where the function U is defined in (4.5), and

$$Z_{\alpha,\beta,G,N} = \sum_{\mathbf{x} \in \Lambda_N^V} e^{W(\mathbf{x})}.$$

By the ergodic theorem for finite irreducible CTMC's the distribution of $\hat{X}(t)$ converges to the stationary distribution (4.13), as $t \to \infty$.

Remark 4.3. Note that if $N = 1$ (in which case the parameter α is redundant) the measure (4.13) is equivalent to a special case of the celebrated Ising model on the graph G. Indeed, the change of variables $y_v = 2x_v - 1$ induces a probability measure on $\{-1, 1\}^V$ that is proportional to $\exp\left(\frac{\beta}{4}\left(\sum_{v\sim u} y_v y_u + 2\sum_v y_v\right)\right)$. The latter corresponds to the Ising model with the inverse temperature $\beta/4$ and the external field $h = \beta/2$ on the graph G.

In the rest of this section we show that, under certain assumptions, the probability measure (4.13) possesses monotonicity properties that are similar to those of the ferromagnetic Ising model.

We start with recalling some necessary definitions by adopting those from [6]. Let $G = (V, E)$ be an arbitrary graph (not necessarily finite), and let, as before, $\Lambda_N = \{0, \dots, N\}^V$. Let $\mathcal{F}_{G,N}$ be a standard σ-algebra of subsets of Λ_N generated by cylinder sets (if the graph $G = (V, E)$ is finite, then $\mathcal{F}_{G,N}$ is just a set of all subsets of Λ_N). Define a partial order on the set Λ_N. Given $\mathbf{x} = (x_v,\, v \in V) \in \Lambda_N$ and $\mathbf{x}' = (x'_v,\, v \in V) \in \Lambda_N$ we write $\mathbf{x} \le \mathbf{x}'$, if $x_v \le x'_v$ for all $v \in G$. A probability measure μ on $(\Lambda_N, \mathcal{F}_{G,N})$ is said to be monotone if

$$\mu(x_v \ge k | \mathbf{x} = \mathbf{z} \text{ off } v) \le \mu(x_v \ge k | \mathbf{x} = \mathbf{y} \text{ off } v), \tag{4.14}$$

for all $v \in V$, $k \in \{0, \dots, N\}$ and $\mathbf{z}, \mathbf{y} \in \Lambda_{V\setminus\{v\},N}$ such that $\mathbf{z} \le \mathbf{y}$, $\mu(\mathbf{x} = \mathbf{z} \text{ off } v) > 0$ and $\mu(\mathbf{x} = \mathbf{y} \text{ off } v) > 0$.

Theorem 4.2. *Let $\beta > 0$. Then the probability measure $\mu^{(N)}_{\alpha,\beta,G}$ is monotone.*

Proof of Theorem 4.2. Start with an auxiliary statement (which generalises Lemma 3.1 in [25]).

Proposition 4.1. *Let* $\mathsf{P} = (p_k, k \in \mathbb{Z}_+)$ *and* $\mathsf{Q} = (q_k, k \in \mathbb{Z}_+)$ *be discrete probability measures on* $\mathbb{Z}_+$. *If* $p_i q_j \le p_j q_i$ *for all* $0 \le j < i$, *then* $\mathsf{P}(\{i : i \ge k\}) \le \mathsf{Q}(\{i : i \ge k\})$ *for* $k \ge 1$, *i.e. the measure* Q *stochastically dominates the measure* P.

Proof. A direct computation gives that

$$\begin{aligned}\mathsf{P}(\{i : i \ge k\}) - \mathsf{Q}(\{i : i \ge k\}) &= \sum_{i=k}^{\infty} p_i - \sum_{i=k}^{\infty} q_i \pm \left(\sum_{i=k}^{\infty} p_i\right)\left(\sum_{i=k}^{\infty} q_i\right) \\ &= \sum_{i=k}^{\infty} p_i \sum_{j=0}^{k-1} q_j - \sum_{i=k}^{\infty} q_i \sum_{j=0}^{k-1} p_j \\ &= \sum_{j=0}^{k-1}\sum_{i=k}^{\infty}(p_i q_j - p_j q_i) \le 0,\end{aligned}$$

for $k \ge 1$, as required. □

Given a vertex $v \in V$ and configurations $\mathbf{y}, \mathbf{z} \in \Lambda_{N,V\setminus\{v\}} = \{0, 1, \dots, N\}^{V\setminus\{v\}}$, such that $\mathbf{y} \le \mathbf{z}$, define probability distributions

$$\mathsf{P} = (p_k = \mu^{(N)}_{\alpha,\beta,G}(x_v = k | \mathbf{x} \equiv \mathbf{y} \text{ off } v,\ k = 0, \dots, N)$$

and

$$\mathsf{Q} = (q_k = \mu^{(N)}_{\alpha,\beta,G}(x_v = k | \mathbf{x} \equiv \mathbf{z} \text{ off } v,\ k = 0, \dots, N)$$

and show that

$$\mathsf{P}(\{k, N\}) \le \mathsf{Q}(\{k, N\}) \quad \text{for} \quad k \in \{0, \dots, N\}. \tag{4.15}$$

A direct computation gives that

$$p_k = \frac{e^{\frac{\alpha k(k-1)}{2} + k\beta(\mathcal{A}\mathbf{y})_v}}{\sum_{i=0}^{N} e^{\frac{\alpha i(i-1)}{2} + i\beta(\mathcal{A}\mathbf{y})_v}} \quad \text{and} \quad \frac{e^{\frac{\alpha k(k-1)}{2} + k\beta(\mathcal{A}\mathbf{z})_v}}{\sum_{i=0}^{N} e^{\frac{\alpha i(i-1)}{2} + i\beta(\mathcal{A}\mathbf{z})_v}}. \tag{4.16}$$

Therefore

$$p_i q_j - p_j q_i = \frac{e^{\alpha\frac{i(i-1)+j(j-1)}{2}} e^{i\beta(\mathcal{A}\mathbf{y})_v + j(\mathcal{A}\mathbf{z})_v}\left(1 - e^{(i-j)\beta(\mathcal{A}(\mathbf{z}-\mathbf{y}))_v}\right)}{\left[\sum_{i=0}^{N} e^{\frac{\alpha i(i-1)}{2} + i\beta(\mathcal{A}\mathbf{y})_v}\right]\left[\sum_{i=0}^{N} e^{\frac{\alpha i(i-1)}{2} + i\beta(\mathcal{A}\mathbf{z})_v}\right]}.$$

