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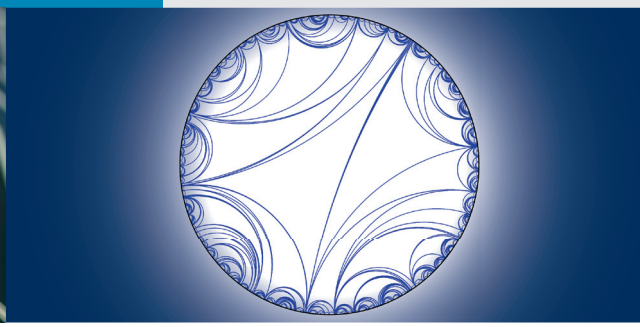

Suren Poghosyan | Mathias Rafler | Sylvie Roelly (Eds.)

Proceedings of the XI international conference Stochastic and Analytic Methods in Mathematical Physics

Lectures in Pure and Applied Mathematics | 6

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Bibliographic information published by the Deutsche Nationalbibliothek
The Deutsche Nationalbibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data are available online
at http://dnb.dnb.de.

Potsdam University Press 2020
http://verlag.ub.uni-potsdam.de/

Am Neuen Palais 10, 14469 Potsdam
Tel.: +49 (0)331 977 2533 / Fax: 2292
E-Mail: verlag@uni-potsdam.de

The series **Lectures in Pure and Applied Mathematics** is edited by the Institute of Mathematics of the University of Potsdam.

ISSN (print) 2199-4951
ISSN (online) 2199-496X

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Cover images:
1. Thomas Roese, ZIM | Building of the Institute at Campus Golm
2. Nicolas Curien, Wendelin Werner | Random hyperbolic triangulation
Published at: Journal of the European Mathematical Society, Volume 15, Issue 4, 2013, pp. 1309–1341, DOI: 10.4171/JEMS/393

Published online in the Institutional Repository of the University of Potsdam:
https://doi.org/10.25932/publishup-45919
https://nbn-resolving.org/urn:nbn:de:kobv:517-opus4-459192

Simultaneously published in print:
ISBN 978-3-86956-485-2

Preface

Stochastic and Analytic Methods in Mathematical Physics

Today the stream of ideas from both mathematics and physics to mathematical physics is increasing dramatically. The scientific meetings in such fields give excellent opportunities for exchange of ideas and information.

The tradition of holding such forums in Armenia started in 1982 when the first conference *Probabilistic methods in modern statistical physics* took place in Tsaghkadzor. These regular meetings in Armenia were always supported by all the organizers of the famous Moscow "Dobrushin-Malyshev-Minlos-Sinai Seminar". R. L. Dobrushin, R. A. Minlos and Y. G. Sinai were often invited by the Yerevan State University and Institute of Mathematics of Armenian Academy of Sciences to give lecture courses on statistical mechanics. They all had Ph.D. students working at the Institute of Mathematics in Yerevan. They participated in two more meetings until 1988, before the collapse of the USSR. The conferences restarted at the international level with the meeting in Nor-Amberd in September 1995. This was one of the last conferences in which R. L. Dobrushin participated. He died soon after.

The eleventh international conference *Stochastic and analytic methods in mathematical physics* was held in Yerevan from 2–7 September in 2019 (the title of the conference was changed in 2012). It was dedicated to the memory of the great mathematician **Robert Adol'fovich Minlos** who passed away in January 2018. R. A. Minlos was a permanent member of the Programme Committee in this series of conferences. He participated with his students in all the conferences including the one in Lake Sevan in 2006. He was one of the main speakers who formulated new problems, generated interesting ideas, questions and discussions. One round table entitled *Robert Adol'fovich Minlos: Life, work, and legacy* was organised on Tuesday, 3 September 2019. Colleagues and former students

were sharing their special memories of R. A. Minlos (see the commemorative chapter). A retrospective short film about his life was presented by his son, Philip Minlos.

Scientific activities of the eleventh conference included talks and discussions of a wide range of problems: classical and quantum statistical physics, quantum dynamics, mathematical methods in quantum mechanics, stochastic analysis, applications of point processes in statistical physics. Participants were specialists from Armenia, Czech Republic, Denmark, France, Germany, Italy, Japan, Lithuania, Russia, the UK and Uzbekistan. A particular focus lied on young scientists' presentations. The traditionally welcoming and warm atmosphere at the conference made it an excellent platform for exchanging experience and generating new ideas.

At this point it is our pleasure to thank all speakers for their significant contribution to the conference. We also would like to thank the members of the Scientific Committee and the members of the Local Organising Committee. A particularly warm thanks to Linda Khachatryan who made sure that the conference went smoothly for everybody. Much gratitude to our sponsors: International Association of Mathematical Physics, the Chair of Probability of University of Potsdam, Annales Henri Poincaré, Research Mathematics Fund (Armenia), Science Committee of the Ministry of Education and Science of the Republic of Armenia. Special thanks to the Akian College of Science and Engineering of American University of Armenia which hosted the conference and provided the facilities.

Special thanks go to Mathias Rafler who supervised the edition of this book by pouring the raw texts in its beautiful LaTeXshape.

Potsdam, Yerevan, March 2020 Sylvie Rœlly, Suren Poghosyan

Participants of the conference during the excursion at Ghegard monastery.

"What we call the beginning is often the end
And to make an end is to make a beginning.
The end is where we start from."

Little Gidding, T. S. Elliot

You may notice that the contributions are not in the usual alphabetical order. Indeed, we thought to award those colleagues, who are always placed at the end of lists because of their name, by placing them first.

Contents

Robert Adol’fovich Minlos

Robert Adol'fovich Minlos (1931–2018) His Work and Legacy

The renowned mathematician Professor Robert Adol'fovich Minlos passed away on 9 January 2018, at the age of 86. An eminent researcher and outstanding teacher, he was a world-renowned specialist in the area of functional analysis, probability theory, and contemporary mathematical physics.

R. A. Minlos was born on 28 February 1931 into a family with a strong connection to the humanities. His father, Adol'f Davidovich Miller, was known as a lecturer and was the author of English dictionaries and manuals. His mother, Nora Romanovna (Robertovna) Minlos, was a historian-ethnographer. This is perhaps why Robert Adol'fovich loved poetry, wrote verses himself, was a fervent theater-goer from his school years, and was began painting seriously at the age of 40.

Nothing foreshadowed a mathematical future, but when he was 15, the young Robert accidentally saw a poster about the Moscow Mathematical Olympiad for schoolchildren. He participated in it, obtained the second prize and, inspired by that, began to attend the school club led by E. B. Dynkin. In 1949 Robert already entered the Faculty of Mechanics and Mathematics of the Moscow State University. He continued to participate in Dynkin's seminar, which together with A. S. Kronrod's seminar, had a great influence on him as an undergraduate student.

R. A. Minlos prepared his first scientific paper (equivalent to a master's degree thesis) in 1950 while participating in the Moscow State University seminar on the theory of

Still life with flowers. R. A. Minlos.

functions of a real variable under the leadership of A. S. Kronrod. But the real scientific interests of the young mathematics student began to form after he became acquainted with I. M. Gelfand. Their joint publication "Solution of the equations of quantum fields" (Doklady Akad. Nauk SSSR, n.s., 97, 209–212, 1954) became Minlos' Diploma thesis in mathematics. It was devoted to the *functional*, or, in mathematical physics language, the *path* integral, which has a direct relation to quantum physics.

As Minlos himself admitted: "My further life in mathematics was predetermined by that work, because I was subsequently mainly occupied with mathematical physics. There were, nevertheless, more works on random processes, on measure theory, and on functional analysis." Very soon one of his papers "Extension of a generalised random process to a completely additive measure" (Doklady Akad. Nauk SSSR, 119, 439–442, 1958) brought Minlos worldwide fame. It became the basis of his Candidate (equivalent to PhD) dissertation "Generalised random processes and their extension to a measure", which was published in Trudy MMO, 8, 497–518, 1959. This result, which is important for the theory of random processes as well as for functional analysis, is now known as the *Minlos theorem* on the extension of cylindrical measures to Radon measures on the continuous dual of a nuclear space, i. e. the continuation of a process to a measure on spaces adjoint to nuclear spaces.

The connection of Minlos to mathematical physics at that time was manifested by the publication (jointly with I. M. Gelfand and Z. Ya. Shapiro) of the monograph "Representations of the rotation and Lorentz groups and their applications" (1958), which was later translated from the Russian by Pergamon, London, in 1964.

From 1956 to 1992, R. A. Minlos was employed by the Department of the Theory of Functions and Functional Analysis of the Faculty of Mechanics and Mathematics at the Moscow State University (MSU). In that period, there was a need to organise a joint seminar with F. A. Berezin, primarily to discuss the mathematical problems of quantum mechanics and of quantum field theory.

A real advance of activity in the field of mathematical physics at the Faculty of Mechanics and Mathematics of MSU was achieved with R. A. Minlos and R. L. Dobrushin's organisation of a seminar on statistical physics in 1962. It soon became widely known in the Soviet Union and abroad as the *Dobrushin-Malyshev-Minlos-Sinai* seminar. The quantum aspects of statistical mechanics at the seminar were primarily associated with the name of R. A. Minlos. The seminar lasted until 1994 and had a huge impact on the

R. A. Minlos with H. Zessin and S. Poghosyan, Bielefeld 2005.

world of modern mathematical physics. Almost all celebrated specialists in this field visited Moscow during the lifespan of the seminar.

The beginning of the 1960s was extremely fruitful for Robert Adol'fovich. In the first place, this concerns new results obtained jointly with L. D. Faddeev on the quantum mechanical description of three particles (1961). It was followed by two articles devoted to study of the thermodynamic limit in classical statistical physics (1967). There R. A. Minlos suggested the first rigorous mathematical definition of the limiting Gibbs distributions for an infinite system of interacting classical particles and also analysed the properties of such distributions (Funct. Anal. Appl., 1, 140–150 and 206–217, 1967). This result anticipated the origin of the Markovian understanding of the Gibbs random fields in the sense of *Dobrushin-Lanford-Ruelle* (1968).

The result (together with Ya. G. Sinai) of the appearance of phase separation in lattice systems at low temperatures (Math. USSR-Sb., 2, 335–395, 1967; Trudy MMO, 17, 213–242, 1967 and 19, 113–178, 1968) was of fundamental importance for the mathematical theory of phase transitions. It formed the basis of Minlos' doctoral dissertation, which he submitted for habilitation in 1968. In another joint work with Ya. G. Sinai (Theor. Math. Phys., 2, 167–176, 1970) the foundation was laid for a new approach to the study of the spectral properties of many-particle systems. In combination with the cluster expansions, this approach drove significant progress in the description of the properties of such infinite systems, including the spectrum of elementary particles of quantum fields and the mathematical description of the *quasi-particle* picture in statistical physics.

R. A. Minlos with participants of the conference, Tsaghkadzor 2002.

The new powerful method of cluster expansions was, from the very beginning, central in the list of interests of Robert Adol'fovich. He proposed to develop further the cluster expansion method so that it could be applied to the study of what he called cluster functions.

These are correlation functions, truncated correlation functions, semi-invariants and the Ursell functions. It was his idea to use the so-called Ursell kernel for the representation of the cluster functions. In his paper with S. Poghosyan (1977) a fundamental forest graph estimate of the Ursell kernel, which contains as a special case the well-known tree graph estimate, was obtained. The forest graph estimate was used later by S. Poghosyan and D. Ueltschi to develop an abstract cluster expansion method. Similarly, S. Poghosyan and H. Zessin developed the large volume geometric expansion of the log-partition function for the models of classical and quantum physics and for construction of the Gibbs processes.

The results of a large series of papers on cluster expansions by R. A. Minlos, V. A. Malyshev, and by their students have been summarised in two monographs "Gibbs random fields: Cluster expansions" (Springer 1991, translation of 1985 Russian edition) and "Linear infinite-particle operators" (Amer. Math. Soc. 1995, translation from the Russian edition of 1994). As was outlined in the book "Gibbs random fields", the method of cluster expansions provides not only a construction of the limiting Gibbs measure but

R. A. Minlos with participants during the excursion, Tsaghkadzor 2002.

also cluster representations of the projections of the limiting Gibbs measure onto bounded regions.

A famous peculiarity of the Dobrushin-Malyshev-Minlos-Sinai seminar was not only its duration of about four hours, which was amazing for foreign guests, or the assertive directness in communicating with lecturers, but also the opportunity to obtain from the discussions some interesting problems to be solved. In essence, the seminar was functioning as a *machine*, generating questions and a possible way to convert them into answers. Robert Adol'fovich was always one of the sources of interesting questions and open problems. The list of projects thus originated includes, for example, the cluster expansions and their applications to the problem of uniqueness/non-uniqueness of the Gibbs states, the quantum three-particle problem, the Trotter product formula for Gibbs semigroups, the study of infinite-particle operators spectra, the analysis of quasi-particle picture in statistical physics, and many others.

In their book "Linear infinite-particle operators" V. A. Malyshev and R. A. Minlos proposed a description of a quasi-particle picture based on the construction by cluster expansions of the lower branches of the spectrum of infinite many-body system with a good clustering. This idea goes back to the paper by R. A. Minlos and Ya. G. Sinai "Investigation of the spectra of some stochastic operators arising in the lattice gas models" (1970). If the system possesses a good clustering one can construct separated translation-invariant two-, three-, and more (interacting) quasi-particles excited states, which are combinations of branches with bands of continuum spectra. Robert Adol'fovich called this property of excitations "The *corpuscular* structure of the spectra of operators describing large systems" (title of his paper in *Mathematical Physics* 2002, Imperial Coll. Press 2000).

In addition to the Dobrushin-Malyshev-Minlos-Sinai seminar in the 1970s, there was a regular tutorial seminar, which was led by Robert Adol'fovich once a week. This was a very good opportunity to learn elements of topological vector spaces, in particular the Minlos theorem about the extension of a generalized random process to a measure on spaces adjoint to nuclear spaces. The seminar also covered elements of mathematical statistical physics in the spirit of the famous "Lectures on statistical physics" in Uspekhi Math. Nauk (1968).

R. A. Minlos as well as Ya. G. Sinai and R. L. Dobrushin were often invited by the Institute of Mathematics in Yerevan to participate in regular conferences under the name

R. A. Minlos with participants of the conference, Lake Sevan 2006.

"Probabilistic methods in modern statistical physics". The first one was held in 1982 and the last one in 1988, three years before the collapse of the Soviet Union.

The conferences restarted in 1995 at the international level. Robert Adol'fovich participated, as a rule with his students, in all of them, including the conference in Lake Sevan in 2006.

In the early nineties Robert Adol'fovich began his collaboration with Italian institutions and mathematicians. He was a guest of the Department of Mathematics at the university of Rome "La Sapienza" many times, and he also visited other institutions in Trieste, Naples, L'Aquila and Camerino.

A first result had been obtained by C. Boldrighini, I. A. Ignatyuk, V. A. Malyshev and A. Pellegrinotti on the annealed model of a discrete-time random walk on a d-dimensional lattice in mutual interaction with a dynamic random environment. Robert Adol'fovich proposed to apply the results that he had obtained, together with V. A. Malyshev and their students, on the spectral analysis of the transfer matrix for perturbed homogeneous random fields.

Robert Adol'fovich was a wonderful teacher, a patient and wise mentor. Directness, accessibility, and enthusiasm attracted numerous students and followers to him. Many of his later PhD students benefited from a direct generous contact with the *Master*. At

R. A. Minlos on the way to Hayravank Monastery, Lake Sevan 2006.

the Faculty of Mechanics and Mathematics at MSU the student seminar was combined with lectures and scientific seminars guided by Robert Adol'fovich first together with F. A. Berezin and then with V. A. Malyshev. The lecture notes gave rise to many nice and popular tutorial books, for example "Introduction to mathematical statistical physics", published by R. A. Minlos in Univ. Lect. Series, vol.19, AMS 2000.

The problems related to the theory of operators and to quantum physics should be especially noted. A long paper ("A system of three quantum particles with point-like interactions", Russian Math. Surveys, 69, 539–564, 2014) was published by R. A. Minlos on this topic. His very last manuscript (with C. Boldrighini, A. Pellegrinotti, and E. A. Zhizhina) was on the subject "Regular and singular continuous time random walk in dynamic random environment".

To his students and collaborators, Robert Adol'fovich was like a brilliant sculptor who, from a shapeless block, cutting off excess, could create a mathematical masterpiece.

Robert Adol'fovich selflessly served science, and in everyday life he was a generous and friendly person. He gladly shared his enthusiasm and energy with his students and colleagues. In addition to the accuracy of reasoning and complicated techniques, there is always a beautiful idea and harmony in his works. To the question "What three math-

ematical formulas are the most beautiful?" Robert Adol'fovich gave the answer: "The Gibbs formula, the Feynman-Kac formula and the Stirling formula."

Always surrounded by relatives and loved ones, and also by loving pupils, colleagues, and friends, Robert Adol'fovich Minlos lived a complete life. In each of those who knew Robert Adol'fovich, he left a bright drop of memory of himself.

C. Boldrighini (Istituto Nazionale di Alta Matematica, Unità locale Università Roma Tre),
V. A. Malyshev (Faculty of Mechanics and Mathematics, Lomonossov MSU),
A. Pellegrinotti (Dipartimento di Matematica e Fisica, Università Roma Tre),
S. K. Poghosyan (Institute of Mathematics of the NAS RA, Yerevan),
Ya. G. Sinai (Department of Mathematics, Princeton University),
V. A. Zagrebnov (Institut de Mathématiques de Marseille),
E. A. Zhizhina (Institute for Information Transmission Problems, Moscow)

A contribution to the conference in commemoration of R. A. Minlos

> *Science and all of us, we have lost an outstanding mathematician. I have lost my best friend and best co-author. But most important, Robert was a reliable friend, kind and human in all life aspects. Nowadays in science (as anywhere else) struggle for power, grants, academic positions, often kills science itself. This I never saw in Robert. I often see now our common past with Robert and this provides me strength to struggle for real science against politicians in science. I feel that he sees all of us from another world. The world that we still even do not try to understand because publishing papers for impact factors takes too much time and energy from us. I am sure he feels strong in that world and is ready to help all of us.*
>
> *Vadim Malyshev*
> *Moscow, September 2019*

Robert Adol'fovich Minlos

1

A Gibbs point process of diffusions: Existence and uniqueness

Alexander Zass[*]

Abstract. *In this work we consider a system of infinitely many interacting diffusions as a marked Gibbs point process. With this perspective, we show, for a large class of stable and regular interactions, existence and (conjecture) uniqueness of an infinite-volume Gibbs process. In order to prove existence we use the specific entropy as a tightness tool. For the uniqueness problem, we use cluster expansion to prove a Ruelle bound, and conjecture how this would lead to the uniqueness of the Gibbs process as solution of the Kirkwood-Salsburg equation.*

1 Introduction and set-up

Consider a Langevin dynamics on $\mathbb{R}^d$ of the form

$$dX_s = dB_s - \frac{1}{2}\nabla V(X_s)ds, \quad s \in [0,2\beta],\ \beta > 0, \tag{1.1}$$

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The author wishes to warmly thank S. Rœlly and H. Zessin for the many discussions and insights into the topic. The research of the author has been partially funded by Deutsche Forschungsgemeinschaft (DFG) – SFB1294/1-318763901 and Deutsch-Französische Hochschule (DFH) – DFDK 01-18.

where B is an $\mathbb{R}^d$-valued Brownian motion, and $V : \mathbb{R}^d \to \mathbb{R}$ is an ultracontractive potential, i. e. outside of some compact subset of $\mathbb{R}^d$,

$$\exists \delta', \mathfrak{a}_1, \mathfrak{a}_2 > 0, \quad V(x) \geq \mathfrak{a}_1 |x|^{d+\delta'} \text{ and } \Delta V(x) - \frac{1}{2}|\nabla V(x)|^2 \leq -\mathfrak{a}_2 |x|^{2+2\delta'}. \tag{1.2}$$

Under these conditions there exists a unique strong solution to (1.1) (see e. g. [12]), which generates an ultracontractive semigroup (see [6],[2]). Moreover, the law of X starting at $X_0 = 0$ is a measure R such that, for any $\delta < \delta'/2$,

$$\int e^{\|m\|_\infty^{d+2\delta}} R(dm) < +\infty. \tag{1.3}$$

For the rest of this work, let $\delta > 0$ as above be fixed.

The question we wish to explore in this work is how to construct a physically meaningful Gibbsian interaction between infinitely many such diffusions starting at random locations. More precisely, we model such a system as a marked Gibbs point process: locations and marks will describe, respectively, starting points and paths of these diffusions. We will then solve the non-trivial questions of existence and uniqueness of the infinite-volume measure for a large class of stable and regular path interactions.

After introducing the Gibbsian framework, we present an existence result via the entropy method of [11]: we use the specific entropy as a tightness tool to prove convergence of a sequence of finite-volume Gibbs measures and show that this limit satisfies the Gibbsian property (that is, the DLR equations). In Section 4 we then use the method of cluster expansion – introduced by S. Poghosyan, D. Ueltschi, and H. Zessin in [8], [10] – and the Kirkwood-Salsburg equation to show a Ruelle bound for a regime of small activity, and conjecture that uniqueness of the constructed infinite-volume Gibbs process associated to path interactions follows.

2 Gibbsian formalism for marked point processes

The state space we consider in this work is $\mathscr{E} = \mathbb{R}^d \times C_0$, where $C_0 := C_0\big([0,2\beta];\mathbb{R}^d\big)$, $\beta > 0$, is the set of continuous paths $m : [0,2\beta] \to \mathbb{R}^d$ with initial value $m(0) = 0$. An element $\mathbf{x} = (x,m) \in \mathscr{E}$ is identified with the path $\big(x + m(t)\big)_{t\in[0,2\beta]}$ of starting point $x \in \mathbb{R}^d$ and trajectory $m \in C_0$.

Denote by $\mathscr{M}$ the set of locally-finite point measures (or *configurations*) on $\mathscr{E}$, which are of the form $\gamma = \sum_i \delta_{(x_i,m_i)} \in \mathscr{M}$; we often identify a configuration γ with its support $\{(x_i,m_i)\}_i \subset \mathscr{E}$.

Let $\mathscr{B}_b(\mathbb{R}^d)$ be the subset of bounded Borel sets of $\mathbb{R}^d$. Let $\mathscr{M}_f$ denote the subset of finite configurations, and for any $\Lambda \in \mathscr{B}_b(\mathbb{R}^d)$, let $\mathscr{M}_\Lambda \subset \mathscr{M}_f$ denote the restriction to starting points inside Λ, and for any configuration $\gamma \in \mathscr{M}$, let $\gamma_\Lambda := \gamma \cap (\Lambda \times C_0) \in \mathscr{M}_\Lambda$.

Let $\mathscr{P}(\mathscr{M})$ denote the set of probability measures on $\mathscr{M}$: these are called *marked point processes*. As reference process we consider, for any $\Lambda \in \mathscr{B}_b(\mathbb{R}^d)$, the marked Poisson point process π^z_Λ on $\mathscr{E}$ with intensity measure $z\,dx_\Lambda \otimes R(dm)$. The coefficient z is a positive real number, dx_Λ is the Lebesgue measure on Λ, and the probability measure R is the path measure of the solution of (1.1) starting at 0. In other words, the starting points are drawn in Λ according to a Poisson process, and the marks are diffusion paths starting at these Poisson points.

We add interaction between the points of a configuration by considering an energy functional that takes into account both the locations and the marks.

Assumption 1.1 For any finite marked point configuration $\gamma = \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \in \mathscr{M}_f$, $N \geq 1$, its *energy* is given by the following functional

$$H(\gamma) = \sum_{i=1}^{N} \Psi(\mathbf{x}_i) + \sum_{i=1}^{N} \sum_{j<i} \Phi(\mathbf{x}_i, \mathbf{x}_j) \in \mathbb{R} \cup \{+\infty\}, \tag{1.4}$$

where

- ◇ The *self-potential* term Ψ satisfies $\inf_{x\in\mathbb{R}^d} \Psi(x,m) \geq -k_\Psi \|m\|_\infty^{d+\delta}$ for some constant $k_\Psi > 0$;
- ◇ The *two-body potential* Φ is defined by

$$\Phi(\mathbf{x}_i, \mathbf{x}_j) = \left(\phi(x_i - x_j) + \int_0^{2\beta} \tilde{\phi}(m_i(s) - m_j(s))ds \right) \mathbb{1}_{\{|x_i - x_j| \leq a_0 + \|m_i\|_\infty + \|m_j\|_\infty\}}, \tag{1.5}$$

where ϕ (acting on on the initial location of the diffusions) is a *radial* (i. e. $\phi(x) = \phi(|x|)$) and *stable* $\mathbb{R}$-valued pair potential in the sense of [13], with stability constant $\mathfrak{c}_\phi \geq 0$, bounded from below, with $\phi(u) \leq 0$ for $u \geq a_0$ (see Figure 1.1); $\tilde{\phi}$ (acting on the dynamics of the diffusions) is a non-negative pair potential.

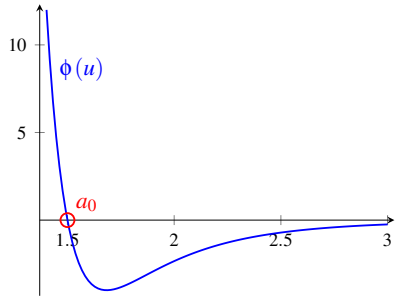

Figure 1.1: An example of radial and stable pair potential ϕ is the *Lennard-Jones* potential $\phi(u) = 16\Big(\big(\frac{3/2}{u}\big)^{12} - \big(\frac{3/2}{u}\big)^{6}\Big)$; its zero is at $a_0 = 3/2$.

Remark 1.2

(i) The stability of the point-interaction potential ϕ and the non-negativity of the mark-interaction potential $\tilde{\phi}$ guarantee stability (in the sense introduced in Lemma 1.5) of the energy H of a marked-point configuration; the fact that ϕ is bounded from below is used to prove the stability of the conditional energy (see Lemma 1.7).

(ii) The indicator function in (1.5) can be interpreted as follows: when the starting points are far enough from each other, the two diffusions do not interact; if their paths do not intersect, they may interact only if $|x_1 - x_2| \leq a_0 + \|m_1\|_\infty + \|m_2\|_\infty$. See Figure 1.2. Notice that the range of interaction is finite but not uniformly bounded.

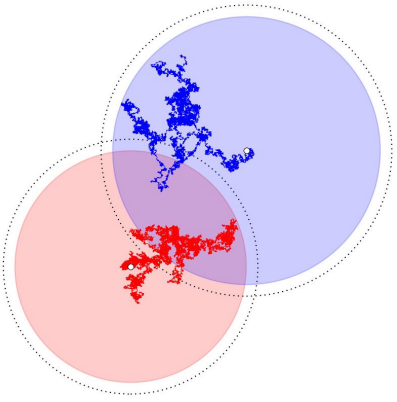

Figure 1.2: The paths of two Langevin diffusions in $\mathbb{R}^2$ which interact. Each circle is centred in the starting point, and its radius corresponds to their maximum displacement in the time interval $[0,1]$. The dotted circles represent the "security" distance $a_0/2$.

Definition 1.3 For any $\Lambda \in \mathscr{B}_b(\mathbb{R}^d)$, the free-boundary-condition *finite-volume Gibbs measure* on Λ with energy H and activity $z > 0$ is the probability measure P_Λ^z on $\mathscr{M}_\Lambda$ defined by

$$P_\Lambda^z(d\gamma) := \frac{1}{Z_\Lambda^z} e^{-H(\gamma_\Lambda)}\, \pi_\Lambda^z(d\gamma). \tag{1.6}$$

In this work we investigate the existence and uniqueness, as Λ increases to cover the whole space $\mathbb{R}^d$, of an infinite-volume Gibbs measure, in the following sense:

Definition 1.4 A probability measure P on $\mathscr{M}$ is said to be an *infinite-volume Gibbs measure* with energy H and activity $z > 0$, denoted by $P \in \mathscr{G}(H,z)$, if it satisfies, for any $\Lambda \in \mathscr{B}_b(\mathbb{R}^d)$ and any positive, bounded, and measurable functional $F : \mathscr{M} \to \mathbb{R}$, the following *DLR equation* (for Dobrushin-Landford-Ruelle)

$$\int_{\mathscr{M}} F(\gamma)\, P(d\gamma) = \int_{\mathscr{M}} \frac{1}{Z_\Lambda^z(\xi)} \int_{\mathscr{M}_\Lambda} F(\gamma_\Lambda \xi_{\Lambda^c}) e^{-H_\Lambda(\gamma_\Lambda \xi_{\Lambda^c})} \pi_\Lambda^z(d\gamma)\, P(d\xi), \tag{DLR}$$

where $H_\Lambda(\gamma)$ is the *conditional energy* of the configuration γ in Λ given its exterior:

$$H_\Lambda(\gamma) := \lim_{r \to +\infty} H\big(\gamma_{\Lambda \oplus B(0,r)}\big) - H\big(\gamma_{\Lambda \oplus B(0,r)\setminus\Lambda}\big), \tag{1.7}$$

with $\Lambda \oplus B(0,r) := \big\{x \in \mathbb{R}^d : \exists y \in \Lambda,\ |y-x| \le r\big\}$.

3 Existence of an infinite-volume Gibbs point process via the entropy method

Under Assumption 1.1 on the energy functional H, the following three lemmas provide the groundwork for the existence theorem.

Lemma 1.5 The following stability condition holds: setting $\mathfrak{c}_H := k_\Psi \vee \mathfrak{c}_\phi$,

$$H(\gamma) \ge -\mathfrak{c}_H \sum_{(x,m)\in\gamma} \big(1 + \|m\|_\infty^{d+\delta}\big), \quad \gamma \in \mathscr{M}_f. \tag{1.8}$$

In order to control the support of the Gibbs point process, we define the subset of *tempered configurations* as the union $\mathscr{M}^{\mathrm{temp}} := \bigcup_{\mathfrak{t}\in\mathbb{N}} \mathscr{M}^{\mathfrak{t}}$, where $\mathscr{M}^{\mathfrak{t}}$ is the set of all configurations $\gamma \in \mathscr{M}$ such that, for all $l \in \mathbb{N}^*$, $\sum_{(x,m)\in\gamma_{B(0,l)}} (1 + \|m\|_\infty^{d+\delta}) \le \mathfrak{t} l^d$.

Lemma 1.6 For any bounded $\Lambda \subset \mathbb{R}^d$ and $\mathfrak{t} \geq 1$, there exists a random variable $\mathfrak{r} = \mathfrak{r}(\gamma_\Lambda, \mathfrak{t}) < +\infty$ such that the limit in (1.7) stabilises, i. e.

$$H_\Lambda(\gamma) = H\big(\gamma_{\Lambda \oplus B(0,\mathfrak{r})}\big) - H\big(\gamma_{\Lambda \oplus B(0,\mathfrak{r}) \setminus \Lambda}\big).$$

We say that $\mathfrak{r}(\gamma_\Lambda, \mathfrak{t})$ is the *finite but random range* of the interaction $H_\Lambda(\gamma)$.

Lemma 1.7 Fix $\Lambda \in \mathscr{B}_b(\mathbb{R}^d)$. For any $\mathfrak{t} \geq 1$, there exists a constant $\mathfrak{c}'(\Lambda, \mathfrak{t}) \geq 0$ such that the following stability of the conditional energy holds: uniformly for all $\xi \in \mathscr{M}^{\mathfrak{t}}$,

$$H_\Lambda(\gamma_\Lambda \xi_{\Lambda^c}) \geq -\mathfrak{c}'(\Lambda, \mathfrak{t}) \sum_{(x,m) \in \gamma_\Lambda} \big(1 + \|m\|_\infty^{d+\delta}\big), \quad \gamma_\Lambda \in \mathscr{M}_\Lambda. \tag{1.9}$$

We endow the set $\mathscr{P}(\mathscr{M})$ of probability measures on $\mathscr{M}$ with the topology of local convergence (see [4], [5]). More precisely,

Definition 1.8 A functional F on $\mathscr{M}$ is called *local* and *tame* if there exist a set $\Delta \in \mathscr{B}_b(\mathbb{R}^d)$ and a constant $a > 0$ such that, for all $\gamma \in \mathscr{M}$, $F(\gamma) = F(\gamma_\Delta)$ and $|F(\gamma)| \leq a\,\big(1 + \sum_{(x,m) \in \gamma_\Delta} (1 + \|m\|_\infty^{d+\delta})\big)$.

We denote by $\mathscr{L}$ the set of all local and tame functionals. The topology $\tau_{\mathscr{L}}$ of *local convergence* on $\mathscr{P}(\mathscr{M})$ is defined as the weak* topology induced by $\mathscr{L}$, i. e. the smallest topology on $\mathscr{P}(\mathscr{M})$ under which all the mappings $P \mapsto \int F\, dP$, $F \in \mathscr{L}$, are continuous.

Let us now recall the concept of specific entropy of a probability measure on $\mathscr{M}$.

Definition 1.9 Given two probability measures Q and Q' on $\mathscr{M}$, the *specific entropy* of Q with respect to Q' is defined by

$$\mathcal{I}(Q|Q') = \lim_{\Lambda_n \nearrow \mathbb{R}^d} \frac{1}{|\Lambda_n|} I_{\Lambda_n}(Q|Q'),$$

where $\Lambda_n = [-n, n)^d$, and the *relative entropy* of Q with respect to Q' on Λ is defined as

$$I_\Lambda(Q|Q') := \begin{cases} \int \log f \, dQ_\Lambda & \text{if } Q_\Lambda \preccurlyeq Q'_\Lambda \text{ with } f := \frac{dQ_\Lambda}{dQ'_\Lambda}, \\ +\infty & \text{otherwise,} \end{cases}$$

where Q_Λ (resp. Q'_Λ) is the image of Q (resp. Q') under the mapping $\gamma \mapsto \gamma_\Lambda$.

The specific entropy with respect to π^z is well-defined as soon as Q is invariant under translations on the lattice. Moreover, we underline that for any $a > 0$, the a-entropy level set

$$\mathscr{P}(\mathscr{M})_{\leq a} := \left\{ Q \in \mathscr{P}(\mathscr{M}) : \mathcal{I}(Q|\pi^z) \leq a \right\}$$

is relatively compact for the local convergence topology $\tau_{\mathscr{L}}$, as proved in [5].

Putting together the technical conditions described in this section yields the existence of an infinite-volume Gibbs measure P^z, for *any* activity $z > 0$.

Theorem 1.10 For any energy functional H as in Assumption 1.1 and any activity $z > 0$, there exists at least one infinite-volume Gibbs measure $P^z \in \mathscr{G}(H, z)$.

Sketch of proof.

(i) For $\Lambda_n = [-n, n)^d$, consider the sequence $(P^z_{\Lambda_n})_{n\geq 1}$ of finite-volume Gibbs measures, and build the empirical field $(\bar{P}^z_n)_{n\geq 1}$ by stationarising it w.r.t. lattice translations.

(ii) Use uniform bounds on the specific entropy to show the convergence, up to a subsequence, to an infinite-volume measure P^z.

(iii) Prove, using an ergodic property, that P^z carries only the space of tempered configurations.

(iv) Noticing that $\bar{P}^z_n$ does not satisfy the (DLR) equations, introduce a new sequence $(\hat{P}^z_n)_n$ asymptotically equivalent to $(\bar{P}^z_n)_n$ but satisfying (DLR).

(v) Use appropriate approximation technique to show that P^z satisfies (DLR) too.

For details, see [11]. □

Example 1.11 Let $d = 2$. A concrete example of functions satisfying the above assumptions is as follows:

Consider as reference diffusion a Langevin dynamics with $V(x) = |x|^4$; the diffusion is ultracontractive with $\delta' = 2$. The invariant measure $\mu(dx) = e^{|x|^4} dx$ is a Subbotin measure (see [15]).

Consider as self interaction $\Psi(\mathbf{x}) = -\|m\|_\infty^{5/2}$; as interaction between the initial locations a *Lennard-Jones* pair potential $\phi(u) = au^{-12} - bu^{-6},\ a, b > 0$; as interaction between the marks any non-negative pair potential $\tilde{\phi}$.

4 Uniqueness of Gibbs measure via cluster expansion

The method of cluster expansion relies on finding a regime of small activity $0 < z \leq \bar{z}$ in which the partition function Z^z_Λ can be written as the exponential of an absolutely converging series of *cluster* terms. It should then be possible to write an equation (the so-called *Kirkwood-Salsburg equation*, see e. g. [14]) for the correlation functions of the infinite-volume Gibbs measure P^z constructed above. We conjecture that under some assumptions, such an equation has a unique solution, which would lead to the uniqueness of the infinite-volume Gibbs measure. Here we use a strategy developed in [9]. For this section, we make the following additional

Assumption 1.12 The potential ϕ (on initial locations of the diffusions) is *integrable* in $\mathbb{R}^d$: $\|\phi\|_1 < +\infty$; the potential $\tilde{\phi}$ (on the dynamics of the diffusions) is *bounded*: $\|\tilde{\phi}\|_\infty < +\infty$.

The partition function is given, for any $\Lambda \subset \mathbb{R}^d$, by

$$Z^z_\Lambda = 1 + \sum_{N\geq 1} \frac{z^N}{N!} \int_{(\Lambda\times C_0)^N} \exp\Bigg\{ - \sum_{1\leq i\leq N} \Psi(x_i, m_i) - \sum_{1\leq i<j\leq N} \Bigg(\phi\big(|x_i - x_j|\big) + \int_0^{2\beta} \tilde{\phi}\big(|m_i(s) - m_j(s)|\big) ds \Bigg) \mathbb{1}_{\{|x_i - x_j| \leq a_0 + \|m_i\|_\infty + \|m_j\|_\infty\}} \Bigg\} dx_1 \cdots dx_N \, R(dm_1) \cdots R(dm_N). \tag{1.10}$$

Theorem 1.13 Consider an energy functional H satisfying Assumption 1.1 and Assumption 1.12. Then the two-body potential Φ satisfies a *modified regularity* condition. Therefore, there exists $\bar{z} > 0$ such that, for any activity $z \leq \bar{z}$, the partition function above converges absolutely and a Ruelle bound holds.

Proof. In order to guarantee the absolute convergence of (1.10), we check whether the pair potential Φ satisfies a *modified* $\mathfrak{c}$*-regularity for the functional* $\mathfrak{a}$ (terminology from [10]; introduced in [8]), i. e. that for any $\mathbf{x}_1 = (x_1, m_1)$, the following inequality holds

$$z e^{\mathfrak{c}} \int e^{\mathfrak{a}(\mathbf{x}_2)} |\Phi(\mathbf{x}_1, \mathbf{x}_2)| e^{-\Psi(\mathbf{x}_2)} dx_2 \, R(dm_2) \leq \mathfrak{a}(\mathbf{x}_1). \tag{1.11}$$

We consider here $\mathfrak{c} = \mathfrak{c}_\phi$, and a function of the form $\mathfrak{a}(x,m) = \mathfrak{a}(m) = a_1(\|m\|^d_\infty \vee 1)$, where

$$a_1 = \|\phi\|_1 + \Big(2\beta \|\tilde{\phi}\|_\infty k_d b_d (a_0^d + 1)\Big),$$

with k_d such that $(x+y+z)^d \le k_d(x^d+y^d+z^d)$, and b_d the volume of the unit ball in $\mathbb{R}^d$. Recalling that the self potential Ψ is such that $\Psi(\mathbf{x}) \ge -k_\Psi \|m\|_\infty^{d+\delta}$. Set $\rho := \int e^{a_1(\|m\|_\infty^d \vee 1)+k_\Psi\|m\|_\infty^{d+2\delta}} R(dm) \overset{(1.3)}{<} +\infty$; the modified regularity condition reads

$$z e^{\mathfrak{C}_\phi} \int_{C_0} e^{a_1(\|m_2\|_\infty^d \vee 1)} \int_{\mathbb{R}^d} \left|\phi(x_2-x_1)\right| + \left(\int_0^{2\beta} \tilde{\phi}(m_2(s)-m_1(s))ds\right) \mathbb{1}_{\{|x_1-x_2|\le a_0+\|m_1\|_\infty+\|m_2\|_\infty\}} dx_2 \, \mathrm{e}^{k_\Psi\|m_2\|_\infty^{d+\delta}} R(dm_2) \le a_1(\|m_1\|_\infty^d \vee 1).$$

Estimating the l. h. s. leads to the following condition:

$$z \le \frac{\|m_1\|_\infty^d \vee 1}{\rho e^{\mathfrak{C}_\phi}(\|m_1\|_\infty^d + 1)},$$

which holds as soon as $z \le (2\rho e^{\mathfrak{C}_\phi})^{-1} =: \bar{z} = \inf_{m_1} \frac{\|m_1\|_\infty^d \vee 1}{\rho e^{\mathfrak{C}_\phi}(\|m_1\|_\infty^d+1)}$. Applying results in [8], this implies the absolute convergence of (1.10). Moreover, in [9] S. Poghosyan and H. Zessin prove that a Ruelle bound also holds. □

The unique step towards uniqueness which is now missing is the proof that the Kirkwood-Salsburg equation has a unique solution. We state the following conjecture:

Conjecture 1.14 For any activity $z \le \bar{z}$, the Kirkwood-Salsburg equation has a unique solution.

Assuming the above conjecture holds true, we obtain the following

Corollary 1.15 For any activity $z \le \bar{z}$, the infinite-volume measure P^z constructed in Theorem 1.10 is the unique Gibbs measure in $\mathscr{G}(H,z)$.

Conclusions and outlook. In [3], D. Dereudre showed the equivalence between the law of an infinite-dimensional interacting SDE with Gibbsian initial law, and a Gibbs point process on the path space, with a certain energy functional.

It is a natural question to ask whether a Gibbs point process with energy functional H as in Assumption 1.1 is the law of infinite dimensional interacting SDE. Using Malliavin derivatives, D. Dereudre proved that Gibbs point processes with regular H are the law of SDEs with a certain non-markovian drift. See [1] and [7] in the lattice case.

The existence and uniqueness results presented here could therefore be useful to obtain a criterium for the solution of infinite-dimensional SDEs. This is a work in progress.

Bibliography

[1] Dai Pra, P., Rœlly, S.: *An existence result for infinite-dimensional Brownian diffusions with non-regular and non-Markovian drift*, Markov Proc. Rel. Fields **10**, 113–136 (2004).

[2] Davies, E. W.: *Heat kernels and spectral theory*, Cambridge University Press (1989).

[3] Dereudre, D.: *Interacting Brownian particles on pathspace*, ESAIM: Probability and Statistics **7**, 251–277 (2003).

[4] Georgii, H.-O.: *Gibbs measures and phase transitions*, De Gruyter studies in Mathematics 9, 2nd ed. (2011).

[5] Georgii, H.-O., Zessin, H.: *Large deviations and the maximum entropy principle for marked point random fields*, Probab. Theory Relat. Fields **96**(2), 177–204 (1993).

[6] Kavian, O., Kerkyacharian, G., Roynette, B.: *Quelques remarques sur l'ultracontractivité*, J. Funct. Anal. **111**, 155–196 (1993).

[7] Minlos, R. A., Rœlly, S., Zessin, H.: *Gibbs states on space-time*, Pot. Anal. **13**, 367–408 (2000).

[8] Poghosyan, S., Ueltschi, D.: *Abstract cluster expansion with applications to statistical mechanical systems*. J. Math. Phys. **50**(5), 053509 (2009).

[9] Poghosyan, S., Zessin, H.: *Penrose-stable interactions in classical statistical mechanics*, manuscript in preparation (2020).

[10] Poghosyan S., Zessin, H.: *Construction of limiting Gibbs processes and the uniqueness of Gibbs processes*, In: Lectures in Pure and Applied Mathematics **6**, Potsdam University Press (2020).

[11] Rœlly, S., Zass, A.: *Marked Gibbs processes with unbounded interaction: an existence result*, arXiv:1911.12800 (2019).

[12] Royer, G.: *An initiation to logarithmic Sobolev inequalities*. AMS (2007).

[13] Ruelle, D.: *Superstable interactions in classical statistical mechanics*, Commun. Math. Phys., **18**(2), 127–159 (1970).

[14] Ruelle, D.: *Statistical mechanics: Rigorous results*. Imperial college Press (1999).

[15] Subbotin, M. T.: *On the law of frequency of error*. Mat. Sb., **31** 296–301 (1923).

2

Trotter product formula on Hilbert and Banach spaces for operator-norm convergence

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Abstract. *We review results on the operator-norm convergence of the Trotter product formula on Hilbert and Banach spaces. We concentrate here on the problem of convergence rates. Some results concerning evolution semigroups are also presented.*

1 Introduction

The product formula for matrices A and B

$$e^{-\tau C} = \lim_{n\to\infty} \left(e^{-\tau A/n} e^{-\tau B/n}\right)^n, \quad \tau \geq 0, \tag{2.1}$$

was established by S. Lie (1875). Here $C \coloneqq A + B$. The proof of formula (2.1) can be easily extended to bounded operators $\mathscr{L}(\mathfrak{H})$ and $\mathscr{L}(\mathfrak{X})$ on Hilbert ($\mathfrak{H}$) and Banach ($\mathfrak{X}$) spaces. Moreover, a straightforward computation shows that the operator norm convergence rate in (2.1) is $O(1/n)$:

$$\sup_{\tau\in[0,T]} \left\| e^{-\tau A/n} e^{-\tau B/n} - e^{-\tau C/n} \right\|_{\mathscr{L}(\cdot)} = O(1/n). \tag{2.2}$$

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H. Trotter [17] has extended this result to unbounded operators A and B on Banach spaces, but now in the (weaker) *strong* operator topology: s-$\lim_{n\to\infty}\mathscr{A}_n=\mathscr{A}\Leftrightarrow\lim_{n\to\infty}\|(\mathscr{A}_n-\mathscr{A})x\|=0$ for any $x\in\mathfrak{X}$. He proved that if A and B are generators of contraction semigroups on a separable Banach space such that the algebraic sum $A+B$ is a densely defined closable operator and the closure $C=\overline{A+B}$ is a generator of a contraction semigroup, then

$$e^{-\tau C}=\text{s-}\lim_{n\to\infty}\left(e^{-\tau A/n}e^{-\tau B/n}\right)^n, \tag{2.3}$$

uniformly in $\tau\in[0,T]$ for any $T>0$. It was a long-time belief that the Trotter formula is valid only in the strong operator topology. But in the *nineties* it was discovered that under certain quite standard assumptions the strong convergence of the product formula (2.3) can be improved to the *operator-norm* convergence: $\lim_{n\to\infty}\|\mathscr{A}_n-\mathscr{A}\|_{\mathscr{L}(\mathfrak{H})}=0\Leftrightarrow\lim_{n\to\infty}\sup_{\{u\in\mathfrak{H}:\|u\|=1\}}\|(\mathscr{A}_n-\mathscr{A})u\|=0$, on a Hilbert space $\mathfrak{H}$.

For the Trotter product formula in the *trace-class ideal* of $\mathscr{L}(\mathfrak{H})$ we refer to [18].

2 Trotter product formula on Hilbert spaces

2.1 Self-adjoint case. Considering the Trotter product formula on a separable Hilbert space $\mathfrak{H}$, T. Kato has shown that for non-negative self-adjoint operators A and B the Trotter formula (2.3) holds in the *strong* operator topology if $\mathrm{dom}(\sqrt{A})\cap\mathrm{dom}(\sqrt{B})$ is dense in the Hilbert space and $C=A\dot{+}B$ is the form-sum of operators A and B. Naturally the problem arises whether Kato's result can be extended to the *operator-norm* convergence. A first attempt in this direction was undertaken by Dzh. Rogava [16]. He claimed that if A and B are non-negative self-adjoint operators such that $\mathrm{dom}(A)\subseteq\mathrm{dom}(B)$ and the operator-sum: $C=A+B$, is *self-adjoint*, then

$$\left\|(e^{-\tau A/n}e^{-\tau B/n})^n-e^{-\tau C}\right\|_{\mathscr{L}(\mathfrak{H})}=O(\ln(n)/\sqrt{n}),\qquad n\to\infty, \tag{2.4}$$

holds. In [12] it was shown that if one substitutes in above conditions the self-adjointness of the operator-sum by the A-smallness of B with a relative bound less then *one*, then (2.4) is true with the rate of convergence improved to

$$\left\|(e^{-\tau A/n}e^{-\tau B/n})^n-e^{-\tau C}\right\|_{\mathscr{L}(\mathfrak{H})}=O(\ln(n)/n),\qquad n\to\infty. \tag{2.5}$$

The problem in its original formulation was finally solved in [7]. There it was shown that the best possible in this general setup rate (2.2) holds if the operator sum: $C = A + B$, is already a self-adjoint operator. Rogava's result, as well as many other results (including [12]), when the operator sum of generators is self-adjoint, are corollary of [7]. A new direction comes due to results for the fractional-power conditions. In [14], with elucidation in [6], it was proven that assuming: $\mathrm{dom}(C^\alpha) \subseteq \mathrm{dom}(A^\alpha) \cap \mathrm{dom}(B^\alpha)$, $\alpha \in (1/2, 1)$, $C = A \dot{+} B$ and $\mathrm{dom}(A^{1/2}) \subseteq \mathrm{dom}(B^{1/2})$ one obtains that

$$\sup_{\tau\in[0,T]} \left\| (e^{-\tau A/n} e^{-\tau B/n})^n - e^{-\tau C} \right\|_{\mathscr{L}(\mathfrak{H})} = O(n^{-(2\alpha-1)}).$$

Notice that formally $\alpha = 1$ yields the rate obtained in [7]. We remark also that the results of [6, 14] do *not* cover the case $\alpha = 1/2$. Although, it turns out that in this case the Trotter product formula converges on the operator norm:

$$\sup_{\tau\in[0,T]} \left\| (e^{-\tau A/n} e^{-\tau B/n})^n - e^{-\tau C} \right\|_{\mathscr{L}(\mathfrak{H})} = o(1),$$

if $\sqrt{B}$ is *relatively compact* with respect to $\sqrt{A}$, i.e. $\sqrt{B}(I + A)^{-1/2}$ is compact, see [13].

2.2 Non-self-adjoint case. Another direction was related with extension of the Trotter, and the Trotter-Kato, product formulae to the case of accretive [1, 2] and non-self-adjoint *sectorial* generators [4, 5]. Let A be a non-negative self-adjoint operator and let B be a maximal *accretive* ($\mathrm{Re}(Bf, f) \geq 0$ for $f \in \mathrm{dom}(B)$) operator, such that

$$\mathrm{dom}(A) \subseteq \mathrm{dom}(B) \quad \text{and} \quad \mathrm{dom}(A) \subseteq \mathrm{dom}(B^*).$$

If B is A-small with a relative bound less than one, then estimate (2.5) holds for generator C which is a well-defined maximal accretive operator-sum: $C = A + B$, see [1].

In [2] this result was generalised as follows. Let A be a non-negative self-adjoint operator and let B be a maximal accretive operator such that $\mathrm{dom}(A) \subseteq \mathrm{dom}(B)$ and B is A-small with relative bound less than one. If the condition

$$\mathrm{dom}\big((C^*)^\alpha\big) \subseteq \mathrm{dom}(A^\alpha) \cap \mathrm{dom}\big((B^*)^\alpha\big), \qquad C = A + B,$$

is satisfied for some $\alpha \in (0,1]$, then the norm-convergent Trotter product formula:

$$\sup_{\tau\in[0,T]} \left\| (e^{-\tau A/n} e^{-\tau B/n})^n - e^{-\tau C} \right\|_{\mathscr{L}(\mathfrak{H})} = O(\ln(n)/n^{\alpha}) \ ,$$

holds as $n \to \infty$. In fact, more results are known about the operator-norm Trotter product formula convergence for non-self-adjoint semigroups with sectorial generators, but *without* the rate estimates, see [3]. A new approach to analysis of the non-self-adjoint case was developed in [5]. Since it is based on holomorphic properties of semigroups, one can apply it even in Banach spaces. Therefore we postpone its presentation to Section 3.

3 Trotter product formula on Banach spaces

3.1 Holomorphic case. There are only few generalisations of the results of Section 2 to Banach spaces. The main obstacle for that is the fact that the concept of self-adjointness is missing. One of solutions is to relax the self-adjointness replacing the non-negative self-adjoint generator A by a generator of the holomorphic semigroup. The following result was proved in [5].

Theorem 2.1 ([5, Theorem 3.6 and Corollary 3.7]) Let A be a generator of a holomorphic contraction semigroup on the separable Banach space $\mathfrak{X}$ and let B be generator of a contraction semigroup on $\mathfrak{X}$.

i) If for some $\alpha \in (0,1)$ the condition $\mathrm{dom}(A^{\alpha}) \subseteq \mathrm{dom}(B)$, holds and $\mathrm{dom}(A^*) \subseteq \mathrm{dom}(B^*)$ is satisfied, then the operator sum $C = A + B$ is generator of a contraction semigroup and for any $T > 0$:

$$\sup_{\tau\in[0,T]} \left\| (e^{-\tau B/n} e^{-\tau A/n})^n - e^{-\tau C} \right\|_{\mathscr{L}(\mathfrak{X})} = O\big(\ln(n)/n^{1-\alpha}\big). \tag{2.6}$$

ii) If for some $\alpha \in (0,1)$ the condition $\mathrm{dom}((A^{\alpha})^*) \subseteq \mathrm{dom}(B^*)$ is satisfied and $\mathrm{dom}(A) \subseteq \mathrm{dom}(B)$ is valid, then $C = A + B$ is generator of a contraction semigroup and

$$\sup_{\tau\in[0,T]} \left\| (e^{-\tau A/n} e^{-\tau B/n})^n - e^{-\tau C} \right\|_{\mathscr{L}(\mathfrak{X})} = O\big(\ln(n)/n^{1-\alpha}\big), \tag{2.7}$$

for any $T > 0$.

Theorem 2.2 ([5, Theorem 3.6 and Corollary 3.7]) Let A be generator of a holomorphic contraction semigroup on $\mathfrak{X}$ and let B be generator of a contraction semigroup on $\mathfrak{X}$. If B is in addition a *bounded* operator, then for any $T > 0$:

$$\sup_{\tau\in[0,T]} \left\|(e^{-\tau B/n}e^{-\tau A/n})^n - e^{-\tau C}\right\|_{\mathscr{L}(\mathfrak{X})} = O\big((\ln(n))^2/n\big),$$
$$\sup_{\tau\in[0,T]} \left\|(e^{-\tau A/n}e^{-\tau B/n})^n - e^{-\tau C}\right\|_{\mathscr{L}(\mathfrak{X})} = O\big((\ln(n))^2/n\big).$$

Theorem 2.2 becomes *false* if the condition that A is generator of a holomorphic semigroup is *dropped*.

3.2 Non-holomorphic: evolution semigroup. Let A and operators $\{B(t)\}_{t\in[0,T]}$ be generators of holomorphic semigroups on a separable Banach space $\mathfrak{X}$. Consider non-autonomous Cauchy problem for $u_0 := u(0)$:

$$\partial_t u(t) = -\big(A + B(t)\big)u(t), \qquad t \in [0,T], \tag{2.8}$$

Assumptions:

(A1) Operator $A \geq I$ is generator of a holomorphic contraction semigroup in $\mathfrak{X}$.

(A2) Let $\{B(t)\}_{t\in[0,T]}$ be a family of closed operators such that for a.e. $t \in [0,T]$ and some $\alpha \in (0,1)$ the condition $\mathrm{dom}(A^\alpha) \subset \mathrm{dom}(B(t))$ is satisfied such that

$$C_\alpha := \operatorname*{ess\,sup}_{t\in[0,T]} \left\|B(t)A^{-\alpha}\right\|_{\mathscr{L}(\mathfrak{X})} < \infty\,.$$

(A3) Let $\{B(t)\}_{t\in[0,T]}$ be a family of generators of contraction semigroups in $\mathfrak{X}$ such that the function $[0,T] \ni t \mapsto \big(B(t) + \xi I\big)^{-1} x \in \mathfrak{X}$ is strongly measurable for any $x \in \mathfrak{X}$ and any $\xi > b$ for some $b > 0$.

(A4) We assume that $\mathrm{dom}(A^*) \subset \mathrm{dom}(B(t)^*)$ and

$$C_1^* := \operatorname*{ess\,sup}_{t\in[0,T]} \left\|B(t)^*(A^*)^{-1}\right\|_{\mathscr{L}(\mathfrak{X}^*)} < \infty,$$

where A^* and $B(t)^*$ denote operators which are adjoint of A and $B(t)$, respectively.

(A5) There exists $\beta \in (\alpha, 1)$ and a constant $L_\beta > 0$ such that for a.e. $t, s \in [0,T]$ one has the estimate:

$$\left\|A^{-1}\big(B(t) - B(s)\big)A^{-\alpha}\right\|_{\mathscr{L}(\mathfrak{X})} \leq L_\beta |t-s|^\beta.$$

(A6) There exists a constant $L_1 > 0$ such that for a.e. $t,s \in [0,T]$ one has the estimate:

$$\left\|A^{-\alpha}\big(B(t)-B(s)\big)A^{-\alpha}\right\|_{\mathscr{L}(\mathfrak{X})} \leq L_1|t-s|.$$

The evolution equation (2.8) is associated with family $\{C(t)\}_{t\in[0,T]}$, $C(t) = A + B(t)$.

We consider the Banach space $L^p([0,T],\mathfrak{X})$ for $p \in [1,\infty)$ and introduce in this space the *multiplication* operators $\mathscr{A}$ and $\mathscr{B}$ generated by A and $\{B(t)\}_{t\in[0,T]}$, see [8, 15]. Similarly, one can introduce the multiplication operator $\mathscr{C}$ induced by the family $\{C(t)\}_{t\in[0,T]}$ which is also a generator of a holomorphic semigroup. Notice that $\mathscr{C} = \mathscr{A} + \mathscr{B}$ and $\mathrm{dom}(\mathscr{C}) = \mathrm{dom}(\mathscr{A})$. Let D_0 the generator of the right-shift *nilpotent* semigroup on $L^p([0,T],\mathfrak{X})$, i.e. $\big(e^{-\tau D_0}f\big)(t) = \chi_{[0,T]}(t-\tau)f(t-\tau), \quad f \in L^p([0,T],\mathfrak{X})$.

Next, we consider the operator

$$\begin{aligned} \widetilde{\mathscr{K}}f &= D_0 f + \mathscr{A}f + \mathscr{B}f, \\ f \in \mathrm{dom}(\widetilde{\mathscr{K}}) &= \mathrm{dom}(D_0) \cap \mathrm{dom}(\mathscr{A}) \cap \mathrm{dom}(\mathscr{B}). \end{aligned} \tag{2.9}$$

Assuming (A1)–(A3) it was shown in [11] that the operator $\widetilde{\mathscr{K}}$ is closable and its closure $\mathscr{K}$ is generator of the *evolution semigroup* $\{e^{-\tau\mathscr{K}}\}_{\tau\geq 0}$ [8, 15], which is also nilpotent and consequently a *non-holomorphic* semigroup. Further we set $\widetilde{\mathscr{K}_0}f = D_0 f + \mathscr{A}f$ for $f \in \mathrm{dom}(\widetilde{\mathscr{K}_0}) = \mathrm{dom}(D_0) \cap \mathrm{dom}(\mathscr{A})$.

In contrast to the Hilbert space the operator $\widetilde{\mathscr{K}_0}$ is not necessary generator of a semigroup. However, the operator $\widetilde{\mathscr{K}_0}$ is closable and its closure $\mathscr{K}_0$ is a generator. Note that $\mathscr{K}$ coincides with the algebraic sum: $\mathscr{K} = \mathscr{K}_0 + \mathscr{B}$.

Theorem 2.3 ([11, Theorem 7.8]) Let the Assumptions (A1)–(A4) be satisfied for some $\alpha \in (0,1)$. If (A5) holds, then one gets for $n \to \infty$ the asymptotic:

$$\sup_{\tau\in[0,T]} \left\| \big(e^{-\tau B/n}e^{-\tau\mathscr{K}_0/n}\big)^n - e^{-\tau\mathscr{K}} \right\|_{\mathscr{L}(L^p([0,T],\mathfrak{X}))} = O\big(1/n^{\beta-\alpha}\big). \tag{2.10}$$

Assuming instead of Assumption (A5) the Assumption (A6) one finds

Theorem 2.4 ([9, Theorem 5.4]) Let the Assumptions (A1)–(A4) be satisfied for some $\alpha \in (1/2,1)$. If (A6) is valid, then for $n \to \infty$ one gets the asymptotic:

$$\sup_{\tau\in[0,T]} \left\| \big(e^{-\tau B/n}e^{-\tau\mathscr{K}_0/n}\big)^n - e^{-\tau\mathscr{K}} \right\|_{\mathscr{L}(L^p([0,T],\mathfrak{X}))} = O\big(1/n^{1-\alpha}\big). \tag{2.11}$$

3.3 Convergence rate for propagators. To construct approximations of solution operators (*propagators*) for the Cauchy problem (2.8), we apply to the problem (2.8) the *evolution semigroup* approach developed in [8, 15, 11]. The idea is to transform the *non-autonomous* Cauchy problem (2.8) into an *autonomous* problem generated by evolution semigroup $\{e^{-\tau\mathscr{K}}\}_{\tau\geq 0}$.

Definition 2.5 ([8, 15]) Linear operator $\mathscr{K}$ in $L^p([0,T],\mathfrak{X})$, $p\in[1,\infty)$, is called *evolution generator* if for multiplication operator $M(\phi)$:

(i) $\mathrm{dom}(\mathscr{K})\subset C([0,T],\mathfrak{X})$ and $M(\phi)\mathrm{dom}(\mathscr{K})\subset\mathrm{dom}(\mathscr{K})$ for $\phi\in W^{1,\infty}([0,T])$;

(ii) $\mathscr{K}M(\phi)f-M(\phi)\mathscr{K}f=M(\partial_t\phi)f$ for $f\in\mathrm{dom}(\mathscr{K})$ and $\phi\in W^{1,\infty}([0,T])$;

(iii) the domain $\mathrm{dom}(\mathscr{K})$ has a dense cross-section, i.e. for each $t\in(0,T]$ the set

$$[\mathrm{dom}(\mathscr{K})]_t := \{x\in\mathfrak{X} : \exists f\in\mathrm{dom}(\mathscr{K}) \text{ such that } x\in f(t)\},$$

is dense in $\mathfrak{X}$. Here for any $\phi\in L^\infty([0,T])$ we denote by $M(\phi)$ a bounded multiplication operator on $L^p([0,T],\mathfrak{X})$ defined as $\big(M(\phi)f\big)(t)=\phi(t)f(t)$, $f\in L^p([0,T],\mathfrak{X})$.

One can check that the operator $\mathscr{K}$ defined as the closure of $\widetilde{\mathscr{K}}$ (2.9) is an evolution generator, cf. [11, Theorem 1.2]. Evolution generators are related to *propagators*, which are defined as follows.

Definition 2.6 Let $\{U(t,s)\}_{(t,s)\in\Delta}$, $\Delta=\{(t,s)\in(0,T]\times(0,T] : s\leq t\leq T\}$, be a strongly continuous family of bounded operators on $\mathfrak{X}$. If the conditions

$$U(t,t)=I \qquad \text{for } t\in(0,T], \tag{2.12}$$

$$U(t,r)U(r,s)=U(t,s) \qquad \text{for } t,r,s\in(0,T] \text{ with } s\leq r\leq t, \tag{2.13}$$

$$\|U\|_\Delta := \sup_{(t,s)\in\Delta}\|U(t,s)\|_{\mathscr{L}(\mathfrak{X})}<\infty \tag{2.14}$$

are satisfied. If $u(t)=U(t,0)u_0$, $t\geq 0$, for $u_0\in\mathrm{dom}(A)$, is solution of the Cauchy problem (2.8), then $\{U(t,s)\}_{(t,s)\in\Delta}$ is called *solution operator*, or *propagator*.

It is known [8, Theorem 4.12] that there is an *one-to-one* correspondence between the set of all evolution generators on $L^p([0,T],\mathfrak{X})$ and the set of all propagators in the sense of Definition 2.6. It is established by equation

$$\big(e^{-\tau\mathscr{K}}f\big)(t)=U(t,t-\tau)\chi_{[0,T]}(t-\tau)f(t-\tau), \qquad f\in L^p([0,T],\mathfrak{X}). \tag{2.15}$$

Let $\mathscr{K}_0$ be generator of evolution semigroup $\{\mathscr{U}_0(\tau)\}_{\tau\geq 0}$ and let $\mathscr{B}$ be multiplication operator induced by a measurable family $\{B(t)\}_{t\in[0,T]}$ of generators of contraction semigroups. Note that in this case the multiplication operator $\mathscr{B}$ is a generator of a contraction semigroup $\left(e^{-\tau\mathscr{B}}f\right)(t) = e^{-\tau B(t)}f(t)$, on the Banach space $L^p([0,T],\mathfrak{X})$. Since $\{\mathscr{U}_0(\tau)\}_{\tau\geq 0}$ is the evolution semigroup, then by (2.15) there exists propagator $\{U_0(t,s)\}_{(t,s)\in\Delta}$ such that the representation: $\left(\mathscr{U}_0(\tau)f\right)(t) = U_0(t,t-\tau)\chi_{[0,T]}(t-\tau)f(t-\tau)$, $f\in L^p([0,T],\mathfrak{X})$, is valid for a. e. $t\in[0,T]$ and $\tau\geq 0$. Then we define

$$Q_j(t,s;n) := U_0\left(s+j\tfrac{(t-s)}{n}, s+(j-1)\tfrac{(t-s)}{n}\right)e^{-\frac{(t-s)}{n}B\left(s+(j-1)\frac{(t-s)}{n}\right)}$$

where $j\in\{1,2,\ldots,n\}$, $n\in\mathbb{N}$, $(t,s)\in\Delta$, and we set for *approximants* $\{V_n(t,s)\}_{n\geq 1}$:

$$V_n(t,s) := \prod_{j=1}^{n\leftarrow} Q_j(t,s;n), \qquad n\in\mathbb{N},\ (t,s)\in\Delta,$$

where the product is increasingly ordered in j from the right to the left. Then by (2.15) a straightforward computation shows that the representation

$$\left(\left(e^{-\tau\mathscr{K}_0/n}e^{-\tau\mathscr{B}/n}\right)^n f\right)(t) = V_n(t,t-\tau)\chi_{[0,T]}(t-\tau)f(t-\tau)\ ,$$

$f\in L^p([0,T],\mathfrak{X})$, holds for each $\tau\geq 0$ and a.e. $t\in[0,T]$.

Similarly we can introduce

$$G_j(t,s;n) = e^{-\frac{t-s}{n}B\left(s+j\frac{t-s}{n}\right)}U_0\left(s+j\tfrac{t-s}{n}, s+(j-1)\tfrac{t-s}{n}\right)$$

where $j\in\{1,2,\ldots,n\}$, $n\in\mathbb{N}$, $(t,s)\in\Delta$. Now let the *approximants* be defined by

$$U_n(t,s) := \prod_{j=1}^{n\leftarrow} G_j(t,s;n), \qquad n\in\mathbb{N},\ (t,s)\in\Delta,$$

where the product is again increasingly ordered in j from the right to the left. Note that

$$\left(\left(e^{-\tau\mathscr{B}/n}e^{-\tau\mathscr{K}_0/n}\right)^n f\right)(t) = U_n(t,t-\tau)\chi_{[0,T]}(t-\tau)f(t-\tau)\ ,$$

$f\in L^p([0,T],\mathfrak{X})$, holds for each $\tau\geq 0$ and a.e. $t\in[0,T]$.

Proposition 2.7 ([10, Proposition 2.1]) Let $\mathscr{K}$ and $\mathscr{K}_0$ be generators of evolution semigroups on the Banach space $L^p([0,T],\mathfrak{X})$ for some $p\in[1,\infty)$. Further, let $\{B(t)\}_{t\in[0,T]}$ be a strongly measurable family of generators of contraction on $\mathfrak{X}$. Then for $n\in\mathbb{N}$,

$$\sup_{\tau\in[0,T]}\left\|e^{-\tau\mathscr{K}}-\left(e^{-\tau\mathscr{K}_0/n}e^{-\tau\mathscr{B}/n}\right)^n\right\|_{\mathscr{L}(L^p([0,T],\mathfrak{X}))}=\operatorname*{ess\,sup}_{(t,s)\in\Delta}\|U(t,s)-V_n(t,s)\|_{\mathscr{L}(\mathfrak{X})},$$
$$\sup_{\tau\in[0,T]}\left\|e^{-\tau\mathscr{K}}-\left(e^{-\tau\mathscr{B}/n}e^{-\tau\mathscr{K}_0/n}\right)^n\right\|_{\mathscr{L}(L^p([0,T],\mathfrak{X}))}=\operatorname*{ess\,sup}_{(t,s)\in\Delta}\|U(t,s)-U_n(t,s)\|_{\mathscr{L}(\mathfrak{X})}.$$

From Theorem 2.3 and Proposition 2.7 one obtains the following assertion.

Theorem 2.8 ([11, Theorem 1.4]) Let the Assumptions (A1)–(A4) be satisfied. If (A5) holds, then for $n\to\infty$ one gets the rate:

$$\operatorname*{ess\,sup}_{(t,s)\in\Delta}\|U_n(t,s)-U(t,s)\|_{\mathscr{L}(\mathfrak{X})}=O\big(1/n^{\beta-\alpha}\big). \tag{2.16}$$

On the other hand, from Theorem 2.4 and Proposition 2.7 we get

Theorem 2.9 ([9, Theorem 5.6]) Let the Assumptions (A1)–(A4) be satisfied for some $\alpha\in(1/2,1)$. If (A6) is valid, then for $n\to\infty$ one obtains a better rate:

$$\operatorname*{ess\,sup}_{(t,s)\in\Delta}\|U_n(t,s)-U(t,s)\|_{\mathscr{L}(\mathfrak{X})}=O\big(1/n^{1-\alpha}\big).$$

4 Example of sharpness

We study bounded perturbations of the evolution generator D_0. To this aim we consider $\mathfrak{X}=\mathbb{C}$ and we denote by $L^2([0,1])$ the Hilbert space $L^2([0,1],\mathbb{C})$.

For $t\in[0,1]$, let $q:t\mapsto q(t)\in L^\infty([0,1])$. Then q induces on the Banach space $L^2([0,1])$ a bounded multiplication operator Q defined as

$$\big(Qf\big)(t):=q(t)f(t),\qquad f\in L^2([0,1]).$$

For simplicity we assume that $q\geq 0$. Then Q generates on $L^2([0,1])$ a contraction semigroup $\{e^{-\tau Q}\}_{\tau\geq 0}$. Since generator Q is bounded, the closed operator $\mathscr{K}:=D_0+Q$, with domain $\operatorname{dom}(\mathscr{K})=\operatorname{dom}(D_0)$, is generator of a semigroup on $L^2([0,1])$. By [17] we get

$$\operatorname*{s-lim}_{n\to\infty}\left(e^{-\tau D_0/n}e^{-\tau Q/n}\right)^n=e^{-\tau(D_0+Q)}.$$

One can easily check that $\mathscr{K}$ is an evolution generator. A straightforward computation shows that

$$\left(e^{-\tau(D_0+Q)}f\right)(t) = e^{-\int_{t-\tau}^{t} q(y)dy}\chi_{[0,1]}(t-\tau)f(t-\tau).$$

This yields that the propagator corresponding to $\mathscr{K}$ is given by

$$U(t,s) = e^{-\int_s^t q(y)dy}, \qquad (t,s)\in\Delta.$$

Now a simple computation shows that

$$\left(\left(e^{-\tau D_0/n}e^{-\tau Q/n}\right)^n f\right)(t) =: V_n(t,t-\tau)\chi_{[0,T]}(t-\tau)f(t-\tau).$$

Then by straightforward calculations we find that

$$V_n(t,s) = e^{-\frac{t-s}{n}\Sigma_{k=0}^{n-1} q(s+k\frac{t-s}{n})}, \qquad (t,s)\in\Delta.$$

Theorem 2.10 ([10, Proposition 3.1]) Let $q\in L^\infty([0,1])$ be non-negative. Then

$$\sup_{\tau\in[0,1]}\left\|e^{-\tau(D_0+Q)} - \left(e^{-\tau D_0/n}e^{-\tau Q/n}\right)^n\right\|_{\mathscr{L}(L^2([0,1]))} \leq O\left(\operatorname*{ess\,sup}_{(t,s)\in\Delta}\left|\int_s^t q(y)dy - \frac{t-s}{n}\sum_{k=0}^{n-1} q(s+k\tfrac{t-s}{n})\right|\right),$$

as $n\to\infty$.

Note that by Theorem 2.10 the operator-norm convergence rate of the Trotter product formula for the pair $\{D_0,Q\}$ coincides with the convergence rate of the integral Darboux-Riemann sum approximation of the Lebesgue integral.

Theorem 2.11 ([10, Theorem 3.2]) If the function: $q\in C^{0,\beta}([0,1])$, $\beta\in(0,1]$, is non-negative, then for $n\to\infty$ one gets

$$\sup_{\tau\in[0,1]}\left\|e^{-\tau(D_0+Q)} - \left(e^{-\tau D_0/n}e^{-\tau Q/n}\right)^n\right\|_{\mathscr{L}(L^2([0,1]))} = O\big(1/n^\beta\big).$$

Theorem 2.12 ([10, Theorem 3.3]) If $q\in C([0,1])$ is continuous and non-negative, then for $n\to\infty$

$$\left\|e^{-\tau(D_0+Q)} - \left(e^{-\tau D_0/n}e^{-\tau Q/n}\right)^n\right\|_{\mathscr{L}(L^2([0,1]))} = o(1)\ . \tag{2.17}$$

It follows that the convergence to zero in (2.17) may be *arbitrarily* slow.

Theorem 2.13 ([10, Theorem 3.4]) Let $\delta_n > 0$ be a sequence with $\delta_n \to 0$ as $n \to \infty$. Then there exists a continuous function $q : [0,1] \to \mathbb{R}$ such that

$$\sup_{\tau\in[0,1]} \left\| e^{-\tau(D_0+Q)} - \left(e^{-\tau D_0/n} e^{-\tau Q/n}\right)^n \right\|_{\mathscr{L}(L^2([0,1]))} = \omega(\delta_n) \,, \tag{2.18}$$

as $n \to \infty$. Here ω is the Landau symbol: $\omega(\delta_n) \Leftrightarrow \limsup_{n\to\infty} |\omega(\delta_n)/\delta_n| = \infty$.

If q is only *measurable*, it can happen that the Trotter product formula for that pair $\{D_0, Q\}$ does *not* converge in the *operator-norm* topology:

Theorem 2.14 ([10, Theorem 3.5]) There is a non-negative measurable function $q \in L^\infty([0,1])$, such that

$$\liminf_{n\to\infty} \sup_{\tau\in[0,1]} \left\| e^{-\tau(D_0+Q)} - \left(e^{-\tau D_0/n} e^{-\tau Q/n}\right)^n \right\|_{\mathscr{L}(L^2([0,1]))} > 0. \tag{2.19}$$

Theorem 2.14 does not exclude the convergence in the *strong* operator topology.

Bibliography

[1] Cachia V., Neidhardt H., Zagrebnov, V. A.: *Accretive perturbations and error estimates for the Trotter product formula*, Integr. Equ. Oper. Theory **39**(4), 396–412 (2001).

[2] Cachia V., Neidhardt H., Zagrebnov, V. A.: *Comments on the Trotter product formula error-bound estimates for nonself-adjoint semigroups*, Integr. Equ. Oper. Theory **42**(4), 425–448 (2002).

[3] Cachia V., Zagrebnov, V. A.: *Operator-norm convergence of the Trotter product formula for sectorial generators*, Lett. Math. Phys. **50**, 203–211 (1999).

[4] Cachia V., Zagrebnov, V. A.: *Operator-norm approximation of semigroups by quasi-sectorial contractions*, J. Funct. Anal. **180**(1), 176–194 (2001).

[5] Cachia V., Zagrebnov, V. A.: *Operator-norm convergence of the Trotter product formula for holomorphic semigroups*, J. Operat. Theor. **46**(1), 199–213 (2001).

[6] Ichinose, T., Neidhardt, H., Zagrebnov, V. A.: *Trotter-Kato product formula and fractional powers of self-adjoint generators*, J. Funct. Anal. **207**(1), 33–57 (2004).

[7] Ichinose, T., Tamura Hideo, Tamura Hiroshi, Zagrebnov V. A.: *Note on the paper: "The norm convergence of the Trotter-Kato product formula with error bound" by T. Ichinose and H. Tamura*, Commun. Math. Phys. **221**(3), 499–510 (2001).

[8] Neidhardt, H.: *On abstract linear evolution equations. I*, Math. Nachr. **103**, 283–298 (1981).

[9] Neidhardt, H., Stephan, A., Zagrebnov, V. A.: *On convergence rate estimates for approximations of solution operators for linear non-autonomous evolution equations*, Nanosyst. Phys. Chem. Math. **8**(2), 202–215 (2017).

[10] Neidhardt, H., Stephan, A., Zagrebnov, V. A.: *Remarks on the operator-norm convergence of the Trotter product formula*, Integr. Equ. Oper. Theory **90:15**, 1–14 (2018).

[11] Neidhardt, H., Stephan, A., Zagrebnov, V. A.: *Convergence rate estimates for Trotter product approximations of solution operators for non-autonomous Cauchy problems*, Publ. RIMS Kyoto Univ. **56**, 1–53 (2020).

[12] Neidhardt, H., Zagrebnov, V. A.: *On error estimates for the Trotter-Kato product formula*, Lett. Math. Phys. **44**(3), 169–186 (1998).

[13] Neidhardt, H., Zagrebnov, V. A.: *Trotter-Kato product formula and operator-norm convergence*, Commun. Math. Phys. **205**(1), 129–159 (1999).

[14] Neidhardt, H., Zagrebnov, V. A.: *Fractional powers of self-adjoint operators and Trotter-Kato product formula*, Integr. Equ. Oper. Theory **35**(2), 209–231 (1999).

[15] Neidhardt, H., Zagrebnov, V. A.: *Linear non-autonomous Cauchy problems and evolution semigroups*, Adv. Differ. Equ. **14**(3-4), 289–340 (2009).

[16] Rogava, Dzh. L.: *Error bounds for Trotter-type formulas for self-adjoint operators*, Funct. Anal. Appl. **27**, 217–219 (1993).

[17] Trotter, H. F.: *On the product of semi-groups of operators*, Proc. Amer. Math. Soc. **10**, 545–551 (1959).

[18] Zagrebnov, V. A.: *Gibbs Semigroups*, Operator Theory Series: Advances and Applications, Vol. 273, Birkhäuser Basel (2019).

3

Semi-recursive algorithm of piecewise linear approximation of two-dimensional function by the method of worst segment dividing

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1 Introduction

In the numerical solution of two-dimensional non-linear boundary value problems of mathematical physics, the finite element method is often used. This method assumes that the domain of the boundary problem is divided into small sub-domains (elements) within which the desired function is assumed to be linear. Thus, the desired function is approximated by a piecewise linear function. Its graph consists of triangles, the projections of which on the OXY plane form a triangular mesh.

In recent years, meshes with variable number of nodes are often used, i.e. the process of successive approximations extends not only to the approximated function, but also to the corresponding grid. At the same time, additional nodes are sequentially added in the worst (in the sense of approximation error) sub-domains. Thus, the mesh is successively improved and the approximation error is minimised.

In [6], an algorithm for an automatic construction of piecewise linear approximations of one-dimensional continuous functions was proposed. The algorithm minimised the approximation error for a given number of lattice points and was based on the principle

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of the worst segment dividing. In [2], the one-dimensional algorithm proposed in [6] was generalised for the two-dimensional case.

For practical reasons, recursive algorithms of mesh generation are preferable. In applications they are very convenient because they are easily programmed using cycle operators. However, the algorithm proposed in [2] was not recursive.

Recursive algorithms. An algorithm is called *recursive*, if each subsequent step does not lead to changes in the parameters obtained in the past. In the case of the construction of meshes with variable number of nodes, the algorithm will be recursive if the addition of each new node leaves the old nodes and old edges (the connections between nodes) in place.

Any one-dimensional uniform lattice cannot be constructed using a recursive algorithm, since when you add a new node, all old lattice nodes are shifted. The algorithm for automatically constructing a one-dimensional piecewise linear approximation with a non-uniform lattice, proposed in [6], is recursive.

In the present paper, a recursive algorithm is proposed for the automated construction of piecewise linear approximations of a two-dimensional continuous function by dividing the worst segment. An improved (but not recursive) algorithm for the automated construction of a two-dimensional piecewise linear approximation by dividing the worst segment was also studied. The improved algorithm can be called semi-recursive, since the addition of each new node leaves in place all the old nodes and almost all edges.

We have constructed a semi-recursive algorithm for constructing a piecewise linear approximation of a two-dimensional function by dividing the worst segment. When adding a new vertex, all previous vertices and almost all edges remain in their places. The edge may change if the "flip" operation is applicable to it: replacing a longer diagonal with a shorter one in a tetragon.

2 Delaunay triangulation

Let $M_n = \{P_i\}_{i=1}^n$ be a finite set of points in the plane. The interior of a domain D we denote by $\operatorname{int} D$. A set $\{D_j\}_{j=1}^m$ of triangles is called *triangle mesh* or *triangle tessellation* with knots M_n, if the following conditions are fulfilled:

1. The interiors of triangles are pairwise disjoint:

$$\operatorname{int} D_j \cap \operatorname{int} D_k = \emptyset, \quad j \neq k.$$

2. The set of all vertices of triangles is the set $\{P_i\}_{i=1}^n$.

3. The union of triangles fills the whole of convex hull of the knots:

$$\bigcup_{j=1}^{m} D_j = \operatorname{conv}\{P_i\}_{i=1}^n.$$

A triangle mesh $\{D_j\}_{j=1}^m$ is called *Delaunay triangulation* with knots $M_n = \{P_i\}_{i=1}^n$, if the following condition is fulfilled (see [1]):

4. For any triangle D_j

$$\operatorname{int} K(D_j) \cap \{P_i\}_{i=1}^n = \emptyset, \quad j = 1, \ldots, m,$$

where $K(D)$ is the circumscribing circle of triangle D.

The Delaunay triangulation with the system of knots M_n we denote by $\mathscr{D}(M_n)$. In [1] it was proved that for any finite set of points M_n there exists a Delaunay triangulation $\mathscr{D}(M_n)$ (not necessarily unique).

3 The method of dividing the worst segment

Let $F(x,y)$ be a two-dimensional continuous function on the plane, the domain of definition of which is the rectangle $[a,b] \times [c,d]$. Our goal is to construct a recursive algorithm for the automated construction of a piecewise linear approximation to the function $F(x,y)$.

First, consider the following recursive algorithm for constructing a sequence of knots $M_n = \{P_1, P_2, \ldots, P_n\}$ and the corresponding mesh S_n. On the rectangle $[a,b] \times [c,d]$, consider the primary set of knots M_4, consisting of 4 vertices: $P_1 = (a,c)$, $P_2 = (b,c)$, $P_3 = (b,d)$, $P_4 = (a,d)$ and the primary mesh S_4 consisting of two triangles $\Delta P_1 P_2 P_3$ and $\Delta P_1 P_3 P_4$ (see Figure 3.1).

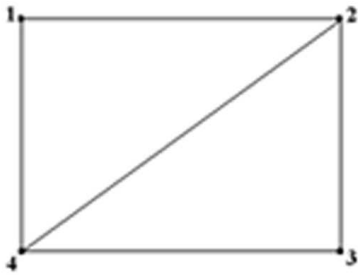

Figure 3.1: The primary mesh S_4.

Note that the mesh S_4 is a Delaunay triangulation with four knots $P_1,\dots,P_4$, i.e. $S_4 = \mathscr{D}(M_4)$. Suppose that the set of nodes $M_{n-1} = \{P_1, P_2, \dots, P_{n-1}\}$ and the corresponding triangle mesh S_{n-1} have already been built. Construct the next point P_n as follows.

Two knots P_i and P_j are called neighbouring and denoted by $P_i \sim P_j$, if they are the endpoints of a side of some triangle of the mesh. Note that in the primary mesh S_4, all pairs of nodes are neighbouring, except for the pair P_2 and P_4.

The pairs of neighbouring knots we call *the edges* of the mesh. Denote by $R(S_{n-1})$ the set of edges of S_{n-1}, i.e.

$$R(S_{n-1}) = \{(P_i, P_j) : \ P_i \sim P_j\}.$$

For any edge $e = (P_i, P_j)$ from $R(S_{n-1})$ with vertices P_i and P_j we calculate the difference $|z_i - z_j|$, where $z_i = F(x_i, y_i)$ is the value of our function F at the point P_i, and (x_i, y_i) are Cartesian coordinates of vertex P_i.

The edge $e = (P_i, P_j) \in R(S_{n-1})$ we call *the worst edge*, if it gives the maximum value of differences $|z_i - z_j|$. In the middle of this edge we add a new node, this is the desired node P_n.

We determine what new edges will appear at the mesh S_n when adding a new vertex P_n. Denote by $\mathrm{conv}(M_n)$ the convex hull of the points $M_n = \{P_1, P_2, \dots, P_n\}$. Two cases are possible:

1) the new vertex P_n belongs to the interior of the hull $\mathrm{conv}(M_n)$. In this case we call P_n an internal knot, and the corresponding worst edge is called diagonal. In this case, when adding a new vertex, two new edges appear (see Figure 3.2);

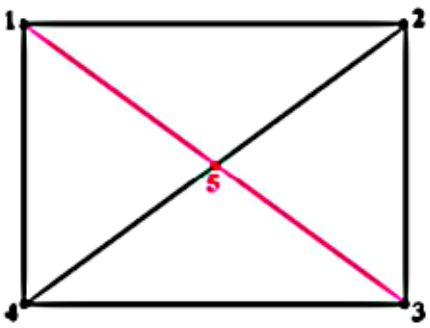

Figure 3.2: The case of an internal knot, the worst edge is P_2P_4.

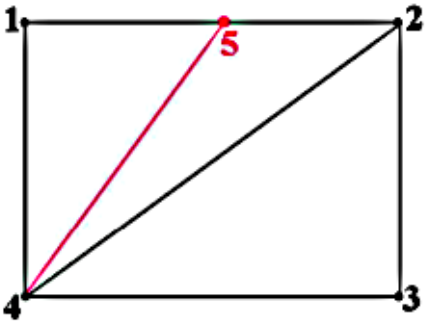

Figure 3.3: The case of a boundary knot, the worst edge is P_1P_2.

2) the new vertex P_n lies on the boundary of the hull $\mathrm{conv}(M_n)$. In this case we call P_n a boundary knot, and the corresponding worst segment is called a boundary edge. In this case, when adding a new vertex, one new edge appears (see Figure 3.3).