Since $z_u - y_u \ge 0$, we have that

$$(\mathcal{A}(\mathbf{z} - \mathbf{y}))_v = \sum_{u\sim v}(z_u - y_u) \ge 0,$$

which gives $1 - e^{(i-j)\beta(\mathcal{A}(\mathbf{z}-\mathbf{y}))_v} \le 0$, and, hence, $p_i q_j \le p_j q_i$ for $0 \le j < i$. Equation (4.15) is now follows from Proposition 4.1. Consequently, the measure $\mu^{(N)}_{\alpha,\beta,G}$ is monotone, as claimed. □

By [6, Theorem 4.11], a monotone probability measure on $(\Lambda_N, \mathcal{F}_{G,N})$ has positive correlations, that is $\mu^{(N)}_{\alpha,\beta,G}(A \cap B) \geq \mu^{(N)}_{\alpha,\beta,G}(A)\mu^{(N)}_{\alpha,\beta,G}(B)$ for any increasing events $A, B \in \mathcal{F}_{G,N}$ (an event $A \in \mathcal{F}_{G,N}$ is said to be increasing if $\mathbf{1}_{\{\mathbf{x}\in A\}} \leq \mathbf{1}_{\{\mathbf{x}'\in A\}}$ for $\mathbf{x} \leq \mathbf{x}'$). It is well known (e.g. see [5], [6]) that positivity of correlations implies existence of the limit for the probability measure (4.13) in the large graph limit, i.e. as the underlying graph G indefinitely expands in an appropriate sense. For example, consider a sequence of graphs G_n given by d-dimensional cubes of volume n centered at the origin. If $\beta > 0$, then the sequence of corresponding model distributions $\mu^{(N)}_{\alpha,\beta,G_n}$ converges to a limit distribution, as n tends to infinity (convergence is understood in the sense of the weak convergence of finite-dimensional distributions). This limit measure corresponds, in terminology of statistical physics, to the so-called empty (zero) boundary conditions. Existence of a limit measure in the case of other *fixed* boundary conditions (e.g. when all spins on the boundary of a graph G_n are equal to N) can be shown similarly. Uniqueness of the limit measure, i.e. that the limit measure does not depend on the boundary conditions, is an open problem.

We are now going to show that the measure $\mu^{(N)}_{\alpha,\beta,G}$ possesses a monotonicity property in the parameter β. Recall that given probability measures μ and μ' on $(\Lambda_N, \mathcal{F}_{G,N})$ the measure μ is said to be dominated by μ' ($\mu \leq \mu'$), if $\mu(A) \leq \mu'(A)$ for every increasing event $A \in \mathcal{F}_{G,N}$.

Theorem 4.3. *If $\beta_1 \leq \beta_2$, then $\mu^{(N)}_{\alpha,\beta_1,G} \leq \mu^{(N)}_{\alpha,\beta_2,G}$.*

Proof. Given $\mathbf{x} \in \Lambda_N$ let $p_k = \mu_{\alpha,\beta_1,N}(x_v = k|\mathbf{x})$ and $q_k = \mu_{\alpha,\beta_2,N}(x_v = k|\mathbf{x})$ for $k = 0, \ldots, N$, and consider probability distributions $\mathsf{P} = (p_k, k = 0, \ldots, N)$ and $\mathsf{Q} = (q_k,\, k = 0, \ldots, N)$ on $\{0, \ldots, N\}$. By the Holley theorem (e.g. Theorem 4.8 in [6]), it suffices to show that $\mathsf{P} \leq \mathsf{Q}$, i.e. $\mathsf{P}(\{k, N\}) \leq \mathsf{Q}(\{k, N\})$ for $k = 0, \ldots, N-1$. Using equation (4.16), as in the proof of Theorem 4.2, we obtain that $p_k \sim e^{\frac{\alpha k(k-1)}{2} + k\beta_1(\mathcal{A}\mathbf{x})_v}$ and $q_k \sim e^{\frac{\alpha k(k-1)}{2} + k\beta_2(\mathcal{A}\mathbf{x})_v}$, $k = 0, \ldots, N$. Since $\beta_2 - \beta_1 \geq 0$ we have that $\beta_2(\mathcal{A}\mathbf{x})_v - \beta_1(\mathcal{A}\mathbf{x})_v = (\beta_2 - \beta_1)\sum_{u\in V} x_u \geq 0$, and, hence,

$$p_i q_j - p_j q_i \sim \exp\Big\{\alpha\frac{i(i-1)+j(j-1)}{2}\Big\}\exp\{i\beta_1(\mathcal{A}\mathbf{x})_v + j\beta_2(\mathcal{A}\mathbf{x})_v\} \times \big(1 - \exp\big\{(i-j)[\beta_2(\mathcal{A}\mathbf{x})_v - \beta_1(\mathcal{A}\mathbf{x})_v]\big\}\big) \leq 0, \text{ if } 0 \leq j < i.$$

By Proposition 4.1, $\mathsf{P} \leq \mathsf{Q}$, and the theorem follows. □

5. CSA point process

In this section we consider a point process motivated by the CSA model. We call this process by the CSA point process. The construction of the CSA

point process is reminiscent to the CSA time series model in Section 2. The key difference between the two models is that the CSA point process is a model for *unordered* point patterns, while the CSA time series model is a model for *sequential* point patterns.

The CSA point process is defined, similarly to other point processes, as a probability measure on the set of finite point configurations of a subset of Euclidean space. Such a measure is usually specified by a density with respect to the Poisson point process with the unit intensity.

Start with some notations and definitions. Let D be a compact convex subset of $\mathbb{R}^d$ that has a positive Lebesgue measure. For $n \geq 1$ define n-point configuration in D as unordered set of points $\mathbf{x} = \{x_1, \ldots, x_n\}$, $x_i \in D$, $i = 1, \ldots, n$, such that $x_i \neq x_j$ $i \neq j$. Let F be a set of all finite point configurations in D including the empty set $\emptyset$ (the empty set corresponds to $n = 0$). Let $\mathcal{F}$ be a σ-algebra of subsets of F, such that all maps $\mathbf{x} \to |\mathbf{x} \cap B|$, where $B \subseteq D$ and $|\cdot|$ is the cardinality of a discrete set, are measurable with respect to $\mathcal{F}$.

Let P_Π be the distribution of Poisson point process with the unit intensity on the set D, i.e. it is the probability measure on $(F, \mathcal{F})$ given by

$$\mathsf{P}_\Pi(A) = e^{-|D|}\Big(\mathbf{1}_{\{\emptyset \in A\}} + \sum_{n=1}^{\infty} \frac{1}{n!} \int\limits_{D^n} 1_{\{\{x_1,\ldots,x_n\} \in A\}} dx_1 \ldots dx_n\Big),\ A \in \mathcal{F}, \quad (5.1)$$

where $\mathbf{1}_B$ denotes the indicator function of set B.