We will continue to add knots by dividing in half the worst edge P_i, P_j corresponding to the largest of the values of the differences $|z_i - z_j|$ until the number of knots reaches a given value n. Note that the resulting mesh from the application of the proposed recursive algorithm will not necessarily be a Delaunay triangulation, it depends on the form of the approximate function $F(x,y)$. So the mesh in Figure 3.2 is a Delaunay triangulation, while the mesh in Figure 3.3 is not a Delaunay triangulation.

Having a triangular mesh S_n with a system of knots $M_n = \{P_1, P_2, \ldots, P_n\}$, we construct the approximation $F_n(x,y)$ to the function $F(x,y)$ as follows. The approximation $F_n(x,y)$ is a piecewise linear function; its graph consists of flat triangles whose projections onto the coordinate plane OXY form the mesh S_n. At the points $P_1, P_2, \ldots, P_n$ the values of the functions $F(x,y)$ and $F_n(x,y)$ coincide. By E_n we denote the approximation error:

$$E_n = \max_{a \le x \le b,\, c \le y \le d} |F(x,y) - F_n(x,y)|.$$

The error E_n can be estimated using the variation V_n, i.e. the largest difference of the values of the function $F(x,y)$ at the knots of the mesh S_n:

$$V_n = \max_{P_i \sim P_j} |z_i - z_j|,$$

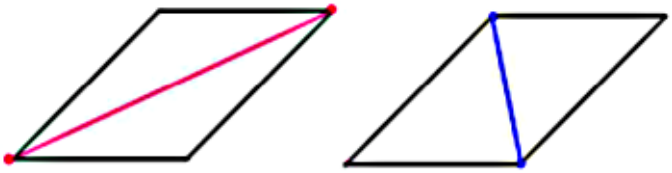

Figure 3.4: Flip operation: long diagonal is replaced by shorter.

where $z_i = F(x_i, y_i)$ and the maximum is taken over all pairs of neighbouring knots of the mesh S_n. It is easy to see that for the proposed recursive algorithm, the sequence V_n monotonically decreases with increasing number of knots n.

Observe that if the sequence V_n tends to zero, then the error E_n may not tend to zero. To ensure that the error tends to zero, we must additionally require the condition of monotonicity.

Proposition 3.1 Let $F(x,y)$ be a smooth function monotonic in both variables. Then for sufficiently large n we have $E_n \approx V_n$, therefore the recursive algorithm leads to vanishing approximation error E_n.

4 Semi-recursive algorithm

Now we modify the proposed recursive algorithm for automated construction of a piecewise-linear approximation of a two-dimensional continuous function by dividing the worst segment by allowing the flip operation, if applicable.

The operation of replacing a longer diagonal in a tetragon with a shorter one is called a "flip" (Figure 3.4). In the mesh in Figure 3.2 there are not four vertices for which the flip operation is applicable, while in Figure 3.3 there is one such set for four knots – these are the vertices P_2, P_3, P_4, P_5. Applying the flip operation to this set of four knots, we obtain the triangulation shown in Figure 3.5. Here the old edge P_2P_4 is replaced by the shorter P_3P_5.

The modified algorithm can be called semi-recursive, since adding each new vertex leaves all old knots and almost all old edges in place, except for one. It is easy to see that the largest edge of the mesh obtained as a result of the semi-recursive algorithm with

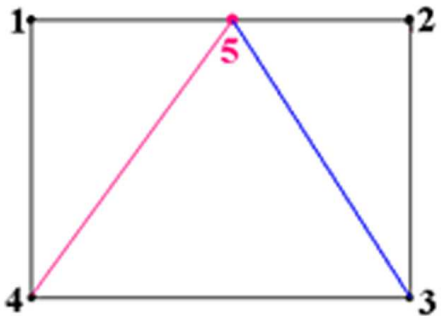

Figure 3.5: The triangulation from Figure 3.3 after the flip operation.

the addition of the flip operation is less than that of the same mesh obtained as a result of the recursive algorithm without the flip operation. Since for smooth monotonic functions $F(x,y)$, the approximation error E_n decreases with decreasing length of the largest edge, we can make the following conjecture.

Conjecture 3.2 As increasing number of knots, the approximation error, resulting from the work of a semi-recursive algorithm for automated construction of a piecewise-linear approximation of a two-dimensional monotonic function by dividing the worst segment with the addition of the flip operation, tends to zero faster than the error obtained as a result of the recursive algorithm without flip operation.

Conjecture 3.2 intuitively seems true and successfully passed the test with numerous practical examples, however the rigorous proof remains open.

It was shown in [3, 4] that the flip operation reduces the sum of the cotangents of the inner angles of a triangular mesh. It is also proved that Delaunay triangulation minimises the sum of the cotangents of the inner angles of the triangulation. From this we obtain the following statement.

Theorem 3.3 For any approximated function and any number of vertices, the mesh resulting from the operation of the semi-recursive algorithm is a Delaunay triangulation.

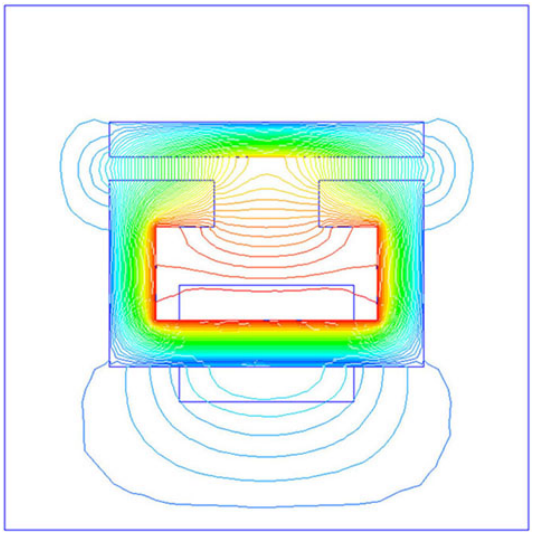

Figure 3.6: The solution of a magnetic field problem.

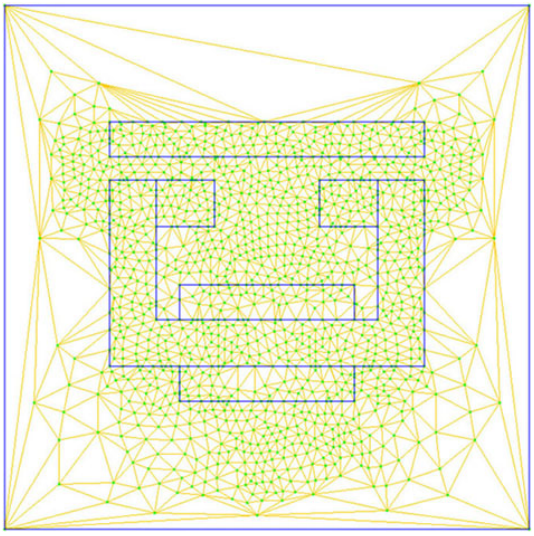

Figure 3.7: The corresponding mesh is Delaunay triangulation.

5 Applications to mathematical physics

Let $F(x,y)$ be an unknown solution of a boundary value problem

$$\begin{cases} L\big(F(x,y)\big) = 0, & (x,y) \in D, \\ F(x,y) = f, & (x,y) \in \partial D, \end{cases}$$

where L is a differential operator acting on rectangle D with boundary ∂D.

Assume that we can construct the piecewise linear approximation of F for given mesh S_n, and we can determine the worst segment of the mesh S_n. Then using the semi-recursive algorithm we obtain a new method of solution of boundary value problem using the meshes with variable number of vertices.

Theorem 3.4 ([5]) For given points, the best mesh for the finite elements approximation for the Maxwell equation of the magnetic field is a Delaunay triangulation.

By Theorems 3.3 and 3.4 we obtain

Theorem 3.5 For the construction of a mesh for the numerical approximation of the Maxwell equation of the magnetic field by the finite elements method, the semi-recursive algorithm is better than algorithms that do not lead to Delaunay triangulation.

Example 3.6 We solve the Maxwell equation for magnetic field using the semi-recursive algorithm. Figure 3.6 shows the solution, while Figure 3.7 shows the corresponding mesh.

Bibliography

[1] Delaunay, B. N.: *On emptiness of sphere*, Izv. AN SSSR **4**, 793–800 (1934).

[2] Melkonyan, T. R., Sukiasyan, H. S.: *On piecewise-linear approximation of two-dimensional function with irregular lattice*, Proceedings of NAS RA and NPUA, series of Technical Sciences, **71**(1), 80–85 (2018).

[3] Sukiasyan, H. S.: *An extremal property of Delaunay triangulation and its applications for fields problems*, Izv. NAN Armenii, ser. tekh. nauk **67**(4), 452–457 (2014).

[4] Sukiasyan, H. S.: *On Extremal property of the sum of cotangents and its applications in Mathematical Physics*, Lobachevskii J. Math., **40**(8), 1137–1140 (2019).

[5] Terzyan, A. A., Sukiasyan, H. S., Akopyan, A. E., Gevorgyan, A. A.: *On construction of optimal mesh for computation of fields problems by finite elements method*, Izv. NAN Armenii, ser. tekh. nauk, **63**(3), 319–327 (2010).

[6] Yenokyan, K. R., Alaei, M. E., Sukiasyan, H. S.: *On automatic construction of piecewise-linear approximation with irregular lattice*, Proceedings of NAS RA and NPUA, series of Technical Sciences, **70**(4), 511–518 (2017).

4

Pinned Gibbs processes

Mathias Rafler[*]

Abstract. *Finite Gibbs processes are conditioned on the barycentre of the point configurations being at a certain location. An integration-by-parts formula is derived from a classical one for such a pinned Gibbs process along with a characterisation. This entails a stochastic domination result for the total number of points as well as a simulation scheme for conditioned point processes.*

1 Pinning Gibbs processes

Classical integration-by-parts formulas for point processes give a dynamic view on point processes identifying certain ones as reversible laws of spatial birth-and-death processes with given birth and death rates. Usually existing points are chosen to disappear independently of each other at rate 1, see e. g. [2] for further possible choices. If, in addition, new points appear independent of the current point configuration, this characterises a Poisson process with intensity given by the birth rate. This property is summarised in Mecke's formula. If this intensity is modified with a term depending on the configuration of points, this yields more general Gibbs processes.

Conforti et al. studied (finite) Poisson processes subject to a pinning of the first moment of the point configurations, i. e. the Poisson process conditioned on an event of probability zero [1]. Clearly, such a conditioned Poisson process cannot satisfy Mecke's

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formula, since typically removing or adding a point changes the first moment of a point configuration. However, they introduced a new kind of dynamic keeping the given condition invariant: They merge three steps of a birth-and-death process, which, suitably chosen, conserve the given condition. Either one point is removed in favour of two new ones, or two points are removed in favour of one new point. Hence, the total number of points increases or decreases by one only.

The idea presented in [1] may be generalised in several ways. Firstly, points may be allowed to interact with each other, i. e. the finite Poisson process is replaced by a finite Gibbs process. Secondly, point configurations are conditioned on a fixed barycentre. Such a condition fails to be linear and transformations need to chosen more carefully.

2 Transformations and invariance

For some $d \in \mathbb{N}$, denote by $\mathscr{M}^{¨}$ the set of locally finite point measures on $\mathbb{R}^d$ as well as $\mathscr{M}_{\mathrm{f}}^{¨}$ its subset of finite point measures, both are Polish spaces. For any atom $x \in \mathbb{R}^d$ of a point measure $\mu \in \mathscr{M}_{\mathrm{f}}^{¨}$, i. e. $\mu(\{x\}) > 0$, write $x \in \mu$.

Denote by $\mathfrak{b} : \mathscr{M}_{\mathrm{f}}^{¨} \to \mathbb{R}^d$ the functional assigning the barycentre to a finite point configuration, i. e.

$$\mathfrak{b}\mu := \frac{1}{\mu(X)} \int x \, \mu(\mathrm{d}x).$$

The barycentre of the empty configuration will be understood as some special element o not contained in $\mathbb{R}^d$.

Of particular interest are transformations replacing a single point by two new ones while leaving the barycentre invariant. A short computation shows that for $z \in \mu$,

$$\mathfrak{b}(\mu + \delta_x + \delta_y - \delta_z) = \mathfrak{b}\mu \qquad \Longleftrightarrow \qquad z = x + y - \mathfrak{b}\mu. \tag{4.1}$$

Whenever a functional is invariant under such a transformation, this pair of functional and transformation is called compatible.

3 Integration by parts

3.1 Unpinned Gibbs processes

Let $\phi_1 : \mathbb{R}^d \to (-\infty, \infty]$ and $\phi_2 : \mathbb{R}^d \times \mathbb{R}^d \to (-\infty, \infty]$ be potentials of single points and pairs of points, both being bounded from below. Then the energy U of a finite point configuration μ is given by

$$U(\mu) = \int \phi_1(x)\mu(\mathrm{d}x) + \frac{1}{2}\int \phi_2(x,y)\mu^{(2)}(\mathrm{d}x,\mathrm{d}y),$$

where $\mu^{(2)}(\mathrm{d}x,\mathrm{d}y) := \big(\mu - \delta_x\big)(\mathrm{d}y)\mu(\mathrm{d}x)$ is the second factorial measure of μ. Integration with respect to $\mu^{(2)}$ means to sum with respect to all pairs of distinct points respecting possible multiplicities. Observe that if $\mu(\mathbb{R}^d) < 2$, then $\mu^{(2)} = 0$, and there is no contribution of a pair interaction. The energy of a point $x \in \mathbb{R}^d$ given a point configuration $\mu \in \mathscr{M}_{\mathrm{f}}^{\cdot\cdot}$ is

$$U(x\,|\,\mu) = \phi_1(x) + \int \phi_2(x,y)\mu(\mathrm{d}y).$$

A finite point process N is a random element in $\mathscr{M}_{\mathrm{f}}^{\cdot\cdot}$, and for a measurable set $B \subseteq \mathbb{R}^d$, N_B is the number of points of N in B. Here both, N and its law $\mathbb{P}$, are called point process. A finite point process N with law $\mathbb{P}$ is called Gibbs process with potentials ϕ_1 and ϕ_2, if its Campbell measure $C_{\mathbb{P}}$ satisfies the (classical) integration-by-parts formula

$$\int h\,\mathrm{d}C_{\mathbb{P}} := \iint h(x,\mu)\mu(\mathrm{d}x)\mathbb{P}(\mathrm{d}\mu) = \iint h(x,\mu+\delta_x)\exp\big(-U(x\,|\,\mu)\big)\,\mathrm{d}x\mathbb{P}(\mathrm{d}\mu) \quad (4.2)$$

for all non-negative, measurable functions h. Equivalently, Equation (4.2) may be written as

$$\mathbf{E}\left[\int h(x,N)N(\mathrm{d}x)\right] = \mathbf{E}\left[\int h(x,N+\delta_x)\exp\big(-U(x\,|\,N)\big)\,\mathrm{d}x\right].$$

Equation (4.2) has a solution if e. g. $\exp(-\phi_1)$ is integrable and ϕ_2 is stable [3]. Subsequently, the potentials shall be chosen such that a finite point process exists as a solution. Note that there is a natural choice of a spatial birth-and-death process on $\mathbb{R}^d$ such that $\mathbb{P}$ is a reversible distribution: Points die independently of each other at rate one, while

new points appear at a rate given by the exponential, see [2] for a discussion. An explicit representation of $\mathbb{P}$ in terms of the kernel is available and given in [4].

Of particular interest is the second order reduced Campbell measure given by

$$\int h \, \mathrm{d}C_{\mathbb{P}}^{(2)} := \mathbf{E}\left[\int h(x,y,N-\delta_x-\delta_y)N^{(2)}(\mathrm{d}x,\mathrm{d}y)\right].$$

Note that a finite point process $\mathbb{P}$ can be reconstructed from $C_{\mathbb{P}}^{(2)}$ only on $\{N_{\mathbb{R}^d} \geq 2\}$.

Subsequently, simplify notation and denote by $\mathfrak{b}$ the barycentre of the point configuration μ. Assume that

$$U(z-y+\mathfrak{b}\,|\,\mu-\delta_z+\delta_y)+U(y\,|\,\mu-\delta_z)<\infty \quad\Longrightarrow\quad U(z\,|\,\mu-\delta_z)<\infty, \qquad z\in\mu,$$

which means that allowing to add points at y and $z-y+\mathfrak{b}$ with a finite energy needs to allow adding a point at z with a finite energy as well.

Proposition 4.1 Let N be a finite Gibbs process with potentials ϕ_1 and ϕ_2. Then

$$\begin{aligned}\mathbf{E}&\left[\int F(x,y,N)N^{(2)}(\mathrm{d}x,\mathrm{d}y)\right]\\ &\qquad=\int \mathbf{E}\left[\int F\big(z-y+\mathfrak{b},y,N+\delta_{z-y+\mathfrak{b}}+\delta_y-\delta_z\big)\sigma(N,y,z)N(\mathrm{d}z)\right]\mathrm{d}y \qquad (4.3)\end{aligned}$$

for all non-negative, measurable functions F, where

$$\sigma(\mu,y,z) := \exp\big(-U(z-y+\mathfrak{b}\,|\,\mu-\delta_z+\delta_y)-U(y\,|\,\mu-\delta_z)+U(z\,|\,\mu-\delta_z)\big), \qquad z\in\mu.$$

Proof. The statement is proven straight forward by an application of integration by parts followed by the substitution $x=z-y+\mathfrak{b}$ and an integration by parts backwards. □

3.2 Pinned Gibbs processes

For a finite point process N with law $\mathbb{P}$ denote by $\tau := \mathbb{P}\circ\mathfrak{b}^{-1}$ the distribution of $\mathfrak{b}$ under $\mathbb{P}$. τ is a distribution on $\mathbb{R}^d\cup\{o\}$ and concentrated on $\mathbb{R}^d$ if and only if N does not charge the empty configuration. Let $\mathbb{P}^a := \mathbb{P}(\,\cdot\,|\,\mathfrak{b}=a)$ be law of the pinned point process

N^a. Note that in any case, if $a \in \mathbb{R}^d$, then necessarily $N^a \neq 0$ almost surely. By the Equivalence (4.1), x, y and z are chosen such that the mapping

$$\mathscr{M}_{\mathrm{f}}^{\cdot\cdot} \to \mathscr{M}_{\mathrm{f}}^{\cdot\cdot}, \qquad \mu \mapsto \mu + \delta_y + \delta_{z-y+\mathfrak{b}\mu} - \delta_z, \qquad z \in \mu,$$

keeps the barycentre invariant.

Proposition 4.2 Let $\mathbb{P}$ be a finite Gibbs process with potentials ϕ_1 and ϕ_2. Then for τ-a.e. $a \in \mathbb{R}^d$, $\mathbb{P}^a$ solves (4.3).

Proof of Proposition 4.2. Let $f : \mathbb{R}^d \cup \{o\} \to \mathbb{R}$ be τ-integrable. Then the statement follows from

$$\int f(a) \int h(x,y,\mu) C^{(2)}_{\mathbb{P}^a}(\mathrm{d}x,\mathrm{d}y,\mathrm{d}\mu)\tau(\mathrm{d}a) = \int f(\mathfrak{b}\mu) h(x,y,\mu) C^{(2)}_{\mathbb{P}}(\mathrm{d}x,\mathrm{d}y,\mathrm{d}\mu)$$

by applying Equation (4.3) respecting the invariance of $\mathfrak{b}$, and the disintegration with respect to τ. □

The pinned point processes inherit the property of solving the second order integration-by-parts formula (4.3). Hence, Equation (4.3) has besides the unpinned Gibbs process at least the parametric family of pinned Gibbs processes as solutions. However, the main statement is that Equation (4.3) together with this pinning characterises the pinned Gibbs processes.

Theorem 4.3 Let Q be a finite point point process such that

1) Q solves (4.3),

2) $Q(\mathfrak{b} = a) = 1$ for some $a \in \mathbb{R}^d$.

Then Q is a pinned Gibbs process subject to the pinning $\mathfrak{b} = a$.

The main steps to prove Theorem 4.3 may be of interest and shall be given and commented on here without too many details.

For a finite point process N, let N^- be the diminished point process, that is N with a uniformly chosen point removed. Since the empty configuration cannot be reduced, it is mapped to a tomb Δ as an extra state added to $\mathscr{M}_{\mathrm{f}}^{\cdot\cdot}$. Note that since $N^a \neq 0$ a.s, $(N^a)^- \neq \Delta$ a.s. and its distribution $(\mathbb{P}^a)^-$ is a probability measure concentrated on $\mathscr{M}_{\mathrm{f}}^{\cdot\cdot}$.

The surprising result is that the law of the diminished pinned Gibbs process has a density with respect to the law of the unpinned Gibbs process.

Proposition 4.4 Let N be a finite Gibbs process with distribution $\mathbb{P}$. Then for τ-a.e. $a \in \mathbb{R}^d$, $(\mathbb{P}^a)^- \ll \mathbb{P}$, and the density is given by

$$\frac{\exp\Big[-U\Big(\big(\mu(\mathbb{R}^d)+1\big)\cdot a - \mu(\mathbb{R}^d)\cdot \mathfrak{b}(\mu)\,\Big|\,\mu\Big)\Big]}{\tau(a)}, \tag{4.4}$$

where $0\cdot\mathfrak{b}(0)=0$.

Observe that the density is essentially an energy, and the argument in the potential shall be interpreted as follows: μ is a diminished point configuration, hence $\big(\mu(\mathbb{R}^d)+1\big)\cdot a$ is the first moment of a point configuration of the Gibbs process pinned at a. Since $\mu(\mathbb{R}^d)\cdot\mathfrak{b}(\mu)$ is the first moment of the diminished point configuration, their difference is the location of the removed point. Consequently, each point configuration is weighted with a factor containing the energy to add the point to get the correct barycentre.

In [1], an approximation argument is used to derive this statement for a certain class of Poisson processes with an absolutely continuous intensity measure. The following sketch of proof uses conditional expectations allowing to replace the absolute continuity with respect to the Lebesgue measure with some reference measure.

Sketch of proof. Let $f : \mathbb{R}^d \cup \{o\} \to \mathbb{R}$ be τ-integrable with $f(o)=0$ and F be $\mathbb{P}$-integrable, then mixing with respect to τ, integration by parts followed by a disintegration yields

$$\begin{aligned}\int f(a)\mathbf{E}\big[F\big((N^a)^-\big)\big]\,\tau(\mathrm{d}a) &= \int f\big(\mathfrak{b}(\mu+\delta_x)\big)\frac{F(\mu)}{\mu(X)+1}\exp\big(-U(x\,|\,\mu)\big)\mathbb{P}^a(\mathrm{d}\mu)\,\tau(\mathrm{d}a)\,\mathrm{d}x\\ &\quad+\int f\big(\mathfrak{b}(\mu+\delta_x)\big)\frac{F(\mu)}{\mu(X)+1}\exp\big(-U(x\,|\,\mu)\big)\mathbb{P}^o(\mathrm{d}\mu)\,\tau(o)\,\mathrm{d}x.\end{aligned}$$

Since $\mathbb{P}^o$ charges the empty configuration only, $f\big(\mathfrak{b}(\mu+\delta_x)\big)=f(x)$ $\mathbb{P}^o$-a.s, and replacing x by b yields that the second integral may be turned into

$$\iint f(b)F(\mu)\frac{\exp\big(-U(b\,|\,\mu)\big)}{\tau(b)}\mathbb{P}^o(\mathrm{d}\mu)\,\tau(o)\,\tau(b)\,\mathrm{d}b.$$

The first integral is evaluated with the aid of two transformations, where the first one pins $\mathfrak{b}(\mu+\delta_x)$ at some $b\in\mathbb{R}^d$ and thus expresses a in terms of b and x, and the second one shifts this expression to a new variable y replacing x. □

An essential observation is that the density (4.4) is positive under the diminished law.

Lemma 4.5 Under the reduced pinned law $(\mathbb{P}^a)^-$,

$$U\Big(\big(\mu(\mathbb{R}^d)+1\big)\cdot a-\mu(\mathbb{R}^d)\cdot\mathfrak{b}(\mu)\,\Big|\,\mu\Big)<\infty$$

for $(\mathbb{P}^a)^-\otimes\tau(\mathrm{d}a)$-a.e. (μ,a), hence the energy is positive almost surely.

Proof. This is shown by proving that the event

$$A:=\big\{(y,\mu)\in\mathbb{R}^d\times\mathscr{M}_{\mathrm{f}}^{\cdot\cdot}\mid U(y\,|\,\mu)=+\infty\big\}$$

has measure 0. Since N^a is pinned at a, $N^a_X\cdot a-(N^a_X-1)\cdot\mathfrak{b}(N^a-\delta_y)=y$. Mixed with respect to τ

$$\begin{aligned}\int\big(\mathbb{P}^a\big)^-(A)\,\tau(\mathrm{d}a)&=\mathbf{E}\left[\frac{1}{N_X}\int 1_A\Big(y,N-\delta_y\Big)N(\mathrm{d}y)\cdot 1_{N>0}\right]\\&=\mathbf{E}\left[\frac{1}{N_X+1}\int 1_{\pi(N,y)=0}\pi(N,y)\,\mathrm{d}y\right].\end{aligned}$$

Since the inner integral vanishes, the claim follows. □

Let Q be a solution of Equation (4.3) such that $Q(\mathfrak{b}=a)=1$ for some $a\in\mathbb{R}^d$. Then one shows that $Q^-\ll\mathbb{P}$ with the density given in (4.4).

Proposition 4.6 Let Q be a finite point process which solves (4.3) and satisfies $Q(\mathfrak{b}=a)=1$ for some $a\in\mathbb{R}^d$. Then $\tilde{Q}$ given by

$$\tilde{Q}(\mathrm{d}\mu):=\frac{\tau(a)}{\exp\Big\{\Big(\big(\mu\big(\mathbb{R}^d\big)+1\big)\cdot a-\mu(\mathbb{R}^d)\cdot\mathfrak{b}(\mu)\Big|\mu\Big)\Big\}}Q^-(\mathrm{d}\mu)$$

is a Gibbs process with potentials ϕ_1 and ϕ_2.

The proof is straightforward by showing that the reduced Campbell measure of $\tilde{Q}$ satisfies a classical integration-by-parts formula (4.2). Note that the Campbell measure of $\tilde{Q}$ turns into a second order Campbell measure for Q allowing the application of (4.3).

What remains is to reconstruct the finite point process Q, or equivalently its reduced Campbell measure from Q^-. Its proof is already given in [1].

Proposition 4.7 Let Q be a finite point process such that $Q(\mathfrak{b} = a) = 1$ for some $\in \mathbb{R}^d$. If $Q^- = \mathbb{P}^-$, where $\mathbb{P}$ is a Gibbs process with potentials ϕ_1 and ϕ_2 conditioned on $\{\mathfrak{b} = a\}$, then $Q = \mathbb{P}$.

4 Applications

4.1 Stochastic domination

A distribution p dominates a distribution q, if the tails of p are heavier than those of q. As shown in [1], a sufficient condition for positive law p on $\mathbb{N}$ dominating q is

$$q(k+1)p(k) \leq q(k)p(k+1) \qquad \text{for all } k \geq 1.$$

Such an inequality can be shown for the law of the total number of points of a pinned Gibbs process N^a and a Poisson distribution conditioned to be positive once

$$\mathbf{E}\big[F(N^a_{\mathbb{R}^d}) \cdot N^a_{\mathbb{R}^d}\big] \leq K \cdot \mathbf{E}\big[F(N^a_{\mathbb{R}^d} + 1)\big] \tag{4.5}$$

is shown for some $K > 0$. The domination then follows in choosing the indicators $F(n) := 1_{\{n+1\}}$ for any $n \in \mathbb{N}$ and completing the conditioned Poisson weights with parameter K.

Equation (4.5) follows from the integration-by-parts formula by choosing functions depending on its parameters via $N^a_{\mathbb{R}^d}$ only, i. e.

$$\mathbf{E}\big[g(N^a_{\mathbb{R}^d})(N^a_{\mathbb{R}^d} - 1)N^a_{\mathbb{R}^d}\big] = \mathbf{E}\left[g(N^a_{\mathbb{R}^d} + 1) \iint \sigma(N^a, y, z)\, \mathrm{d}y N^a(\mathrm{d}z)\right],$$

and the innermost integral can shown to be bounded from above uniformly by K. For a hard-core interaction of particles inside some bounded box, this is satisfied automatically since

$$U(z - y + \mathfrak{b} \,|\, \mu - \delta_z + \delta_y) + U(y \,|\, \mu - \delta_z) - U(z \,|\, \mu - \delta_z) \geq 0.$$

A domination result with the roles exchanged can be shown as soon as the innermost integral is bounded from below by a positive constant.

4.2 Monte Carlo subject to conditions

The integration-by-parts formula allows a dynamic approach to sample approximately from the law of the conditioned point process N^a by running a continuous time Markov chain starting from a single point at $a \in \mathbb{R}^d$. If μ is the current point configuration, then the following jumps occur at the following rates:

1) With rate one each, a pair of distinct points $x, y \in \mu$ is chosen and removed in favour of a single point at $x + y - a$.

2) A rejection method is applied to remove one point in favour of two new points, so assume that $\sigma(\mu, y, z) \leq K$ for some constant K. At rate $K \cdot \mu(\mathbb{R}^d)$, choose a point y uniformly. Choose $z \in \mu$ uniformly, and toss a coin with success probability

$$\frac{\sigma(\mu, y, z)}{K}.$$

In case of success, remove z from μ and add points at y and $z - y + a$. Otherwise, reject any jump.

The barycentre at a is a conserved quantity and does not need to be computed at each step.

Bibliography

[1] Conforti, G., Kosenkova, T., Rœlly, S.: *Conditioned point processes with application to Lévy bridges*. J. Theoret. Probab. **32**(4), 2111–2134 (2019).

[2] Garcia, N., Kurtz, T.: *Spatial birth and death processes as solutions of stochastic equations*. Alea **1**, 281–303 (2006).

[3] Ruelle, D.: *Superstable interactions in classical statistical mechanics*. Commun. Math. Phys. **18**, 127–159 (1970).

[4] Zessin, H.: *Der Papangelou-Prozess*. J. Contemp. Math. Anal. **44**(1), 36–44 (2009).

5

Construction of limiting Gibbs processes and the uniqueness of Gibbs processes

Suren Poghosyan[*] *and Hans Zessin*[†]

Abstract. *For a pair potential* Φ *in a general phase space* X *satisfying some natural and sufficiently general stability and regularity conditions in the sense of Poghosyan and Ueltschi we define by means of the so-called Ursell kernel a function* r *which is shown to be the correlation function of a unique infinitely extended process* P. *Finally, under more restrictive assumptions, we show that the Gibbs process for* Φ*, if it exists, coincides with* P. *Here we use the classical method of Kirkwood-Salsburg equations.*

1 Preliminaries

Let $(X, \mathscr{B}(X), \mathscr{B}_0(X))$ be the underlying phase space where X is a locally compact, second countable Hausdorff topological space, $\mathscr{B}(X)$ its Borel σ-field and $\mathscr{B}_0(X)$ its bounded Borel sets. Let ρ be a Radon measure on X.

Let $\mathscr{M}^{\cdot}(X)$ be the space of Radon point measures on X and $\mathfrak{X}$ be the collection of all finite point measures (finite configurations) ξ in X. $\mathfrak{X}_+$ denotes the collection of all

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non-empty ξ in $\mathfrak{X}$. For $A \in \mathscr{B}_0(X)$ let $\mathfrak{X}(A)$ be the set of finite point measures supported by A. Let $\mathscr{M}_R(X)$, $R > 0$, be the space of simple point measures μ on X having the property that the minimal distance of every pair of points in any configuration μ is R, i. e. $(x, y \in \mu, x \neq y \Rightarrow d(x,y) > R)$ where d is a metric on X. Here all Dirac measures ε_x at the point $x \in X$ and the zero measure o are elements of $\mathfrak{X}$ and $\mathscr{M}_R(X)$.

We call a subset $\mathfrak{X}'$ of $\mathfrak{X}$ an *environment in* X if $(\eta \in \mathfrak{X}', \xi \preceq \eta \Rightarrow \xi \in \mathfrak{X}')$. Here $\xi \preceq \eta$ if $\xi(x) \leq \eta(x)$ for all $x \in X$. Examples are $\mathfrak{X}$ and $\mathfrak{X}_R = \mathscr{M}_R(X) \cap \mathfrak{X}$.

We denote by F_+ the space of $[0, +\infty]$-valued measurable functions on the corresponding space and by $\mathscr{K}$ we denote the collection of continuous functions with compact support. Define a locally finite measure Λ_ρ on $\mathfrak{X}$ by

$$\Lambda_\rho \varphi = \varphi(o) + \sum_{n=1}^{\infty} \frac{1}{n!} \int_X \cdots \int_X \varphi(\varepsilon_{x_1} + \ldots + \varepsilon_{x_n}) \rho(\mathrm{d}x_1) \cdots \rho(\mathrm{d}x_n), \qquad \varphi \in F_+.$$

For a given configuration $\mu \in \mathscr{M}^{\cdot\cdot}$ we define the following measure on $\mathfrak{X}$:

$$\Lambda'_\mu(h) = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{X^n} h(\varepsilon_{x_1} + \ldots + \varepsilon_{x_n}) \widetilde{\mu}^n(\mathrm{d}x_1, \ldots, \mathrm{d}x_n), \qquad h \in F_+, \text{ where}$$
$$\widetilde{\mu}^n(\mathrm{d}x_1, \ldots, \mathrm{d}x_n) = \big(\mu - \varepsilon_{x_1} - \ldots - \varepsilon_{x_{n-1}}\big)(\mathrm{d}x_n) \cdots \big(\mu - \varepsilon_{x_1}\big)(\mathrm{d}x_2) \mu(\mathrm{d}x_1).$$

$\widetilde{\mu}^n$ is called the *factorial measure* of μ of order n, and Λ'_μ the *compound factorial measure built on* μ. The term $n = 0$ of the sum is $h(o)$. Also, $\Lambda'_o(h) = h(o)$.

Below we often use the following important equation, *the Minlos' formula* [3]:

$$\int_{\mathfrak{X}} \int_{\mathfrak{X}} h(\xi, \nu - \xi) \Lambda'_\nu(\mathrm{d}\xi) \Lambda_\rho(\mathrm{d}\nu) = \int_{\mathfrak{X}} \int_{\mathfrak{X}} h(\xi, \nu) \Lambda_\rho(\mathrm{d}\xi) \Lambda_\rho(\mathrm{d}\nu), \qquad h \in F_+, \quad (5.1)$$

which is valid for all h integrable with respect to the measure on the left-hand or the right-hand side of the equation.

Let P be a point process in X that is a probability on $\mathscr{M}^{\cdot\cdot}(X)$. The *moment measure of* P *of order* k is the measure on X^k defined by

$$\nu^k_{\mathsf{P}} f = \int_{\mathscr{M}^{\cdot\cdot}(X)} \mu^{\otimes k}(f) \, \mathsf{P}(\mathrm{d}\mu), \qquad f \in \mathscr{K}(X^k),$$

whereas the *correlation measure (also called factorial moment measure) of* P *of order* k is the measure given by

$$\widetilde{\nu}^k_{\mathsf{P}}(f) = \int_{\mathscr{M}^{\cdot}(X)} \widetilde{\mu}^k(f)\,\mathsf{P}(\mathrm{d}\mu), \qquad f \in \mathscr{K}(X^k).$$

If $\widetilde{\nu}^k_{\mathsf{P}}$ has a density r^k_{P} with respect to some product measure $\rho^{\otimes k}$, where ρ is a Radon measure on X, then we say that r^k_{P} is a *correlation function of* P *of k-th order*. The process P is called *of order* k if ν^k_{P} is a Radon measure. P is called *of infinite order* if it is of order k for every k.

2 Ruelle's algebraic approach

We here follow Ruelle [10]. Let $\mathscr{A}$ be the set of all measurable complex functions on $\mathfrak{X}$. We define a $\star$-multiplication of two functions $h_1, h_2 \in \mathscr{A}$ by

$$h_1 \star h_2(\xi) = \int_{\mathfrak{X}} h_1(\nu) h_2(\xi - \nu)\,\Lambda'_{\xi}(\mathrm{d}\nu), \qquad \xi \in \mathfrak{X}. \tag{5.2}$$

With the $\star$-product $\mathscr{A}$ becomes a commutative algebra with the unit $\mathbb{1}(\xi) = \delta_o(\xi)$. Let $\mathscr{A}_0 = \{f \in \mathscr{A} \mid f(o) = 0\}$. We define the mapping $\Gamma : \mathscr{A}_0 \to \mathbb{1} + \mathscr{A}_0$ (*algebraic exponent*) by

$$\Gamma h = \mathbb{1} + h + \frac{1}{2!}h^{\star 2} + \ldots + \frac{1}{n!}h^{\star n} + \ldots, \qquad h \in \mathscr{A}_0. \tag{5.3}$$

Let Φ be a measurable symmetric function $\Phi : X \times X \to]-\infty, +\infty]$, a pair potential in X. $E(\xi) := \sum_{1 \le i < j \le n} \Phi(x_i, x_j)$ is the *energy* of the configuration $\xi = \varepsilon_{x_1} + \ldots + \varepsilon_{x_n}$; $B := \mathrm{e}^{-E}$ is called the Boltzmann factor. The *conditional energy* at x given the configuration ξ is given by $W_\Phi(x, \xi) := \int_X \Phi(x, y)\,\xi_x(\mathrm{d}y)$, where $\xi_x = \xi$ if $x \notin \xi$ and $\xi = \xi - \varepsilon_x$ otherwise.

We assume that Φ is b-*stable*, i. e. there exists a measurable function $\mathsf{b} : X \to [0, +\infty)$ such that $E(\xi) \ge -\sum_{x \in \xi} \mathsf{b}(x)$, $\xi \in \mathfrak{X}$.

We consider also $\mathscr{P}$-*stable*[1] Φ *with stability function* b in the environment $\mathfrak{X}'$. This means that there exists a measurable function $\mathsf{b} : X \to [0, +\infty)$ such that $W_\Phi(x, \xi_x) \ge -\mathsf{b}(x)$, $x \in \xi \in \mathfrak{X}'$, $\xi_x = \xi - \varepsilon_x$. If Φ is $\mathscr{P}$-stable with function b, then it is b-stable.

Any non-negative Φ is $\mathscr{P}$-stable in the environment $\mathfrak{X}$. Another important example is the *Penrose potential* [7] (see also [5]). Let (X, ρ) be the d-dimensional Euclidean

[1] This notion goes back to Oliver Penrose [7].

space with Lebesgue measure. Let $c, \varepsilon, R > 0$ be constants. Φ is the following hard-core potential: If $|x-y| < R$ then $\Phi(x,y) = +\infty$; and if $|x-y| \geq R$ then $|\Phi|(x,y) \leq c|x-y|^{-(d+\varepsilon)}$. As Penrose has shown this potential is $\mathscr{P}$-stable in the environment $\mathfrak{X}_R$ with a constant stability which can be calculated explicitly.

The Boltzmann factor $B = \mathrm{e}^{-E}$ is an element of the algebra $(\mathscr{A}, \star)$ having an inverse with respect to the $\star$ multiplication, which is denoted by $B_\star^{-1}$. Another important element U of the algebra $\mathscr{A}$ is the *Ursell function* given by

$$U(o) = 0, \qquad U(\varepsilon_x) = 1, \qquad U(\varepsilon_{x_1} + \ldots + \varepsilon_{x_n}) = \sum_{\gamma \in \mathscr{C}_n} \prod_{(i,j)\in\gamma} \omega(x_i, x_j), \quad n \geq 2, \tag{5.4}$$

where $\mathscr{C}_n$ denotes the set of all simple, unoriented, connected graphs γ with n vertices, the product is taken over all edges (i,j) in γ and $\omega(x,y) = \mathrm{e}^{-\Phi(x,y)} - 1$ is the Mayer function.

Note that $U \in \mathscr{A}_0$ and the following important relation is valid $B = \Gamma U$.

3 Ursell kernel
Representation of the correlation function

Here we follow the work of Minlos, Poghosyan [4]. Let $\mathsf{z} : X \to [0, +\infty)$ be measurable. We consider Radon measures of the form $\mathsf{z}.\rho = \rho_{\mathsf{z}}$, where ρ is Radon measure and z is a density function.

Given $A \in \mathscr{B}_0(X)$ we define the finite volume Gibbs process in A as the probability $\mathsf{Q}_{\mathsf{z},A}$ on $\mathfrak{X}(A)$ which is given by

$$\mathsf{Q}_{\mathsf{z},A}(\mathrm{d}\xi) = \frac{1}{\Xi(\mathsf{z},A)} \mathrm{e}^{-E(\xi)} \cdot \Lambda_{\mathsf{z}.\rho_A}(\mathrm{d}\xi)$$

where $\rho_A = 1_A \cdot \rho$ and the normalising constant (*the partition function*) is given by

$$\Xi(\mathsf{z},A) = \int_{\mathfrak{X}(A)} \prod_{x\in\eta} \mathsf{z}(x) \mathrm{e}^{-E(\eta)} \Lambda_{\rho_A}(\mathrm{d}\eta).$$

By stability $\Xi(\mathsf{z},A) \leq \exp\left(\int_A \mathrm{e}^{\mathsf{b}(x)} \mathsf{z}(x)\, \rho(\mathrm{d}x)\right) < \infty$.

It is well known that the *correlation function of the Gibbs process* $\mathsf{Q}_{\mathsf{z},A}$ is given by

$$r_{\mathsf{z},A}(\xi) = \frac{\prod_{x\in\xi}\mathsf{z}(x)}{\Xi(\mathsf{z},A)}\int_{\mathfrak{X}(A)} \mathrm{e}^{-E(\xi+\eta)}\,\Lambda_{\mathsf{z}.\rho_A}(\mathrm{d}\eta), \qquad \xi\in\mathfrak{X}(A).$$

Proposition 5.1 The correlation function has the following remarkable representation:

$$r_{\mathsf{z},A}(\xi) = \prod_{x\in\xi}\mathsf{z}(x)\int_{\mathfrak{X}(A)} G(\xi,\eta)\,\Lambda_{\mathsf{z}.\rho_A}(\mathrm{d}\eta), \qquad \xi\in\mathfrak{X}(A) \tag{5.5}$$

where the *Ursell kernel* $G:\mathfrak{X}^2\to\mathbb{R}$ is given by $G(\xi,\eta) = (B_\star^{-1}\star D_\xi B)(\eta)$, $\xi,\eta\in\mathfrak{X}$ and $D_\xi B(\nu) = B(\xi+\nu)$, $\nu\in\mathfrak{X}$. In particular $G(\varepsilon_x,\eta) = U(\varepsilon_x+\eta)$ where U is the Ursell function.

For the proof we note that by the Minlos' formula

$$\frac{1}{\Xi(\mathsf{z},A)}\Lambda_{\mathsf{z}.\rho_A}(D_\xi B) = \frac{1}{\Xi(\mathsf{z},A)}\Lambda_{\mathsf{z}.\rho_A}(B\star B_\star^{-1}\star D_\xi B) = \Lambda_{\mathsf{z}.\rho_A}(B_\star^{-1}\star D_\xi B).$$

For a given pair potential Φ let $\overline{\Phi}=\Phi$ if Φ is finite and $\overline{\Phi}=1$ if $\Phi=+\infty$. Let a, b, c be non-negative functions on X. We will say that Φ satisfies

- ◇ c-*regularity*, if there exists a function a such that

$$\int_X \big|\omega\big|(x,y)\mathrm{e}^{(\mathsf{c}+\mathsf{a})(y)}\,\rho_{\mathsf{z}}(\mathrm{d}y)\le \mathsf{a}(x), \qquad x\in X. \tag{5.6}$$

- ◇ *Modified* b-*regularity*, if there exists a function a such that

$$\int_X \big|\overline{\Phi}\big|(x,y)\mathrm{e}^{\mathsf{b}(y)+\mathsf{a}(y)}\,\rho_{\mathsf{z}}(\mathrm{d}y)\le \mathsf{a}(x), \qquad x\in X. \tag{5.7}$$

Both assumptions (5.6) and (5.7) are introduced in [8].

Theorem 5.2 Let Φ be a b-stable pair interaction. Assume also that Φ is $2\mathsf{b}$-*regular* for a. Then the function

$$r_{\mathsf{z}}(\xi) = \prod_{x\in\xi}\mathsf{z}(x)\int_{\mathfrak{X}} G(\xi,\eta)\,\Lambda_{\rho_{\mathsf{z}}}(\mathrm{d}\eta), \qquad \xi\in\mathfrak{X} \tag{5.8}$$

is well defined and satisfies the following *Ruelle bound*

$$r_{\mathsf{z}}(\xi) \le \prod_{x\in\xi} \mathsf{z}(x) \int_{\mathfrak{X}} \big|G\big|(\xi,\eta)\,\Lambda_{\rho_{\mathsf{z}}}(\mathrm{d}\eta) \le \prod_{x\in\xi} \mathsf{z}(x)\mathrm{e}^{(2\mathsf{b}+\mathsf{a})(x)}, \qquad \xi\in\mathfrak{X}. \tag{5.9}$$

If Φ is $\mathscr{P}$-stable and b-regular for a then (5.9) holds with $\mathrm{e}^{(\mathsf{b}+\mathsf{a})(x)}$ instead of $\mathrm{e}^{(2\mathsf{b}+\mathsf{a})(x)}$. Moreover $r_{\mathsf{z}}(\xi) = \lim_{A\uparrow X} r_{\mathsf{z},A}(\xi)$.

The proof of this theorem is based on the so-called *forest graph estimate*. For $\xi,\eta\in\mathfrak{X}$ let $\mathscr{F}(\xi,\eta)$ be the collection of forests with the set of vertices $\xi+\eta$ and roots ξ. An unoriented simple graph is called *rooted forest* if its connected components are *rooted trees*, i. e. trees where one vertex is specified as a root.

We consider the case of b-stable Φ. The $\mathscr{P}$-stable case is entirely the same, one only needs to replace $\mathrm{e}^{2\mathsf{b}}$ by e^{b}. If Φ is modified regular, then one has to pass from ω to $\overline{\Phi}$ using the formula $\big|\omega\big|(x,y) \le \big|\overline{\Phi}\big|(x,y)\mathrm{e}^{\Phi^-(x,y)}$.

Lemma 5.3 ([4]) For $\xi\neq o$,

$$\big|G\big|(\xi,\eta) \le \prod_{x\in\xi+\eta} \mathrm{e}^{2\mathsf{b}(x)} \sum_{\gamma\in\mathscr{F}(\xi,\eta)} \prod_{(x,y)\in\gamma} \big|\omega\big|(x,y). \tag{5.10}$$

Denoting the right-hand side of (5.10) by $H(\xi,\eta)$ one can show that

$$H(\varepsilon_{x_1}+\ldots+\varepsilon_{x_n},\eta) = H\big(x_1,\cdot\big)\star\cdots\star H\big(x_n,\cdot\big)(\eta).$$

Then an application of the Minlos' formula and Theorem 2.1 from [8] completes the proof of Theorem 5.2.

In particular Lemma 5.3 gives the famous tree graph estimate of the Ursell function:

$$\big|U\big|(\eta) = \big|G\big|(\varepsilon_x,\eta-\varepsilon_x) \le \prod_{x\in\eta} \mathrm{e}^{2\mathsf{b}(x)} \sum_{\gamma\in\mathscr{T}(\eta)} \prod_{(x,y)\in\gamma} \big|\omega\big|(x,y), \qquad x\in\eta. \tag{5.11}$$

Here $\mathscr{T}(\eta)$ is the set of trees with the set of vertices η.

4 Construction of limiting Gibbs processes

Theorem 5.4 Let Φ be a $\mathscr{P}$-stable pair potential in X which is b-regular for a. If $\mathrm{e}^{\mathsf{b}+\mathsf{a}}\rho$ is a Radon measure, then there exists a unique process P_{z} in X of infinite order having

correlation function r_{z}, which is the limiting Gibbs process of the sequence $(\mathsf{Q}_{\mathsf{z},A_n})_n$ in the weak sense.

The proof of this theorem is based on the following lemma.

Lemma 5.5 ([11]) Let $(\mathsf{P}_n)_n$ be a sequence of point processes in X of infinite order satisfying the conditions: for each k the limits $\widetilde{\nu}^k(f) = \lim_{n\to\infty} \widetilde{\nu}^k_{\mathsf{P}_n}(f)$, $f \in \mathscr{K}(X^k)$, exist and $\sum_{\ell=1}^{\infty} \nu^\ell(A^\ell)^{-\frac{1}{2\ell}} = +\infty$ for each bounded A. Here $\nu^\ell(A^\ell) = \sum_{\mathscr{J}} \widetilde{\nu}^{|\mathscr{J}|}(A^{|\mathscr{J}|})$, where the summation is over all partitions of $\{1,\dots,\ell\}$ into non-empty subsets. Then there exists one and only one point process P in X of infinite order such that $\mathsf{P}_n \Rightarrow \mathsf{P}$ and $\widetilde{\nu}^k_{\mathsf{P}} = \widetilde{\nu}^k$ for each k.

Lemma 5.5 combined with the Ruelle bound completes the proof of Theorem 5.4. We consider below the case where $\mathsf{z}(x) \equiv z > 0$, $x \in X$.

Proposition 5.6 Under the conditions of Theorem 5.4, $r_z(\xi) = z^{|\xi|} \int_{\mathfrak{X}} G(\xi,\eta)\Lambda_{\rho_z}(\mathrm{d}\eta)$ satisfies the Kirkwood-Salsburg (K-S) equation:

$$(\mathsf{K}\Sigma_{z\rho}) \qquad r_z(\xi) = z\mathrm{e}^{-W_\Phi(x,\xi)} \cdot \int_{\mathfrak{X}} K(x,\eta) r_z(\xi_x+\eta)\,\Lambda_\rho(\mathrm{d}\eta), \qquad x \in \xi \neq o,$$

where $K(x,\eta) := \prod_{y\in\eta} \omega(x,y)$.

The proof follows from Theorem 5.2, Minlos' formula and the fact that the Ursell kernel satisfies the equations ([PU09], [Ru69]): $G(o,\eta) = \delta_{o,\eta}$ and

$$G(\xi,\eta) = \mathrm{e}^{-W_\Phi(x,\xi_x)} \int_{\mathfrak{X}} K(x,\nu) G(\xi_x+\nu, \eta-\nu)\,\Lambda'_\eta(\mathrm{d}\nu), \qquad x \in \xi \neq o.$$

Theorem 5.7 Let Φ be a $\mathscr{P}$-stable b-regular potential for a. If $\mathrm{e}^{\mathsf{b}+\mathsf{a}}\rho$ is a Radon measure and $\sup_x \mathsf{a}(x) = C < \infty$ and if the activity satisfies $0 < z < (\mathrm{e}C)^{-1}$, the $(\mathsf{K}\Sigma_{z\rho})$ equation has a unique solution and the correlation function r_z of the process P_z is this unique solution.

Proof. We follow [10] and [3]. Let $\mathscr{E}_\delta$, $\delta > 0$, be the Banach space of all complex valued measurable functions $\varphi : \mathfrak{X}_+ \to \mathbb{C}$ such that

$$\|\varphi\|_\delta = \sup_{\xi\in\mathfrak{X}_+} \frac{|\varphi|(\xi)}{\delta^{|\xi|} \prod_{x\in\xi} \mathrm{e}^{(\mathsf{a}+\mathsf{b})(x)}} < +\infty, \tag{5.12}$$

where $|\xi| = \xi(X)$ denotes the number of particles in ξ. Since r_z satisfies the *Ruelle bound* (5.9), the correlation function r_z belongs to $\mathscr{E}_\delta$ with the norm ≤ 1 if $z \le \delta$.

We define on $\mathscr{E}_\delta$ the linear operator K by

$$\mathsf{K}\varphi(\varepsilon_x) = z\int_{\mathfrak{X}_+} K(x,\eta)\varphi(\eta)\,\Lambda_\rho(\mathrm{d}\eta), \qquad x\in X, \tag{5.13}$$

$$\mathsf{K}\varphi(\xi) = z\mathrm{e}^{-W_\Phi(x,\xi)}\cdot\int_{\mathfrak{X}} K(x,\eta)\varphi(\eta+\xi_x)\Lambda_\rho(\mathrm{d}\eta), \qquad x\in\xi\neq o. \tag{5.14}$$

Using the operator K, we can write the K-S equation as an integral equation in the Banach space $\mathscr{E}_\delta$: $r_z = \mathsf{K}r_z + \alpha_z$, where $\alpha_z(\xi) = 0$ if $\xi(X) > 1$ and $\alpha_z(\varepsilon_x) = z$. For sufficiently small $z > 0$ the operator K is bounded. Indeed let $\varphi\in\mathscr{E}_\delta$ with $\|\varphi\|\le 1$. Then by $\mathscr{P}$-stability and b-regularity of Φ for every $x\in\xi\in\mathfrak{X}$,

$$\begin{aligned}\big|(\mathsf{K}\varphi)\big|(\xi) &\le z\mathrm{e}^{\mathsf{b}(x)}\int_{\mathfrak{X}}\big|\omega_x\big|(\eta)\delta^{|\eta|+|\xi|-1}\mathrm{e}^{(\eta+\xi_x)(\mathsf{b}+\mathsf{a})}\Lambda_\rho(\mathrm{d}\eta)\\ &\le z\delta^{|\xi|-1}\mathrm{e}^{\xi(\mathsf{b}+\mathsf{a})}\cdot\exp\Big(\delta\rho\big(|\omega_x|\mathrm{e}^{\mathsf{b}+\mathsf{a}}\big)\Big) \le \frac{z\mathrm{e}^{\delta C}}{\delta}\delta^{|\xi|}\mathrm{e}^{\xi(\mathsf{b}+\mathsf{a})}.\end{aligned}$$

Thus, if the parameters z and δ satisfy the condition $z\mathrm{e}^{\delta C}\delta^{-1} < 1$, then $\|\mathsf{K}\|_\delta < 1$ and the K-S equation has a unique solution. In particular, if we take $\delta = \frac{1}{C}$, this condition on z becomes $0 < z < (\mathrm{e}C)^{-1}$. A more detailed discussion of the choice of δ can be found in [3]. □

5 Uniqueness of Gibbs processes

In a final step we show that Gibbs processes G for Φ with activity z have correlation functions which solve the K-S equation in the same range of the parameter z. This implies that the Gibbs process G, if it exists, coincides with P_z.

We use the notion of Gibbs process introduced in [6] as a solution of an integration-by-parts formula. A point processes G is called a *Gibbs process for* (Φ,ρ), if for all $h\in F_+$

$$(\Sigma_\rho)\quad \int_{\mathscr{M}^{\cdot}}\int_X h(x,\mu)\,\mu(\mathrm{d}x)\,\mathsf{G}(\mathrm{d}\mu) = \int_{\mathscr{M}^{\cdot}}\int_X h(x,\mu+\varepsilon_x)\exp\big(-W_\Phi(x,\mu)\big)\,\rho(\mathrm{d}x)\,\mathsf{G}(\mathrm{d}\mu).$$

We then write $\mathsf{G}\in\mathscr{G}(\Phi,\rho)$. This is equivalent to saying that G is a Gibbs process for (Φ,ρ) in the sense of Dobrushin, Lanford and Ruelle, cf. [6].

From now on we assume that Φ is $\mathscr{P}$-stable, modified b-regular for a and $\mathrm{e}^{\mathsf{b}+\mathsf{a}}\rho$ is a Radon measure. Then

Lemma 5.8 ([6]) Every $\mathsf{G} \in \mathscr{G}(\Phi, \rho_z)$ is of infinite order and its correlation function is given by

$$g_z(\xi) = z^{|\xi|} \int_{\mathscr{M}^{\cdot}} \exp\bigl(-W_\Phi(\xi, \mu)\bigr)\, \mathsf{G}(\mathrm{d}\mu), \qquad \xi \in \mathfrak{X}. \tag{5.15}$$

Furthermore, G is uniquely determined by its correlation functions.

Note that by modified regularity of Φ the conditional energy $W_\Phi(x, \mu)$ can be extended to the whole $\mathscr{M}^{\cdot}(X)$ and remains $\mathscr{P}$-stable with the same function b. Due to the $\mathscr{P}$-stability, the Ruelle bound takes the form $g_z(\xi) \le z^{|\xi|} \prod_{x\in\xi} \mathrm{e}^{\mathsf{b}(x)}$. Using ideas of Sabine Jansen [1], we then obtain

Proposition 5.9 Let G_z be a Gibbs process in X for (Φ, ρ_z). Then its correlation function g_z solves the $(\mathsf{K}\Sigma_{z\rho})$ equation.

In the view of the Ruelle bound we are in the situation as we had been above for the correlation function r_z.

Lemma 5.10 Let Φ be a $\mathscr{P}$-stable pair potential satisfying above mentioned conditions. Assume also $0 < z < (\mathrm{e}C)^{-1}$. Then g_z coincides with r_z which implies that G_z coincides with the limiting Gibbs process P_z.

Thus we arrive at the main result of this paper

Theorem 5.11 For all $0 < z < (\mathrm{e}C)^{-1}$ the collection $\mathscr{G}(\Phi, \rho_z)$ of Gibbs processes is either empty or the singleton $\{\mathsf{P}_z\}$.

For a large class of hard-core potentials we show in [9] that indeed for all $0 < z < (\mathrm{e}C)^{-1}$ the set $\mathscr{G}(\Phi, \rho_z)$ is not empty and therefore reduced to a unique element constructed as the limiting Gibbs process.

Acknowledgement. The authors are grateful to the referee for several proposals which improved the presentation of our contribution.

Bibliography

[1] Jansen, S.: *Cluster expansion for Gibbs point processes*, Adv. Appl. Prob. **51**, 1129–1178 (2019).

[2] Minlos, R. A.: *Limiting Gibbs distribution*, translated from Funktsional'nyi Analiz i Ego Prilozheniya **1**, 60–73 (1967).

[3] Minlos, R. A.: *Lectures on statistical physics*, Russ. Math. Surv. **23**(1), 137–194 (1968).

[4] Minlos, R. A., Poghosyan, S.: *Estimates of Ursell functions, group functions, and their derivatives*, Theor. Math. Phys. **31**, 1–62 (1980).

[5] Morrey, Ch. B.: *On the derivation of the equations of hydrodynamics from statistical mechanics*, Commun. Pure Appl. Math. **8**, 279–326 (1955).

[6] Nguyen, X. X., Zessin, H.: *Integral and differential characterizations of the Gibbs process*, Math. Nachr. **88**, 105–115 (1979).

[7] Penrose, O.: *Convergence of fugacy expansions for fluids and lattice gases*, J. Math. Phys. **4**, 1312 (1963).

[8] Poghosyan, S., Ueltschi, D.: *Abstract cluster expansion with applications to statistical mechanics*, J. Math. Phys. **50**, 053509 (2009).

[9] Poghosyan, S., Zessin, H.: *Penrose-stable interactions in classical statistical mechanics*, manuscript in preparation (2020).

[10] Ruelle, D.: *Statistical mechanics*, W. A. Benjamin, Massachusetts (1969).

[11] Zessin, H.: *The method of moments for random measures*, Z. Wahrscheinlichkeitstheorie verw. Gebiete **62**, 395–409 (1983).

6

Non-local convolution type parabolic equations with fractional and regular time derivative

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Abstract. *This note deals with the fundamental solutions of parabolic equations for convolution type non-local operators. Our goal is to compare the large time asymptotics of these fundamental solutions with that of the classical Gaussian heat kernel. A similar problem is considered for evolution equations with a fractional time derivative.*

1 Introduction

Parabolic equations with non-local elliptic operators play an important role in the study of population dynamics models. The presence of a non-local operator on the right-hand side of the equation reflects the fact that the interaction in these models has a non-local character. One of these models is the so-called contact model in $\mathbb{R}^d$, see e. g. [5, 6]. It is a continuous time birth and death Markov process in a continuum defined on the space of infinite (but locally finite) configurations $\gamma \in \Gamma$ lying in the space $\mathbb{R}^d$: $\gamma \subset \mathbb{R}^d$. The process is characterised by the birth and death rates. Each point $x \in \gamma$ of a configuration γ might create an offspring y independently of other points of the configuration. The

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offspring location is distributed in the space with the density $a(x-y)$ (so-called dispersal kernel), and we assume $\int_{\mathbb{R}^d} a(z)dz = 1$. In addition, any point of the configuration has an independent exponentially distributed random life time determined by the mortality rate $m(x) > 0$, and in the general case the mortality rate is a spatially inhomogeneous function $m(x) \geq 0$. The formal generator of the dynamics of this process takes the form

$$LF(\gamma) = \sum_{x\in\gamma} \int_{\mathbb{R}^d} a(x-y)\big(F(\gamma\cup y) - F(\gamma)\big)dy + \sum_{x\in\gamma} m(x)\big(F(\gamma\backslash x) - F(\gamma)\big).$$

The case of homogeneous mortality $m(x) \equiv \kappa$ has been studied in detail in the paper [5]. In the most interesting case $\kappa = 1$ (the critical regime) a family of stationary distributions exist.

One of the remarkable properties of the contact model is the fact that the first correlation function $\rho(x)$ (the so-called density of configurations) satisfies an evolution equation which is decoupled and can be considered separately. It should be noted that evolutions of the higher order correlation functions have more complicated hierarchical structure.

The dynamics of the first correlation function is described by the following Cauchy problem:

$$\frac{\partial\rho}{\partial t} = A\rho, \quad \rho = \rho(t,x), \quad x \in \mathbb{R}^d,\, t \geq 0, \qquad \rho(0,x) = \rho_0(x) \geq 0, \qquad \text{where} \quad (6.1)$$

$$A\rho(x) = -m(x)\rho(x) + \int_{\mathbb{R}^d} a(x-y)\rho(y)dy. \quad (6.2)$$

If $m(x) \equiv 1$, then the operator A takes the form

$$A\rho(x) = -\rho(x) + \int_{\mathbb{R}^d} a(x-y)\rho(y)dy = \int_{\mathbb{R}^d} a(x-y)\big(\rho(y) - \rho(x)\big)dy. \quad (6.3)$$

Thus we obtain parabolic equation (6.1) with a convolution operator on the right-hand side.

Notice that correlation functions in the contact model, as well as in other models of the population dynamics, need not vanish at infinity. Thus to study the behaviour of correlation functions we have to consider the Cauchy problem for evolution equations (6.1)–(6.3) in the classes of functions that satisfy suitable growth conditions at infinity. Then the information about the point-wise asymptotics or two-sided bounds of the corresponding fundamental solution becomes very important not only in the region where the central limit theorem applies but also in other space-time regions.

In this note we compare the large time behaviour of the fundamental solutions of problem (6.1)–(6.3) with that of the classical Gaussian heat kernel.

We also make a similar comparison of the Gaussian heat kernel and the fundamental solution of evolution equations with a fractional time derivative.

An essential part of the estimates used in this note is borrowed from our previous works [4] and [7]. However, the lower bounds for the studied fundamental solutions in the region of super-large deviations are new. For these bounds we provide a detailed proof.

2 Convolution type operators

We consider a zero order convolution type operator A in $L^2(\mathbb{R}^d)$, $d \geq 1$, defined by

$$Af(x) = \int_{\mathbb{R}^d} a(x-y)\big(f(y)-f(x)\big)dy,$$

where the convolution kernel a is a non-negative integrable function. If $\int_{\mathbb{R}^d} a(z)\,dz = 1$, then A is the generator of a continuous time Markov jump process with the jump distribution $a(z)$: $Af = a * f - f$. We assume that the convolution kernel $a(\cdot)$ has the following properties:

- ◇ Boundedness
$$a(x) \geq 0, \qquad a(x) \in L^\infty(\mathbb{R}^d) \cap L^1(\mathbb{R}^d). \tag{6.4}$$
- ◇ Symmetry
$$a(x) = a(-x) \quad \text{for all } x \in \mathbb{R}^d. \tag{6.5}$$
- ◇ Normalisation and second moments
$$\int_{\mathbb{R}^d} a(x)dx = 1, \qquad \int_{\mathbb{R}^d} |x|^2 a(x)dx < \infty. \tag{6.6}$$
- ◇ (Super)exponential decay
$$0 \leq a(x) \leq Ce^{-b|x|^p}, \quad \text{with } p \geq 1, b > 0, C > 0, \tag{6.7}$$
we also consider the case of compactly supported $a(x)$.

3 Non-local parabolic problem

We study the large time behaviour of the fundamental solution of the following parabolic problem

$$\begin{aligned} \partial_t u(x,t) &= Au(x,t) = a * u - u, \qquad (x,t) \in \mathbb{R}^d \times (0,+\infty), \\ u(x,0) &= \delta(x). \end{aligned} \tag{6.8}$$

Remark 6.1 Let $\xi^0(t)$ be a continuous time jump Markov process with jump intensity equal to 1 and with jump distribution $a(\cdot)$, and assume that $\xi^0(0)=0$. Then $u(\cdot,t)$ is the law of $\xi^0(t)$.

Since A is a bounded operator in $L^2(\mathbb{R}^d)$ we have

$$e^{tA}=e^{-t}\,e^{ta\star}=e^{-t}\sum_{k=0}^{\infty}t^k\frac{a^{\star k}}{k!}=e^{-t}\mathbb{1}+e^{-t}\sum_{k=1}^{\infty}t^k\frac{a^{\star k}}{k!}$$

and

$$u(x,t)=e^{tA}\delta(x)=e^{-t}\delta(x)+e^{-t}\sum_{k=1}^{\infty}\frac{t^k}{k!}a^{\star k}(x). \tag{6.9}$$

Observe that $u(x,t)$ consists of a singular part at zero $e^{-t}\delta(x)$ and a regular part $v(x,t)\in L^\infty(\mathbb{R}^d)\cap L^1(\mathbb{R}^d)$:

$$v(x,t)=e^{-t}\sum_{k=1}^{\infty}\frac{t^k}{k!}a^{\star k}(x). \tag{6.10}$$

We focus on obtaining point-wise upper and lower bounds for the regular part $v(x,t)$ as $t\to\infty$.

Let us briefly recall some of the existing results on heat kernels. The heat kernel of the classical heat equation in $\mathbb{R}^d$

$$\partial_t g-\Delta g=0,\qquad g|_{t=0}=\delta_x,$$

is given by the Gauss-Weierstrass function

$$g_t(x,y)=\frac{1}{(4\pi t)^{d/2}}\exp\left(-\frac{|x-y|^2}{4t}\right). \tag{6.11}$$

For the heat kernel of a more general parabolic equation $\partial_t g-Lg=0$ with a uniformly elliptic second-order divergence form operator L the well-known Aronson estimates hold, see [1],

$$g_t(x,y)\asymp\frac{C}{t^{d/2}}\exp\left(-\frac{|x-y|^2}{ct}\right).$$

One of the simplest non-local heat equation is

$$\partial_t g+(-\Delta)^{\alpha/2}g=0,\qquad \text{where } 0<\alpha<2.$$

Its heat kernel satisfies the following estimates, see e. g. [2],

$$g_t(x,y)\asymp\frac{C}{t^{d/\alpha}}\left(1+\frac{|x-y|}{t^{1/\alpha}}\right)^{-(d+\alpha)} \tag{6.12}$$

Remark 6.2 Note that $(-\Delta)^{\alpha/2}$ is an integro-differential operator of the form

$$(-\Delta)^{\alpha/2} f(x) = c_{d,\alpha}\, \text{p.v.} \int_{\mathbb{R}^d} \frac{f(x)-f(y)}{|x-y|^{d+\alpha}} dy. \tag{6.13}$$

The heavy tail of the heat kernel in estimate (6.12) is a consequence of slow decay of the integral kernel in (6.13).

4 Asymptotics of $v(x,t)$ as $t \to \infty$

In this section we present results from the paper [4], where the large time behaviour of the fundamental solution to the problem (6.8) has been obtained. This asymptotic behaviour depends crucially on the relation between $|x|$ and t. We consider separately four different regions in the (x,t) space. Namely,

I. $|x| \le r t^{1/2}\big(1+o(1)\big)$ (standard deviations region)

II. $|x| = r t^{1+\delta/2}\big(1+o(1)\big)$, $\delta \in (0,1)$ (moderate deviations region)

III. $|x| = r t\big(1+o(1)\big)$ ($\delta = 1$) (large deviations region)

IV. $|x| = r t^{1+\delta/2}\big(1+o(1)\big)$, $\delta > 1$ ("extra-large" deviations region)

4.1 Normal and moderate deviations region

We begin with the case when x belongs to regions I. or II.

Theorem 6.3 (see [4]) Assume that $a(\cdot)$ satisfies conditions (6.4)–(6.7). Then for the function $v(x,t)$ defined by (6.10) the following asymptotic relation holds as $t \to \infty$:

1) if $|x| \le r t^{1/2}$ for some $r > 0$, then

$$v(x,t) = (2\pi t)^{-d/2}\big(\det(\sigma)\big)^{-1/2}\, e^{-\frac{(\sigma^{-1}x,x)}{2t}}\big(1+o(1)\big) \tag{6.14}$$

with $\sigma^{ij} = \displaystyle\int_{\mathbb{R}^d} x_i x_j\, a(x)\, dx$.

2) if $x = r t^{1+\delta/2}\big(1+o(1)\big)$ with $0 < \delta < 1$ and $r \in R^d \setminus \{0\}$, then the following asymptotic relation holds as $t \to \infty$:

$$v(x,t) = e^{-\frac{(\sigma^{-1}x,x)}{2t}(1+o(1))} = e^{-\frac{1}{2}(\sigma^{-1}r,r)t^{\delta}(1+o(1))}. \tag{6.15}$$

It should be noted that the Gaussian form of the asymptotics (6.14) in the region of standard deviations is the immediate consequence of the local limit theorem for processes with independent increments. Formula (6.14) can also be derived from the asymptotic representation of the corresponding Fourier transform. In the moderate deviations region the asymptotics (6.15) of the fundamental solution still coincide with that in the standard deviations region, but only in the logarithmic order. For the pre-exponential factor we can only state the sub-exponential rate of decay.

4.2 Large deviations region

In order to formulate the result in the region $|x| \sim t$ we should first introduce a number of auxiliary quantities. Let X be a random vector in $\mathbb{R}^d$ with distribution $a(\cdot)$. If condition (6.7) is fulfilled with some $p \geq 1$ then X has finite exponential moment $\Lambda(\gamma) = \mathbb{E}e^{\gamma \cdot X}$ at least for small enough $\gamma \in \mathbb{R}^d$.

We define the cumulant generating function $L(\gamma) = \ln \Lambda(\gamma)$, and introduce $I(r)$, $r \in \mathbb{R}^d$, as its Legendre transform: $I(r) = \sup_{\gamma} \big(\gamma \cdot r - L(\gamma)\big)$, $r, \gamma \in R^d$. Denote by ξ_r a positive solution of the equation

$$\ln \xi = I(\xi r) - \xi r \cdot \nabla I(\xi r), \qquad \xi \in R.$$

Lemma 6.4 Let $a(x)$ satisfy conditions (6.4)–(6.7). Then for any $r \in R^d \backslash \{0\}$ the above equation has a unique solution ξ_r, and $0 < \xi_r < 1$.

Let us define the rate function

$$\Phi(r) = 1 - \frac{1}{\xi_r}\big(1 + \ln \xi_r - I(\xi_r r)\big). \tag{6.16}$$

We introduce now some additional technical conditions on the kernel.

- $(\mathbf{A}_1)$ $p = 1$ and for any $b_1 > b$ and any $\theta \in S^{d-1}$ we have $\mathbb{E}e^{b_1(X,\theta)} = \infty$, where b is the same constant as in (6.7).
- $(\mathbf{A}_1^{\mathbf{s}})$ $p = 1$ and $\mathbb{E}|X|e^{b(X,\theta)} = \infty$ for any $\theta \in S^{d-1}$.
- $(\mathbf{A}_p)$ $p > 1$ and for any $\theta \in S^{d-1}$

$$L(\gamma) = \ln \mathbb{E}e^{\gamma(X,\theta)} = C(b,p)|\gamma|^{p/(p-1)}\big(1 + o(1)\big), \qquad \text{as } |\gamma| \to \infty,$$

where $C(b,p) = \frac{p-1}{p}(bp)^{-1/(p-1)}$ is a constant appearing in the logarithmic asymptotics of the Laplace transform of $e^{-b|x|^p}$.

Remark 6.5 Condition $(\mathbf{A}_p)$, $p \geq 1$, can be treated as a sort of soft lower bound for $a(x)$. In particular, it holds if $a(x)$ satisfies the following two-sided estimate

$$C_0 e^{-b|x|^p} \leq a(x) \leq C_1 e^{-b|x|^p}, \qquad p \geq 1. \tag{6.17}$$

Also, Condition $(\mathbf{A}_p)$ implies that $a(x)$ could not have a bounded support.

Theorem 6.6 (see [4]) Let conditions (6.4)–(6.7) be fulfilled, and assume additionally that in the case $p = 1$ condition $(\mathbf{A}_\mathbf{1}^\mathbf{s})$ holds. Then for $x = rt\big(1+o(1)\big)$ with $r \in R^d \backslash \{0\}$ we have

$$v(x,t) = e^{-\Phi(r)t(1+o(1))} \qquad \text{as } t \to \infty, \tag{6.18}$$

where $\Phi(r)$ is defined by (6.16).

The rate function $\Phi(r)$ possesses the following important properties: Φ is a convex function, $\Phi(0) = 0$, $\Phi(r) > 0$ for $r \neq 0$, and

$$\Phi(r) = \frac{1}{2}\,\sigma^{-1} r \cdot r \,\big(1+o(1)\big), \qquad \text{as } r \to 0; \tag{6.19}$$

$$\Phi(r) \to \infty, \qquad \text{as } r \to \infty. \tag{6.20}$$

If $a(x)$ has a finite support, then

$$\Phi(r) \geq c|r| \ln |r|, \qquad \text{as } |r| \to \infty.$$

Furthermore, if $p = 1$ and condition $(\mathbf{A_1})$ holds, then

$$\Phi(r) = b|r| \,\big(1+o(1)\big), \qquad \text{as } |r| \to \infty; \tag{6.21}$$

if $p > 1$ and condition $(\mathbf{A_p})$ holds, then

$$\Phi(r) = \frac{p}{p-1}\big(b(p-1)\big)^{1/p} |r| \,(\ln |r|)^{\frac{p-1}{p}} \,\big(1+o(1)\big), \qquad \text{as } |r| \to \infty. \tag{6.22}$$

Remark 6.7 It should be also emphasised that in the case $p = 1$ conditions $(\mathbf{A_1})$, $(\mathbf{A}_\mathbf{1}^\mathbf{s})$ are required for proving the main result on the asymptotics of the heat kernel, while in the case $p > 1$ condition $(\mathbf{A}_p)$ is only used for determining the asymptotic behaviour of the function $\Phi(r)$ for large r.

4.3 Extra-large deviations region

In the region $|x| \gg t$ only an upper bound for $v(x,t)$ was obtained in [4].

Theorem 6.8 (see [4]) Assume that $a(x)$ satisfies conditions (6.4)–(6.7). Then for $|x| = rt^{1+\delta/2}\big(1+o(1)\big)$ with $\delta > 1$ and $r \neq 0$ the following asymptotic upper bound holds:

$$v(x,t) \le e^{-c_p t^{\delta+1/2}(\ln t)^{p-1/p}(1+o(1))} \qquad \text{as } t \to \infty, \tag{6.23}$$

where the constant $c_p = c_p(b,r)$ depends on b, r and p. If $a(\cdot)$ has a finite support, then for $|x| = rt^{\delta+1/2}\big(1+o(1)\big)$ with $\delta > 1$ we have

$$v(x,t) \le e^{-\tilde{c} t^{\delta+1/2}\ln t(1+o(1))} \qquad \text{as } t \to \infty,$$

where $\tilde{c}$ depends on r, δ and the support of $a(\cdot)$.

Here, for $a(x)$ satisfying two-sided estimate (6.17), we prove that a similar lower bound holds.

Theorem 6.9 Let Conditions (6.4)–(6.6) be fulfilled, and assume that bound (6.17) holds. Then in the region of "extra-large" deviations with $|x| \gg t$ the following two-sided bound holds for all sufficiently large t:

$$\exp\left\{-\tilde{C}_1|x|\left(\ln\left|\frac{x}{t}\right|\right)^{\frac{p-1}{p}}\right\} \le v(x,t) \le \exp\left\{-\tilde{C}_2|x|\left(\ln\left|\frac{x}{t}\right|\right)^{\frac{p-1}{p}}\right\}. \tag{6.24}$$

Proof. The upper bound in (6.24) is a direct consequence of estimate (6.23). To obtain the lower bound in (6.24) we consider an auxiliary operator

$$\big(\tilde{A}u\big)(x) = \int_{\mathbb{R}^d} C_0\tilde{a}_p(x-y)u(y)dy - C_1\int_{\mathbb{R}^d}\tilde{a}_p(y)dy\cdot u(x),$$

where $\tilde{a}_p(x) = e^{-b|x|^p}$ and C_0, C_1 are the same constants as in (6.17). Let us represent $\tilde{u}(x,t) = e^{t\tilde{A}}\delta(x)$ in the same way as (6.9):

$$\tilde{u}(x,t) = e^{-C_1\alpha_p t}\delta(x) + e^{-C_1\alpha_p t}\sum_{k=1}^{\infty}\frac{(C_0t)^k}{k!}\tilde{a}_p^{\star k}(x),$$

where $\alpha_p = \int_{\mathbb{R}^d}\tilde{a}_p(y)dy$. Thus the regular part of $\tilde{u}(x,t)$ equals to

$$\tilde{v}(x,t) = e^{-C_1\alpha_p t}\sum_{k=1}^{\infty}\frac{(C_0t)^k}{k!}\tilde{a}_p^{\star k}(x), \tag{6.25}$$

and we conclude using (6.17) that $v(x,t) \ge \tilde{v}(x,t)$ for all $x \in \mathbb{R}^d$. Therefore, it suffices to obtain the lower bound in (6.24) for the function $\tilde{v}(x,t)$. To this end we first estimate $\tilde{a}_p^{\star k}(x)$ for $k = \left(\ln\frac{|x|}{t}\right)^{-1/p}|x|$. Divide the one-dimensional segment $[0,x]$ into k equal

parts and denote by z_j, $j=1,\dots,k$, the centers of corresponding subsegments $[r_{j-1},r_j]$, $r_j=\frac{x}{k}j$. Notice that

$$|r_j-r_{j-1}|=\frac{|x|}{k}=\Big(\ln\frac{|x|}{t}\Big)^{1/p}\to\infty \qquad \text{as } t\to\infty.$$

Let $B_1(z)\subset\mathbb{R}^d$ be a ball of the unit volume with the center at z. If $x_j\in B_1(z_j)$, $x_{j-1}\in B_1(z_{j-1})$, then

$$|x_j-x_{j-1}|\le|r_j-r_{j-1}|+2=\frac{|x|}{k}\big(1+o(1)\big).$$

Consequently

$$\tilde a_p^{\star k}(x)\ge\int\limits_{B_1(z_1)}\cdots\int\limits_{B_k(z_k)}e^{-|x_1-x_2|^p-\dots-|x_k-x|^p}dx_1\cdots dx_k\ge e^{-c_1\left(\frac{|x|}{k}\right)^p k} \tag{6.26}$$

with some constant $c_1>0$. Finally keeping in representation (6.25) for $\tilde v(x,t)$ only one term with $k=\big(\ln\frac{|x|}{t}\big)^{-1/p}|x|$ and considering estimate (6.26) we obtain the desired low bound in (6.24). □

5 Time fractional equations

In this section we present results of our work [7] where the asymptotic behaviour of solution $w_\alpha(x,t)$ of the following fractional time parabolic problem has been studied

$$\partial_t^\alpha w_\alpha=a*w_\alpha-w_\alpha,\qquad w_\alpha\big|_{t=0}=\delta_0.$$

Here ∂_t^α is the fractional derivative (the Caputo derivative) of the order α, $0<\alpha<1$, and $a(x)$ is the same convolution kernel as that in Section 2.

As follows from [3] the solution $w_\alpha(x,t)$ admits the following representation in terms of the fundamental solution $u(x,t)$ of a non-local heat equation:

$$w_\alpha(x,t)=\int_0^\infty u(x,r)d_r\mathbb{P}(S_r\ge t)=\int_0^\infty u(x,r)G_t^\alpha(r)dr,$$

here $S=\{S_r,r\ge0\}$ is the α-stable subordinator with the Laplace transform $\mathbb{E}e^{-\lambda S_r}=e^{-r\lambda^\alpha}$, and $G_t^\alpha(r)=d_r\Pr\{V_t^\alpha\le r\}$ is the density of the inverse α-stable subordinator V_t^α. Using the representation for the Laplace transform of V_t^α: $\mathbb{E}e^{-\lambda V_t^\alpha}=E_\alpha(-\lambda t^\alpha)$, E_α is the Mittag-Leffler function, and representation (6.9) for the non-local heat kernel

$$u(x,t)=e^{-t}\delta_0(x)+v(x,t)\qquad\text{with } v(x,t)=\sum_{k=1}^\infty\frac{a^{*k}(x)}{k!}t^k e^{-t}$$

we obtain $w_\alpha(x,t) = E_\alpha(-t^\alpha)\delta_0(x) + p_\alpha(x,t)$, where the regular part of $w_\alpha(x,t)$ equals

$$p_\alpha(x,t) = \sum_{k=1}^{\infty} \frac{a^{*k}(x)}{k!} t^{\alpha k} E_\alpha^{(k)}(-t^\alpha)$$

It turned out that in contrast with the equations studied in Section 4.1 in the case of equations with fractional time derivatives we should divide (x,t) space in 6 regions in order to describe the large time behaviour of the corresponding fundamental solutions. These regions are

- ◇ $|x|$ is bounded;
- ◇ (Subnormal deviations) $1 \ll |x| \ll t^{\frac{\alpha}{2}}$ or equivalently, $|x(t)| \to \infty$ and there exists an increasing function $r(t)$, $r(0) = 0$, $\lim\limits_{t\to\infty} r(t) = +\infty$ such that $r(t) \le |x| \le \big(r(t)+1\big)^{-1} t^{\alpha/2}$ for all sufficiently large t;
- ◇ (Normal deviations) $x = vt^{\alpha/2}\big(1+o(1)\big)$ with an arbitrary $v \in \mathbb{R}^d \setminus \{0\}$;
- ◇ (Moderate deviations) $x = vt^\beta\big(1+o(1)\big)$ with $\frac{\alpha}{2} < \beta < 1$ and $v \in \mathbb{R}^d \setminus \{0\}$;
- ◇ (Large deviations) $x = vt\big(1+o(1)\big)$ with $v \in \mathbb{R}^d \setminus \{0\}$;
- ◇ (Extra large deviations) $|x| \gg t$, i. e. $\lim\limits_{t\to\infty} \frac{|x(t)|}{t} = \infty$.

The main result from [7] is the following point-wise asymptotic formula for $p_\alpha(x,t)$ as $t \to \infty$.

- ◇ If $|x|$ is bounded, then

$$\begin{aligned} \mathsf{c}_- t^{-\alpha/2} \le p_\alpha(x,t) \le \mathsf{c}_+ t^{-\alpha/2} \qquad & \text{if } d = 1, \\ \mathsf{c}_- t^{-\alpha}\log t \le p_\alpha(x,t) \le \mathsf{c}_+ t^{-\alpha}\log t \qquad & \text{if } d = 2, \\ \mathsf{c}_- t^{-\alpha} \le p_\alpha(x,t) \le \mathsf{c}_+ t^{-\alpha} \qquad & \text{if } d \ge 3. \end{aligned}$$

- ◇ If $1 \ll |x| \ll t^{\alpha/2}$, then

$$\begin{aligned} \mathsf{c}_- t^{-\alpha/2} \le p_\alpha(x,t) \le \mathsf{c}_+ t^{-\alpha/2} \qquad & \text{if } d = 1, \\ \mathsf{c}_- t^{-\alpha}\log\frac{t^\alpha}{|x|^2} \le p_\alpha(x,t) \le \mathsf{c}_+ t^{-\alpha}\log\frac{t^\alpha}{|x|^2} \qquad & \text{if } d = 2, \\ \mathsf{c}_- t^{-\alpha}|x|^{2-d} \le p_\alpha(x,t) \le \mathsf{c}_+ t^{-\alpha}|x|^{2-d} \qquad & \text{if } d \ge 3. \end{aligned}$$

◇ If $x = vt^{\alpha/2}\big(1+o(1)\big)$ with $v \in \mathbb{R}^d \setminus \{0\}$, then

$$p_\alpha(x,t) = t^{-\frac{d\alpha}{2}} \int_0^\infty W_\alpha(s)\Psi(v,s)\,ds\,\big(1+o(1)\big), \qquad \text{where}$$

$$\Psi(v,s) = \frac{1}{|\det\sigma|^{1/2}(2\pi s)^{d/2}} \exp\left(-\frac{(\sigma^{-1}v,v)}{s}\right)$$

and $W_\alpha(s)$ is the Wright function that is expressed via the density $G_t^\alpha(r)$ of the inverse subordinator.

◇ If $x = vt^\beta\big(1+o(1)\big)$ with $\alpha/2 < \beta < 1$ and $v \in \mathbb{R}^d \setminus \{0\}$, then

$$p_\alpha(x,t) = \exp\Big\{-K_v t^{2\beta-\alpha/2-\alpha}\big(1+o(1)\big)\Big\}$$

with a constant K_v depending on α and v.

◇ If $x = vt\big(1+o(1)\big)$ with $v \in \mathbb{R}^d \setminus \{0\}$, then

$$p_\alpha(x,t) = \exp\big\{-\mathtt{F}(v)t\big(1+o(1)\big)\big\}.$$

◇ If $|x| \gg t$, then, combining the approach developed in [7] with the statement of Theorem 6.9, we obtain

$$\exp\left\{-\mathtt{c}_-\,|x|\,\left(\log\left|\frac{x}{t}\right|\right)^{p-1/p}\right\} \le p_\alpha(x,t) \le \exp\left\{-\mathtt{c}_+\,|x|\,\left(\log\left|\frac{x}{t}\right|\right)^{p-1/p}\right\}.$$

6 Conclusions

1. Comparing classical heat kernel (6.11) and the regular part of the fundamental solution of the non-local parabolic problem (6.8) we observe that crucial modifications of the Gaussian form of the asymptotics occurs in the region of large deviations, when $x = rt$. It is there, at the distances of order t, that the non-local character of the operator A starts to play an important role. As seen from (6.19), the fundamental solution is still close to the Gaussian function for small r, but it differs essentially from the corresponding Gaussian function for sufficiently large r, see (6.21), (6.22). In the "extra-large" deviations region this difference is further enhanced. It follows from estimate (6.24) that the non-local fundamental solution $v(x,t)$ has more heavy tail at infinity than the classical heat kernel (6.11).
2. Comparing $p_\alpha(x,t)$ and $v(x,t)$ we notice that

- ◇ in the regions of normal and moderate deviations the asymptotics of $p_\alpha(x,t)$ strongly depends on α, and in the region of subnormal deviations it additionally depends on the dimension;
- ◇ in the region of large deviations $|x| \sim t$ the form of the asymptotics of $p_\alpha(x,t)$ is similar to that of $v(x,t)$, however the rate functions are different;
- ◇ in the region of extra large deviations the asymptotic upper bounds for $p_\alpha(x,t)$ and for $v(x,t)$ are the same.