The CSA point process with the interaction radius $R > 0$ and parameters $(\beta_m \geq 0,\ m \in \mathbb{Z}_+)$ is a probability measure on $(F, \mathcal{F})$ specified by the following density (with respect to measure (5.1))

$$f(\mathbf{x}) = Z^{-1} \prod_{x_k \in \mathbf{x}} \beta_{\nu(x_k, \mathbf{x})}, \quad (5.2)$$

where $\nu(x_k, \mathbf{x})$ is the number of neighbours of a point x_k in a finite point configuration $\mathbf{x} = \{x_1, \ldots, \}$ (defined in (2.1)),

$$Z = e^{-|D|}\Big(1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int\limits_{D^n} \prod_{k=1}^{n} \beta_{\nu(x_k, \mathbf{x})} dx_1 \ldots dx_n\Big), \quad (5.3)$$

i.e. Z is the normalising constant.

The process is well defined if $Z < \infty$. It was shown in [8, Lemma 1] that, if there exists a constant $C > 0$, such that $\beta_m \leq C m^\alpha$ for all m with some $\alpha < 1$, then the CSA point process (5.2) is well-defined.

It turns out that the CSA point process is a special case of the class of interacting neighbours (INP) point process (introduced in [7]). An INP process is specified by a density (with respect to the Poisson point process with the unit intensity) proportional to a function of the form $\prod\limits_{x_k \in \mathbf{x}} g(x_k, \mathbf{x})$, where, in turn,

$g : D \times F \to \mathbb{R}_+$ is a non-negative measurable function. The density (5.2) is obtained by setting

$$g(x, \mathbf{z}) = \sum_{m \geq 0} \beta_m 1_{\{|\mathbf{z}|=m\}}.$$

It is easy to see that the construction of the CSA point process is reminiscent to the construction of CSA model for time series of spatial locations in Section 2. By this similarity the CSA point process is also useful for modelling a wide spectrum of point configurations from regular ones to various clustered point patterns.

Some special cases of the CSA point process are the well known in spatial statistics point processes. Consider several examples.

1. A Poisson point process in the domain D with the intensity $\beta > 0$ is obtained for $\beta_i \equiv \beta$, $i \geq 0$.

2. Assume that $\beta_0 = \beta$ and $\beta_i = 0$ for $i \geq 1$. The corresponding process is the well known process with hard core interaction of intensity β and the interaction radius R. Realisations of a hard processes are point patterns, in which the distance between any two points is not less than the interaction radius R, i.e. a point has no neighbours.

3. A natural generalisation of the process with the hard core interaction is the CSA process with a finite number of non zero parameters, that is $\beta_i > 0$ for $0 \leq i \leq N$ and $\beta_i = 0$ for $i > N$, where $N \geq 0$ is a given integer (if $N = 0$, then we obtain the process with the hard core interaction). Realisations of such a process are point patterns, in which a point can have no more than N neighbours.

4. The famous in spatial statistics Strauss point process with the parameters $\alpha > 0$ and $0 < \gamma < 1$ is obtained by setting $\beta_i = \alpha\gamma^{i/2}$, $i \geq 0$. Traditionally, its distribution is specified by a density (with respect to Poisson point process with the unit intensity) proportional to the function $\alpha^{|\mathbf{x}|}\gamma^{s(\mathbf{x})}$, where $s(\mathbf{x})$ is the number of pairs of neighbours in the configuration $\mathbf{x}$. It is easy to see that $s(\mathbf{x}) = 1/2 \sum_{x_k \in \mathbf{x}} \nu(x_k, \mathbf{x})$, i.e. the density (5.2) is the density of the Strauss process for the indicated choice of the parameters.

Consider the CSA point process with a finite number of non zero β-parameters, i.e. the process in the item 3 above. Parameters of this process can be estimated by adopting the estimation procedure described in the case of the CSA time series model in Section 2.3. Namely, assume, as in Section 2.3 that the interaction radius R is known (or, somehow estimated). Then, given an observation $\mathbf{x} = \{x_1, \ldots, x_n\}$ the parameter N (the number of non-zero β-parameters) can be estimated by $\widehat{N} = \max_{x \in \mathbf{x}} \nu(x, \mathbf{x})$. Non-zero parameters β

can be estimated by using MLE. However, unlike the CSA time series model, the computation of MLE estimators here is not so straightforward. The difficulty is that the computation of the model likelihood in the case of the CSA point process requires the computation of the normalising constant (5.3) which is not analytically tractable. This is the well-known common problem in MLE estimation of parameters of a point process given by a density with respect to the Poisson point process. The normalising constant can be computed/estimated numerically by using the Markov chain Monte-Carlo method. Implementation of the latter is not straightforward for point processes and requires advanced simulation techniques (e.g. the method of perfect simulation). This is in contrast to the case of the CSA time series model, where the classic Monte-Carlo is rather effective (see Remark 2.4).

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Markov Processes and **Related Fields**

Diffusion Approximation for Symmetric Birth-and-Death Processes with Polynomial Rates

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Abstract. The symmetric birth and death stochastic process on the non-negative integers $x \in \mathbb{Z}_+$ with polynomial rates $x^\alpha, \alpha \in [1,2], x \neq 0$, is studied. The process moves slowly and spends more time in the neighborhood of the state 0. We prove the convergence of the scaled process to a solution of stochastic differential equation without drift. Sticking phenomenon appears at the limiting process: trajectories, starting from any state, take finite time to reach 0 and remain there indefinitely.

Keywords: birth-death processes, stochastic differential equations, diffusion approximation

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1. Introduction

A birth-and-death process is a continuous-time Markov process with states $x \in \mathbb{Z}_+ := \{0, 1, 2, \ldots\}$ (representing the population size) and with transitions

occurring between neighboring states: from a given state $x \in \mathbb{Z}_+$ the process jumps to a neighbouring state $x+1$ with a rate $\lambda(x)$, and to $x-1$ with a rate $\mu(x)$. Such simple processes are commonly accessible for analytical studies and they serve as valuable tools for modelling a wide range of phenomena, encompassing various fields, owing to their versatility and simplicity.

Mathematically, birth-death processes offer a foundational framework for investigating diverse facets of limiting theorems within non-homogeneous spatial settings. Our previous studies [1–4] on large deviations of birth-death processes have been dedicated to the case of polynomial transition rates $\lambda(x) = \lambda x^l, \mu(x) = \mu x^m$. In all these papers we used the technique (changes of measures) introduced in [4]. Curiously, this technique encounters limitations when dealing with the symmetric case where $\lambda(x) = \mu(x)$.

Recently, in our work [5], we achieved significant progress by studying the case $\lambda(x) = \mu(x) = x \in \{1, 2, \dots, N\}$, employing a large deviation technique described in [6]. The model is symmetric in transition rates and spatially inhomogeneous, resulting in a deceleration of the process dynamics near the state $x = 1$. The scaling employed (with respect to N) leads to a concentration of the process around the initial point. However, it is important to note that the invariant measure tends to localize at zero. Consequently, we hypothesized that utilizing the diffusion scaling, (2.2) (see, (2.1) for the generator of the scaled process) could be a promising approach to achieve a limiting process capable of localizing or exhibiting "sticking" behavior at zero.