Bibliography

[1] Aronson, D. G.: *Bounds for the fundamental solution of a parabolic equation*, Bull. Amer. Math. Soc. **73**, 890–896 (1967).

[2] Bendikov, A.: *Asymptotic formulas for symmetric stable semigroups*, Expo. Math. **12**, 381–384 (1994).

[3] Chen, Z.-Q., Kim, P., Kumagai, T., Wang, J.: *Heat kernel estimates for time fractional equations*, Forum Math. **30**(5), 1163–1192 (2018).

[4] Grigor'yan, A., Kondratiev, Yu., Piatnitski, A., Zhizhina, E.: *Pointwise estimates for heat kernels of convolution type operators*, Proc. London Math. Soc. **117**(4), 849–880 (2018). dx.doi.org/10.1112/plms.12144.

[5] Kondratiev, Yu., Kutoviy, O., Pirogov, S.: *Correlation functions and invariant measures in continuous contact model*, Infin. Dimens. Anal. Quantum Probab. Relat. Top. **11**(2), 231–258 (2008).

[6] Kondratiev, Yu., Molchanov, S., Pirogov S., Zhizhina E.: *On ground state of some non local Schrödinger operator*, Appl. Anal. **96**(8), 1390–1400 (2017). https://doi.org/10.1080/00036811.2016.1192138.

[7] Kondratiev, Yu., Piatnitski, A., Zhizhina, E.: *Asymptotics of fundamental solutions for time fractional equations with convolution kernels* (2019). https://arxiv.org/abs/1907.08677.

7

Large emissions. Hawking-Penrose black hole model

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Abstract. *We propose a formalism about the large deviations of emissions. As an example we study the large deviations asymptotics for an introduced stochastic version of the Hawking-Penrose black hole model with special attention to the large emission regime. One of our goals is to find the most probable trajectory corresponding to a certain amount of the emission during the time interval.*

1 Introduction

This paper is devoted to applications of the large deviations theory. The large deviations theory is an area of probability theory studying rare events with vanishing positive probability. It means that such an event may occur but very rarely. It can happen as a catastrophic event like an overload of the queueing system or a crisis phenomenon in the

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The researches of E. Pechersky and S. Pirogov were carried out at the Institute for Information Transmission Problems (IITP), Russian Academy of Science. E. Pechersky thanks FAPESP for the financial support via grant 2019/07192-9.

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A. Yambartsev thanks CNPq (grant 301050/2016-3) and FAPESP (2017/10555-0, 2019/07192-9) for the financial support.

economy. Rare events also naturally appear in nature. Perhaps there are processes with a stochastic component in their dynamics such that some rare event drastically changes the behaviour of the process forever.

In this paper, we briefly review our previous results and continue our research on rare large emissions [8]–[7]. In general, the emission can be represented as a function of a base (original) process: the emission counts the occurrence of some set of specific transitions of an original process. Conditioning on a large emission event changes the behaviour of the original process. This change is characterised by a rate function. We study here the rate function for the proposed stochastic version of the Hawking-Penrose black hole model.

2 General settings

Markov processes. Markov processes ξ are the basic object of our studies in this work. The processes are pure jumps on the finite time interval $[0,T]$. We consider the processes having a finite state space $\mathcal{N} = \{0,1,\dots,N\}$. The process paths are right-continuous step functions

$$x \in \mathcal{X}; \quad x\colon [0,T] \to \mathcal{N}.$$

The jumps of any $x \in \mathcal{X}$ are equal to -1 or $+1$ only. We suppose that the corresponding rate transitions can be represented in the following form: for any state $k \in \mathcal{N}$

$$r_+(k,N) = \lambda_N k^{\gamma_+} u_+(k,N)\big(1-\delta(N-k)\big), \tag{7.1}$$

$$r_-(k,N) = \mu_N k^{\gamma_-} u_-(k)\big(1-\delta(k-1)\big), \tag{7.2}$$

where $\delta(m) = 1$ for $m = 0$ and $\delta(m) = 0$ otherwise. The power functions k^{γ_+} and k^{γ_-} describe the main functional part of the intensities of the jumps. Real numbers $\lambda_N > 0$ and $\mu_N > 0$ depend on N only. The functions $u_+(k,N)$ and $u_-(k)$ present some linear dependence on N and k of the intensities. We will restrict ourselves here only to two cases for the functions $u_\pm$: $u_+(k,N) = N-k$ or $u_+(k,N) \equiv 1$, and $u_-(k) = k$ or $u_-(k) \equiv 1$. The multipliers $\big(1-\delta(N-k)\big)$ and $\big(1-\delta(k-1)\big)$ do not allow the process to go out of $\mathcal{N}$.

The rate $r_+(k,N)$ corresponds to the jump $k \to k+1$, and the rate $r_-(k,N)$ corresponds to the jump $k \to k-1$. The infinitesimal operator on the function set $\mathbf{F}$; $f \in \mathbf{F} : \mathcal{N} \to \mathbb{R}$ is

$$\mathbf{L}f(k) = r_+(k,N)\big[f(k+1)-f(k)\big] + r_-(k,N)\big[f(k-1)-f(k)\big]. \tag{7.3}$$

Particle systems. Particle systems are the main interpretation of the studied Markov processes. The particle system is a set $\mathfrak{P}$ of $N = |\mathfrak{P}|$ particles. Each particle $\mathfrak{p} \in \mathfrak{P}$ can be in one of two states from $S = \{0,1\}$. Let $s_{\mathfrak{p}} \in S$ be the state of the particle $\mathfrak{p}$. The state $s_{\mathfrak{p}} = 0$ is a *ground state* of the particle $\mathfrak{p}$. The state $s_{\mathfrak{p}} = 1$ is an *excited* state of the particle. The state $s_{\mathfrak{p}}$ of any particle is random variable changing over time, $s_{\mathfrak{p}} \equiv s_{\mathfrak{p}}(t)$. For this settings, the values of the Markov process ξ are the number of the excited particles

$$\xi(t) = \sum_{\mathfrak{p}\in\mathfrak{P}} s_{\mathfrak{p}}(t).$$

The physical terminology is commonly used in order to characterise the particle state. This terminology is related to the energy of the system. However, in our example of the stochastic version of the black hole, the state of a particle will be interpreted in other terms: the excited state 1 means that the particle is located inside of the black hole, and the ground state 0 means that the particle is out of the black hole.

Large deviations. Our aim is to study an emission of the particle system. More exactly, we would like to understand behaviour of the probability of the large emission on the interval $[0,T]$. The emissions in terms of the process $\xi(t)$ are negative jumps of the process: the emission occurs at the moment $\tau \in [0,T]$ means that $\xi(\tau) - \xi(\tau - 0) = -1$.

We introduce a process $\eta(t), t \in [0,T]$, of the emissions in the following way. Let

$$\Theta_-(t) = \{t_i : \ t_i \le t \text{ and } \xi(t_i) - \xi(t_i - 0) = -1\}$$

be the set of the time instances of the emissions during $[0,t]$, $t \le T$. Then

$$\eta(t) = |\Theta_-(t)| \tag{7.4}$$

is the number of the emissions occurred during $[0,t]$. The process $\eta(t)$ takes its values in $\mathbb{Z}_+$ and it is the monotone increasing process. Further, we consider the pair $\big(\xi(t), \eta(t)\big)$ of dependent processes. The infinitesimal generator of the joint process is

$$\mathbf{L}^r f(k,m) = r_+(k,N)\big[f(k+1,m) - f(k,m)\big] + r_-(k,N)\big[f(k-1,m+1) - f(k,m)\big], \tag{7.5}$$

where $k \in \mathcal{N}, m \in \mathbb{Z}_+$.

The large emission, which we study, is the event

$$\big\{\eta(T) \ge \widetilde{B}T\big\}, \tag{7.6}$$

where $\widetilde{B} > 0$ is large. The event (7.6) is a rare event arising during stochastic dynamics of the processes $\big(\xi(t), \eta(t)\big)$. The study of rare events is the subject of the large devia-

tions theory. The answer which can be obtained by this theory has an asymptotic form. Therefore instead of one process, a sequence of scaled processes is considered, where the sequence is defined by a scaling parameter connected to the original process. In the large deviation theory, the probabilities of the rare events are being found asymptotically under the scaling parameter. We will take as the scaling parameter for our case the number N of the particles in the system.

Therefore we will consider the scaled version of our problem where the scaling is taken by growing N, $N \to \infty$. The scaled processes are

$$\big(\xi_N(t), \eta_N(t)\big) = \left(\frac{\xi(t)}{N}, \frac{\eta(t)}{N}\right). \tag{7.7}$$

The jumps of $\xi_N(t)$ are $\pm\frac{1}{N}$ and the jumps of $\eta_N(t)$ are equal to $\frac{1}{N}$.

The intensities of the processes $\big(\xi_N(t), \eta_N(t)\big)$ are as follows

$$R_+\left(\frac{k}{N}, N\right) = \lambda_N N^{\gamma_+ + \mathrm{e}_+} u_+\left(\frac{k}{N}, 1\right)\left(\frac{k}{N}\right)^{\gamma_+}\left(1 - \delta\left(1 - \frac{k}{N}\right)\right),$$
$$R_-\left(\frac{k}{N}, N\right) = \mu_N N^{\gamma_- + \mathrm{e}_-} u_-\left(\frac{k}{N}\right)\left(\frac{k}{N}\right)^{\gamma_-}\left(1 - \delta\left(\frac{k-1}{N}\right)\right),$$

where

$$\mathrm{e}_+ = \begin{cases} 1, \text{ if } u_+(k,N) = N-k, \\ 0, \text{ if } u_+(k,N) \equiv 1, \end{cases} \qquad \mathrm{e}_- = \begin{cases} 1, \text{ if } u_+(k) = k, \\ 0, \text{ if } u_+(k) \equiv 1. \end{cases} \tag{7.8}$$

It is convenient to put $\widetilde{B} = NB$ in the scaled version of the system, where $B > 0$ is large enough. The large emission $\widetilde{B}$ is large if NB is large which is the same as large N. In terms of the scaled processes the event (7.6) is

$$\big\{\eta_N(T) \geq BT\big\}, \tag{7.9}$$

where B is large enough.

The theory of the large deviations also allows to extract a large deviation path of the process which produces the given deviation of the large emissions during the interval $[0,T]$. We apply the large deviations theory in a topological space of paths $\mathbf{F}_2 : \mathbb{D} \to \mathbb{R}$ on $[0,T]$, where $\mathbb{D} = [0,1] \times \mathbb{R}_+$. The paths $\big(\mathbf{x}(\cdot), \mathbf{y}(\cdot)\big) \in \mathbf{F}_2$ satisfy the following conditions

1) the paths $\big(\mathbf{x}(\cdot), \mathbf{y}(\cdot)\big)$ are real-valued right-continuous paths defined on $[0,T]$ with left-hand limits;

2) the path $\mathbf{y}(\cdot)$ is non-negative and non-decreasing;

3) a topology in $\mathbf{F}_2$ is defined by Lindvall metric ([1]).

The theory of large deviations allows one to solve both mentioned tasks: to find the asymptotics of the large emission probability as $N \to \infty$ as well as the path of the dynamics that realises the large deviation on the interval $[0,T]$. Solving these problems by the method of large deviations we follow constructions and results in [3].

Further, we assume that

$$\lim_{N\to\infty} \lambda_N N^{\gamma_+ + e_+ - 1} = \lambda^R, \qquad \lim_{N\to\infty} \mu_N N^{\gamma_- + e_- - 1} = \mu^R,$$

where $\lambda^R > 0$ and $\mu^R > 0$ are parameters of the model.

For any $x \in (0,1)$, sequences of integers k such that $\frac{k}{N} \to x$ as $N \to \infty$ then

$$\begin{aligned} R_+(x) &:= \lim_{N\to\infty} R_+\left(\frac{k}{N}, N\right) = \lambda^R u_+(x) x^{\gamma_+}, \\ R_-(x) &:= \lim_{N\to\infty} R_-\left(\frac{k}{N}, N\right) = \mu^R u_-(x) x^{\gamma_-}. \end{aligned} \tag{7.10}$$

The *principle of the large deviations* introduced by Varadhan is a basic construction of the large deviations theory (see [10]). To have the large deviations principle means to know a *rate function* I. In our case it is the function $I : \mathbb{D} \to \mathbb{R}_+$, which has the following integral functional form

$$I(\mathbf{x},\mathbf{y}) = \int_0^T \sup_{\varkappa_1,\varkappa_2} \left(\varkappa_1 \dot{\mathbf{x}} + \varkappa_2 \dot{\mathbf{y}} - R_+(\mathbf{x})[e^{\varkappa_1} - 1] - R_-(\mathbf{x})[e^{-\varkappa_1+\varkappa_2} - 1]\right) \mathrm{d}t. \tag{7.11}$$

The function $\mathbf{x} : [0,T] \to [0,1]$ is a density of excited particles, the non-decreasing function $\mathbf{y} : [0,T] \to \mathbb{R}_+$ is the dynamics of the emissions. The functions $\varkappa_1$ and $\varkappa_2 : [0,T] \to \mathbb{R}$ are dual variables to $\mathbf{x}$ and $\mathbf{y}$ accordingly.

Generally speaking, the functions $\mathbf{x}$ and $\mathbf{y}$ from $\mathbf{F}_2$ can be discontinuous. However, the rate function I in (7.11) has finite values on the absolutely continuous $\mathbf{x}$ and $\mathbf{y}$ only.

Main information on the rare events is contained in the rate function I, (7.11). According to the large deviations theory, we can estimate the probability of the event (7.9) by the rate function as the following

$$\lim_{N\to\infty} \frac{1}{N} \ln \Pr(\eta_N \geq BT) = -\inf_{(x,y)\in\mathscr{B}} I(\mathbf{x},\mathbf{y}), \tag{7.12}$$

where $\mathscr{B} = \{(\mathbf{x},\mathbf{y}) : \mathbf{y}(0) = 0, \mathbf{y}(T) = BT\}$ is a set of the paths describing the event (7.9). If we have found a path $(\mathbf{x}_B, \mathbf{y}_B)$ such that

$$I(\mathbf{x}_B, \mathbf{y}_B) = \inf_{(\mathbf{x},\mathbf{y})\in\mathscr{B}} I(\mathbf{x},\mathbf{y}) \tag{7.13}$$

then this path is a mean path of a conditioned process under the event (7.9).

Remark that expression (7.12) holds only if

$$\inf_{(\mathbf{x},\mathbf{y})\in\mathscr{B}^o} I(\mathbf{x},\mathbf{y}) = \inf_{(\mathbf{x},\mathbf{y})\in\overline{\mathscr{B}}} I(\mathbf{x},\mathbf{y}), \tag{7.14}$$

where $\mathscr{B}^o$ is interior and $\overline{\mathscr{B}}$ is closure of $\mathscr{B}$. If (7.14) does not hold we only obtain bounds for $\lim_{N\to\infty} \frac{1}{N} \ln \Pr(\eta_N \geq BT)$.

The rate function (7.11) is Legendre transform of the Hamiltonian

$$H(\mathbf{x},\mathbf{y},\varkappa_1,\varkappa_2) = R_+(\mathbf{x})[e^{\varkappa_1} - 1] + R_-(\mathbf{x})[e^{-\varkappa_1+\varkappa_2} - 1]. \tag{7.15}$$

If the pair $(\mathbf{x}_B, \mathbf{y}_B)$ satisfies (7.13), then it is a solution of the Hamiltonian system

$$\begin{cases} \dot{\mathbf{x}} = \dfrac{\partial H}{\partial \varkappa_1} = R_+(\mathbf{x})\exp\{\varkappa_1\} - R_-(\mathbf{x})\exp\{-\varkappa_1+\varkappa_2\}, \\ \dot{\mathbf{y}} = \dfrac{\partial H}{\partial \varkappa_2} = R_-(\mathbf{x})\exp\{-\varkappa_1+\varkappa_2\}, \\ \dot{\varkappa}_1 = -\dfrac{\partial H}{\partial x} = -R'_+(\mathbf{x})[e^{\varkappa_1} - 1] - R'_-(\mathbf{x})[e^{-\varkappa_1+\varkappa_2} - 1], \\ \dot{\varkappa}_2 = -\dfrac{\partial H}{\partial y} = 0, \end{cases} \tag{7.16}$$

where $R'_\omega(x), \omega \in \{+,-\}$ is the derivative over x.

To find $(\mathbf{x}_B, \mathbf{y}_B)$, (see (7.13)) we have to solve this system under suitable boundary conditions. For the considered cases, the boundary conditions are $\mathbf{y}(0) = 0,\ \mathbf{y}(T) = BT$ and arbitrary $\mathbf{x}(0) = x_0$.

In many cases when $R_+(x)$ and $R_-(x)$ depend on x, finding the solution is a rather difficult problem. Peculiar properties of the system can facilitate the search of the solutions. These facilitating properties are that the right sides of every equation do not depend on y and that $\varkappa_2$ is a constant.

A general property of the solutions is in the following equation followed from (7.16)

Lemma 7.1

$$\frac{\mathrm{d}}{\mathrm{d}t} \ln \dot{\mathbf{y}} = (\dot{\mathbf{x}} + \dot{\mathbf{y}}) \frac{\mathrm{d}}{\mathrm{d}x} \ln \big(R_+(\mathbf{x}) R_-(\mathbf{x})\big) - R'_+(\mathbf{x}) - R'_-(\mathbf{x}). \tag{7.17}$$

Proposition 7.2 If $\mathbf{x}$ is constant, then $\mathbf{y}$ is linear on $[0,T]$.

For the next proposition denote $A(\mathbf{x}) = \frac{\mathrm{d}}{\mathrm{d}x} \ln \big(R_+(\mathbf{x})R_-(\mathbf{x})\big)$ and $C(\mathbf{x}) = B \cdot \frac{\mathrm{d}}{\mathrm{d}x} \ln \big(R_+(\mathbf{x})R_-(\mathbf{x})\big) - R'_+(\mathbf{x}) - R'_-(\mathbf{x})$.

Proposition 7.3 If $\dot{\mathbf{y}} = B$, then the solution of (7.17) in the form $\mathbf{x}(t) \equiv x_0$, $\mathbf{y}(t) = Bt$ exists, where x_0 is a root of the equation $C(x) = 0$.

3 Hawking-Penrose black hole

In this section, we apply the general settings described above to the Hawking-Penrose black hole model. The goal here is to investigate of the large emissions of the black hole. This model is one of the earliest and simplest descriptions of Schwarzschild black hole (see [4, 9]). The black hole both emits and absorbs the matter. The absorption is the result of the gravitation, and the emission is the result of the Hawking radiation.

The model we propose is as follows. There is the *Universe* composed by a finite piece of a space and a matter in the space. The matter is a finite set $\mathfrak{P}$ of particles. Some part of Universe space is a specific area which is called the *black hole*. Some portion $\mathfrak{P}_1 \subseteq \mathfrak{P}$ of the particles of the matter is located in the black hole. The remaining portion $\mathfrak{P}_2 = \mathfrak{P} \setminus \mathfrak{P}_1$ is located in the Universe outside the black hole. The Schwarzschild black hole has the shape of a ball. The radius of the ball is proportional to the number of the particles in $\mathfrak{P}_1$.

There is a dynamic of the particles between the parts $\mathfrak{P}_1$ and $\mathfrak{P}_2$.

We construct a stochastic dynamic of the particle jumps between $\mathfrak{P}_1$ and $\mathfrak{P}_2$. The particle jumps are described by a Markov process. The change of the particle number in the black hole that is of the set $\mathfrak{P}_1$, changes the radius of the black hole. One of the features of this stochastic dynamic is that the surface value of the black hole affects the laws of the jumps thereby determining the properties of the Markov processes. In physics, this feature is explained by the so-called *holographic principle* which means that the black hole surface (*horizon*) contains all the information about the black hole state. Our main interest is the big emission of the black hole, that is the large number of jumps $\mathfrak{P}_1 \to \mathfrak{P}_2$.

Formal descriptions: Markov process. The dynamics of the particles between the sets $\mathfrak{P}_1$ and $\mathfrak{P}_2$ is defined by a Markov process $\xi(t)$, where the value of $\xi(t)$ is number of the particles in the set $\mathfrak{P}_1$, $\xi(t) = |\mathfrak{P}_1|$. We consider the jump dynamics on the finite interval $[0,T]$ driven by the Markov process $\xi(t)$ taking its values in $\mathcal{N} \setminus \{0\} = \{1,\dots,N\}$. It

means that the number of the particle in Universe is N. Here we exclude the point 0 from the state space $\mathcal{N}$. It means that the black hole contains at least one particle, and does not disappear.

As in the general setting described above, the jumps of the process are $+1$ or -1. The jump $+1$ means the increment of the set $\mathfrak{P}_1$ (the matter in the black hole) by one particle, and -1 is the decrement of the same set by one particle.

The intensities of the jumps of ξ depend on the size of the horizon, which in turn depends on the amount of matter in the black hole. Let $\xi(t) = k, t \in [0,T]$, that is k particles are located in the black hole at the moment t. Then the jump intensities are

$$r_+(k,N) = \lambda_N k^2 (N-k)\big(1-\delta(N-k)\big),$$
$$r_-(k,N) = \mu_N k^{-2}\big(1-\delta(k-1)\big),$$

(cf. (7.1) and (7.2)).

For studying the large emission from the black hole, we introduce the process $\eta(t)$ (see (7.4)) as described in the section *Large deviations*. Next, we have to study the scaled version of the processes

$$\big(\xi_N(t), \eta_N(t)\big) = \left(\frac{\xi(t)}{N}, \frac{\eta(t)}{N}\right)$$

(see (7.7)). The intensities of the scaled version of the processes are

$$R_+(x) = \lim_{N\to\infty} R_+\left(\frac{k}{N}, N\right) = \lambda^R x^2 (1-x),$$
$$R_-(x) = \lim_{N\to\infty} R_-\left(\frac{k}{N}, N\right) = \mu^R x^{-2},$$

assuming that $k/N \to x \in (0,1)$.

According the general settings of Section 2, we obtain the rate function

$$I(\mathbf{x},\mathbf{y}) = \int_0^{\mathscr{T}} \sup_{\varkappa_1(t),\varkappa_2(t)} \Big\{ \varkappa_1(t)\dot{\mathbf{x}}(t) + \varkappa_2(t)\dot{\mathbf{y}}(t) - \lambda^R \mathbf{x}^2(t)(1-\mathbf{x}(t))[e^{\varkappa_1(t)}-1] - \mu^R \tfrac{1}{\mathbf{x}^2(t)}[e^{-\varkappa_1(t)+\varkappa_2(t)}-1] \Big\} \mathrm{d}t, \tag{7.18}$$

where $\mathbf{x}(t)$ is a density of the particles in the black hole at the moment $t \in [0,T]$, and $\mathbf{y}(t)$ is a path of the particle emission on the interval $[0,T]$ which means the number of the particles emitted on the interval $[0,t]$.

As in the general case, the rate function is Legendre transform of the Hamiltonian

$$H(\mathbf{x},\mathbf{y},\varkappa_1,\varkappa_2)=\lambda^R\mathbf{x}^2(1-\mathbf{x})[e^{\varkappa_1}-1]+\mu^R\mathbf{x}^{-2}[e^{-\varkappa_1+\varkappa_2}-1].$$

In order to find the probability $\Pr\big(\eta_N(T)\geq BT\big)$, and an optimal path $\big(\mathbf{x}_B(\cdot),\mathbf{y}_B(\cdot)\big)$ on $[0,T]$, we have to find a solution of the equation system with suitable boundary conditions.

$$\begin{cases} \dot{\mathbf{x}}= \dfrac{\partial H}{\partial\varkappa_1}=\lambda(1-\mathbf{x})\mathbf{x}^2\exp\{\varkappa_1\}-\mu\frac{1}{\mathbf{x}^2}\exp\{-\varkappa_1+\varkappa_2\},\\ \dot{\mathbf{y}}= \dfrac{\partial H}{\partial\varkappa_2}=\mu\frac{1}{\mathbf{x}^2}\exp\{-\varkappa_1+\varkappa_2\},\\ \dot{\varkappa}_1=-\dfrac{\partial H}{\partial x}=-\lambda\big(2(1-\mathbf{x})\mathbf{x}-\mathbf{x}^2\big)[e^{\varkappa_1}-1]+\mu\frac{2}{\mathbf{x}^3}[e^{-\varkappa_1+\varkappa_2}-1],\\ \dot{\varkappa}_2=-\dfrac{\partial H}{\partial y}=0, \end{cases} \tag{7.19}$$

These solutions are extremals of the integral functional (7.18). We need the solution which finds the extremal hitting the infimum of (7.12). The event $\mathscr{B}$ defines the corresponding boundary conditions. That is $\mathbf{y}(0)=0$, $\mathbf{y}(T)=BT$ and $\mathbf{x}(0)=x_0$ is chosen such that it gives the minimum of (7.18).

The solution of (7.19) under prescribed boundary conditions is a rather difficult problem because of the high non-linearity of the system.

We find the extremal determining a solution $\big(\mathbf{x}_B,\mathbf{y}_B\big)$, where $\mathbf{x}_B$ is a constant and $\mathbf{y}_B$ is a linear function, (see Propositions 7.2 and 7.3). It means that the corresponding conditional processes (ξ_N,η_N) considered at large N has its average values $\mathbf{x}_B$ and $\mathbf{y}_B$.

Definition 7.4 For a constant $B>0$, the path $(\mathbf{x}_B(t),\mathbf{y}_B(t))$ is called a *stationary emission regime* if

1) there is a constant x_B such that $\mathbf{x}_B(t)\equiv x_B$, for all $t\in[0,T]$,

2) $\mathbf{y}_B(t)=Bt$, for all $t\in[0,T]$,

3) the path $\big(\mathbf{x}_B(t),\mathbf{y}_B(t)\big)$ are extremal of I with the boundary conditions $\mathbf{x}_B(0)=\mathbf{x}_B(T)=x_B$ and $\mathbf{y}_B(0)=0$, $\mathbf{y}_B(T)=BT$.

According the above definition of stationary emission regime, using Propositions 7.2 and 7.3 we obtain the following theorem [8].

Theorem 7.5 For any $B > 0$, there exists a constant x_B such that the paths $\mathbf{x}(t) \equiv x_B$, $\mathbf{y}(t) = Bt$ realise the stationary emission regime. We have $x_B \to 0$ as $B \to \infty$ with the asymptotics

$$x_B \sim \left(\frac{2\mu}{B}\right)^{\frac{1}{3}}.$$

Bibliography

[1] Billingsley, P.: *Convergence of probability measures*, Second edition, John Wiley and Sons, Inc., (1999).

[2] van Enter, A. C. D., Fernandez, R., den Hollander, F., Redig, F.: *A large-deviation view on dynamical Gibbs-non-Gibbs transitions*, Mosc. Math. J. **10**(4), 687–711, (2010).

[3] Feng, J., Kurtz, T. G.: *Large deviations for stochastic processes*, AMS, (2006).

[4] Hawking, S.W.: *Particle creation by black holes*, Commun. Math. Phys. **43**(3), 199–220, (1975).

[5] Pechersky, E., Pirogov S., Schütz, G. M., Vladimirov, A., Yambartsev, A.: *Large emission regime in mean field luminescence*, Mosc. Math. J. **19**(1), 107–120, (2019).

[6] Pechersky, E., Pirogov S., Schütz, G. M., Vladimirov, A., Yambartsev, A.: *Large fluctuations in two-level systems with stimulated emission*, Theoret. and Math. Phys. **198**(1), 118–128, (2019).

[7] Pechersky, E., Pirogov, S., Schütz, G. M., Vladimirov, A., Yambartsev, A.: *Large fluctuations of radiation in stochastically activated two-level systems*, J. Phys. A, Math. Theor. **50**(45), 455203, (2017).

[8] Pechersky, E., Pirogov S., Yambartsev, A.: *Hawking-Penrose black hole model. Large emission regime*, Preprint arXiv:1906.08309, (2019).

[9] Penrose, R.: *Singularity and time-asymmetry*, in General relativity: an Einstein centenary survey, eds Israel, Hawking, Cambridge, 581–638, (1979).

[10] Varadhan, S. S.: *Asymptotic probabilities and differential equations*, Commun. Pure Appl. Math. **19**(3), 261–286, (1966).

8

On an approximation of 2-D stochastic Navier-Stokes equations

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Abstract. *We describe a full-discrete explicit approximation scheme for the process solution of the two-dimensional incompressible stochastic Navier-Stokes equations driven by additive noise with periodic boundary conditions. We focus on the properties which play a role in the proof of the strong convergence towards the mild solution of the equation.*

1 Introduction

Often (stochastic) evolution equations, such as stochastic Navier-Stokes equations, are mathematical models for dynamics and phenomena in physics. Therefore, the simulation of the solutions with implementable approximation schemes has become of great interest. The approximations should converge in some sense and possibly reflect the behaviour of the solutions. A *strongly convergent* scheme (i. e., in mean square) "respects", for instance, the mean of the process.

In general terms, the explicit and the linear-implicit Euler schemes do not converge strongly to the solutions of many stochastic evolution equations (see e. g. [7, Theorem 2.1]) and convergent implicit schemes have higher computational costs (for more details see, e. g. [8]). Therefore recently, different versions of the Euler method have

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been proven to converge strongly for (specific cases of) evolution equations. The techniques are different according to the specificity of the coefficients and the dimension: truncation of the drift, taming, etc.

In the case of two-dimensional stochastic Navier-Stokes equations driven by additive or multiplicative noise, several existence and uniqueness results and (strongly) convergent approximation schemes are available. We refer to [4] and references therein for existence and uniqueness results and an overview on numerical approximations such as the strong convergent ones in [5] (in the additive noise case). Other relevant strongly convergent schemes are the fully implicit and also the semi-implicit Euler schemes introduced in [3] and the splitting scheme of [1]. This list is far from extensive. We refer for instance to the introduction of the recent article [6] for a state-of-the-art summary.

In this article we describe an *explicit full-discrete non-linearity-truncated accelerated exponential Euler-type scheme* (DTAEE scheme, see Equation (8.5) below) which has been proven in [11] to converge strongly to the *mild solutions*[1] of the two-dimensional incompressible stochastic Navier-Stokes equations on the torus driven by some trace class noise in Equation (8.3). We focus on the description of the approximation scheme stressing the properties leading to the already mentioned strong convergence result. The contribution of this document is therefore a deeper insight on the properties of the DTAEE scheme.

This paper is organised as follows: We first introduce the stochastic Navier-Stokes equations under consideration (see Section 2). In Section 3 we focus on the numerical approximation scheme DTAEE. Finally in Section 3.2 we comment on the strong convergence of the approximation towards the solution.

2 The framework: 2-D stochastic Navier-Stokes equations

2.1 The 2-D stochastic Navier-Stokes equations with periodic boundary conditions on the torus and trace class noise

Let $T \in (0,\infty)$, let $\lambda_{(0,1)^2}$ denote the Lebesgue measure on $(0,1)^2$, and let $H_0 \subset H_1 \subset H \subset L^2(\lambda_{(0,1)^2};\mathbb{R}^2)$ be appropriate Hilbert subvector spaces of the Hilbert space $L^2(\lambda_{(0,1)^2};\mathbb{R}^2)$

[1] Weaker notion of solution with respect to the classical strong and weak one: any strong/weak solution is also a mild solution.

to be precised in Section 2.2. In particular, H is the separable Hilbert space having an orthonormal basis consisting of divergence-free functions with periodic boundary. Let P be the projection on H of elements of $L^2(\lambda_{(0,1)^2};\mathbb{R}^2)$, and let W be an Id_H-cylindrical Wiener process.

Let $\varepsilon_0, \varepsilon \in (0,\infty)$ and $\xi \in H_0$. It is known that the process $X\colon [0,T]\times\Omega \to H_1$ satisfying for all $t \in [0,T]$ that $\mathbb{P}$-a.s.

$$X_t = \mathrm{e}^{tA}\xi + \int_0^t \mathrm{e}^{(t-s)A}\big(F(X_s) + \varepsilon_0 X_s\big)\,ds + \int_0^t \mathrm{e}^{(t-s)A}(-A)^{-1/2-\varepsilon}\,dW_s \tag{8.1}$$

is a *mild solution* to the following stochastic partial differential equation

$$\begin{cases} dX_t(x) = \big(\Delta X_t(x) + F\big(X_t\big)(x)\big)dt + (-A)^{-1/2-\varepsilon}\,dW_t(x), \quad x \in (0,1)^2, t \in [0,T], \\ \quad X_0 = \xi \in H_0, \end{cases} \tag{8.2}$$

with *incompressibility* (i. e. divergence-free) condition $\operatorname{div} X_t = 0$ and where $A = \Delta - \varepsilon_0$, Δ is the Laplacian with periodic boundary conditions, and $F(X_s) = c_1 X_s + c_2 P(-\nabla X_s \cdot X_s)$ with $c_1, c_2 \in \mathbb{R}$.

This is a two-dimensional stochastic Navier-Stokes equations on the torus $(0,1)^2$ with periodic boundary conditions driven by some trace class noise. Indeed $(-A)^{-1/2-\varepsilon}$, $\varepsilon \in (0,\infty)$ is a Hilbert-Schmidt operator, so we are actually considering as noise a Wiener process on the Hilbert space H with covariance matrix $(-A)^{-1-2\varepsilon}$. Note that we could change the noise and/or the operator A up to a multiplicative constant, or consider a more regular noise. For simplicity, from now on, we take $c_1 = -\varepsilon_0$, $c_2 = 1$. Hence the mild solution (8.1) rewrites

$$X_t = \mathrm{e}^{tA}\xi + \int_0^t \mathrm{e}^{(t-s)A}P(-\nabla X_s \cdot X_s)\,ds + \int_0^t \mathrm{e}^{(t-s)A}(-A)^{-1/2-\varepsilon}\,dW_s. \tag{8.3}$$

To conclude, note that the mild solution expresses the process as a stochastic evolution equation. The right-hand side of equation is the sum of a Bochner integral, resulting from the convolution of the semigroup and the non-linearity, with a stochastic integral which is the noise part, also called the *stochastic convolution* process.

2.2 The state space

Let us now construct the Hilbert space of square-integrable divergence-free functions with periodic boundary conditions $H \subset L^2(\lambda_{(0,1)^2};\mathbb{R}^2)$. (Recall that $\lambda_{(0,1)^2}$ denotes the Lebesgue measure on $(0,1)^2$).

For all $k \in \mathbb{Z}$ let $\varphi_k \in C\big((0,1),\mathbb{R}\big)$ be the function

$$\varphi_k(x) := \mathbb{1}_{\{0\}}(k) + \mathbb{1}_{\mathbb{N}}(k)\sqrt{2}\cos(2k\pi x) + \mathbb{1}_{\mathbb{N}}(-k)\sqrt{2}\sin(-2k\pi x), \qquad x \in (0,1).$$

Let the following elements of $L^2(\lambda_{(0,1)^2};\mathbb{R}^2)$:

$$e_{0,0,0} \equiv (1,0), \qquad e_{0,0,1} \equiv (0,1), \quad \text{and} \quad e_{k,l,0}\colon (x,y) \mapsto \left(\frac{l\varphi_k(x)\varphi_l(y)}{\sqrt{k^2+l^2}}, \frac{k\varphi_{-k}(x)\varphi_{-l}(y)}{\sqrt{k^2+l^2}}\right)$$

for all $k,l \in \mathbb{Z}^2 \setminus \{(0,0)\}$.

Let $H \subseteq U$ be the closed subvector space of $L^2(\lambda_{(0,1)^2};\mathbb{R}^2)$ with orthonormal basis $\mathbb{H} = \{e_{0,0,1}\} \cup \{e_{i,j,0}\colon i,j \in \mathbb{Z}\}$.

In addition consider the eigenvalues of the perturbed Laplace operator $\varepsilon_0 - \Delta$:

$$\lambda_{e_{0,0,1}} = \lambda_{e_{0,0,0}} = \varepsilon_0, \quad \lambda_{e_{k,l,0}} = \varepsilon_0 + 4\pi^2(k^2+l^2), \qquad k,l \in \mathbb{Z}.$$

Note that the operator $\varepsilon_0 - \Delta$ is a diagonal operator on the basis $\mathbb{H}$ with point spectrum $\{\lambda_h\colon h \in \mathbb{H}\}$: for all v in the domain of $(\varepsilon_0 - \Delta)$

$$(\varepsilon_0 - \Delta)v = \sum_{h\in\mathbb{H}} \lambda_h \langle v,h\rangle_H.$$

Let ρ_0, ρ be positive real numbers satisfying $1/2 < \rho_0 < \rho < 1/2 + \varepsilon$, $\gamma \in (\rho,\infty)$, $\kappa \geq 0$ and let H_0, H_1, H_ρ be respectively the domains of the following fractional powers of the operator $(\kappa - \Delta)$: $(\kappa-\Delta)^\gamma$, $(\kappa-\Delta)^\rho$ and $(\kappa-\Delta)^{\rho_0}$. Therefore $\|h\|_{H_1}^2 = \sum_{v\in\mathbb{H}} (\kappa - \varepsilon_0 + \lambda_v)^{2\rho} \langle h,v\rangle^2$ for every $h \in H_1$. For simplicity we take here $\kappa = \varepsilon_0$, hence

$$\|h\|_{H_1}^2 = \sum_{v\in\mathbb{H}} \lambda_v^{2\rho} \langle h,v\rangle^2$$

for every $h \in H_1$.

3 The explicit full-discrete non-linearity-truncated accelerated exponential Euler-type scheme

In this section we will need the following notation: For every $n \in \mathbb{N}$, let $\mathbf{H}_n$ be the finite dimensional subspace of H spanned by

$$\mathbb{H}_n := \{e_{0,0,1}\} \cup \{e_{k,l,0} \colon k,l \in \mathbb{Z} \text{ and } k^2 + l^2 < n^2\} \subseteq \mathbb{H}$$

and $P_n \colon H \to H$ the projection on $\mathbf{H}_n$

$$P_n(u) := \sum_{h \in \mathbb{H}_n} \langle h, u \rangle_H \, h, \quad u \in H.$$

3.1 Step-by-step construction

The DTAEE scheme approximating in the strong sense the mild solution (8.3) can be constructed as follows in several steps. First, one considers a *spectral Galerkin approximation* (see [2]) combined with truncation of the non-linearity, obtaining the approximation scheme (8.4) below. Then one discretises the time, obtaining (8.5) below, and finally one notices that the quantities can be computed explicitly with the known square integrable functions belonging to the orthonormal basis $\mathbb{H}$.

Let $(h_m)_{m \in \mathbb{N}}$ be a sequence of positive real numbers converging to 0 and let P_n be projections on increasing finite dimensional spaces $\mathbf{H}_n \subseteq H_1$ specified in Section 2.2. Let $\mathscr{O}^n, \mathscr{X}^n \colon [0,T] \times \Omega \to \mathbf{H}_n$ be the stochastic processes satisfying for all $n \in \mathbb{N}$, $t \in [0,T]$:

$$\begin{aligned} \mathscr{O}_t^n &= \int_0^t P_n \mathrm{e}^{(t-s)A} (-A)^{-1/2-\varepsilon} \, dW_s + P_n e^{tA} \xi \\ \mathscr{X}_t^n &= \mathscr{O}_t^n + \int_0^t P_n \mathrm{e}^{(t-s)A} \, \mathbb{1}_{\left\{ \| \mathscr{X}^n_{\lfloor s \rfloor_{h_n}} \|_{H_1} + \| \mathscr{O}^n_{\lfloor s \rfloor_{h_n}} \|_{H_1} \leq h_n^{-\chi} \right\}} \big(-\nabla \mathscr{X}^n_{\lfloor s \rfloor_{h_n}} \cdot \mathscr{X}^n_{\lfloor s \rfloor_{h_n}} \big) \, ds \end{aligned} \tag{8.4}$$

$\mathbb{P}$-a.s., where $\chi \in \big(0, \min\{ \frac{1-\rho_0}{5}, \frac{\rho-\rho_0}{3} \}\big)$, $\lfloor t \rfloor_{h_n} := \max\big((-\infty, t] \cap \{0, h_n, -h_n, 2h_n, -2h_n, \ldots\} \big)$ denotes the so-called round-ground function.

The latter scheme is not full-discrete, but the fact that we know precisely how the operator acts on elements of (the orthonormal basis $\mathbb{H}$ of) H yields its fully explicit space-

time discrete version. We call it DTAEE scheme and it is derived by taking for all $n \in \mathbb{N}$ the sequence $\left(\mathscr{X}^n_{(k+1)h_n}\right)_{k\in(-1,T/h_n-1)\cap\mathbb{N}}$ and making explicit the projections P_n.

Let us first consider the time discretisation: For all $n = 1,2,\ldots$, $k \in (-1, T/h_n - 1)\cap\mathbb{N}$ let $\mathbf{X}^n_0 := \mathbf{O}^n_0 := P_n\xi = \sum_{v\in\mathbb{H}_n}\langle v,\xi\rangle v$ and

$$\begin{aligned}
\mathbf{O}^n_{(k+1)h_n} &= \mathrm{e}^{h_nA}\mathbf{O}^n_{kh_n} + \int_{kh_n}^{(k+1)h_n} P_n\mathrm{e}^{((k+1)h_n-s)A}(-A)^{-1/2-\varepsilon}\,dW_s,\\
\mathbf{X}^n_{(k+1)h_n} &= \mathrm{e}^{h_nA}\mathbf{X}^n_{kh_n} + \mathbf{O}^n_{(k+1)h_n} - \mathrm{e}^{h_nA}\mathbf{O}^n_{kh_n}\\
&\quad + \int_{kh_n}^{(k+1)h_n} P_n\mathrm{e}^{((k+1)h_n-s)A}\,\mathbb{1}_{\left\{\|\mathbf{X}^n_{kh_n}\|_{H_1}+\|\mathbf{O}^n_{kh_n}\|_{H_1}\le h_n^{-\chi}\right\}}(-\nabla\mathbf{X}^n_{kh_n}\cdot\mathbf{X}^n_{kh_n})\,ds.
\end{aligned} \tag{8.5}$$

We can explicate further the approximation scheme in (8.5) for two-dimensional stochastic Navier-Stokes equations. Indeed, one of the main features of the scheme (8.4) is that it does not discretise the semigroup and yet a discretisation of the noise part is allowed in the following sense. Let us consider $(\beta^v)_{v\in\mathbb{H}}$ a sequence of independent standard Brownian motions such that the cylindrical Wiener process can be seen as $W = \sum_{v\in\mathbb{H}}\beta^v v$. Let us rewrite the approximation of the noise in (8.5) as

$$\mathbf{O}^n_{(k+1)h_n} = \sum_{v\in\mathbb{H}_n}\left(\mathrm{e}^{-h_n\lambda_v}\langle\mathbf{O}^n_{kh_n},v\rangle + \int_{kh_n}^{(k+1)h_n}\mathrm{e}^{-((k+1)h_n-s)\lambda_v}(\lambda_v)^{-1/2-\varepsilon}\,d\beta^v_s\right)v. \tag{8.6}$$

For every $v\in\mathbb{H}$ it holds that $\int_{kh_n}^{(k+1)h_n}\mathrm{e}^{-((k+1)h_n-s)\lambda_v}(\lambda_v)^{-1/2-\varepsilon}\,d\beta^v_s$ is independent of $\mathbf{O}^n_{kh_n}$ and is distributed as a Gaussian random variable with mean 0 and variance $\frac{1-\mathrm{e}^{-2h_n\lambda_v}}{2\lambda_v^{2(1+\varepsilon)}}$.