Here we develop this idea. Furthermore, we extend the model by considering polynomial transition rates of the form $\lambda(x) = \mu(x) = x^\alpha$, where $\alpha \geq 0$. The case $\alpha = 1$ corresponds to the model discussed in [5]. Our primary objective is to examine the limiting behaviour of the process near zero, depending on the parameter α. To facilitate this analysis, we have expanded the state space of the birth-death process to include all non-negative integers on a half-line $\mathbb{Z}_+$. We are constrained to the case where α falls within the interval $[1, 2]$.

Utilizing the martingale techniques [7] we establish that under the scaling (2.2) the limit of this process is a solution to the stochastic differential equation (SDE) (2.4). The solution is proven to be unique when α lies within the interval $[1, 2]$. Notably, for all $\alpha \in [1, 2)$, this unique solution possesses a remarkable property: once the process reaches the boundary at 0, it remains there indefinitely. On the other hand, if $\alpha = 2$ the (well-known) solution of (2.4) will never reach zero, when starting from a positive initial state.

Another motivation for our study of this process comes from the field of physics. The study [5] offers a perspective on the famous matter-antimatter imbalance problem. The matter-antimatter imbalance, an intriguing and unsolved problem in Physics, continues to captivate attention. We propose that the observed imbalance originates from the inhomogeneity within stochastic competition between matter and antimatter.

To model this competition, in [5] we employ a birth-death process, where the rescaled states

$$\left\{\frac{1}{N}, \frac{2}{N}, \ldots, \frac{N-1}{N}, 1\right\}$$

represent the relative amount of antimatter with respect to the total matter in the Universe of size N. More precisely, if the relative amount of antimatter is $\frac{k}{N}$, then the absoulut amount of the antimatter and matter are $\frac{k}{N+k}N$ and $\frac{N}{N+k}N$, respectively, and the transition rate in each neighbour state is k. When the scaled process is close to 1, it signifies an almost equal amount of matter and antimatter, leading to high-frequency transitions between nearest states, typically of order N. Conversely, when the relative amount of antimatter is low, corresponding to a small states (near 0) in the scaled process, the transition frequency slows down.

Here we extend the modelling of (relative) antimatter processes originally considered in [5]. The state space of the resulting process is the set of non-negative real numbers $\mathbb{R}_{\geq 0}$, unlike the process in [5] with the states in interval $[0, 1]$. However, the behaviour near zero for both processes remains to be the same. When $\alpha = 1$, this extension retains the interpretation provided previously. Furthermore, in the context of matter-antimatter balance, the resulting diffusion process reveals that when the antimatter proportion approaches zero, it will persist at that level indefinitely. This may explain the scarcity of antimatter in the Universe.

The rest of the paper consists of three sections. In Section 2, we formulate and prove the main results for $\alpha \in [1, 2]$. In Section 3 we briefly discuss the case when $\alpha \notin [1, 2]$. Auxiliary results are in Section 4.

2. Definition and main results

Consider a homogeneous in time Markov process $\xi(t)$, $t \geq 0$ (continuous time), with state space $E := \{0\} \cup \mathbb{N}$, whose transition probabilities satisfy the following system of equalities for $\Delta \to 0$

$$\mathbf{P}(\xi(t+\Delta) = y \mid \xi(t) = x) = \begin{cases} \lambda x^\alpha \Delta + o(\Delta), \ y = x \pm 1, \ x \neq 0, \\ b\Delta + o(\Delta), \ y = 1, \ x = 0, \\ 1 - 2\lambda x^\alpha \Delta + o(\Delta), \ y = x, \ x \neq 0, \\ 1 - b\Delta + o(\Delta), \ y = 0, \ x = 0, \end{cases}$$

where $\lambda > 0, b > 0$ and $\alpha \geq 0$ are parameters of the process. In order to find a proper scaling, we choose the space scaling $N \in \mathbb{N}$, and find suitable time-scaling by calculating generator. Let $N^\gamma > 0$ be the time-scaling which corresponds to the space-scaling N. Consider the process

$$\xi_N(t) = \frac{\xi(N^\gamma t)}{N}, \quad t \in [0, T],$$

with its generator G_N on the state space $E_N = \frac{1}{N}E$, such that for a given $x_N \in E_N$ we have

$$\begin{aligned} G_N f(x_N) &:= \lim_{\Delta\to 0} \frac{1}{\Delta}\Big(\mathbb{E}(f(\xi_N(\Delta))) - f(x_N)\Big) \\ &= \lim_{\Delta\to 0} \frac{1}{\Delta}\Big(\big(f(x_N + \tfrac{1}{N}) - f(x_N)\big)\lambda(Nx_N)^\alpha N^\gamma \Delta \\ &\qquad + \big(f(x_N - \tfrac{1}{N}) - f(x_N)\big)\lambda(Nx_N)^\alpha N^\gamma \Delta + o(N^\gamma\Delta)\Big) \\ &= N^2(f(x_N + \tfrac{1}{N}) - 2f(x_N) + f(x_N - \tfrac{1}{N}))\lambda N^{-2}(Nx_N)^\alpha N^\gamma. \end{aligned}$$

Here f is a twice differentiable function with compact support. Observe that if $\alpha + \gamma - 2 = 0$, and $x_N \to x$, then

$$\lim_{N\to\infty} G_N f(x_N) = \lambda x^\alpha f''(x). \tag{2.1}$$

This tells us that the correct time scaling should be

$$\gamma = 2 - \alpha.$$

Further, we deal with the scaled process

$$\xi_N(t) = \frac{\xi(N^{2-\alpha}t)}{\sqrt{\lambda}N}, \quad t \in [0,T], \tag{2.2}$$

where $N \in \mathbb{N}$ is increasing to infinity scaling parameter, $T > 0$ is a fixed positive constant. We are interested in limiting distribution for this sequence of scaled processes. To not overload the notation, we will omit the symbol α in the scaled process (2.2). However, it will be evident in each case that α is considered.

Assume the sequence of initial states $\xi_N(0) = x_N$ satisfies

$$\lim_{N\to\infty} x_N = x, \tag{2.3}$$

where x non-negative real number.

The main result here concerns convergence of the scaled process (2.2) under the condition (2.3). For a given positive T, let $\mathbf{D}[0,T]$ denote the set of càdlàg functions on the time interval $[0,T]$, equipped with the Skorokhod metric. We prove the following theorem.