The other term can be explicated as follows: $\mathbf{X}^n_{(k+1)h_n} = \sum_{v\in\mathbb{H}_n}\langle\mathbf{X}^n_{(k+1)h_n},v\rangle v$ with

$$\begin{aligned}
\langle\mathbf{X}^n_{(k+1)h_n},v\rangle &= \mathrm{e}^{-h_n\lambda_v}\langle\mathbf{X}^n_{kh_n},v\rangle + \langle\mathbf{O}^n_{(k+1)h_n},v\rangle - \mathrm{e}^{-h_n\lambda_v}\langle\mathbf{O}^n_{kh_n},v\rangle + \frac{1-\mathrm{e}^{-h_n\lambda_v}}{\lambda_v}\times\\
&\quad\times\mathbb{1}_{\left\{\sqrt{\sum_{w\in\mathbb{H}_n}\lambda_w^{2\rho}\langle\mathbf{X}^n_{kh_n},w\rangle^2}+\sqrt{\sum_{w\in\mathbb{H}_n}\lambda_w^{2\rho}\langle\mathbf{O}^n_{kh_n},w\rangle^2}\le h_n^{-\chi}\right\}}\langle-\nabla\mathbf{X}^n_{kh_n}\cdot\mathbf{X}^n_{kh_n},v\rangle.
\end{aligned} \tag{8.7}$$

Note that this is a recursive formulation of the approximation scheme.

Finally note that the scheme in (8.4) and the derived discretised one are adaptations to the specific stochastic Navier-Stokes equation (8.2) of a type of approximation method which have been proven to converge strongly to a large class of infinite-dimensional

stochastic evolution equations with non-globally monotone non-linearity (see e. g. Theorem 3.5 in [10] and references therein). The specific result in the case of (8.2) is discussed in Section 3.2.

3.2 Properties of the approximation scheme

In this section we analyse the properties of the 2-D stochastic Navier-Stokes equations we consider and the DTAEE approximation scheme which yield the following strong convergence result:

Theorem 8.1 (cf. [11]) Let X the mild solution in (8.3), and $\mathscr{X}^n$, $n \in \mathbb{N}$ as in (8.4). Then for all $p \geq 1$

$$\limsup_{n\to\infty} \sup_{s\in[0,T]} \mathsf{E}\big[\|X_s - \mathscr{X}_s^n\|_H^p\big] = 0.$$

This is strong convergence uniform in time. From the statement of the result it is clear that the same convergence holds with the (DTAEE) more explicit version of the scheme (8.5): take $\mathbf{X}_t^n$ to be the process with continuous sample paths obtained, e. g., by interpolation from $\mathbf{X}_{h_n k}^n$ (given in recursive formulation in Equations (8.6)–(8.7)). Indeed, the approximation processes have continuous sample paths which coincide a.s. on a dense countable subset of $[0,T]$.

One of the difficulties in proving the strong convergence follows from the fact that the non-linearity F, although $F \in C(H_\rho, H)$, is not globally Lipschitz. Indeed, it is only Lipschitz on bounded sets: there exists a non-negative real number $\theta \in [0,\infty)$ such that for all $v, w \in H_\rho$ it holds that

$$\|F(v) - F(w)\|_H \leq \theta\big(1 + \|v\|_{H_\rho} + \|w\|_{H_\rho}\big)\|v - w\|_{H_\rho} < \infty$$

(see [11] for the proof). However note that, roughly speaking, the approximation scheme controls the Lipschitz constant by truncating the non-linearity. In other words, the truncation prevents strong divergence (see (8.8) below).

The lack of global Lipschitzianity for the non-linear functional F has been compensated by the fact that the non-linearity satisfies the following coercivity-type condition.

For all $\delta > 0$, $v, w \in H_\rho$ it holds that

$$|\langle v, F(v+w)\rangle_H| \leq \left(\frac{3}{2}\varepsilon_0 + \frac{1}{2\delta}\left[\sup_{x\in(0,1)^2} |\underline{w}(x)|_2^2\right]\right)\|v\|_H^2 + 2\delta\|(\varepsilon_0 - \Delta)^{1/2}v\|_H^2 + \left(\frac{\varepsilon_0}{2}\left[\sup_{x\in(0,1)^2} |\underline{w}(x)|_2^2\right] + \frac{1}{2\delta}\left[\sup_{x\in(0,1)^2} |\underline{w}(x)|_2^4\right]\right),$$

where $\underline{v}, \underline{w}$ are the continuous functions belonging to the equivalence class $v, w \in H_\rho$ which exist by Sobolev's embedding. (See [11] for the proof).

The coercivity-type condition, combined with the Lipschitzianity on bounded sets above and some Gronwall-type argument, yields a-priori estimates for the approximation scheme involving a transformation of the noise part $\mathscr{O}^n$, say $\mathbb{O}^n$ (see e. g. [10, Corollary 2.6]).

To prove the strong convergence based on the mentioned a-priori bounds for $\|\mathscr{X}_t^n\|_H$, one needs to prove suitable exponential integrability properties of the process $\mathbb{O}^n$, related to the uniform norms involved in the coercivity-type condition. More precisely, given $p > 4$, there exists $\eta \in [0,\infty)$ such that $\mathbb{O}_t^n = \int_0^t P_n \mathrm{e}^{(t-s)(A-\eta)}(-A)^{-1/2-\varepsilon} dW_s + P_n \mathrm{e}^{t(A-\eta)}\xi$ and

$$\sup_{m\in\mathbb{N}} \mathsf{E}\left[\int_0^T \exp\left(\int_s^T p\left(\sup_{x\in(0,1)^2} |\mathbb{O}^m_{\lfloor u\rfloor_{h_m}}(x)|^2\right) du\right) \cdot \max\left\{1, \sup_{x\in(0,1)^2} \left|\mathbb{O}^m_{\lfloor s\rfloor_{h_m}}(x)\right|^{2p}, \left\|\mathbb{O}^m_s\right\|_H^p, \int_0^T \left\|\mathscr{O}^m_u + P_m\left(\mathrm{e}^{u(A-\eta)} - e^{uA}\right)\xi\right\|_{H_\rho}^{6p} du\right\} ds\right] < \infty.$$

The proof of this statement (we refer to [11]) is quite technical but kind of natural since the noise is a Gaussian process. Indeed one of the main tools is Fernique's theorem.

The a-priori bounds are then used to prove that the approximation scheme does not explode:

$$\limsup_{n\to\infty} \sup_{t\in[0,T]} \mathsf{E}\left[\|\mathscr{X}_t^n\|_H^p\right] < \infty, \qquad p \geq 1. \tag{8.8}$$

Once obtained these uniform moments bounds for the approximation, it suffices to prove the convergence in probability uniformly in time of $\mathscr{X}^n$ towards the mild solution X in (8.3) to obtain the desired strong convergence uniform in time (see [9, Proposition 4.5]).

The coercivity-type condition satisfied by the drift is not required in the proof of the convergence in probability uniformly in time (based e. g. on [9, Proposition 3.3]). Instead,

local Lipschitzianity and the following convergence for the noise are relevant. It can be easily shown that $\sup_{t\in[0,T]} \mathsf{E}\big[\|O_t - \mathscr{O}_t^n\|_{H_\rho}^p\big]$ converges to 0 for all $p \geq 1$ with an explicit polynomial rate, where the process O denotes the sum of the initial condition and the stochastic convolution in (8.3). This is not surprising either because the approximation of the noise term is essentially Galerkin approximation.

We examined here the properties of the approximation scheme (8.4) relevant for the strong convergence uniform in time towards the mild solution (8.3) of two-dimensional Navier-Stokes equations (8.2). To conclude, we would like to mention that the rate of convergence for this approximation scheme has not been proven yet. Recent results based on some stochastic non-linear integration-by-parts formulas seem promising, but have not yet been exploited in the case of 2-D Navier-Stokes equations.

Bibliography

[1] Bessaih, H., Brzeźniak, Z., Millet, A.: *Splitting up method for the 2D stochastic Navier-Stokes equations*, Stoch. Partial Differ. Equ., Anal. Comput. **2**(4), 433–470 (2014).

[2] Breckner, H.: *Galerkin approximation and the strong solution of the Navier-Stokes equation*, J. Appl. Math. Stochastic Anal. **13**(3), 239–259 (2000).

[3] Carelli, E., Prohl, A.: *Rates of convergence for discretizations of the stochastic incompressible Navier-Stokes equations*, SIAM J. Numer. Anal. **50**(5), 2467–2496 (2012).

[4] Carelli, E.: *Numerical Analysis of the Stochastic Navier-Stokes Equations*, Dissertation zur Erlangung des Grades eines Doktors der Naturwissenschaften, Tübingen (2011).

[5] Dörsek, P.: *Semigroup splitting and cubature approximations for the stochastic Navier-Stokes equations*, SIAM J. Numer. Anal. **50**(2), 729–746 (2012).

[6] Hausenblas, E., Randrianasolo, T. A.: *Time-discretization of stochastic 2-D Navier-Stokes equations with a penalty-projection method*, Numer. Math. **143**(2), 339–378 (2019).

[7] Hutzenthaler, M., Jentzen, A., Kloeden, P. E.: *Strong and weak divergence in finite time of Euler's method for stochastic differential equations with non-globally Lipschitz continuous coefficients*, Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences, The Royal Society (2010).

[8] Hutzenthaler, M., Jentzen, A., Kloeden, P. E.: *Strong convergence of an explicit numerical method for SDEs with nonglobally Lipschitz continuous coefficients* Ann. Appl. Prob., **22**(4), 1611–1641 (2012).

[9] Hutzenthaler, M., Jentzen, A., Salimova, D.: *Strong convergence of full-discrete nonlinearity-truncated accelerated exponential Euler-type approximations for stochastic Kuramoto-Sivashinsky equations*, Commun. Math. Sci. **16**(6), 1489–1529 (2018).

[10] Jentzen, A. and Salimova, D., Welti, T.: *Strong convergence for explicit space-time discrete numerical approximation methods for stochastic Burgers equations*, J. Math. Anal. Appl. **469**(2), 661–704 (2019).

[11] Mazzonetto, S.: *Strong convergence for explicit space-time discrete numerical approximation for 2D stochastic Navier-Stokes equations*, arXiv:1809.01937 (2018).

9

When bounded chaos becomes unbounded

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Abstract. *We consider infinite particle systems with deterministic Newtonian dynamics. Assuming that initial conditions are uniformly bounded, we find examples and general conditions when coordinates and/or velocities remain bounded and when they can grow infinitely in time.*

1 Introduction

Here we present our first results in the field which could be called non-equilibrium deterministic mechanics of infinite systems. We hope that this field can provide a lot of models describing some qualitative phenomena in physical and biological systems. Obviously, the main interesting interaction for such models is Coulomb interaction. However, it remains difficult and as of yet unknown. That is why we use quadratic interaction, which is natural when each particle spends all its time in some potential well. Assuming that initial conditions are uniformly bounded, we find examples and general conditions when the coordinates and velocities remain bounded and when they can grow infinitely in time. Our conclusion is: when the initial deviations from the equilibrium strongly fluctuate,

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then they grow infinitely in time, and when they are sufficiently smooth, they stay uniformly bounded forever. However, we could not get necessary and sufficient conditions for this.

We consider here a countable system of point particles with unit masses on $\mathbb{R}$ with coordinates $\{x_k\}_{k\in\mathbb{Z}}$ and velocities $\{v_k\}_{k\in\mathbb{Z}}$. We define a formal energy (hamiltonian) by the following formula:

$$H = \sum_{k\in\mathbb{Z}} \frac{v_k^2}{2} + \frac{\omega_0^2}{2} \sum_{k\in\mathbb{Z}} \big(x_k(t) - ka\big)^2 + \frac{\omega_1^2}{2} \sum_{k\in\mathbb{Z}} \big(x_k(t) - x_{k-1}(t) - a\big)^2,$$

with parameters $a > 0$, $\omega_1 > 0$, $\omega_0 \geqslant 0$. Particle dynamics is defined by the infinite system of ODE:

$$\ddot{x}_k(t) = -\frac{\partial H}{\partial x_k} = -\omega_0^2\big(x_k(t) - ka\big) + \omega_1^2\big(x_{k+1}(t) - x_k(t) - a\big) - \omega_1^2\big(x_k(t) - x_{k-1}(t) - a\big), \qquad k \in \mathbb{Z} \quad (9.1)$$

with initial conditions $x_k(0)$, $v_k(0)$. The equilibrium state (minimum of the energy) is

$$x_k = ka, \quad v_k = 0, \qquad k \in \mathbb{Z}.$$

This means that if the initial condition is the equilibrium state, then the system will not evolve, i.e. $x_k(t) = ka$, $v_k(t) = 0$ for all $t \geqslant 0$. Let us introduce the deviation variables:

$$q_k(t) = x_k - ka, \qquad p_k(t) = \dot{q}_k(t) = v_k(t).$$

It is easy to see that $q_k(t)$ satisfies the following system of ODE:

$$\ddot{q}_k = -\omega_0^2 q_k + \omega_1^2(q_{k+1} - q_k) - \omega_1^2(q_k - q_{k-1}), \quad k \in \mathbb{Z}. \quad (9.2)$$

The system of coupled harmonic oscillators (9.2) and its generalisations is a classical object in mathematical physics. The existence of a solution and its ergodic properties were studied in [12]. There has been an extensive research on convergence to equilibrium for an infinite harmonic chain coupled with a heat bath ([1, 7, 15, 2]). The property of uniform boundedness of particle coordinates (by time t and index k) is crucial in some applications. For instance, uniform boundedness in finite harmonic chains allows to derive Euler equations and Chaplygin gas without any stochastics (see in [13]). Uniform boundedness of a one-side non-symmetrical harmonic chain plays an important role in some traffic flow models [14]. We should also cite some physical papers [11, 8, 9]. The

most closely related works to our results are [5, 6], where the author studied weighted l_2 norms of infinite harmonic chains, whereas our main interest is a max-norm.

Remark. Proofs of all forthcoming theorems will appear in the second issue of the new journal "Structure of Mathematical Physics", 2020, No. 2.

2 l_2 initial conditions

Introduce the following function spaces on $\mathbb{Z}$:

$$l_\infty := l_\infty(\mathbb{Z}) = \{f : \mathbb{Z} \to \mathbb{R} : \sup_{k\in\mathbb{Z}} |f(k)| < \infty\}, \qquad |f|_\infty = \sup_{k\in\mathbb{Z}} |f(k)|,$$
$$l_2 := l_2(\mathbb{Z}) = \{f : \mathbb{Z} \to \mathbb{R} : \sum_{k\in\mathbb{Z}} |f(k)|^2 < \infty\}, \qquad |f|_2 = \sqrt{\sum_{k\in\mathbb{Z}} |f(k)|^2}.$$

If $q(0)$, $p(0) \in l_2(\mathbb{Z})$, then there exists unique solution $q(t)$, $p(t)$ of (9.2) which belongs to $l_2(\mathbb{Z})$, i.e. $q(t)$, $p(t) \in l_2(\mathbb{Z})$ for all $t \geqslant 0$. This assertion is well known (see [12, 3, 4]), and easily follows from the boundedness of the operator W on $l_2(\mathbb{Z})$:

$$(Wq)_k = -\omega_0^2 q_k + \omega_1^2(q_{k+1} - q_k) - \omega_1^2(q_k - q_{k-1}).$$

The first question of our interest is uniform boundedness (in k and time $t \geqslant 0$) of $|q_k(t)|$. Define the max-norm of $q_k(t)$, $M(t) := \sup_k |q_k(t)|$. We shall say that the system has the property of uniform boundedness, if $\sup_{t\geqslant 0} M(t) < \infty$.

Theorem 9.1 The following assertions hold:

1) If $\omega_0 > 0$, then $\sup_{t\geqslant 0} M(t) < \infty$.

2) If $\omega_0 = 0$,

then we have several results:

a) For all $t \geqslant 0$ the following inequality holds:

$$M(t) \leqslant \frac{2}{\sqrt{\omega_1}} \|p(0)\|_2 \sqrt{t} + \|q(0)\|_2 \tag{9.3}$$

b) Suppose that $\sum_{k\neq 0} |p_k(0)| \ln|k| < \infty$. Then there is constant $c > 0$ such that for all $t \geqslant 0$:

$$M(t) \leqslant \frac{\sqrt{2}}{\omega_1 \pi} |P| \ln(t) + \|q(0)\|_2 + c, \qquad P = \sum_k p_k(0)$$

c) For all $\delta > 1/2$, there exists at least one initial condition $q(0) = 0$, $p(0) \in l_2(\mathbb{Z})$ such that

$$\lim_{t\to\infty} \frac{q_0(t)}{\sqrt{t}} \ln^{\delta} t = \Gamma(\delta) > 0,$$

where Γ is the gamma function.

From case 9.1 a) we see that if $\omega_0 = 0$ and the initial velocities of the particles are all zero, then $|q_k(t)|$ are uniformly bounded. The assertions 9.1 c) is an attempt to answer the question on the accuracy in the basic inequality (9.3) from 9.1 a) with respect to the rate of growth in t.

Next we will formulate theorems concerning asymptotic behavior of $q_k(t)$ in several cases. Define Fourier transform of the sequence $u = \{u_k\} \in l_2(\mathbb{Z})$, $\widehat{u}(\lambda) = \sum_k u_k e^{ik\lambda}$, $\lambda \in \mathbb{R}$. Note that $\widehat{u}(\,\cdot\,) \in L_2([0,2\pi])$, i.e. $\int_0^{2\pi} |\widehat{u}(\lambda)|^2 \, d\lambda = 2\pi \sum_k |u_k|^2 < \infty$.

Further on we will use the Fourier transform of the initial conditions $Q(\lambda) = \widehat{q(0)}(\lambda)$, $P(\lambda) = \widehat{p(0)}(\lambda)$.

For complex valued functions f and g on $\mathbb{R}$ and a constant $c \in \mathbb{C}$ we will write $f(x) \asymp c + \frac{g(x)}{\sqrt{x}}$, if $f(x) = c + \frac{g(x)}{\sqrt{x}} + \bar{\bar{o}}\left(\frac{1}{\sqrt{x}}\right)$ as $x \to \infty$.

Theorem 9.2 ($\omega_0 > 0$) Suppose that $\omega_0 > 0$ and Q, P are of the class $C^n(\mathbb{R})$ for some $n \geqslant 2$. Then

1) For any fixed $t \geqslant 0$ we have $q_k(t) = O(k^{-n})$.

2) For any fixed $k \in \mathbb{Z}$ and $t \to \infty$ we have the following asymptotic formula:

$$q_k(t) \asymp \frac{1}{\sqrt{t}} \Big(C_1 \cos\big(\omega_1(t)\big) + S_1 \sin\big(\omega_1(t)\big) + (-1)^k C_2 \cos\big(\omega_2(t)\big) + (-1)^k S_2 \sin\big(\omega_2(t)\big) \Big),$$

where

$$C_1 = \frac{1}{\omega_1}\sqrt{\frac{\omega_0}{2\pi}} Q(0), \qquad S_1 = \frac{1}{\omega_1 \omega_0}\sqrt{\frac{\omega_0}{2\pi}} P(0)$$

$$C_2 = \frac{1}{\omega_1}\sqrt{\frac{\omega_0'}{2\pi}} Q(\pi), \qquad S_2 = \frac{1}{\omega_1 \omega_0'}\sqrt{\frac{\omega_0'}{2\pi}} P(\pi),$$

$$\omega_1(t) = t\omega_0 + \frac{\pi}{4}, \qquad \omega_2(t) = t\omega_0' - \frac{\pi}{4}, \qquad \omega_0' = \sqrt{\omega_0^2 + 4\omega_1^2}.$$

3) Let $t = \beta|k|$, $\beta > 0$ and $k \to \infty$. Put $\gamma(\beta) = \beta^2\omega_1^2 - 1 - \beta\omega_0$.

a) If $\gamma(\beta) > 0$, then

$$q_k(t) \asymp \frac{1}{\sqrt{|k|}} \left(\mathscr{F}_k^+[Q] - i\mathscr{F}_k^- \left[\frac{P(\lambda)}{\omega(\lambda)} \right] \right),$$

where for a complex valued function $g(\lambda)$ defined on the real line we introduce the following functionals:

$$\mathscr{F}_k^{\pm}[g] = c_+ \left(g(\mu_+) e^{i\omega_+(k)} \pm g(-\mu_+) e^{-i\omega_+(k)} \right) + c_- \left(g(\mu_-) e^{i\omega_-(k)} \pm g(-\mu_-) e^{-i\omega_-(k)} \right)$$

$$\omega_\pm(k) = k\big(\mu_\pm + \beta\,\omega(\mu_\pm)\big) \pm \frac{\pi}{4}\operatorname{sign}(k), \qquad c_\pm = \frac{1}{2}\sqrt{\frac{\beta\,\omega(\mu_\pm)}{2\pi\Delta}},$$

$$\mu_\pm = -\arccos \frac{1}{\beta^2\omega_1^2}(1 \pm \Delta),$$

$$\Delta = \sqrt{(\beta^2\omega_1^2 - 1)^2 - \beta^2\omega_0^2}, \qquad \omega(\lambda) = \sqrt{\omega_0^2 + 2\omega_1^2(1 - \cos\lambda)}.$$

b) If $\gamma(\beta) = 0$ and $n \geqslant 3$, then $q_k(t) = O(k^{-3})$.

c) If $\gamma(\beta) < 0$ then $q_k(t) = O(k^{-n})$ for n defined above.

Recall that a sufficient condition on $z \in l_2(\mathbb{Z})$ for $\widehat{z} \in C^n(\mathbb{R})$ is $\sum_k |k|^n |z_k| < \infty$. Thus if the following series converge for some $n \geqslant 2$:

$$\sum_k |k|^n |q_k(0)| < \infty \qquad \text{and} \qquad \sum_k |k|^n |p_k(0)| < \infty,$$

then Theorem 9.2 holds.

Theorem 9.3 ($\omega_0 = 0$) Suppose that $\omega_0 = 0$ and $Q, P \in C^n(\mathbb{R})$, $n \geqslant 6$ then

1) For any fixed $t \geqslant 0$ we have $q_k(t) = O(k^{-n})$.

2) For any fixed $k \in \mathbb{Z}$ and $t \to \infty$ one has:

$$q_k(t) \asymp \frac{P(0)}{2\omega_1} + \frac{(-1)^k}{\sqrt{t}} \Big(C\cos\big(2\omega_1 t - \tfrac{\pi}{4}\big) + S\sin\big(2\omega_1 t - \tfrac{\pi}{4}\big) \Big),$$

where

$$C = \frac{1}{\sqrt{\pi\omega_1}} Q(\pi), \qquad S = \frac{1}{2\omega_1\sqrt{\pi\omega_1}} P(\pi).$$

3 l_∞ initial conditions

Our next concern will be the uniform boundedness in k and t of the solution. Denote $p(t) = \dot{q}(t)$. Further on we always assume that $q(0) \in l_\infty$, $p(0) = 0$, that is $\sup_k |q_k(0)| < \infty$, $p_k(0) = 0$. The following result follows from Theorem 9.1.

Proposition 9.4 Let $q(0) \in l_2(\mathbb{Z})$, $p(0) = 0$, then $|q(t)|_\infty \leqslant |q(0)|_2$.

Thus the solution will be uniformly bounded. The situation drastically changes if we consider l_∞ initial conditions. Namely, the following theorem holds.

Theorem 9.5

1) Let $q(0) \in l_\infty(\mathbb{Z})$, $p(0) = 0$, then for any $t \geqslant 0$:

$$|q(t)|_\infty \leqslant \left(\sqrt{2\gamma\omega_1 t} + 2\right) |q(0)|_\infty,$$

where $\gamma > 0$ is the root of the equation $\frac{1}{\gamma} e^{\frac{1}{\gamma}} = \frac{1}{e}$.

2) For any $k \in \mathbb{Z}$ there exists a constant $c > 0$, initial conditions $q(0) \in l_\infty(\mathbb{Z})$, $p(0) = 0$ and increasing sequence of time moments $t_1 < t_2 < \ldots$, $t_n \to \infty$ as $n \to \infty$ such that

$$q_k(t_{2n}) \geqslant c\sqrt{t_{2n}}, \qquad q_k(t_{2n+1}) \leqslant -c\sqrt{t_{2n+1}}, \qquad n = 1, 2, \ldots.$$

Corollary 9.6 For any $k \in \mathbb{Z}$ there is initial condition $q(0) \in l_\infty(\mathbb{Z})$, $p(0) = 0$ such that

$$\limsup_{t\to\infty} \frac{q_k(t)}{\sqrt{t}} = c_1 > 0, \qquad \liminf_{t\to\infty} \frac{q_k(t)}{\sqrt{t}} = c_2 < 0.$$

for some constants c_1, c_2 depending on k.

Define the following operator on l_∞,

$$(Vq)_k = -\omega_1^2 (\Delta q)_k = -\omega_1^2 (q_{k+1} - 2q_k + q_{k-1}).$$

It is clear that $|V|_\infty \leqslant 4\omega_1^2$. Thus the following operator $C(t)$ is also bounded in l_∞:

$$C(t) \doteqdot \cos\left(t\sqrt{V}\right) = \sum_{k=0}^{\infty} (-1)^k \frac{t^{2k} V^k}{(2k)!}. \tag{9.4}$$

Theorem 9.7 There exist constants $a, b > 0$ such that for all $t \geqslant 0$ the following inequalities hold:

$$a\sqrt{t} + 1 \leqslant \left|\cos\left(t\sqrt{V}\right)\right|_\infty \leqslant b\sqrt{t} + 1$$

We will need some definitions. For sequence $q \in l_\infty$ define new sequence:

$$q^\Delta = -\Delta q, \quad q_k^\Delta = 2q_k - q_{k+1} - q_{k-1}, \qquad k \in \mathbb{Z}.$$

Let $l^\Delta \subset l_\infty(\mathbb{Z})$ be the set of sequences $q \in l_\infty(\mathbb{Z})$, for which the following conditions hold:

1) $q^\Delta \in l_2(\mathbb{Z})$. Then the Fourier transform of q^Δ, $Q^\Delta(\lambda) = \sum_k e^{ik\lambda} q_k^\Delta$ belongs to $L_2([0,2\pi])$.

2) For some real number $A \in \mathbb{R}$ the function

$$\phi(\lambda) = \frac{1}{\sin\frac{\lambda}{2}} \left(\frac{Q^\Delta(\lambda)}{\sin\frac{\lambda}{2}} - iA \right) \tag{9.5}$$

belongs to $L_1[0,\pi]$, where $i^2 = -1$, that is $\int_0^\pi |\phi(\lambda)| d\lambda < \infty$.

Then l^Δ becomes a linear vector space over $\mathbb{R}$.

Theorem 9.8 Assume that $q(0) \in l^\Delta$, $p(0) = 0$, then the solution $\{q_k(t)\}$ is uniformly bounded that is $\sup_{t \geqslant 0} \sup_{k \in \mathbb{Z}} |q_k(t)| < \infty$.

Theorem 9.9 Assume that $q(0) \in l^\Delta$, $p(0) = 0$, then there exists $\nu \in \mathbb{R}$ such that for any $k \in \mathbb{Z}$ the following equality holds: $\lim_{t \to \infty} q_k(t) = \nu$.

Relation of the number ν with the limit $q_k(0)$ at infinity is given in Theorem 9.11 below.

We now give examples of sequences $q \in l^\Delta$.

1) Sign sequence. Put

$$q_k = \operatorname{sign}(k) = \begin{cases} 1, & k > 0, \\ 0, & k = 0, \\ -1, & k < 0 \end{cases}.$$

It is clear that $q_k^\Delta = 0$ for $|k| > 1$. Then $q_1^\Delta = 1$, $q_{-1}^\Delta = -1$, $q_0^\Delta = 0$. That is why $Q^\Delta(\lambda) = \left(e^{i\lambda} - e^{-i\lambda}\right) = 2i\sin(\lambda)$. Put $A = 4$ in (9.5). Then

$$\phi(\lambda) = \frac{1}{\sin\frac{\lambda}{2}} \left(\frac{2\sin(\lambda)}{\sin\frac{\lambda}{2}} - 4 \right) = \frac{4}{\sin\frac{\lambda}{2}} \left(\cos\frac{\lambda}{2} - 1 \right).$$

It is clear that $\phi(\lambda) \in L_1[0,\pi]$. Thus, $\operatorname{sign}(k) \in l^\Delta$. See Figure 9.1 for the solution with intial condition $q_k(0) = \operatorname{sign}(k)$, $p(0) = 0$. and $\omega = 1/2$: Both particles, (with

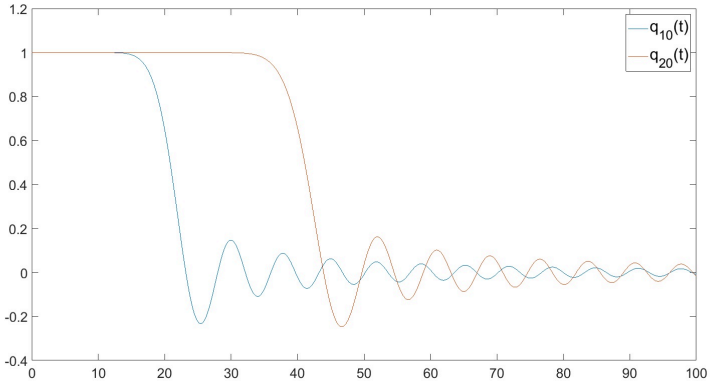

Figure 9.1: Solution with initial condition $q_k(0) = \text{sign}(k)$, $p(0) = 0$

numbers 10 and 20), until $t \ll 2n$, oscillate around point 1 with exponentially small amplitude. However, such fluctuations are not visible on the picture

Then they quickly fall into a regime of relaxation oscillations around the equilibrium point. In such a case the solution is given by the formula:

$$q_n(t) = J_0(t) + 2\sum_{k=1}^{n-1} J_{2k}(t) + J_{2n}(t) = 1 + J_{2n}(t) - 2\sum_{k=2n}^{\infty} J_{2k}(t), \qquad n \geqslant 1, \quad (9.6)$$

where

$$J_n(t) = \frac{1}{\pi}\int_0^{\pi} \cos(nx - t\sin x)dx, \qquad t \geqslant 0$$

is the Bessel function of first kind. In Equality (9.6) we used the known formula ([10]):

$$2\sum_{k=1}^{\infty} J_{2k}(t) + J_0(t) = 1.$$

2) Now consider as example the in some sense opposite to the Sign sequence:

$$q_k = \begin{cases} 1, & k \neq 0 \\ b, & k = 0 \end{cases},$$

for some $b \in \mathbb{R}$. Then

$$Q^\Delta(\lambda) = e^{i\lambda}(2-b-1) + 2b - 2 + e^{-i\lambda}(2-b-1) \\ = 2(b-1)(1-\cos\lambda) = 4(b-1)\sin^2\frac{\lambda}{2}.$$

Put $A = 0$ in (9.5). Then $\phi(\lambda) = 4(b-1)$. Again we see that $\phi(\lambda) \in L_1[0,\pi]$ and then $q_k \in l^\Delta$.

3) Consider the sequence $q_k = (-1)^k$. Then $(\Delta q)_k = (-1)^k(-1-1-2) = -4q_k$. And thus, $q \notin l^\Delta$. Nevertheless one can prove the uniform boundedness of solution with such initial conditions. It is known that $q(t) = \cos\big(t\sqrt{V}\big)q(0)$ and $V = -\omega_1^2\Delta$. Thus

$$q(t) = \sum_{k=0}^{\infty}(-1)^k\frac{t^{2k}V^k}{(2k)!}q = \sum_{k=0}^{\infty}(-1)^k\frac{(4\omega_1^2)^k t^{2k}}{(2k)!}q = \cos(2\omega_1 t)q.$$

Uniform boundedness of $q(t)$ follows.

Theorem 9.10 Assume that

$$\sum_{k\neq 0}|q_k^\Delta|\cdot|k|\ln|k| < \infty, \tag{9.7}$$

then $q \in l^\Delta$.

As an example, consider the sequence

$$q_k = \frac{\sin\big(\ln\ln|k|\big)}{\ln^2\big(|k|\big)} \quad \text{if } |k| > 1$$

and $q_k = 0$ for $|k| \leqslant 1$. It is not difficult to see that

$$q_k^\Delta = O\left(\frac{1}{k^2\ln^3|k|}\right).$$

Thus the conditions of (9.7) hold, and then $q \in l^\Delta$.

Theorem 9.11 Assume that $q \in l^\Delta$, then there exist finite limits

$$\lim_{k\to+\infty} q_k = L_+, \qquad \lim_{k\to-\infty} q_k = L_-$$

and the following equalities hold as well:

$$L_+ - L_- = \frac{A}{2}, \qquad \frac{L_+ + L_-}{2} = \nu,$$

where number A is defined in (9.5), and ν was introduced in Theorem 9.9.

Bibliography

[1] Bogolyubov, N. N: *On some statistical methods in mathematical physics*, Academy of science of USSR, Kiev (1945).

[2] Boldrighini, C., Pellegrinotti, A., Triolo, L.: *Convergence to stationary states for infinite harmonic systems*, J. Stat. Phys. **30**(1), 123–155 (1983).

[3] Dalecki, Ju. L., Krein, M. G.: *The stability of the solutions of differential equations in a Banach space*, Moscow, Nauka (1970). [Russian].

[4] Deimling, K.: *Ordinary differential equations in Banach spaces*, Springer (1977).

[5] Dudnikova, T.: *Behavior for large time of a two-component chain of harmonic oscillators*, Russ. J. Math. Phys. **25**(4), 470–491 (2018).

[6] Dudnikova, T.: *Long-time asymptotics of solutions to a hamiltonian system on a lattice*, J. Math. Sci. **219**(1), 69–85 (2016).

[7] Dudnikova, T., Komech, A., Spohn, H.: *On the convergence to statistical equilibrium for harmonic crystals*, J. Math. Phys. **44**(6), 2596–2620 (2003).

[8] Fox, R.: *Long-time tails and diffusion*, Phys. Rev. A **27**(6), 3216–3233 (1983).

[9] Florencio, J., Howard Lee, M.: *Exact time evolution of a classical harmonic-oscillator chain*, Phys. Rev. A **31**(5), 3221–3236 (1985).

[10] Gradshteyn, L. S., Ryzhik, I. M.: *Table of integrals, series, and products*, 5th ed. (1994).

[11] Hemmen, J.: *Dynamics and ergodicity of the infinite harmonic crystal*, Phys. Rep. **65**(2), 43–149 (1980).

[12] Lanford, O., Lebowitz, J.: *Time evolution and ergodic properties of harmonic systems*, in: Moser J. (eds) Dynamical Systems, Theory and Applications. Lecture Notes in Physics, vol 38. Springer, Berlin, Heidelberg (1975).

[13] Lykov, A., Malyshev, V.: *From the N-body problem to Euler equations*, Russ. J. Math. Phys. **24**(1), 79–95 (2017).

[14] Lykov, A., Malyshev, V., Melikian, M.: *Phase diagram for one-way traffic flow with local control*, Phys. A **486**, 849–866 (2017).

[15] Spohn, H., Lebowitz, J.: *Stationary non-equilibrium states of infinite harmonic systems*, Commun. Math. Phys. **54**, 97–120 (1977).

10

On direct and inverse problems in the description of lattice random fields

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Abstract. *Various systems of finite-dimensional distributions parameterised by boundary conditions are considered. For such systems solutions to direct and inverse problems of description of lattice random fields are given.*

1 Introduction

Let P be a random field on the integer lattice $\mathbb{Z}^d$ ($d \geq 1$) with state space X, that is, a probability measure on the σ-algebra generated by all cylinder sets of $X^{\mathbb{Z}^d}$.

Since it is quite difficult to work directly with the probability measure P defined on the infinite product of state space X (often called *infinite-volume* measure), its study usually reduced to the analysis of a suitable system Q_P of probability distributions generated by P and defined on finite products of X. The natural requirement for such a system Q_P is that Q_P must uniquely *determine* (*restore*) the random field P, i. e., any random field P' such

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that $\mathrm{Q}_{P'} = \mathrm{Q}_P$ must coincide with P. In this case it is necessary to note that the random field P was restored by the system Q_P, we will use the following notation: P_{Q_P}.

For a given random field P, the problem of the existence of a system Q_P for which $P_{\mathrm{Q}_P} = P$ we call the *direct problem* in the description of random fields. We will say that a system Q_P is a solution to the direct problem for a given random field P if $P_{\mathrm{Q}_P} = P$. Note that for a given random field there may exist various solutions to the direct problem.

If the direct problem is solved, the following question naturally arises: does the system Q_P possess such specific properties (consistency conditions) which allow restoring the random field P without taking into account the fact that the elements of Q_P are generated by the random field P? In the case such consistency conditions are found, it is quite possible that for any system Q endowed by these properties, there exists a random field P whose system of finite-dimensional distributions Q_P coincides with Q.

For a given system Q of finite-dimensional distributions, the problem of the existence of a random field P for which $\mathrm{Q}_P = \mathrm{Q}$ we call the *inverse problem* in the description of random fields. We will say that a random field P is a solution to the inverse problem for a given system Q if $\mathrm{Q}_P = \mathrm{Q}$. For a given system Q, any solution to the inverse problem will be denoted by P_{Q}, so that $\mathrm{Q}_{P_{\mathrm{Q}}} = \mathrm{Q}$.

By solving the direct problem, we obtain the possibility to define classes of random fields and to study their main properties; while the solution to the inverse problem makes it possible to construct models of random fields with required properties.

Historically, Kolmogorov was the first one who considered both the direct and the inverse problems of description of random processes (see [7], originally published in German in 1933). His subject of consideration was a consistent system of unconditional finite-dimensional distributions. This system, which uniquely determines a random field, is a very general one, and specific classes of random processes are defined by the corresponding restrictions on its elements. For example, by corresponding restrictions on Kolmogorov's system, classes of Gaussian processes, processes with independent increments as well as stationary processes are defined.

Over time, it became clear that in many cases it is convenient to impose restrictions not only on unconditional distributions but also on their relations, that is, on conditional distributions. This type of restrictions leads to other important classes of random processes, namely Markov processes, Gibbs random fields, martingales, etc.

It should be noted that, generally speaking, an inverse problem may have more than one solution, i. e., be incorrect. If for a given system Q the inverse problem of description of random fields is correct (has a unique solution), we will say that the system Q *specifies* (uniquely defines) a random field. Note, that Kolmogorov's system characterises a random field. However, in some cases incorrect problems lead to very interesting and useful results. For example, in the Dobrushin's theory of description of Gibbs random fields, the non-correctness of the inverse problem (non-uniqueness of its solution) is interpreted as the presence of a phase transition in the model under study (see the seminal paper [6]).

In the present work we restrict ourselves to the case of positive lattice random fields with finite state space X. We consider various systems of conditional distributions generated by a random field as well as autonomously defined consistent systems of finite-dimensional distributions parametrised by boundary conditions. For such objects solutions to the direct and the inverse problems in the description of random fields are given.

2 Preliminaries

Let $S \subset \mathbb{Z}^d$ and let $W(S) = \{V \subset S, 0 < |V| < \infty\}$ be the set of all (non-empty) finite subsets of S. For $S = \mathbb{Z}^d$ we use a simpler notation W. In some cases the braces in the notation of one-point sets $\{t\}$, $t \in \mathbb{Z}^d$, are omitted. For any function $f(\Lambda)$, $\Lambda \in W(S)$, the notation $\lim\limits_{\Lambda \uparrow S} f(\Lambda) = a$ will mean that for any increasing sequence $\{\Lambda_n\}_{n \geq 1}$ of finite sets converging to S (that is, $\Lambda_n \in W(S)$, $\Lambda_n \subset \Lambda_{n+1}$ and $\bigcup\limits_{n=1}^{\infty} \Lambda_n = S$), we have $\lim\limits_{n \to \infty} f(\Lambda_n) = a$.

Denote by $X^S = \{(x_t, t \in S)\}$, $x_t \in X$, the set of all functions (configurations) on S taking values in X. If $S = \emptyset$, we assume $X^{\emptyset} = \{\underline{o}\}$, where $\underline{o}$ is the empty configuration. For any $S, T \subset \mathbb{Z}^d$ such that $S \cap T = \emptyset$ and any $x \in X^S$, $y \in X^T$ we denote xy the concatenation of x and y defined as the configuration on $S \cup T$ equal to x on S and to y on T. If $T \subset S$, by x_T we denote the restriction of the configuration $x \in X^S$ on T.

Let P be a random field, that is, a probability measure on $X^{\mathbb{Z}^d}$. We denote by P_V the restriction of P on X^V, i. e., $P_V(A) = \big(P\big)_V(A) = P\big(\{x \in X^{\mathbb{Z}^d} : x_V \in A\}\big)$, where $A \subset X^V$, $V \in W$. A random field P is called positive if $P_V(x) > 0$ for all $x \in X^V$ and $V \in W$.

For a positive random field P, its conditional probability Q_V^z on X^V under finite condition $z \in X^S$, $S \in W(\mathbb{Z}^d \backslash V)$, is defined as $Q_V^z(x) = P_{V \cup S}(xz) \big/ P_S(z)$, $x \in X^V$, $V \in W$. In the case of infinite boundary condition $z \in X^S$, $S \subset \mathbb{Z}^d \backslash V$, $S \notin W(\mathbb{Z}^d \backslash V)$, we put

$Q_V^z(x) = \lim_{\Lambda \uparrow S} Q_V^{z_\Lambda}(x)$, $x \in X^V$, $V \in W$, where the limit exists for almost all (with respect to P) configurations z.

3 Kolmogorov's system

In [7] Kolmogorov showed that any random field P is determined by its system of finite-dimensional unconditional distributions $K_P = \{P_V, V \in W\}$, and thus K_P is a solution to the direct problem.

Among the properties of the restoring system K_P, Kolmogorov singled out the following one as a consistency condition: for all $V, I \in W$, $V \cap I = \emptyset$ and $x \in X^V$

$$\sum_{y \in X^I} P_{V \cup I}(xy) = P_V(x). \tag{10.1}$$

He proved that the system $K = \{p_V, V \in W\}$ of probability distributions p_V on X^V, $V \in W$, whose elements are consistent in the sense (10.1), characterises a random field P_K, i. e., there exists a unique solution to the inverse problem for the system K.

4 Systems of probability distributions parameterised by boundary conditions

Below we examine both the direct and the inverse problems for various consistent systems of finite-dimensional distributions parameterised by boundary conditions.

Note that if a system Q defines a random field P_{Q} then the system $\mathrm{Q}_{P_{\mathrm{Q}}}$ (which coincides with Q) is a solution to the direct problem for the random field P_{Q}. Thus, further, we will mainly focus on the inverse problem.

4.1 Conditional distribution of a random field

In this section we consider the widest system of conditional probability distributions generated by a random field.