Theorem 2.1. *Let $\alpha \in [1,2]$, and suppose that the condition (2.3) holds. Then the sequence $\xi_N(t)$ weakly converges (when $N \to \infty$) in $\mathbf{D}[0,T]$ to the solution of the following stochastic equation*

$$X(t) = x + \sqrt{2}\int_0^t X^{\alpha/2}(s)dw(s), \quad t \in [0,T]. \tag{2.4}$$

Note that the equation (2.4) has the unique strong solution with finite second moment only if $\alpha \in [1,2]$ or $\alpha = 0$ (see, for example, [8, Chapter 4, Theorem 2.4, Theorem 3.2]). Indeed, [8, Theorem 2.4, Chapter 4], when applied to one-dimensional SDE of the form:

$$dX(t) = b(X(t))dt + \sigma(X(t))dw(t),$$

establishes the finiteness of the second moment of the solution for any $t > 0$ and ensures that the explosion time is infinite, provided the following condition holds:

$$|b(x)|^2 + |\sigma(x)|^2 \le K(1 + |x|^2),$$

for some constant K. Notably, in our case, with $b(x) \equiv 0$, $\sigma(x) = \sqrt{2}x^{\alpha/2}$, this condition is satisfied when $\alpha \le 2$. This essentially establishes the existence of the solution of (2.4).

The uniqueness condition is provided by [8, Theorem 3.2, Chapter 4], which asserts that if there exists a strictly increasing function $\rho(u)$ on $[0,\infty)$ such that $\rho(0) = 0$ and for a small $\varepsilon > 0$, the integral

$$\int_0^\varepsilon \frac{du}{\rho^2(u)} = \infty$$

and

$$|\sigma(x) - \sigma(y)| \le \rho(|x - y|),$$

for all x, y, then pathwise uniqueness of solutions is guaranteed. These conditions hold when we choose $\rho(u) = \sqrt{2}u^{\alpha/2}$, providing a lower bound for the parameter $\alpha \ge 1$.

Note that if $x = 0$ and $\alpha \ge 1$, there exists a unique solution $X(t) = 0$ for all $t > 0$, meaning that once the process reaches the state of zero, it will remain at zero indefinitely.

Proof of Theorem 2.1

Consider an auxiliary random process $\tilde{\xi}(t)$ extending the original process on $\mathbb{Z}$. The transition probabilities satisfiy the following system:

$$\mathbf{P}(\tilde{\xi}(t+\Delta) = y \mid \tilde{\xi}(t) = x) = \begin{cases} \lambda|x|^\alpha\Delta + o(\Delta),\ y = x \pm 1,\ x \neq 0, \\ \dfrac{b}{2}\Delta + o(\Delta),\ y = \pm 1,\ x = 0, \\ 1 - 2\lambda|x|^\alpha\Delta + o(\Delta),\ y = x,\ x \neq 0, \\ 1 - b\Delta + o(\Delta),\ y = 0,\ x = 0. \end{cases}$$

It is easy to see that thanks to the symmetry $\xi(\cdot) \stackrel{d}{=} |\tilde{\xi}(\cdot)|$. Thus, if the sequence of random processes

$$\tilde{\xi}_N(t) = \frac{\tilde{\xi}(N^{2-\alpha}t)}{\sqrt{\lambda}N}, \quad t \in [0,T] \tag{2.5}$$

converges to some process $\tilde{X}(\cdot)$ as $N \to \infty$ in the space $\mathbf{D}[0,T]$, then the sequence $\xi_N(\cdot)$ converges to $|\tilde{X}(\cdot)|$.

Thus, we will show that the sequence $\tilde{\xi}_N(\cdot)$ weakly converges in $\mathbf{D}[0,T]$ to the solution of the stochastic equation

$$\tilde{X}(t) = x + \sqrt{2}\int_0^t |\tilde{X}(s)|^{\alpha/2} dw(s), \quad t \in [0,T]. \tag{2.6}$$

In order to prove this, we use the following alternative representation $\eta(\cdot)$ for the $\tilde{\xi}(\cdot)$:

$$\eta(t) := \tilde{\xi}(0) + \sum_{k=-\infty}^{\infty} \int_0^t \mathbf{I}(\eta(s-) = k)\nu_k(ds) - \sum_{k=-\infty}^{\infty} \int_0^t \mathbf{I}(\eta(s-) = k)\mu_k(ds), \tag{2.7}$$

where the Poisson processes ν_k, μ_k, $k \in \mathbb{Z}$ with rates

$$\mathbf{E}\nu_k(1) = \mathbf{E}\mu_k(1) = \lambda k^\alpha, \quad k \in \mathbb{Z} \setminus \{0\},$$

and

$$\mathbf{E}\nu_0(1) = \mathbf{E}\mu_0(1) = \frac{b}{2},$$

are independent. Lemma 4.1 proves that indeed

$$\tilde{\xi}(\cdot) \stackrel{d}{=} \eta(\cdot).$$

Thus, if the limit of the sequence (2.5) exists, then it should coincide with the limit of the sequence of processes

$$\eta_N(t) := \frac{\eta(N^{2-\alpha}t)}{\sqrt{\lambda}N}, \quad t \in [0,T],$$

where $\eta(\cdot)$ is defined by (2.7).

Remark 2.2. It is easy to see that

$$\eta(t) = \tilde{\xi}(0) + \sum_{k=-\infty}^{\infty} \int_0^t \mathbf{I}(\xi(s-) = k)\tilde{\nu}_k(ds) - \sum_{k=-\infty}^{\infty} \int_0^t \mathbf{I}(\xi(s-) = k)\tilde{\mu}_k(ds),$$

where

$$\tilde{\nu}_k(ds) = \nu_k(ds) - \lambda|k|^\alpha ds, \quad \tilde{\mu}_k(ds) = \mu_k(ds) - \lambda|k|^\alpha ds, \qquad k \in \mathbb{Z},$$
$$\tilde{\nu}_0(ds) = \nu_0(ds) - \frac{b}{2}ds, \quad \tilde{\mu}_0(ds) = \mu_0(ds) - \frac{b}{2}ds.$$

Thus, the random process $\eta(t)$ is a martingale with respect to the generated filtration.