For a random field P, the system $Q_P = \{Q_V^z, z \in X^S, \emptyset \neq S \subset \mathbb{Z}^d \setminus V, V \in W\}$ of conditional probabilities Q_V^z on X^V under boundary conditions z outside V, $V \in W$, we call *conditional distribution of the random field P*.

Any random field P is restored by its conditional distribution Q_P. Thus, the conditional distribution Q_P of a random field P is a solution to the direct problem. Now let us consider the inverse problem.

We call a set $Q = \{q_V^z, z \in X^S, \emptyset \neq S \subset \mathbb{Z}^d \setminus V, V \in W\}$ of probability distributions q_V^z on X^V parametrised by boundary conditions z outside V, $V \in W$, *(general) specification* if its elements satisfy the following consistency conditions:

1. for any disjoint sets $V, I \in W$, $\emptyset \neq S \subset \mathbb{Z}^d \setminus (V \cup I)$ and $x \in X^V$, $y \in X^I$, $z \in X^S$

$$q_{V \cup I}^z(xy) = q_V^z(x) q_I^{zx}(y); \tag{10.2}$$

2. for all $V \in W$ and $\emptyset \neq S \subset \mathbb{Z}^d \setminus V$ it holds

$$q_V^z(x) = \lim_{\Lambda \uparrow S} q_V^{z_\Lambda}(x), \qquad x \in X^V, z \in X^S. \tag{10.3}$$

The consistency condition (10.2) in the case of infinite boundary conditions was considered for the first time in [1]. A specification Q will be called positive if all its elements are strictly positive.

It is not difficult to see that for any random field P, the elements of its conditional distribution Q_P satisfy the consistency conditions (10.2) and (10.3) for almost all (with respect to P) boundary conditions. However, any random field has a version of its conditional distribution Q_P being the specification.

For a given specification, there is a unique solution to the inverse problem of description of random fields.

Theorem 10.1 Let Q be a positive specification. Then there exists a unique random field P such that its conditional distribution Q_P coincides with Q.

Proof. For any $V \in W$ put

$$p_V(x) = \frac{q_V^y(x)}{q_I^x(y)} \left(\sum_{\alpha \in X^V} \frac{q_V^y(\alpha)}{q_I^\alpha(y)} \right)^{-1}, \qquad x \in X^V, \tag{10.4}$$

where $y \in X^I$, $I \in W(\mathbb{Z}^d \setminus V)$. Using (10.2) one can show that the function p_V does not depend on the choice of I and y. It is not difficult to see that the system of probability distributions $\{p_V, V \in W\}$ is consistent in Kolmogorov's sense and hence defines a unique random field P such that $K_P = \{p_V, V \in W\}$. Moreover, it can be shown that $Q_P = Q$. $\square$

4.2 One-point conditional distribution

For a given random field P, the system $Q_1(P) = \{Q_t^z, z \in X^S, \emptyset \neq S \subset \mathbb{Z}^d \setminus \{t\}, t \in \mathbb{Z}^d\}$ we call *one-point conditional distribution of the random field P*. Any random field P can be restored by its one-point conditional distribution $Q_1(P)$.

We call a system $Q_1 = \{q_t^z, z \in X^S, \emptyset \neq S \subset \mathbb{Z}^d \setminus \{t\}, t \in \mathbb{Z}^d\}$ of one-point probability distributions parametrised by boundary conditions *(general) 1-specification* if its elements satisfy the following consistency conditions:

1. for all $t, s \in \mathbb{Z}^d$, $S \subset \mathbb{Z}^d \setminus \{t, s\}$ and $x, u \in X^{\{t\}}$, $y, v \in X^{\{s\}}$, $z \in X^S$

$$q_t^{zy}(x) q_s^{zx}(v) q_t^{zv}(u) q_s^{zu}(y) = q_s^{zx}(y) q_t^{zy}(u) q_s^{zu}(v) q_t^{zv}(x); \tag{10.5}$$

2. for all $t \in \mathbb{Z}^d$, $\emptyset \neq S \subset \mathbb{Z}^d \setminus \{t\}$ and $x \in X^{\{t\}}$, $z \in X^S$ it holds $q_t^z(x) = \lim\limits_{\Lambda \uparrow S} q_t^{z_\Lambda}(x)$.

Theorem 10.2 Let Q_1 be a positive 1-specification. Then there exists a unique random field P such that its one-point conditional distribution $Q_1(P)$ coincides with Q_1.

Proof. Let us construct a Kolmogorov's system $K_{Q_1} = \{p_V, V \in W\}$ as follows. For $V = \{t\}$, $t \in \mathbb{Z}^d$, put

$$p_t(x) = \frac{q_t^y(x)}{q_s^x(y)} \left(\sum_{\alpha \in X^{\{t\}}} \frac{q_t^y(\alpha)}{q_s^\alpha(y)} \right)^{-1}, \qquad x \in X^{\{t\}}, \tag{10.6}$$

where $y \in X^{\{s\}}$, $s \in \mathbb{Z}^d \setminus \{t\}$. Further, for any $V \in W$, $t \in \mathbb{Z}^d \setminus V$ and $x \in X^V$, $z \in X^{\{t\}}$ put

$$p_{t \cup V}(zx) = p_t(z) q_V^z(x),$$

$$q_V^z(x) = \prod_{j=1}^n \frac{q_{t_j}^{z(xu)_j}(x_{t_j})}{q_{t_j}^{z(xu)_j}(u_{t_j})} \cdot \left(\sum_{\alpha \in X^V} \prod_{j=1}^n \frac{q_{t_j}^{z(\alpha u)_j}(\alpha_{t_j})}{q_{t_j}^{z(\alpha u)_j}(u_{t_j})} \right)^{-1}. \tag{10.7}$$

Here $(xu)_j = x_{t_1} \dots x_{t_{j-1}} u_{t_{j+1}} \dots u_{t_n}$ for $1 < j < n$ and $(xu)_1 = u_{t_2} \dots u_{t_n}$, $(xu)_n = x_{t_1} \dots x_{t_{n-1}}$, $n = |V|$, $V = \{t_1, t_2, \dots, t_n\}$ is some enumeration of the points of the set V, and $u \in X^V$ is an arbitrary configuration. By virtue of (10.5), p_t and q_V^z are correctly defined. It is not difficult to see that the elements of the system K_{Q_1} are consistent in Kolmogorov's sense, and hence K_{Q_1} defines a random field P such that $K_P = K_{Q_1}$. Moreover, one can verify that $Q_1(P) = Q_1$. □

4.3 Finite-conditional distribution of a random field

For a given random field P, the system $Q^{\text{fin}}(P) = \{Q_V^z, z \in X^S, S \in W(\mathbb{Z}^d \backslash V), V \in W\}$, introduced in [3], is called *finite-conditional distribution of the random field P*. The system $Q^{\text{fin}}(P)$ restores the random field P.

We call a set $Q^{\text{fin}} = \{q_V^z, z \in X^S, S \in W(\mathbb{Z}^d \backslash V), V \in W\}$ of probability distributions parametrised by finite boundary conditions *specification with finite boundary conditions* if its elements satisfy the following consistency condition: for any disjoint sets $V, I, S \in W$ and configurations $x \in X^V$, $y \in X^I$, $z \in X^S$ it holds $q_{V \cup I}^z(xy) = q_V^z(x) q_I^{zx}(y)$.

Theorem 10.3 Let Q^{fin} be a positive specification with finite boundary conditions. Then there exists a unique random field P such that $Q^{\text{fin}}(P) = Q^{\text{fin}}$.

The proof of this result is similar to the proof of Theorem 10.1.

4.4 One-point finite-conditional distribution of a random field

For a given random field P, the system $Q_1^{\text{fin}}(P) = \{Q_t^z, z \in X^S, S \in W(\mathbb{Z}^d \backslash \{t\}), t \in \mathbb{Z}^d\}$, introduced in [4], is called *one-point finite-conditional distribution of the random field P*. The system $Q_1^{\text{fin}}(P)$ restores the random field P.

We call a set $Q_1^{\text{fin}} = \{q_t^z, z \in X^S, S \in W(\mathbb{Z}^d \backslash \{t\}), t \in \mathbb{Z}^d\}$ of one-point probability distributions parametrised by finite boundary conditions *1-specification with finite boundary conditions* if its elements satisfy the following consistency condition: for all $t, s \in \mathbb{Z}^d$, $S \in W\left(\mathbb{Z}^d \backslash \{t,s\}\right)$ and $x, u \in X^{\{t\}}$, $y, v \in X^{\{s\}}$, $z \in X^S$

$$q_t^{zy}(x) q_s^{zx}(v) q_t^{zv}(u) q_s^{zu}(y) = q_s^{zx}(y) q_t^{zy}(u) q_s^{zu}(v) q_t^{zv}(x). \tag{10.8}$$

Theorem 10.4 Let Q_1^{fin} be a positive 1-specification with finite boundary conditions. Then there exists a unique random field P such that $Q_1^{\text{fin}}(P) = Q_1^{\text{fin}}$.

The proof of this result is similar to the proof of Theorem 10.2.

Note that in [4] the inverse problem for the system Q_1^{fin} was solved under the following (equivalent to (10.8)) consistency conditions:

1. for all $t,s \in \mathbb{Z}^d$, $S \in W\left(\mathbb{Z}^d \backslash \{t,s\}\right)$ and $x \in X^{\{t\}}$, $y \in X^{\{s\}}$, $z \in X^S$

$$q_t^z(x) q_s^{zx}(y) = q_s^z(y) q_t^{zy}(x);$$

2. for all $t,s \in \mathbb{Z}^d$ and $x,u \in X^{\{t\}}$, $y,v \in X^{\{s\}}$

$$q_t^y(x) q_s^x(v) q_t^v(u) q_s^u(y) = q_s^x(y) q_t^y(u) q_s^u(v) q_t^v(x).$$

4.5 Palm-type conditional distribution of a random field

For a given random field P, the system $Q^{\Pi}(P) = \left\{Q_V^z, z \in X^{\{t\}}, t \in \mathbb{Z}^d \backslash V, V \in W\right\}$ of conditional probabilities under condition at a point we call *Palm-type conditional distribution of the random field P*. The system $Q^{\Pi}(P)$ restores the random field P.

We call a set $Q^{\Pi} = \left\{q_V^z, z \in X^{\{t\}}, t \in \mathbb{Z}^d \backslash V, V \in W\right\}$ of probability distributions parametrised by boundary condition at a point *Palm specification* if its elements satisfy the following consistency conditions:

1. for any disjoint sets $V,I \in W$ and $z \in X^{\{t\}}$, $t \in \mathbb{Z}^d \backslash (V \cup I)$

$$\sum_{y \in X^I} q_{V \cup I}^z(xy) = q_V^z(x), \qquad x \in X^V; \tag{10.9}$$

2. for any $t,s \in \mathbb{Z}^d$, $V \in W(\mathbb{Z}^d \backslash \{t,s\})$ and $x \in X^{\{t\}}$, $y \in X^{\{s\}}$, $u \in X^V$

$$q_t^y(x) q_{s \cup V}^x(yu) = q_s^x(y) q_{t \cup V}^y(xu). \tag{10.10}$$

Theorem 10.5 Let Q^{Π} be a positive Palm specification. Then there exists a unique random field P such that $Q^{\Pi}(P) = Q^{\Pi}$.

Proof. For any $V \in W$ put $p_V(x) = p_t(x_t) q_{V \backslash \{t\}}^{x_t}(x_{V \backslash \{t\}})$, $x \in X^V$, $t \in V$, where p_t is defined by (10.6). By virtue of (10.10), the probability distribution p_V does not depend on the choice of the point $t \in V$. According to (10.9), the system $\{p_V, V \in W\}$ is consistent

in Kolmogorov sense, and hence there exists a unique random field P such that $K_P = \{p_V, V \in W\}$. Moreover, it can be shown that $Q^{\Pi}(P) = Q^{\Pi}$. □

4.6 Dobrushin's conditional distribution of a random field

Among the conditional distributions of a random field P under infinite boundary conditions, there is a system, introduced by Dobrushin in [5], which has a special place.

For a given random field P, the system $Q^{\mathrm{D}}(P) = \{Q^z_V, z \in X^{\mathbb{Z}^d \setminus V}, V \in W\}$ of conditional probabilities on X^V under a boundary condition everywhere outside V, $V \in W$, we call *Dobrushin's conditional distribution of the random field P*.

Generally speaking, Dobrushin's system does not solve the direct problem, since there may exist various random fields with the same Dobrushin's conditional distribution (see [6]). However, there are random fields which can be restored by Dobrushin's conditional distributions (see Theorem 2 in [5]).

We call a set $Q^{\mathrm{D}} = \{q^z_V, z \in X^{\mathbb{Z}^d \setminus V}, V \in W\}$ of probability distributions parametrised by infinite boundary conditions *Dobrushin's specification* if its elements satisfy the following consistency condition: for all disjoint sets $V, I \in W$ and $x \in X^V$, $y \in X^I$, $z \in X^{\mathbb{Z}^d \setminus (V \cup I)}$

$$q^z_{V \cup I}(xy) = q^{zx}_I(y) \sum_{v \in X^I} q^z_{V \cup I}(xv).$$

For a given specification Q^{D}, Dobrushin in [5] presented a condition (quasilocality) under which there exists a random field P such that $Q^{\mathrm{D}}(P) = Q^{\mathrm{D}}$. But there may exist more than one random field whose conditional distribution $Q^{\mathrm{D}}(P)$ coincides with Q^{D}, i. e., for Dobrushin's specification the inverse problem is incorrect. However, there are conditions under which such a random field is unique (see, for example, Theorem 2 in [5]).

4.7 One-point Dobrushin-type conditional distribution of a random field

For a given random field P, the system $Q^{\mathrm{D}}_1(P) = \{Q^z_t, z \in X^{\mathbb{Z}^d \setminus \{t\}}, t \in \mathbb{Z}^d\}$ was considered in [2]. We will call it *one-point Dobrushin-type conditional distribution of the random field P*. The system $Q^{\mathrm{D}}_1(P)$, generally speaking, does not solve the direct problem for the random field P.

We call a set $Q_1^{\mathrm{D}} = \{q_t^z, z \in X^{\mathbb{Z}^d\setminus\{t\}}, t \in \mathbb{Z}^d\}$ of one-point probability distributions parametrised by infinite boundary conditions *Dobrushin-type 1-specification* if its elements satisfy the following consistency condition: for all $t,s \in \mathbb{Z}^d$ and $x,u \in X^{\{t\}}$, $y,v \in X^{\{s\}}$, $z \in X^{\mathbb{Z}^d\setminus\{t,s\}}$

$$q_t^{zy}(x)q_s^{zx}(v)q_t^{zv}(u)q_s^{zu}(y) = q_s^{zx}(y)q_t^{zy}(u)q_s^{zu}(v)q_t^{zv}(x).$$

In [2] it was shown that for a given quasilocal Dobrushin-type 1-specification Q_1^{D} there exists a random field P such that $Q_1^{\mathrm{D}}(P) = Q_1^{\mathrm{D}}$; the conditions of uniqueness of P are the same as for Q^{D}.

Authors are grateful to S. Rœlly for useful remarks.

Bibliography

[1] Arzumanyan, V. A., Nahapetian, B. S.: *Consistent systems of finite dimensional distributions*, Armen. J. Math. **7**(2), 146–163 (2015).

[2] Dachian, S., Nahapetian, B. S.: *Description of random fields by means of one–point conditional distributions and some applications*, Markov Process. Relat. Fields **7**, 193–214 (2001).

[3] Dachian, S., Nahapetian, B. S.: *On Gibbsiannes of random fields*, Markov Process. Relat. Fields **15**, 81–104 (2009).

[4] Dalalyan, A., Nahapetian, B. S.: *Description of random fields by means of one-point finite conditional distribution*, J. Contemp. Math. Anal. Arm. Acad. Sci. **46** (2), 113–119 (2011).

[5] Dobrushin, R. L.: *The description of a random field by means of conditional probabilities and conditions of its regularity*, Theory Probab. Appl. **13** (2), 197–224 (1968).

[6] Dobrushin, R. L.: *The problem of uniqueness of a gibbsian random field and the problem of phase transitions*, Funct. Anal. Appl. **2** (4), 302–312, (1968).

[7] Kolmogorov, A. N.: *Foundations of the theory of probability*, Oxford, England: Chelsea Publishing Co. (1950).

11

The peak model for finite rank supersingular perturbations

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Abstract. *We review the peak model for finite rank supersingular perturbations of a lower semibounded self-adjoint operator by comparing the main aspects with the A-model. The exposition utilies the techniques based on the notion of boundary triples.*

1 Introduction

Given a densely defined symmetric operator in a Hilbert space, there always exists a self-adjoint extension to a Hilbert space containing the initial one as a subspace. Adapting the present principle to the symmetric operator which is essentially self-adjoint, non-trivial extensions are constructed by extension-restriction procedure with respect to the triplet extensions in scales of Hilbert spaces of an initially given self-adjoint operator. Having found the Hilbert subspace in which the symmetric operator has non-trivial but finite defect numbers, one extends that subspace by a suitable finite dimensional linear space, and then considers triplet extensions restricted to the resultant space, which is equipped with an appropriate metric.

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The research is supported by the Research Council of Lithuania. The European Social Fund Grant No. 09.3.3-LMT-K-712-13-0025.

Depending on the inner structure of an additional linear space, and hence on the metric of a resultant space, one deals with the triplet extensions restricted to either Pontryagin or Hilbert space. Following [12], the Pontryagin space models are referred to as the B-models, while those which admit both indefinite and non-negative metrics are called A-models. The A- and B-models constitute the cascade models, since an additional finite-dimensional linear space in these models contains singular elements of different order of singularity, which therefore belong to different spaces from the scale. For the symmetric operator with defect numbers $(1,1)$ (in a subspace of an initial Hilbert space), the cascade models are developed in [12, 13, 16, 7]; see also the references therein.

Due to the indefiniteness of the metric in the cascade models, the so-called peak model was suggested in [18] as an alternative. The present model is purely Hilbert space model, but it has its own limitations, simply because the model does not apply to all operators (see the next paragraph for details).

In the present paper, we review the peak model for the restricted symmetric operator with defect numbers (d,d), $d \in \mathbb{N}$, which is developed in [14]. In parallel, we remark the key differences between the present model and the A-model. The results are presented using the techniques from the theory of boundary triples [8, 11, 10, 9].

2 The peak model versus A-model

In this section we construct non-trivial realisations of a symmetric operator that is essentially self-adjoint in the reference Hilbert space. The main results are the Krein-Naimark resolvent formula (11.1) and the computed Weyl function (11.3).

2.1 Triplet adjoint

As is well-known, non-trivial realisations of a symmetric operator $L_{\min}$ that is essentially self-adjoint in the reference Hilbert space $\mathfrak{H}_0$ are considered in an extended Hilbert space by means of the compressions of their resolvents. Thus, given a self-adjoint operator L in $\mathfrak{H}_0$, let $(\mathfrak{H}_n)_{n\in\mathbb{Z}}$ be the scale of Hilbert spaces [3, 1] associated with L. To simplify the present exposition, the operator L is lower semibounded. The scalar product in $\mathfrak{H}_n$ is defined by $\langle\cdot,\cdot\rangle_n := \langle\cdot, b_n(L)\cdot\rangle_0$, where $b_0(L) := I$ and $b_m(L) := (L-z_1)\cdots(L-z_m)$ and

$b_{-m}(L) \coloneqq b_m(L)^{-1}$ for $m \in \mathbb{N}$. The real numbers $z_1, \dots, z_m$ from the resolvent set $\operatorname{res} L$ are fixed and referred to as the model parameters.

Let $L_{\min} \subseteq L$ be the symmetric restriction to $\mathfrak{H}_m$ with defect numbers (d,d), and the deficiency subspace spanned by the elements $\{G_\sigma(z) \in \mathfrak{H}_m \smallsetminus \mathfrak{H}_{m+1}\}$, $z \in \operatorname{res} L$, with σ ranging over an index set $\mathscr{S}$ of cardinality $d \in \mathbb{N}$. One considers the triplet adjoint $L_{\max}$ of $L_{\min}$ for the Hilbert triple $\mathfrak{H}_m \subseteq \mathfrak{H}_0 \subseteq \mathfrak{H}_{-m}$. The operator $L_{\max}$ in $\mathfrak{H}_{-m}$ extends $L\,|_{\mathfrak{H}_{-m+2}}$ to the domain $\mathfrak{H}_{-m+2} \dotplus \mathfrak{N}_z(L_{\max})$ (direct sum), where the eigenspace $\mathfrak{N}_z(L_{\max})$ is the linear span of the singular elements $\{g_\sigma(z) \coloneqq b_m(L) G_\sigma(z) \in \mathfrak{H}_{-m} \smallsetminus \mathfrak{H}_{-m+1}\}$. These elements are also represented as the generalised vectors $g_\sigma(z) = (L-z)^{-1}\varphi_\sigma$ by means of linearly independent singular functionals $\{\varphi_\sigma \in \mathfrak{H}_{-m-2} \smallsetminus \mathfrak{H}_{-m-1}\}$. The action of φ_σ on $\mathfrak{H}_{m+2}$ is realised via the duality pairing $\langle \varphi_\sigma, \cdot \rangle$ in a usual way [2, Eq. (1.17)]. Because $m \geq 1$, rank-d perturbations of L are called supersingular [17]; this is an allusion to the heuristic form $L + \sum_{\sigma,\sigma' \in \mathscr{S}} C_{\sigma\sigma'} \langle \varphi_{\sigma'}, \cdot \rangle \varphi_\sigma$ with some matrix $(C_{\sigma\sigma'})$ in $\mathbb{C}^d$. In what follows we also use the vector notation $\langle \varphi, \cdot \rangle \coloneqq (\langle \varphi_\sigma, \cdot \rangle)\colon \mathfrak{H}_{m+2} \to \mathbb{C}^d$.

2.2 Intermediate space

To construct non-trivial realisations of $L_{\min}$, the space $\mathfrak{H}_{-m}$ in which $L_{\max}$ is defined turns out to be too large. Thus one defines the so-called intermediate space $\mathscr{H}$, in the sense that $\mathfrak{H}_m \subseteq \mathscr{H} \subseteq \mathfrak{H}_{-m}$, and considers the range restriction $A_{\max}$ to $\mathscr{H}$ of $L_{\max}$. As a linear space, $\mathscr{H}$ is the direct sum of $\mathfrak{H}_m$ and a md-dimensional linear space $\mathfrak{K} \subseteq \mathfrak{H}_{-m}$ such that $\mathfrak{K} \cap \mathfrak{H}_{m-1} = \{0\}$. Since $\mathfrak{K}$ is in bijective correspondence with $\mathbb{C}^{md}$, each element $k \in \mathfrak{K}$ is uniquely determined by the vector $d(k) \in \mathbb{C}^{md}$. Depending on the inner structure of $\mathfrak{K}$, the set $\mathscr{H}$ is made into either Hilbert or Pontryagin space by completing it with respect to the metric

$$\langle f + k, f' + k' \rangle_{\mathscr{H}} \coloneqq \langle f, f' \rangle_m + \langle d(k), \mathscr{G} d(k') \rangle_{\mathbb{C}^{md}}$$

for $f, f' \in \mathfrak{H}_m$ and $k, k' \in \mathfrak{K}$, and some Hermitian matrix $\mathscr{G}$ in $\mathbb{C}^{md}$, referred to as the Gram matrix. For a suitable $\mathscr{G}$, the operator $A_{\max}$ is the adjoint in $\mathscr{H}$ of a densely defined, closed, symmetric, and simple operator $A_{\min}$; hence one applies to $A_{\min}$ a standard extension theory by means of $A_{\min} \subseteq A_\Theta \subseteq A_{\max}$, where a (closed) proper extension A_Θ is uniquely determined by a (closed) linear relation Θ in $\mathbb{C}^d$. Let $(\mathbb{C}^d, \Gamma_0, \Gamma_1)$ be an ordinary boundary triple (OBT) [11, Definition 7.11] for $A_{\max} = A_{\min}^*$, let γ and M be the

corresponding γ-field and the Weyl function; then the Krein-Naimark resolvent formula for an extension A_Θ defined on $f \in \mathrm{dom} A_{\max}$ such that $(\Gamma_0 f, \Gamma_1 f) \in \Theta$ reads

$$(A_\Theta - z)^{-1} = (A_0 - z)^{-1} + \gamma(z)\big(\Theta - M(z)\big)^{-1}\gamma(\overline{z})^* \tag{11.1}$$

for $z \in \mathrm{res} A_\Theta \cap \mathrm{res} A_0$, where $A_0 := A_{\{0\}\times\mathbb{C}^d}$ is one of the two distinguished self-adjoint extensions of $A_{\min}$. From here one deduces the formula for the compression of the resolvent to $\mathfrak{H}_m$.

2.3 Gram matrix

In the cascade models, an Hermitian matrix $\mathscr{G}$ is initially chosen arbitrarily and the set $\mathfrak{K}$ is the linear span of the singular elements $h_\alpha := b_j(L)^{-1}\varphi_\sigma \in \mathfrak{H}_{-m-2+2j} \ominus \mathfrak{H}_{-m-1+2j}$, with $\alpha = (\sigma, j)$ ranging over $\mathscr{S} \times J$, $J := \{1, \dots, m\}$. However, the definition $A_{\min} := A_{\max}^*$ requires in addition that $\mathscr{G}$ be invertible. Moreover, to make $A_{\min}$ symmetric, the computation of the boundary form of $A_{\max}$ shows that $\mathscr{G}$ must satisfy a certain commutation relation. For example, when $d = 1$ and $z_1 = \ldots = z_m$, it must hold $\mathscr{G}\mathfrak{M} = \mathfrak{M}^*\mathscr{G}$ with a Hankel (anti-triangular) matrix $\mathfrak{M}$, i. e. the matrix with the entries $\mathfrak{M}_{jj'} := \delta_{jj'}z_1 + \delta_{j+1,j'}$ ($j \in J \ominus \{m\}$, $j' \in J$) and $\mathfrak{M}_{mj'} := \delta_{j'm}z_1$; for $m = 1$ one puts $\mathfrak{M} := z_1$. It follows in particular that, for $m \geq 2$, one cannot put $\mathscr{G} = \mathscr{G}_* := \big(\langle h_\alpha, h_{\alpha'}\rangle_{-m}\big)$, because $\langle h_{\sigma 1}, h_{\sigma 1}\rangle_{-m} > 0$ (this statement applies to $d \in \mathbb{N}$; see also [15]).

In contrast, in the peak model, the origin of $\mathscr{G}$ is clear. Namely, the Gram matrix $\mathscr{G}$ of the peak model is made of the entries $\mathscr{G}_{\alpha\alpha'} := \langle g_\alpha, g_{\alpha'}\rangle_{-m}$, where $g_\alpha := g_\sigma(z_j)$; hence it is Hermitian and positive definite provided that $z_j \neq z_{j'}$ for $j \neq j'$. The set $\mathfrak{K}$ is defined as the linear span of the singular elements of the same order of singularity, namely $\{g_\alpha \in \mathfrak{H}_{-m} \ominus \mathfrak{H}_{-m+1}\}$. It follows that each $k \in \mathfrak{K}$ is in bijective correspondence with $d(k) = \big(d_\alpha(k)\big) \in \mathbb{C}^{md}$ via

$$k = \sum_\alpha d_\alpha(k) g_\alpha, \qquad d_\alpha(k) = \sum_{\alpha'} \big[\mathscr{G}^{-1}\big]_{\alpha\alpha'} \langle g_{\alpha'}, k\rangle_{-m}.$$

In particular, using that

$$b_m(L)^{-1} = \sum_j b_j'(z_j)^{-1}(L - z_j)^{-1}, \qquad b_j'(\cdot) := \prod_{j' \in J \ominus \{j\}} (\cdot - z_{j'})$$

and putting $d_{\sigma j}(k) = c_\sigma b'_j(z_j)^{-1}$ for some $c = (c_\sigma) \in \mathbb{C}^d$, one deduces that the set $\mathfrak{K}_{\min} := \mathfrak{K} \cap \mathfrak{H}_{m-2} \setminus \mathfrak{H}_{m-1}$ is the linear span of $\{b_m(L)^{-1}\varphi_\sigma\}$, and is referred to as the minimal subset of $\mathfrak{K}$. An element $k \in \mathfrak{K}_{\min}$ is thus of the form $k = k_{\min}(c)$, where

$$k_{\min}(c) := \sum_\sigma c_\sigma b_m(L)^{-1}\varphi_\sigma = \sum_\alpha \big[\mathscr{G}^{-1}\mathscr{G}_b c\big]_\alpha g_\alpha.$$

The matrix $\mathscr{G}_b$ from $\mathbb{C}^d$ to $\mathbb{C}^{md}$ is formed by the entries

$$\big[\mathscr{G}_b\big]_{\alpha\sigma'} := \sum_{j'} \mathscr{G}_{\alpha,\sigma' j'}\, b'_{j'}(z_{j'})^{-1}$$

and has the trivial kernel.

2.4 Symmetric operator in intermediate space

The maximal operator $A_{\max}$ in the peak model is then the operator in the Hilbert space $\mathscr{H}$ which extends A_0 to the domain $\mathrm{dom}A_0 \dotplus \mathfrak{N}_z(A_{\max})$ for $z \in \mathrm{res}A_0 = \mathrm{res}L \setminus \{z_j \,|\, j \in J\}$, where the eigenspace of $A_{\max}$ coincides with that of $L_{\max}$ (but for $z \in \mathrm{res}A_0$). The minimal operator $A_{\min}$ is made symmetric iff $\mathscr{G}$ is diagonal in $j \in J$, in which case $A_{\max}$ is closed and equals $A_{\max} = A^*_{\min}$ (this is in contrast to the A-model, where $A_{\max}$ is automatically closed by construction, provided that the Gram matrix of the model is invertible):

$$\mathrm{dom}A_{\min} = \{f^\# + k \in \mathfrak{H}_{m+2} \dotplus \mathfrak{K} \,|\, \langle\varphi, f^\#\rangle = \mathscr{G}_b^* d(k)\},$$
$$\mathrm{dom}A_{\max} = \mathrm{dom}A_0 \dotplus \mathfrak{N}_z(A_{\max}) = \mathfrak{H}_{m+2} \dotplus \mathfrak{N}_z(L^*_{\min}) \dotplus \mathfrak{K}$$

and

$$A_{\max}\big(f^\# + G_z(c) + k\big) = A_0(f^\# + k) + zG_z(c) + k_{\min}(c), \tag{11.2}$$
$$G_z(c) := \sum_\sigma c_\sigma G_\sigma(z), \qquad c = (c_\sigma) \in \mathbb{C}^d, \qquad z \in \mathrm{res}A_0$$

where the self-adjoint operator A_0 on $\mathrm{dom}A_0 = \mathfrak{H}_{m+2} \dotplus \mathfrak{K}$ is defined by

$$A_0(f^\# + k) = Lf^\# + \sum_\alpha \big[Z_d d(k)\big]_\alpha g_\alpha.$$

For brevity, Z_d denotes the matrix direct sum of d diagonal matrices $\mathrm{diag}\{z_j; j \in J\}$.

On one hand, the diagonality of $\mathscr{G}$ significantly simplifies the computations, but on the other hand, the condition is not satisfied for some operators L with perturbations of class $\mathfrak{H}_{-m-2} \setminus \mathfrak{H}_{-m-1}$ with $m \geq 2$; see e. g. [15] for $m = 2$.

2.5 Weyl function

In the peak (resp. cascade) model, the Weyl function M is represented by the sum of a Nevanlinna function associated with $L_{\min}$ in $\mathfrak{H}_m$ and the Krein Q-function associated with the Gram matrix $\mathscr{G}$ (resp. the generalszed Nevanlinna function – due to the indefiniteness of $\mathscr{G}$ – associated with the multiplication operator in a reproducing kernel Pontryagin space [5, 4, 6]). More specifically, the γ-field and the Weyl function associated with the OBT

$$\Gamma_0(f^\# + G_z(c) + k) \coloneqq c, \qquad \Gamma_1(f^\# + G_z(c) + k) \coloneqq \langle \varphi, f^\# \rangle + R(z)c - \mathscr{G}_b^* d(k)$$

for $A_{\max}$ are given by

$$\gamma(z) = b_m(z)^{-1} b_m(L) G_z(\,\cdot\,), \qquad M(z) = R(z) + Q_{\mathscr{G}}(z) \tag{11.3}$$

for $z \in \operatorname{res} A_0$. Here R is the Weyl function associated with the OBT for $L_{\min}^*$, which is obtained from $\Gamma \coloneqq (\Gamma_0, \Gamma_1)$ by restriction to $\operatorname{dom} L_{\min}^* = \mathfrak{H}_{m+2} \dotplus \mathfrak{N}_z(L_{\min}^*)$. Note that the γ-field associated with this OBT for $L_{\min}^*$ is $G_z(\cdot)$. The Q-function associated with $\mathscr{G}$ is the matrix in $\mathbb{C}^d$ whose entries are defined by

$$\big[Q_{\mathscr{G}}(z)\big]_{\sigma\sigma'} \coloneqq \sum_j \frac{\big[\mathscr{G}_b^*\big]_{\sigma,\sigma' j}}{(z_j - z) b_j'(z_j)} = \sum_j \frac{\mathscr{G}_{\sigma j,\sigma' j}}{(z_j - z) b_j'(z_j)^2}.$$

The second equality accounts for the condition that $\mathscr{G}$ is diagonal in $j \in J$; for $d = 1$, see also [18, Theorem 6.1].

2.6 Renormalised Weyl function

Ignoring formally that $\mathscr{G}$ is diagonal in j for $m \geq 2$, one can perform a kind of renormalisation of $Q_{\mathscr{G}}(z)$. For this purpose, put $z_j = z_1 - \delta_{j-1}$, $\delta_{j-1} \neq 0$, $j \in J \setminus \{1\}$, in the first

formula of $Q_{\mathscr{G}}(z)$, take the limits $\delta_j \to \delta_{j-1}$, as well as $\delta_1 \to 0$, and deduce by induction that the matrix $Q_{\mathscr{G}}(z)$ is "renormalised" to the matrix $Q_*(z)$ whose entries are given by

$$\big[Q_*(z)\big]_{\sigma\sigma'} := -\sum_j \frac{\big[\mathscr{G}_*\big]_{\sigma m,\sigma' j}}{(z-z_1)^{m-j+1}}.$$

An interesting observation is that the corresponding Weyl function M, denoted now by M_*, is, up to a constant, the Weyl function M_{A} of $A_{\max}$ in the A-model with model parameters $z_j = z_1$, provided that the entries at the m-th row of the Gram matrix of the A-model satisfy $\mathscr{G}_{\sigma m,\sigma' j} = \big[\mathscr{G}_*\big]_{\sigma m,\sigma' j}$. In this case, with a suitable choice of the OBT for $A_{\max}$ in the A-model, one has

$$M_*(z) = R_*(z_1) + M_{\mathrm{A}}(z)$$

for $z \in \operatorname{res} L \setminus \{z_1\}$. In the above formula R_* is obtained from R by simply replacing all $\{z_j\}$ in $b_m(L)$ by z_1; that is, the entries

$$\big[R_*(z) - R_*(z_1)\big]_{\sigma\sigma'} = (z-z_1)\,\langle \varphi_\sigma, b_m(L)^{-1}(L-z)^{-1}(L-z_1)^{-1}\varphi_{\sigma'}\rangle$$

for $z \in \operatorname{res} L$, constitute the matrix valued Q-function which is associated with $L_{\min}$ in $\mathfrak{H}_m$, where now $b_m(L) := (L-z_1)^m$.

3 Transformation preserving the Weyl function

According to [19], if Q-functions of two densely defined, closed, symmetric, and simple operators in (possibly) distinct Hilbert spaces coincide, then the operators are unitarily equivalent. In this paragraph we extend the latter statement to a not necessarily unitary transformation, which becomes unitary, however, in the special case.

Let $P_{\mathscr{H}}$ be a bounded operator from a Hilbert space $\mathfrak{H}_{-m}$ to a Hilbert space $\mathscr{H}$; let $P^*_{\mathscr{H}}$ be its adjoint, considered as a bounded operator from $\mathscr{H}$ to $\mathfrak{H}_{-m}$. Let $\Omega := P_{\mathscr{H}} b_m(L)^{1/2}$ be a bounded operator from $\mathfrak{H}_0$ to $\mathscr{H}$; then the operator $\Omega^* = b_m(L)^{-1/2} P^*_{\mathscr{H}}$, considered as a bounded operator from $\mathscr{H}$ to $\mathfrak{H}_0$, is the adjoint of Ω. Define also a bounded, non-negative, self-adjoint operator in $\mathscr{H}$ by $\iota := \Omega\Omega^* = P_{\mathscr{H}} P^*_{\mathscr{H}}$.

Let A_Θ be a (closed) proper extension of the symmetric operator $A_{\min}$ in $\mathscr{H}$ as described above, and define the operator $\boldsymbol{A}_\Theta := \Omega^* A_\Theta \Omega$ in $\mathfrak{H}_0$ on its natural domain. A direct computation shows that the adjoint in $\mathfrak{H}_0$ is the operator $\boldsymbol{A}_{\Theta^*}$. Let also $\boldsymbol{A}_{\min} := \Omega^* A_{\min} \Omega$,

and similarly for $\boldsymbol{A}_{\max}$. Then $\boldsymbol{A}_\Theta$ is a proper extension of a densely defined, closed, symmetric, and simple operator $\boldsymbol{A}_{\min}$. The domain of $\boldsymbol{A}_\Theta$ can be described in terms of Θ as the set of $u \in \mathrm{dom}\boldsymbol{A}_{\max}$ such that $(\boldsymbol{\Gamma}_0 u, \boldsymbol{\Gamma}_1 u) \in \Theta$, where $\boldsymbol{\Gamma} := (\boldsymbol{\Gamma}_0, \boldsymbol{\Gamma}_1)\colon \mathrm{dom}\boldsymbol{A}_{\max} \to \mathbb{C}^d \times \mathbb{C}^d$ is defined according to $\boldsymbol{\Gamma} = \Gamma\Omega$. Because $\Omega\mathrm{dom}\boldsymbol{A}_{\max} \subseteq \mathrm{dom}A_{\max}$ the operator $\boldsymbol{\Gamma}$ is not surjective, in general, so the present parametrisation of $\mathrm{dom}\boldsymbol{A}_\Theta$ applies to not all Θ, and the triple $\boldsymbol{\Pi} := (\mathbb{C}^d, \boldsymbol{\Gamma}_0, \boldsymbol{\Gamma}_1)$ is only an isometric boundary triple [8, Definition 1.8] for $\boldsymbol{A}_{\max}$. To make $\boldsymbol{\Pi}$ an OBT, we assume that $P_{\mathscr{H}}$ leaves $\mathrm{dom}A_{\max}$ invariant, because in this case $\Omega\mathrm{dom}\boldsymbol{A}_{\max} = \mathrm{dom}A_{\max}$. Then the following result holds.

Theorem 11.1 Let $\boldsymbol{M}$ be the Weyl function of $\boldsymbol{A}_{\min}$ corresponding to the OBT $\boldsymbol{\Pi}$ for $\boldsymbol{A}_{\max}$. Then $\boldsymbol{M}(z) = M(z)$, $z \in \mathrm{res}A_0$, iff

$$(\forall c \in \mathbb{C}^d)\,(\forall z \in \Sigma_\iota)\,\big[(A_0 - z)^{-1} - (\iota A_0 - z)^{-1}\iota\big]k_{\min}(c) \\ - (\iota A_0 - z)^{-1}(\iota - I)zG_z(c) \in \mathrm{dom}A_{\min}.$$

Here $\Sigma_\iota := \mathrm{res}A_0 \cap \mathrm{res}(\iota A_0)$. For $\iota = I$, one recovers that $P_{\mathscr{H}}$ (and hence Ω) is unitary, which is the case considered in [19, Theorem 2.2].

Proof. First, observe that $\mathfrak{N}_z(\iota A_{\max}) = H_z(\mathbb{C}^d)$, $z \in \Sigma_\iota$, where

$$H_z(c) := \big[I - z(\iota A_0 - z)^{-1}(\iota - I)\big]G_z(c) - (\iota A_0 - z)^{-1}\iota k_{\min}(c).$$

Indeed, since $f \in \mathfrak{N}_z(\iota A_{\max})$ belongs to $\mathrm{dom}A_{\max}$, it follows from (11.2) that

$$0 = \big(\iota A_0 - z\big)(f^{\#} + k) + (\iota - I)zG_z(c) + \iota k_{\min}(c).$$

By using $(L - z)G_z(c) = k_{\min}(c)$ the assertion follows.

Second, the graph of the γ-field $\boldsymbol{\gamma}$ associated with an OBT $\boldsymbol{\Pi}$ consists of the pairs $(c, u_z) \in \mathbb{C}^d \times \mathfrak{N}_z(\boldsymbol{A}_{\max})$ such that $\Omega u_z = H_z(c)$. Indeed, by definition, $\boldsymbol{\gamma}$ contains (c, u_z) such that $\boldsymbol{\Gamma}_0 u_z = c$. Since $\Omega\mathfrak{N}_z(\boldsymbol{A}_{\max}) \subseteq \mathfrak{N}_z(\iota A_{\max})$, the assertion follows by using the first claim. To verify that $\boldsymbol{\gamma}$ is the graph, let us compute its multivalued part; it is the set of $u_z \in \mathfrak{N}_z(\boldsymbol{A}_{\max}) \cap \ker\Omega = \ker(\boldsymbol{\Gamma}_0 \,|\, _{\mathfrak{N}_z(\boldsymbol{A}_{\max})}) = \{0\}$.

Third, the Weyl function $\boldsymbol{M}$ associated with $\boldsymbol{\Pi}$ is given by $\boldsymbol{M}(z) = \Gamma_1 H_z(\,\cdot\,)$ (on $\mathbb{C}^d$) for $z \in \Sigma_\iota$, which is seen from the second claim. Using in addition that

$$Q_{\mathscr{G}}(z)c = -\Gamma_1\big[(A_0 - z)^{-1}k_{\min}(c)\big]$$

one gets that

$$\boldsymbol{M}(z) = M(z) + \Delta(z)$$

with

$$\Delta(z)c \coloneqq \Gamma_1\big\{\big[(A_0 - z)^{-1} - (\imath A_0 - z)^{-1}\imath\big]k_{\min}(c) - (\imath A_0 - z)^{-1}(\imath - I)zG_z(c)\big\}.$$

Thus $\boldsymbol{M}(z) = M(z)$ iff $\Delta(z)$ vanishes; in this case the equality for the analytic Weyl functions extends to the domain of analyticity of $M(z)$, namely, $\operatorname{res} A_0$.

Finally, $(\forall c)\ \Delta(z)c = 0$ iff the term in $\{\ \}$, which belongs to $\operatorname{dom} A_0$ by construction, also belongs to $\ker\Gamma_1$, i. e. iff it belongs to $\operatorname{dom} A_0 \cap \ker\Gamma_1 = \operatorname{dom} A_{\min}$. □

To this end we remark that a similar theorem can be formulated in the A-model as well, but now the situation is more delicate, because M in the A-model might belong to the class of generalised Nevanlinna families with a finite number κ of negative squares, while $\boldsymbol{M}$ associated with the OBT for the Hilbert space (i. e. $\mathfrak{H}_0$) adjoint of a symmetric operator belongs to the class of Nevanlinna families, i. e. $\kappa = 0$. Thus a different meaning has to be given to the adjoint of $P_{\mathscr{H}}$ (and hence Ω). The details will be presented elsewhere.