Further, without loss of generality, we will assume $\lambda = 1$. According to Remark 2.2, we obtain

$$\begin{aligned}\eta_N(t) = \frac{\eta(N^{2-\alpha}t)}{N} &= x_N + \frac{1}{N}\sum_{k=-\infty}^{\infty}\int_0^{N^{2-\alpha}t}\mathbf{I}(\eta(s-)=k)\tilde{\nu}_k(ds)\\ &\quad - \frac{1}{N}\sum_{k=-\infty}^{\infty}\int_0^{N^{2-\alpha}t}\mathbf{I}(\eta(s-)=k)\tilde{\mu}_k(ds)\\ &= x_N + \frac{1}{N}\sum_{k=-\infty}^{\infty}\int_0^{t}\mathbf{I}\left(\eta_N(s-)=\frac{k}{N}\right)\tilde{\nu}_k(dN^{2-\alpha}s)\\ &\quad - \frac{1}{N}\sum_{k=-\infty}^{\infty}\int_0^{t}\mathbf{I}\left(\eta_N(s-)=\frac{k}{N}\right)\tilde{\mu}_k(dN^{2-\alpha}s).\end{aligned} \tag{2.8}$$

Let us find the quadratic characteristic of martingale $\eta_N(\cdot)$. Using Itô's formula (see, for example, [7, Chapter 2, §3, Theorem 1]) and (2.8), we obtain

$$\begin{aligned}(\eta_N(t))^2 = x_N^2 &+ \sum_{k=-\infty}^{\infty}\int_0^t\left(\left(\eta_N(s)+\frac{\mathbf{I}\left(\eta_N(s)=\frac{k}{N}\right)}{N}\right)^2-\eta_N^2(s)\right.\\ &\left.-2\eta_N(s)\frac{\mathbf{I}\left(\eta_N(s)=\frac{k}{N}\right)}{N}\right)N^{2-\alpha}|k|^\alpha ds\\ &+\int_0^t\left(\left(\eta_N(s)+\frac{\mathbf{I}\left(\eta_N(s)=0\right)}{N}\right)^2-\eta_N^2(s)\right.\\ &\left.-2\eta_N(s)\frac{\mathbf{I}\left(\eta_N(s)=0\right)}{N}\right)N^{2-\alpha}\frac{b}{2}ds\\ &+\sum_{k=-\infty}^{\infty}\int_0^t\left(\left(\eta_N(s)-\frac{\mathbf{I}\left(\eta_N(s)=\frac{k}{N}\right)}{N}\right)^2-\eta_N^2(s)\right.\\ &\left.+2\eta_N(s)\frac{\mathbf{I}\left(\eta_N(s)=\frac{k}{N}\right)}{N}\right)N^{2-\alpha}|k|^\alpha ds\\ &+\int_0^t\left(\left(\eta_N(s)-\frac{\mathbf{I}\left(\eta_N(s)=0\right)}{N}\right)^2-\eta_N^2(s)\right.\\ &\left.+2\eta_N(s)\frac{\mathbf{I}\left(\eta_N(s)=0\right)}{N}\right)N^{2-\alpha}\frac{b}{2}ds\\ &+\sum_{k=-\infty}^{\infty}\int_0^t\left(\left(\eta_N(s-)+\frac{\mathbf{I}\left(\eta_N(s-)=\frac{k}{N}\right)}{N}\right)^2-\eta_N^2(s-)\right)\tilde{\nu}_k(dN^{2-\alpha}s)\end{aligned}$$

$$+\sum_{k=-\infty}^{\infty}\int_0^t\left(\left(\eta_N(s-)-\frac{\mathbf{I}\left(\eta_N(s-)=\frac{k}{N}\right)}{N}\right)^2-\eta_N^2(s-)\right)\tilde{\mu}_k(dN^{2-\alpha}s)$$

$$=\frac{2}{N^\alpha}\sum_{k=-\infty}^{\infty}\int_0^t\mathbf{I}\left(\eta_N(s)=\frac{k}{N}\right)|k|^\alpha ds$$

$$+\frac{b}{N^\alpha}\int_0^t\mathbf{I}\left(\eta_N(s)=0\right)ds+M_N(t),$$

where the martingale $M_N(t)$ is

$$M_N(t):=x_N^2$$

$$+\sum_{k=-\infty}^{\infty}\int_0^t\left(\left(\eta_N(s-)+\frac{\mathbf{I}\left(\eta_N(s-)=\frac{k}{N}\right)}{N}\right)^2-\eta_N^2(s-)\right)\tilde{\nu}_k(dN^{2-\alpha}s)$$

$$+\sum_{k=-\infty}^{\infty}\int_0^t\left(\left(\eta_N(s-)-\frac{\mathbf{I}\left(\eta_N(s-)=\frac{k}{N}\right)}{N}\right)^2-\eta_N^2(s-)\right)\tilde{\mu}_k(dN^{2-\alpha}s).$$

Thus, the martingale $\eta_N(\cdot)$ has the following quadratic characteristic

$$\langle\eta_N(t)\rangle=\frac{2}{N^\alpha}\sum_{k=-\infty}^{\infty}\int_0^t\mathbf{I}\left(\eta_N(s)=\frac{k}{N}\right)|k|^\alpha ds+\frac{b}{N^\alpha}\int_0^t\mathbf{I}\left(\eta_N(s)=0\right)ds. \tag{2.9}$$

According to [7, Chapter 8, §3, Theorem 1] it is sufficient to show that

$$\lim_{N\to\infty}x_N=x \tag{2.10}$$

and for any $\varepsilon>0$

$$\lim_{N\to\infty}\mathbf{P}\left(\sup_{t\in[0,T]}|\eta_N(t)-\eta_N(t-)|\geq\varepsilon\right)=0, \tag{2.11}$$

$$\lim_{N\to\infty}\mathbf{P}\Big(\sup_{t\in[0,T]}\left|\langle\eta_N(t)\rangle-2\int_0^t|\eta_N(s)|^\alpha ds\right|\geq\varepsilon\Big)=0. \tag{2.12}$$

Statement (2.10) is exactly the condition (2.3), while (2.11) holds thanks to the fact that a value of any increments of the process $\eta_N(\cdot)$ is equal to $\frac{1}{N}$. Let us show that the equality (2.12) holds too. Let us transform the first term on the right in (2.9):

$$\frac{2}{N^\alpha}\sum_{k=-\infty}^{\infty}\int_0^t\mathbf{I}\left(\eta_N(s)=\frac{k}{N}\right)|k|^\alpha ds$$

$$= 2\sum_{k=-\infty}^{\infty}\int_0^t \mathbf{I}\left(\eta_N(s)=\frac{k}{N}\right)\left(\frac{|k|}{N}\right)^{\alpha} ds$$
$$= 2\sum_{k=-\infty}^{\infty}\left(\frac{|k|}{N}\right)^{\alpha}\mathbf{L}\left(\left\{s\in[0,t]:\eta_N(s)=\frac{k}{N}\right\}\right)$$
$$= 2\int_0^t |\eta_N(s)|^{\alpha} ds, \tag{2.13}$$

where $\mathbf{L}(\cdot)$ Lebesgue measure.

Using (2.9) and (2.13), for any $\varepsilon>0$, $\alpha\in[1,2)$ we obtain

$$\lim_{N\to\infty}\mathbf{P}\left(\sup_{t\in[0,T]}\left|\langle\eta_N(t)\rangle - 2\int_0^t|\eta_N(s)|^{\alpha}ds\right|\geq\varepsilon\right)$$
$$= \lim_{N\to\infty}\mathbf{P}\left(\frac{b}{N^{\alpha}}\int_0^T \mathbf{I}\left(\eta_N(s)=0\right)ds\geq\varepsilon\right)$$
$$\leq \lim_{N\to\infty}\mathbf{P}\left(\frac{bT}{N^{\alpha}}\geq\varepsilon\right)=0.$$

Thus, the conditions (2.10)–(2.12) hold and the sequences $\tilde{\xi}_N(\cdot)$ and $\xi_N(\cdot)$ converge weakly in the space $\mathbf{D}[0,T]$ to the random processes $\tilde{X}(\cdot)$ and $|\tilde{X}(\cdot)|$, correspondingly. Moreover, the limiting process $\tilde{X}(\cdot)$ allows for the representation (2.6)

$$\tilde{X}(t)=x+\sqrt{2}\int_0^t|\tilde{X}(s)|^{\alpha/2}dw(s),\quad t\in[0,T].$$

It remains to show that $|\tilde{X}(\cdot)|\stackrel{d}{=}X(\cdot)$ (recall, $X(\cdot)$ is the solution of the equation (2.4)).

Applying the Tanaka's formula (see, for example, [10, Chapter 9, Proposition 9.2]), we obtain

$$|\tilde{X}(t)|=x+\sqrt{2}\int_0^t\operatorname{sign}(\tilde{X}(s))|\tilde{X}(s)|^{\alpha/2}dw(s)+L_0^{\tilde{X}}(t), \tag{2.14}$$

where $L_0^{\tilde{X}}(t)$ is the local time at zero of the process $\tilde{X}(\cdot)$, and

$$\operatorname{sign}(y)=\begin{cases}1, & \text{if } y\geq 0,\\ -1, & \text{if } y<0.\end{cases}$$

We will prove that $L_0^{\tilde{X}}(t)\equiv 0$. To prove this, according to [11, Chapter 9, §3, Lemma 3.3], we must to provide a Borel function ρ from $(0,\infty)$ into itself such that for any small $\varepsilon>0$

$$\int_0^{\varepsilon}\rho(y)dy=\infty, \tag{2.15}$$

and for any $t \in (0, T]$, the following condition should holds

$$\int_0^t \mathbf{I}(\tilde{X}(s) \in (0, \varepsilon))\rho(\tilde{X}(s))d\langle\tilde{X}(s)\rangle < \infty,$$

where $\langle\tilde{X}(\cdot)\rangle$ is the quadratic characteristic of the martingale $\tilde{X}(\cdot)$.

Indeed, choosing $\rho(y) = 1/|y|^\alpha$ the condition (2.15) holds for all $\alpha \in [1, 2]$, and we will have

$$\int_0^t \mathbf{I}(\tilde{X}(s) \in (0, \varepsilon))\rho(\tilde{X}(s))d\langle\tilde{X}(s)\rangle = 2\int_0^t \mathbf{I}(\tilde{X}(s) \in (0, \varepsilon))ds < \infty \text{ a.s.}, \quad (2.16)$$

where in our case $d\langle\tilde{X}(s)\rangle = 2|X(s)|^\alpha ds$. Thus, from [11, Chapter 9, §3, Lemma 3.3] and (2.16), (2.15) it follows that $L_0^{\tilde{X}}(t) \equiv 0$ and

$$|\tilde{X}(t)| = x + \sqrt{2}\int_0^t \text{sign}(\tilde{X}(s))|\tilde{X}(s)|^{\alpha/2}dw(s). \quad (2.17)$$

It is easy to see that the random process

$$\tilde{w}(t) = \int_0^t \text{sign}(\tilde{X}(s))dw(s) \quad (2.18)$$

is Wiener process. From (2.17), (2.18) it follows that

$$|\tilde{X}(t)| = x + \sqrt{2}\int_0^t |\tilde{X}(s)|^{\alpha/2}d\tilde{w}(s).$$

Thus, the random process $|\tilde{X}(\cdot)|$ has the same distribution as the solution of the equation (2.4). □

Remark 2.3. In the case when $\alpha \in (0, 1)$ we assume that the limit process for the sequence $\xi_N(\cdot)$ will satisfy the equation (2.4). However, for such α the solution of this equation will not be unique even in a weak sense (see, for example, [9, Chapter 1, §3, Example 1.22]). Therefore, we cannot apply Theorem 1 [7, Chapter 8, §3] which requires that the limit equation has a unique solution. Apparently, in this case there will be a weak convergence to one of the solutions.

Remark 2.4. Note that the proposed method of the proof of Theorem 2.1 can also consider the case $\alpha = 0$ (essentially, this will be a generalized Poisson process with reflection at zero, built on a classical random walk). In this case, the limiting process will be the solution to the stochastic equation

$$X(t) = x + \sqrt{2}w(t) + L_0^X(t), \quad t \in [0, T],$$

where $L_0^X(t)$ is the local time at zero of the process $X(\cdot)$.

Remark 2.5. Let

$$\tau = \inf\{t \geq 0 : X(t) = 0\}$$

and

$$\kappa = \inf\{t \geq 0 : X(t) = \infty\}.$$

The condition (3) of [8, Theorem 3.2, Chapter 6, §3] holds. It implies that for any initial $x \geq 0$ the probability $\mathbf{P}(\tau \wedge \kappa < \infty) = 1$. Moreover, we observe that the condition (2) [8, Theorem 3.1, Chapter 6, §3] is also satisfied, that implies $\mathbf{P}(\tau < \kappa) = 1$. Thus, when $\alpha \in [1, 2)$, a trajectory reaches 0 within a finite time.

3. Discussion

Let us briefly discuss the case when $\alpha \notin [1, 2]$. The method we employed for the proof, specifically [7, Chapter 8, §3, Theorem 1], allowed us to establish convergence for all $\alpha \leq 2$. Therefore, when $\alpha \in (0, 1)$, the existence of a solution of the equation (2.4) can be confirmed by [8, Theorem 2.4, Chapter 4], for example. However, we have not been able to prove its uniqueness (see for more detail [9, Chapter 1, §3, Example 1.22]). It's worth noting that the absence of uniqueness is also a well-known phenomenon.

Simultaneously, the diffusion coefficient is locally Lipschitz outside the boundary even in the case $\alpha \in (0, 1)$. This property enables us to establish uniqueness up to the hitting time at zero. We hypothesize that the resulting limiting process "extracts" from the set of solutions one that reflects at zero and it is unique. It would indicate the absence of a localization phenomenon at zero. Proof of this we leave for a future work.

We do not have a proof of convergence when $\alpha > 2$. This limitation may attributed to the absence of the finiteness of the second moment. If the second moment is infinite, the quadratic characteristic is infinite as well. Nevertheless, we can establish that the solution of the equation (2.4) does not explode, it is unique, and never reaches zero when starting from a positive number. It is also the focus of our future research.

The matter-antimatter imbalance, an intriguing and unsolved problem in physics, continues to captivate the attention of researchers. We also address the matter-antimatter imbalance in the Universe in [5]. We believe the same martingale techniques can be applied to the birth-death process restricted to the set $0, 1, \ldots, N$. One may expect the same diffusion equations without drift will hold on the space interval $[0, 1]$. However, this should be a subject of a separate study.

4. Auxiliary results

Recall that the process η is defined by (2.7)

Lemma 4.1. *The following holds true* $\tilde{\xi}(\cdot) \stackrel{d}{=} \eta(\cdot)$.

Proof. Define recursively the jump instances:

$$t_1 := \min\left\{t \in [0,\infty) : \max\left(\nu_{\eta(0)}(t) - \nu_{\eta(0)}(t-), \mu_{\eta(0)}(t) - \mu_{\eta(0)}(t-)\right) = 1\right\},$$

and for $k \geq 2$

$$t_k := \min\big\{t \in (t_{k-1},\infty) : \max\big(\nu_{\eta(t_{k-1})}(t) - \nu_{\eta(t_{k-1})}(t-), \mu_{\eta(t_{k-1})}(t) - \mu_{\eta(t_{k-1})}(t-)\big) = 1\big\}.$$

Denote by τ_k, $k \in \mathbb{N}$ the time when the process $\tilde{\xi}(\cdot)$ makes the kth jump.

It is sufficient to show that for any $k \in \mathbb{N}$

$$\begin{aligned}(t_1, t_2 - t_1, \ldots, t_k - t_{k-1}, \eta(t_1), \ldots, \eta(t_k)) \\ \stackrel{d}{=} (\tau_1, \tau_2 - \tau_1, \ldots, \tau_k - \tau_{k-1}, \tilde{\xi}(\tau_1), \ldots, \tilde{\xi}(\tau_k)).\end{aligned} \tag{4.1}$$

Let us prove (4.1) by mathematical induction. Using (2.7), we obtain

$$\eta(t) = \tilde{\xi}(0) + \nu_{\tilde{\xi}(0)}(t) - \mu_{\tilde{\xi}(0)}(t), \text{ if } t \in [0, t_1].$$

By definition t_1 has the exponential distribution with rate $2\lambda\tilde{\xi}(0)$, when $\tilde{\xi}(0) \neq 0$; and with the rate b, if $\tilde{\xi}(0) = 0$ (the minimum of two independent random variables with exponential distribution). At time t_1 the state of process $\eta(\cdot)$ increases or decreases by 1 depending on which process $\nu_{\tilde{\xi}(0)}(\cdot)$ or $\mu_{\tilde{\xi}(0)}(\cdot)$ has the jump at the time t_1, therefore

$$\mathbf{P}(\eta(t_1) = \tilde{\xi}(0) - 1) = \mathbf{P}(\eta(t_1) = \tilde{\xi}(0) + 1) = \frac{1}{2}.$$

Thus, $(t_1, \eta(t_1)) \stackrel{d}{=} (\tau_1, \tilde{\xi}(\tau_1))$.

Suppose for fixed $k \in \mathbb{N}$ the following equality holds

$$\begin{aligned}(t_1, t_2 - t_1, \ldots, t_k - t_{k-1}, \eta(t_1), \ldots, \eta(t_k)) \\ \stackrel{d}{=} (\tau_1, \tau_2 - \tau_1, \ldots, \tau_k - \tau_{k-1}, \tilde{\xi}(\tau_1), \ldots, \tilde{\xi}(\tau_k)).\end{aligned}$$

We will show that the equality holds also for $k+1$.

Using (2.7), we obtain

$$\eta(t) = \eta(t_k) + (\nu_{\eta(t_k)}(t) - \nu_{\eta(t_k)}(t_k)) - (\mu_{\eta(t_k)}(t) - \mu_{\eta(t_k)}(t_k)), \text{ if } t \in [t_k, t_{k+1}].$$

By definition $t_{k+1} - t_k$ has the exponential distribution with rate $2\lambda\eta^{\alpha}(t_k)$, if $\eta(t_k) \neq 0$, with rate b, if $\eta(t_k) = 0$. At time t_{k+1} the process $\eta(\cdot)$ changes its state by 1 or -1 depending on which process $\nu_{\eta(t_k)}(\cdot)$ or $\mu_{\eta(t_k)}(\cdot)$ made a jump

$$\mathbf{P}(\eta(t_{k+1}) = \eta(t_k) - 1) = \mathbf{P}(\eta(t_{k+1}) = \eta(t_k) + 1) = \frac{1}{2}.$$

Thus, we proved that if $\eta(t_k) = x$, then thee joint distribution of random variables $t_{k+1} - t_k$ and $\eta(t_{k+1})$ depends on only the value of x and coincides with the joint distribution of random variables $\tau_{k+1} - \tau_k$ and $\tilde{\xi}(\tau_{k+1})$ under the condition $\tilde{\xi}(\tau_k) = x$. Using this fact by induction for any reals $y_1, \dots, y_{k+1}, v_1, \dots, v_{k+1}$ we will have

$$\begin{aligned}
&\mathbf{P}\left(t_1 < y_1, t_2 - t_1 < y_2, \dots, t_{k+1} - t_k < y_{k+1}, \eta(t_1) < v_1, \dots, \eta(t_{k+1}) < v_{k+1}\right) \\
&\quad = \sum_{x=-\infty}^{v_k} \mathbf{P}(t_{k+1} - t_k < y_{k+1}, \eta(t_{k+1}) < v_{k+1} \mid \eta(t_k) = x) \\
&\qquad\qquad \times \mathbf{P}\left(t_1 < y_1, \dots, t_{k+1} - t_k < y_{k+1}, \eta(t_1) < v_1, \dots, \eta(t_k) = x\right) \\
&\quad = \sum_{x=-\infty}^{v_k} \mathbf{P}\left(\tau_{k+1} - \tau_k < y_{k+1}, \tilde{\xi}(\tau_{k+1}) < v_{k+1} \mid \tilde{\xi}(\tau_k) = x\right) \\
&\qquad\qquad \times \mathbf{P}\left(\tau_1 < y_1, \dots, \tau_{k+1} - \tau_k < y_{k+1}, \tilde{\xi}(\tau_1) < v_1, \dots, \tilde{\xi}(\tau_k) = x\right) \\
&\quad = \mathbf{P}(\tau_1 < y_1, \tau_2 - \tau_1 < y_2, \dots, \tau_{k+1} - \tau_k < y_{k+1}, \tilde{\xi}(\tau_1) < v_1, \dots, \tilde{\xi}(\tau_{k+1}) < v_{k+1}).
\end{aligned}$$

□

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