Bibliography

[1] Albeverio, S., Kurasov, P.: *Rank one perturbations of not semibounded operators*, Integr. Equ. Oper. Theory **27**, 379–400 (1997).

[2] Albeverio, S, Kurasov, P.: *Singular perturbations of differential operators*, London Mathematical Society Lecture Note Series 271. Cambridge University Press, UK (2000).

[3] Albeverio, S, Kuzhel, S., Nizhnik, L.: *Singularly perturbed self-adjoint operators in scales of Hilbert spaces*, Ukr. J. Math. **59**(6), 787–810 (2007).

[4] Behrndt, J., Hassi, S., de Snoo, H.: *Boundary relations, unitary colligations, and functional models*, Compl. Anal. Oper. Theory **3**(1), 57–98 (2009).

[5] Behrndt, J., Hassi, S., de Snoo, H.: *A realization theorem for generalized Nevanlinna families*, Oper. Matrices **5**(4), 679–706 (2011).

[6] Derkach, V.: *Abstract interpolation problem in Nevanlinna classes*, Modern Analysis and Applications **190**, 197–236 (2009).

[7] Derkach, V., Hassi, S., de Snoo, H.: *Singular perturbations of self-adjoint operators*, Math. Phys. Anal. Geom. **6**(4), 349–384 (2003).

[8] Derkach, V., Hassi, S., Malamud, M.: *Generalized boundary triples, Weyl functions and inverse problems*, *arXiv:1706.07948v1* (2017).

[9] Derkach, V., Hassi, S., Malamud, M., de Snoo, H.: *Boundary relations and their Weyl families*, Trans. Amer. Math. Soc. **358**(12), 5351–5400 (2006).

[10] Derkach, V., Hassi, S., Malamud, M., de Snoo, H.: *Boundary relations and generalized resolvents of symmetric operators*, Russ. J. Math. Phys. **16(1)**, 17–60 (2009).

[11] Derkach, V., Hassi, S., Malamud, M., de Snoo, H.: *Boundary triplets and Weyl functions. Recent developments*, In Seppo Hassi, Hendrik S. V. de Snoo, and Franciszek Hugon Szafraniec, editors, *Operator Methods for Boundary Value Problems, London Math. Soc. Lecture Note Series*, volume 404, chapter 7, pages 161–220. Cambridge University Press, UK (2012).

[12] Dijksma, A., Kurasov, P., Shondin, Yu.: *High order singular rank one perturbations of a positive operator*, Integr. Equ. Oper. Theory **53**, 209–245 (2005).

[13] Dijksma, A., Langer, H., Shondin, Yu.: *Rank one perturbations at infinite coupling in Pontryagin spaces*, J. Func. Anal. **209**(1), 206–246 (2004).

[14] Juršėnas, R.: *The peak model for the triplet extensions and their transformations to the reference Hilbert space in the case of finite defect numbers*, *arXiv:1810.07416* (2018).

[15] Juršėnas, R.: *On some extensions of the A-model*, *arXiv:1909.07078* (2019).

[16] Kurasov, P.: *$\mathfrak{H}_{-n}$-perturbations of self-adjoint operators and Krein's resolvent formula*, Integr. Equ. Oper. Theory **45**(4), 437–460 (2003).

[17] Kurasov, P.: *Singular and supersingular perturbations: Hilbert space methods*, Contemp. Math. **340**, 185–216 (2003).

[18] Kurasov, P.: *Triplet extensions I: Semibounded operators in the scale of Hilbert spaces*, J. Anal. Math. **107**(1), 252–286 (2009).

[19] Langer, H., Textorius, B.: *On generalized resolvents and Q-functions of symmetric linear relations (subspaces) in Hilbert space*, Pac. J. Math. **72**(1), 135–165 (1977).

12

Mayer expansion for the Asakura-Oosawa model of colloid theory

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Abstract. *We present a convergence criterion for the activity expansion of the Asakura-Oosawa model of penetrable hard-spheres, a popular toy model in colloid theory. The model consists of a binary mixture of large and small spheres where small spheres may freely overlap with each other but the interaction is hard-core otherwise. Our convergence criterion is formulated in terms of an effective activity for large objects that takes into account excluded volume effects.*

1 The Asakura-Oosawa model. Depletion attraction

Consider a binary mixture of small spheres of radius $r > 0$ and large spheres of radius $R > r$, with respective activities $z_r > 0$ and $z_R > 0$. Two large spheres cannot overlap, a small sphere and a large sphere cannot overlap either, but two small spheres are allowed

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to overlap. Let $\Lambda = [0,L]^d$ with $L > 2(R+r)$. The grand-canonical partition function for the Asakura-Oosawa model [2] in the box Λ is

$$\Xi_\Lambda(z_R,z_r) = \sum_{n_1,n_2=0}^{\infty} \frac{z_R^{n_1}}{n_1!}\frac{z_r^{n_2}}{n_2!} \int_{\Lambda^{n_1}} \left\{ \int_{\Lambda^{n_2}} \left(\prod_{1\le i<j\le n_1} \mathbb{1}_{\{|x_i-x_j|>2R\}} \right) \times \left(\prod_{\substack{1\le i\le n_1\\ 1\le j\le n_2}} \mathbb{1}_{\{|x_i-y_j|>R+r\}} \right) \mathrm{d}\boldsymbol{y} \right\} \mathrm{d}\boldsymbol{x}.$$

Integrals with zero integration variables are set to be equal to 1; in particular, the summand for $n_1 = n_2 = 0$ is 1.

Since small spheres do not interact, the integration over the y-variables can be carried out explicitly, which yields

$$\Xi_\Lambda(z_R,z_r) = \mathrm{e}^{z_r|\Lambda|} \sum_{n_1=0}^{\infty} \frac{z_R^{n_1}}{n_1!} \int_{\Lambda^{n_1}} \left(\prod_{1\le i<j\le n} \mathbb{1}_{\{|x_i-x_j|>2R\}} \right) \times \exp\left(-z_r \Big| \Lambda \cap \bigcup_{i=1}^{n} B(x_i,R+r) \Big| \right) \mathrm{d}x$$

where $|A|$ denotes the Lebesgue measure of a set $A \subset \mathbb{R}^d$, $|x-y|$ is the Euclidean distance in $\mathbb{R}^d$, and $B(x_i,R+r)$ is the closed ball of radius $R+r$ centered at x_i. In order to get rid of the Λ-dependence inside the last exponential, we switch to periodic boundary conditions: let $d(x_1,x_2) \equiv d_L(x_1,x_2) := \inf_{k\in\mathbb{Z}^d} |x_1 - x_2 + kL|$ and

$$\Xi_\Lambda^{\mathrm{per}}(z_R,z_r) = \mathrm{e}^{z_r|\Lambda|} \sum_{n_1=0}^{\infty} \frac{z_R^{n_1}}{n_1!} \int_{\Lambda^{n_1}} \left(\prod_{1\le i<j\le n} \mathbb{1}_{\{d(x_i,x_j)>2R\}} \right) \times \exp\left(-z_r \Big| \bigcup_{i=1}^{n} B_d(x_i,R+r) \Big| \right) \mathrm{d}x.$$

Here $B_d(x_i,R+r)$ is a closed ball with respect to the metric $d = d_L$ that takes into account the periodic boundary conditions. Set

$$W_k(x_1,\dots,x_k;z_r) := z_r(-1)^{k-1} \Big| \bigcup_{i=1}^{n} B_d(x_i,R+r) \Big|.$$

By inclusion-exclusion, the area covered by the union of the balls is equal to

$$\left|\bigcup_{i=1}^{n} B_d(x_i,R+r)\right| = n\left|B_d(0,R+r)\right| + \sum_{k=2}^{n}(-1)^{k-1}\sum_{1\le i_1<\cdots<i_k\le n}\left|\bigcap_{\ell=1}^{k} B_d(x_{i_\ell},R+r)\right|.$$

Further set

$$\widehat{z}_R \equiv \widehat{z}_R(z_r) := z_R \exp\Big(-z_r\left|B_d(0,R+r)\right|\Big),$$

$v(x_1,x_2) := \infty\cdot\mathbb{1}_{\{|x_1-x_2|\le 2R\}}$, and

$$H_n(x_1,\dots,x_n;z_r) := \sum_{1\le i<j\le n} v(x_i,x_j) + \sum_{k=2}^{n}\sum_{1\le i_1<\dots<i_k\le n} W_k(x_{i_1},\dots,x_{i_k};z_r).$$

The grand-canonical partition function with periodic boundary conditions becomes

$$\Xi_\Lambda^{\mathrm{per}}(z_R,z_r) = \mathrm{e}^{z_r|\Lambda|}\left(1+\sum_{n=1}^{\infty}\frac{\widehat{z}_R(z_r)^n}{n!}\int_{\Lambda^n}\mathrm{e}^{-H_n(x_1,\dots,x_n;z_r)}\,\mathrm{d}x\right).$$

Notice that $\exp\big(z_r|\Lambda|\big) = \Xi_\Lambda^{\mathrm{per}}(0,z_r)$. Thus we have found that the full partition function $\Xi_\Lambda^{\mathrm{per}}(z_R,z_r)$, divided by the partition function $\Xi_\Lambda^{\mathrm{per}}(0,z_r)$ that has small spheres only, is equal to the grand-canonical partition function of an effective model. The effective model sees only large spheres with a new effective activity $\widehat{z}_R$. In addition to the hard-core interaction that large spheres may not overlap, there are multibody interaction terms $W_k(\,\cdot\,;z_r)$ that correspond to effective interactions mediated by the small spheres. The effective interactions kick in only when the *depletion layers* $B(x_i,R+r)$ overlap. Moreover the new effective interaction is negative,

$$\sum_{k=2}^{n}\sum_{1\le i_1<\dots<i_k\le n} W_k(x_{i_1},\dots,x_{i_k};z_r) = z_r\left|\bigcup_{i=1}^{n} B_d(x_i,R+r)\right| - z_r\sum_{i=1}^{n}\left|B_d(x_i,R+r)\right| \le 0,$$

a phenomenon called *depletion attraction* [2].

2 Cluster expansion

A *hypergraph* $\mathfrak{h}$ is a pair $\mathfrak{h}=(V,E)$ consisting of a finite set V and a set $E\equiv E(\mathfrak{h})\subset\{J\mid J\subset V,\#J\ge 2\}$. Elements of V are called *vertices*, elements of E *hyperedges*. A

hypergraph is *connected* if for every pair of vertices $v, w \in V$, there exists a finite sequence $J_1, \dots, J_\ell \in E$ of hyperedges such that $v \in J_1$, $w \in J_m$, and $J_i \cap J_{i+1} \neq \varnothing$ for all $i = 1, \dots, \ell - 1$. Let $\mathfrak{C}_m$ be the set of connected hypergraphs with vertex set $\{1, \dots, n\}$. For $\mathfrak{h} \in \mathfrak{C}_m$ and $x_1, \dots, x_m \in \Lambda$, define the graph weight

$$w(\mathfrak{h}; x_1, \dots, x_m; z_r) := \left(\prod_{\{i,j\} \in E(\mathfrak{h})} \left(\mathrm{e}^{-v(x_i,x_j) - W_2(x_i,x_j;z_r)} - 1 \right) \right) \times \left(\prod_{\substack{J \in E(\mathfrak{h}): \\ \#J \geq 3}} \left(\mathrm{e}^{-W_{\#J}((x_j)_{j \in J}; z_r)} - 1 \right) \right).$$

Finally let

$$\psi_m^{\mathsf{T}}(x_1, \dots, x_m; z_r) := \sum_{\mathfrak{h} \in \mathfrak{C}_m} w(\mathfrak{h}; x_1, \dots, x_m; z_r)$$

and $\psi_1^{\mathsf{T}}(x_1; z_r) := 1$.

Theorem 12.1 Assume that there exist scalars $a, A \geq 0$ such that z_r and $\widehat{z}_R = \widehat{z}_R(z_r)$ satisfy

$$\big|B(0,2R)\big| \, \mathrm{e}^A \widehat{z}_R + \big|B(0,R+r) \setminus B(0,R-r)\big| \, \mathrm{e}^a z_r \leq A,$$
$$\big|B(0,R+r) \setminus B(0,R-r)\big| \, \mathrm{e}^A \widehat{z}_R \leq a.$$

Then for all $L > R + r$,

$$\log \Xi_\Lambda^{\mathrm{per}}(z_R, z_r) = z_r |\Lambda| + \sum_{m=1}^{\infty} \frac{\widehat{z}_R^m}{m!} \int_{\Lambda^m} \psi_m^{\mathsf{T}}(x_1, \dots, x_m; z_r) \, \mathrm{d}x$$

with

$$\sum_{m=2}^{\infty} \frac{\widehat{z}_R^{m-1}}{(m-1)!} \int_{\Lambda^{m-1}} \big| \psi_m^{\mathsf{T}}(x_1, \dots, x_m; z_r) \big| \, \mathrm{d}x_2 \cdots \mathrm{d}x_m \leq \mathrm{e}^A - 1 < \infty \qquad (x_1 \in \Lambda). \quad (12.1)$$

The theorem should be contrasted with the convergence condition

$$\big|B(0,2R)\big| \, \mathrm{e}^A z_R + \big|B(0,R+r)\big| \, \mathrm{e}^a z_r \leq A, \qquad \big|B(0,R+r)\big| \, \mathrm{e}^A z_R \leq a.$$

obtained from a direct application of a convergence condition for non-negative pair potentials by Ueltschi [6] to the original binary mixture. The latter has been extended to attractive pair potentials by Poghosyan and Ueltschi [5], building on the method developed by Minlos and Poghosyan [3]. Our new convergence condition differs in two ways: first, it has $\widehat{z}_R$ instead of z_r; second, it has the shell $B(0,R+r) \setminus B(0,R-r)$ instead of the full ball $B(0,R+r)$.

3 Proof ideas

3.1 From hypergraphs to leaf-constrained bipartite graphs

It is a matter of standard combinatorics to check that

$$\log\left(1+\sum_{n=1}^{\infty}\frac{\widehat{z}_R^m}{m!}\int_{\Lambda^m}\mathrm{e}^{-H_m(x_1,\dots,x_m;z_r)}\,\mathrm{d}x\right)=\sum_{m=1}^{\infty}\frac{\widehat{z}_R^m}{m!}\int_{\Lambda^m}\psi_m^{\mathsf{T}}(x_1,\dots,x_m;z_r)\,\mathrm{d}x$$

holds true as an equality of formal power series in $\widehat{z}_R$. The challenge is to prove absolute convergence of the right-hand side. The first step of the proof is a mapping from hypergraphs on m vertices to graphs with a variable number $m+n$ of new vertices. New vertices represent hyperedges of the original graph. Set

$$f(x_1,x_2):=\mathrm{e}^{-v(x_1,x_2)}-1=-\mathbb{1}_{\{d(x_1,x_2)\le R+r\}},\qquad \zeta(x,y):=-\mathbb{1}_{\{d(x,y)\le 2R\}}.$$

Let $\mathscr{C}^*_{m,n}$ be the set of connected graphs with vertex set $\{1,\dots,m+n\}$ such that (i) there are no edges $\{i,j\}$ linking two vertices $i,j\ge m+1$ and (ii) every vertex $j\in\{m+1,\dots,m+n\}$ connects to at least two distinct vertices $i,i'\in\{1,\dots,m\}$. Graphs in $\mathscr{C}^*_{m,n}$ are usual graphs with edges $\{i,j\}$ (no hyperedges of cardinality $\#J\ge 3$). Define

$$\varphi^{\mathsf{T}}_{m,n,*}(x_1,\dots,x_m;y_{m+1},\dots,y_{m+n}):=\sum_{G\in\mathscr{C}^*_{m,n}}\Bigg(\prod_{\substack{\{i,j\}\in E(G):\\1\le i<j\le m}}f(x_i,x_j)\Bigg)\Bigg(\prod_{\substack{\{i,j\}\in E(G):\\i\le m<j}}\zeta(x_i,y_j)\Bigg).$$

Lemma 12.2 For all $m\ge 2$ and $x_1,\dots,x_m\in\Lambda$,

$$\psi_m^{\mathsf{T}}(x_1,\dots,x_m;z_r)=\sum_{n=0}^{\infty}\frac{z_r^n}{n!}\int_{\Lambda^n}\varphi^{\mathsf{T}}_{m,n,*}(x_1,\dots,x_m;y_{m+1},\dots,y_{m+n})\,\mathrm{d}y_{m+1}\cdots\mathrm{d}y_{m+n}.$$

Proof. Let $\mathfrak{h}\in\mathfrak{C}_m$ be a connected hypergraph. If $J\in E(\mathfrak{h})$ is a hyperedge with cardinality $\#J\ge 3$, we expand

$$\mathrm{e}^{-W_{\#J}((x_j)_{j\in J};z_r)}-1=\sum_{k_J=1}^{\infty}\frac{1}{k_J!}\big(-W_{\#J}((x_j)_{j\in J};z_r)\big)^{k_J}=\sum_{k_J=1}^{\infty}\frac{z_r^{k_J}}{k_J!}\left(\int_{\Lambda}\prod_{j\in J}\zeta(x_j,y)\,\mathrm{d}y\right)^{k_J}.$$

For edges $\{i,j\}\in E(\mathfrak{h})$ of cardinality 2, we expand

$$\mathrm{e}^{-v(x_i,x_j)-W_2(x_i,x_j;z_r)}-1=f(x_i,x_j)+\big(1+f(x_i,x_j)\big)\sum_{k_{ij}=1}^{\infty}\frac{z_r^{k_{ij}}}{k_{ij}!}\left(\int_{\Lambda}\zeta(x_i,y)\zeta(x_j,y)\,\mathrm{d}y\right)^{k_{ij}}.$$

Inserting these expansions into the definition of the weight $w(\mathfrak{h};x_1,\dots,x_m;z_r)$ gives rise to a sum over tuples $(k_J)_{J\in E(\mathfrak{h})}$ of non-zero integers. We group terms with a common

value of $n = \sum_{J\in E(\mathfrak{h})} k_J$ and rearrange the powers of z_r and the factorials as

$$\prod_{J\in E(\mathfrak{h})} \frac{z_r^{k_J}}{k_J!} = \frac{z_r^n}{n!} \times \frac{n!}{\prod_{J\in E(\mathfrak{h})} k_J!}.$$

The multinomial counts the number of mappings $\mathscr{J}$ from the label set $m+1,\dots,m+n$ to the hyperedges of $\mathfrak{h}$ such that exactly k_J labels are mapped to J. Every mapping $\mathscr{J}$ is associated with a bipartite graph G with vertex set $\{1,\dots,m+n\}$ and edge set

$$E(G) = \big\{\{i,j\} \mid i \le m < j, i \in \mathscr{J}(j)\big\},$$

moreover

$$\prod_{J\in E(\mathfrak{h})} \Big(\int_\Lambda \prod_{i\in J} \zeta(x_i,y)\,\mathrm{d}y\Big)^{k_J} = \int_{\Lambda^n} \prod_{\{i,j\}\in E(G')} \zeta(x_i,y_j)\,\mathrm{d}y.$$

Conversely, every bipartite graph G' such that every vertex $j > m$ is linked to at least two distinct vertices $i, i' \in J$ is uniquely associated with a mapping $\mathscr{J}$. As a consequence, if $\mathfrak{h}$ has no edge of cardinality 2, then

$$\psi_m^{\mathsf{T}}(\mathfrak{h};x_1,\dots,x_m;z_r) = \sum_{n=0}^{\infty} \frac{z_r^n}{n!} \int_{\Lambda^n} \sum_{G} \prod_{\{i,j\}\in E(G)} \zeta(x_i,y_j)\,\mathrm{d}y.$$

where the sum runs over bipartite graphs G with degree constraint as above that arise from a mapping $\mathscr{J} : \{m+1,\dots,m+n\} \to E(\mathfrak{h})$ such that $\#\mathscr{J}^{-1}(J) \ge 1$, for all $J \in E(\mathfrak{h})$. If $\mathfrak{h}$ has edges of cardinality 2, a similar formula holds true but with a sum over graphs that may have additional edges $\{i,j\}$ with $1 \le i < j \le m$, associated with an additional factor $f(x_i,x_j)$. Summation over all connected hypergraphs $\mathfrak{h}$ translates into summation over graphs $G \in \mathscr{C}^*_{m,n}$. □

3.2 Tree-graph inequality

The second ingredient to the proof of Theorem 12.1 is a variant of the classical tree-graph inequality due to O. Penrose [4]. Set $\tilde{\zeta}(x_i,y) := -\mathbb{1}_{\{y\in B_d(x_i,R+r)\setminus B_d(x_i,R-r)\}}$. Notice

$$\big(1+f(x_i,x_j)\big)\cdot\big|\zeta(x_i,y)\zeta(x_j,y)\big| \le \big(1+f(x_i,x_j)\big)\cdot\big|\tilde{\zeta}(x_i,y)\tilde{\zeta}(x_j,y)\big|. \tag{12.2}$$

Indeed, if $y \in B_d(x_i,R+r)\cap B_d(x_j,R+r)$ and $B_d(x_i,R)\cap B_d(x_j,R) = \varnothing$, then necessarily $d(x_i,y) \ge d(x_i,x_j) - d(x_j,y) > R-r$. Similarly,

$$\big|\zeta(x_1,y)\big| \prod_{1\le i<j\le k} \big(1+f(x_i,x_j)\big)\cdot \left|\left(\prod_{j=2}^{k}\big(1+\zeta(x_j,y)\big)-1\right)\right| \le \big|\tilde\zeta(x_1,y)\big| \prod_{1\le i<j\le k} \big(1+f(x_i,x_j)\big). \quad (12.3)$$

Proposition 12.3 Set $\mathscr{T}^*_{m,n} \subset \mathscr{C}^*_{m,n}$ be the subset of graphs $G \in \mathscr{C}^*_{m,n}$ that are trees. Then

$$\big|\varphi^{\mathsf{T}}_{m,n,*}(x_1,\dots,x_m.y_{m+1},\dots,y_{m+n})\big| \le \sum_{T\in\mathscr{T}^*_{m,n}} \left(\prod_{\substack{\{i,j\}\in E(T):\\ 1\le i<j\le m}} \big|f(x_i,x_j)\big|\right)\cdot\left(\prod_{\substack{\{i,j\}\in E(T):\\ i\le m<j}} \big|\tilde\zeta(x_i,y_j)\big|\right).$$

Proof sketch. We identify every edge $\{i,j\}$ with the two-letter word ji where $j \ge i$. Let $\prec$ be the reverse lexicographic order, i. e. $ji \prec j'i'$ if and only if either $j \ge j'$ or $j = j'$ and $i \ge i'$. Thus

$$\{m+n,m+n-1\} \prec \{m+n,m+n-1\} \prec \cdots \prec \{m+n,1\} \prec \cdots \{2,1\} \prec \{1,1\}. \quad (12.4)$$

The order lists all edges that include a vertex $j > m$, associated with a y-variable, before the edges $\{i,j\}$, $1 \le i < j \le m$, associated with x-variables only. If $G \in \mathscr{C}^*_{m,n}$, we construct a spanning tree T with Kruskal's algorithm by going through the edges of G in the order dictated by the total order $\prec$, discarding edges that create loops. In the sum over connected graphs G defining $\varphi^{\mathsf{T}}_{m,n,*}$ we group together graphs that are mapped to the same spanning tree T. The proposition follows by carefully revisiting classical arguments on tree partition schemes, taking into account the precise choice (12.4) of the order $\prec$ and the inequalities (12.2) and (12.3), which allow us to replace $\zeta(x_i,y_j)$ with $\tilde\zeta(x_i,y_j)$. See [1, Proposition 5.4] for a detailed proof in a more general context. □

3.3 Proof of convergence

Armed with Lemma 12.2 and Proposition 12.3 we can sketch the proof of the inequality (12.1) in Theorem 12.1. Set $\mathscr{P} := \Lambda \times \{R,r\}$ and define $h : \mathscr{P}\times\mathscr{P} \to [-1,0]$ by

$$h(P_1,P_2) := \begin{cases} f(x_1,x_2), & P_1 = (x_1,R),\ P_2 = (x_2,R)\\ \tilde\zeta(x_1,y_2), & P_1 = (x_1,R),\ P_2 = (y_2,r),\\ \tilde\zeta(x_2,y_1), & P_1 = (y_1,r),\ P_2 = (x_2,R),\\ 0, & P_1,P_2 \in \Lambda\times\{r\}. \end{cases}$$

Further let $b : \mathscr{P} \to \mathbb{R}_+$ be given by $b(x,R) = A$ and $b(x,r) = a$ for all $x \in \Lambda$. For $B \subset \mathscr{P}$ let $\lambda(B) := \widehat{z}_R \big|B \cap (\Lambda \times \{R\})\big| + z_r \big|B \cap (\Lambda \times \{r\})\big|$. The conditions of the theorem ensure that

$$\int_{\mathscr{P}} |h(P,Q)| \mathrm{e}^{b(Q)} \lambda(\mathrm{d}Q) \leq b(P),$$

for all $P \in \mathscr{P}$. Let $\mathscr{T}_n^\circ$ denote the set of trees with vertex set $\{0,1,\dots,n\}$. Proceeding as in [6], we see that for all $P_0 \in \mathscr{P}$,

$$\sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathscr{P}^n} \sum_{T \in \mathscr{T}_n} \prod_{\{i,j\} \in E(T)} \big|h(P_i,P_j)\big| \, \lambda^n\big(\mathrm{d}(P_1,\dots,P_n)\big) \leq \mathrm{e}^{b(P_0)} - 1.$$

The theorem then follows from Lemma 12.2 and Proposition 12.3.

Bibliography

[1] Jansen, S., Tsagkarogiannis, D.: *Cluster expansions with renormalized activities and applications to colloids*, Ann. Inst. H. Poincaré Online first (2019).

[2] Lekkerkerker, H. N. W., Tuinier, R.: *Colloids and the Ddpletion interaction*. Lect. Notes Phys., vol. 833. Springer, Berlin (2011).

[3] Minlos, R. A., Pogosyan, S. K.: *Estimates of Ursell functions, group functions and their derivatives.* Teor. Mat. Fiz. **31**, 408–418 (1977).

[4] Penrose, O.: *Convergence of fugacity expansions for classical systems.* In: Bak, T. A. (ed.) Statistical Mechanics: Foundations and Applications, proceedings of the I. U. P. A. P. Meeting, Copenhagen, 1966, p. 101. W., A. Benjamin, Inc., New York (1967).

[5] Poghosyan, S., Ueltschi, D.: *Abstract cluster expansion with applications to statistical mechanical systems*, J. Math. Phys. **50**, 053509, 17 pp. (2009).

[6] Ueltschi, D.: *Cluster expansions and correlation functions*, Mosc. Math. J. **4**, 511–522 (2004).

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Virial inversion for inhomogeneous systems

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Abstract. *We prove a novel inversion theorem for functionals given as power series in infinite-dimensional spaces and apply it to the inversion of the density-activity relation for inhomogeneous systems. This provides a rigorous framework to prove convergence for density functionals with applications in classical density function theory, liquid crystals, molecules with various shapes or other internal degrees of freedom.*

1 Introduction

One of the main challenges in statistical mechanics is to derive functional expressions for thermodynamic quantities from microscopic models which are based on physical principles. In particular, for systems in classical density functional theory, liquid crystals, heterogeneous materials, colloids and in general of molecules with internal degrees of freedom the key point is to consider non-constant densities and hence non-translation

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invariance. One first mathematically rigorous result for homogeneous systems was the proof of the convergence of the virial expansion by Lebowitz and Penrose in 1964 [6], building on the previously established convergence of the activity expansion of the pressure and of the density. The goal of this paper is to establish the validity of the inversion formulas for inhomogeneous fluids with applications in the above cases. We view the latter as systems of uncountably many species, by considering the position $x \in \Lambda \subset \mathbb{R}^d$ as species. In this way, we can treat at the same time systems with internal degrees of freedom without increasing the complexity of the arguments involved.

At first sight, one may try to use inverse function theorems in complex Banach spaces, applied to the functional that maps the activity profile $\big(z(x)\big)_{x\in\Lambda}$ to the density profile $\big(\rho(x)\big)_{x\in\Lambda}$. This works well for inhomogeneous systems of e. g. objects of bounded size, e. g., hard spheres of fixed radius. It turns out, however, that Banach inversion fails for mixtures of objects of finite but unlimited size, for a precise example see [4] as well as [3]. As a way out, mixtures of countably many species were treated with the help of Lagrange-Good inversion in [5], leaving the case of uncountably many species wide open.

Our main result is a novel inversion theorem (Theorem 13.3) that addresses the above-mentioned difficulties and bypasses both Banach and Lagrange-Good inversion. The novelty is two-fold. First, we work on the level of formal series and relate the formal inverse to generating functions of trees or equivalently, solutions of certain formal fixed point problems (Proposition 13.4). This part is inspired by the combinatorial proof of the Lagrange-Good formula for finitely many variables given in [2]. Second, we provide sufficient conditions for the convergence of the formal inverse, i. e., of a generalised tree generating functions (Theorem 13.2).

2 Main theorem

Let $(\mathbb{X}, \mathscr{X})$ be a measurable space and $\mathfrak{M}(\mathbb{X}, \mathscr{X})$ the set of σ-finite non-negative measures on $(\mathbb{X}, \mathscr{X})$. Further let $\mathfrak{M}_{\mathbb{C}}(\mathbb{X}, \mathscr{X})$ be the set of complex linear combinations of measures in $\mathfrak{M}(\mathbb{X}, \mathscr{X})$. When there is no risk of confusion, we shall write $\mathfrak{M}$ and $\mathfrak{M}_{\mathbb{C}}$ for short. Suppose we are given a family of measurable functions $A_n : \mathbb{X} \times \mathbb{X}^n \to \mathbb{C}$,

$\big(q,(x_1,\dots,x_n)\big) \mapsto A_n(q;x_1,\dots,x_n)$. We assume that each A_n is symmetric in the x_j's, i. e.,

$$A_n(q;x_{\sigma(1)},\dots,x_{\sigma(n)}) = A_n(q;x_1,\dots,x_n), \tag{13.1}$$

for all permutations $\sigma \in \mathfrak{S}_n$. When we say that a power series converges absolutely, we mean that

$$\sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} \big|A_n(q;x_1,\dots,x_n)\big|\, |z|(\mathrm{d}x_1)\cdots|z|(\mathrm{d}x_n) < \infty, \tag{13.2}$$

where $|z|$ is the total variation of $z \in \mathfrak{M}_{\mathbb{C}}$. Let $\mathcal{D}(A) \subset \mathfrak{M}_{\mathbb{C}}$ be the domain of convergence of the associated power series, that is $z \in \mathcal{D}(A)$ if and only if the power series converges absolutely in the above sense. We set

$$A(q;z) := \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} A_n(q;x_1,\dots,x_n) z(\mathrm{d}x_1)\cdots z(\mathrm{d}x_n) \qquad (z \in \mathcal{D}(A)). \tag{13.3}$$

We are interested in maps of the form

$$\mathfrak{M}_{\mathbb{C}} \supset \mathcal{D}(A) \to \mathfrak{M}_{\mathbb{C}}, \quad z \mapsto \rho[z] \tag{13.4}$$

given by

$$\rho[z](\mathrm{d}q) \equiv \rho(\mathrm{d}q;z) := \mathrm{e}^{-A(q;z)} z(\mathrm{d}q), \tag{13.5}$$

where $\rho(\mathrm{d}q;z)$ is just a notation for $\rho[z](\mathrm{d}q)$. The latter is useful whenever one wants to stress the q instead of the z dependence. Thus $\rho[z]$ is absolutely continuous with respect to z with Radon-Nikodým derivative $\exp\big(-A(q;z)\big)$. (Note that for the case of an inhomogeneous gas this corresponds to the one-particle density as a function of position and activity.) We want to determine the inverse map $\nu \mapsto \zeta[\nu]$,

$$\nu = \rho[z] \Leftrightarrow z = \zeta[\nu].$$

Suppose for a moment that such an inverse map exists. Clearly z is equivalent to $\nu = \rho[z]$ with Radon-Nikodým derivative $\exp(A(q;z))$. Consequently we should have

$$\zeta[\nu](\mathrm{d}q) \equiv \zeta(\mathrm{d}q;\nu) = \mathrm{e}^{A(q;\zeta[\nu])} \nu(\mathrm{d}q). \tag{13.6}$$

This observation is the starting point for our inversion result, namely the family of power series $(T_q^\circ)_{q\in\mathbb{X}}$ given by

$$T_q^\circ(\nu) \equiv T^\circ(q;\nu) = \mathrm{e}^{A(q;\zeta[\nu])} \tag{13.7}$$

should solve

$$\zeta[\nu](\mathrm{d}q) = T_q^\circ(\nu)\nu(\mathrm{d}q) = \mathrm{e}^{A(q;\nu T_q^\circ(\nu))}\nu(\mathrm{d}q) \tag{13.8}$$

and therefore

$$T_q^\circ(\nu) = \exp\left(\sum_{n=1}^{\infty}\frac{1}{n!}\int_{\mathbb{X}^n} A_n(q;x_1,\dots,x_n)\,T_{x_1}^\circ(\nu)\cdots T_{x_n}^\circ(\nu)\,\nu(\mathrm{d}x_1)\cdots\nu(\mathrm{d}x_n)\right). \tag{FP}$$

In Proposition 13.4 below we provide a combinatorial interpretation of T_q° as the exponential generating function for coloured rooted, labeled trees whose root is a ghost of colour q (i. e., the root does not come with powers of ν in the generating function). For our main inversion theorem, however, it is enough to know that the fixed point equation (FP) determines the power series $(T_q^\circ)_{q\in\mathbb{X}}$ uniquely.

Lemma 13.1 There exists a uniquely defined family of formal power series

$$T_q^\circ(\nu) = 1 + \sum_{n=1}^{\infty}\frac{1}{n!}\int_{\mathbb{X}^n} t_n(q;x_1,\dots,x_n)\,\nu(\mathrm{d}x_1)\cdots\nu(\mathrm{d}x_n) \qquad (q\in\mathbb{X}) \tag{13.9}$$

with $t_n : \mathbb{X}\times\mathbb{X}^n \to \mathbb{C}$ measurable and symmetric in the x_j's, that solves (FP) in the sense of formal power series.

As the above expressions are interpreted in the sense of formal power series, neither the series need to converge nor the integrals need to exist.

Proof. Set $t_0 := 1$. Let $B_n(q;x_1,\dots,x_n)$ be the coefficients of the series in the exponential in (FP), i. e., each $B_n : \mathbb{X}\times\mathbb{X}^n \to \mathbb{C}$ is measurable, and we have

$$\sum_{n=1}^{\infty}\frac{1}{n!}\int_{\mathbb{X}^n} B_n(q;x_1,\dots,x_n)\nu(\mathrm{d}x_1)\cdots\nu(\mathrm{d}x_n)$$
$$= \sum_{n=1}^{\infty}\frac{1}{n!}\int_{\mathbb{X}^n} A_n(q;x_1,\dots,x_n)\,T_{x_1}^\circ(\nu)\cdots T_{x_n}^\circ(\nu)\,\nu(\mathrm{d}x_1)\cdots\nu(\mathrm{d}x_n)$$

in the sense of formal power series. It follows that

$$B_n(q;x_1,\dots,x_n)=\sum_{m=1}^{n}\sum_{\substack{J\subset[n]\\ \#J=m}} A_m\big(q;(x_j)_{j\in J}\big)\sum_{\substack{(V_j)_{j\in J}:\\ \dot\cup_{j\in J}V_j=[n]\setminus J}}\prod_{j\in J} t_{\#V_j}\big(x_j;(x_v)_{v\in V_j}\big). \tag{13.10}$$

Note that the third sum is over ordered partitions $(V_j)_{j\in J}$ of $[n]\setminus J$, indexed by J, into $\#J$ disjoint sets V_j, with $V_j=\varnothing$ explicitly allowed. For example,

$$\begin{aligned} B_1(q;x_1)&=A_1(q;x_1),\\ B_2(q;x_1,x_2)&=A_2(q;x_1,x_2)+A_1(q;x_1)t_1(x_1;x_2)+A_1(q;x_2)t_1(x_2;x_1). \end{aligned}$$

More generally, $B_n(q;\cdot)$ depends on $t_1(q;\cdot),\dots,t_{n-1}(q;\cdot)$ alone. This is the only aspect of (13.10) that enters the proof of this lemma.

For $n\in\mathbb{N}$, let $\mathscr{P}_n$ be the collection of set partitions of $\{1,\dots,n\}$. The family $(T_q^\circ)_{q\in\mathbb{X}}$ solves (FP) in the sense of formal power series if and only if for all $n\in\mathbb{N}$ and $q,x_1,\dots,x_n\in\mathbb{X}^n$, we have

$$t_n(q;x_1,\dots,x_n)=\sum_{m=1}^{n}\sum_{\{J_1,\dots,J_m\}\in\mathscr{P}_n}\prod_{\ell=1}^{m} B_{\#J_\ell}\big(q;(x_j)_{j\in J_\ell}\big). \tag{13.11}$$

In particular,

$$\begin{aligned} t_1(q;x_1)&=B_1(q;x_1)=A_1(q;x_1)\\ t_2(q;x_1,x_2)&=B_2(q;x_1,x_2)+B_1(q;x_1)B_1(q;x_2) \end{aligned}$$

which determines t_1 and t_2 uniquely. A straightforward induction over n, exploiting that the right-hand side of (13.11) depends on $t_1,\dots,t_{n-1}$ alone (via $B_1,\dots,B_n$), shows that the system of equations (13.11) has a unique solution $(t_n)_{n\in\mathbb{N}}$. □

Next we provide a sufficient condition for the absolute convergence of the series $T_q^\circ(\nu)$.

Theorem 13.2 Let $T_q^\circ(\nu)$ be the unique solution of (FP) from Lemma 13.1. Assume that for some measurable function $b:\mathbb{X}\to[0,\infty)$, the measure $\nu\in\mathfrak{M}_{\mathbb{C}}$ satisfies, for all $q\in\mathbb{X}$,

$$\sum_{n=1}^{\infty}\frac{1}{n!}\int_{\mathbb{X}^n}|A_n(q;x_1,\dots,x_n)|\mathrm{e}^{\sum_{j=1}^n b(x_j)}|\nu|(\mathrm{d}x_1)\cdots|\nu|(\mathrm{d}x_n)\le b(q). \tag{$\mathcal{S}_b$}$$

Then, for all $q \in \mathbb{X}$, we have that

$$1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_{\mathbb{X}^n} |t_n(q;x_1,\dots,x_n)| \; |\nu|(\mathrm{d}x_1)\cdots|\nu|(\mathrm{d}x_n) \le \mathrm{e}^{b(q)} \qquad (\mathcal{M}_b)$$

and the fixed point equation (FP) holds true as an equality of absolutely convergent series.

Proof. The inductive proof is similar to [8, 7]. Let $S_q^N(\nu)$, $N \in \mathbb{N}_0$, be the partial sums for the left-hand side of $(\mathcal{M}_b)$,

$$S_q^N(\nu) := 1 + \sum_{n=1}^{N} \frac{1}{n!} \int_{\mathbb{X}^n} |t_n(q;x_1,\dots,x_n)| \; |\nu|(\mathrm{d}x_1)\cdots|\nu|(\mathrm{d}x_n).$$

We prove $S_q^N(\nu) \le \mathrm{e}^{b(q)}$ by induction on N, building on the proof of Lemma 13.1. The estimate for the full series then follows by a passage to the limit $N \to \infty$.

For $N = 0$, we have $S_q^0(\nu) = 1$ and the inequality $S_q^0(\nu) \le \exp\bigl(b(q)\bigr)$ is trivial. Now assume $S_q^{N-1}(\nu) \le \exp\bigl(b(q)\bigr)$. The triangle inequality applied to Eqs. (13.10) and (13.11) yields the same iterative formula for $|t_n(q;x_1,\dots,x_n)|$ as for $t_n(q;x_1,\dots,x_n)$ just with $A_n(q;x_1,\dots,x_n)$ replaced by $\bigl|A_n(q;x_1,\dots,x_n)\bigr|$. We noted before that, if we consider $S_q^N(\nu)$ and hence only $|t_n(q;x_1,\dots,x_n)|$ for $n \le N$, then on the right-hand side only $|t_n(q;x_1,\dots,x_n)|$ with $n \le N-1$ appear. However, there are some terms on the right-hand side, which as well only contain $|t_n(q;x_1,\dots,x_n)|$ with $n \le N-1$ but which come from some term $|t_n(q;x_1,\dots,x_n)|$ on the left-hand side for $n > N$. Adding these missing terms, we reconstruct an exponential on the right-hand side. As all of these additional terms are non-negative, we get the following inequality, instead of an equality

$$\begin{aligned} S_q^N(\nu) &\le \exp\left(\sum_{n=1}^{N-1} \frac{1}{n!} \int_{\mathbb{X}^n} \bigl|A_n(q;x_1,\dots,x_n)\bigr| \, S_{x_1}^{N-1}(\nu)\cdots S_{x_n}^{N-1}(\nu) \, |\nu|(\mathrm{d}x_1)\cdots|\nu|(\mathrm{d}x_n) \right) \\ &\le \exp\left(\sum_{n=1}^{N-1} \frac{1}{n!} \int_{\mathbb{X}^n} \bigl|A_n(q;x_1,\dots,x_n)\bigr| \, \mathrm{e}^{b(x_1)+\cdots+b(x_n)} \, |\nu|(\mathrm{d}x_1)\cdots|\nu|(\mathrm{d}x_n) \right) \\ &\le \mathrm{e}^{b(q)}. \end{aligned}$$

The induction is complete. It follows that $(\mathcal{M}_b)$ holds true. In particular, the series $T_q^\circ(\nu)$ is absolutely convergent and satisfies $|T_q^\circ(\nu)| \le \exp\bigl(b(q)\bigr)$. By condition $(\mathcal{S}_b)$, the right-hand side of the fixed point equation (FP) is absolutely convergent as well. Therefore

Eq. (FP) holds true not only as an identity of formal power series but in fact as an identity of well-defined complex-valued functions. □

Now that we have addressed the convergence of the series T_q°, we may come back to the inversion of the map $\mathcal{D}(A) \ni z \mapsto \rho[z]$. For measurable $b : \mathbb{X} \to [0,\infty)$, let

$$\mathcal{V}_b := \{\nu \in \mathfrak{M}_\mathbb{C} \mid \nu \text{ satisfies condition } (\mathcal{S}_b)\}. \tag{13.12}$$

For $\nu \in \mathcal{V}_b$, define $\zeta[\nu] \in \mathfrak{M}_\mathbb{C}$ by

$$\zeta[\nu](\mathrm{d}q) = \zeta(\mathrm{d}q;\nu) := T_q^\circ(\nu)\nu(\mathrm{d}q). \tag{13.13}$$

Theorem 13.3 For every weight function $b : \mathbb{X} \to \mathbb{R}_+$, there is a set $\mathcal{U}_b \subset \mathcal{D}(A)$ such that $\rho : \mathcal{U}_b \to \mathcal{V}_b$, defined in (13.5), is a bijection with inverse ζ.

Proof. Let $\mathcal{U}_b$ be the image of $\mathcal{V}_b$ under ζ. By Theorem 13.2, the set $\mathcal{U}_b$ is contained in $\mathcal{D}(A)$, in particular if $z = \zeta[\nu]$ with $\nu \in \mathcal{V}_b$, then $\rho[z]$ is well-defined with

$$\begin{aligned}\rho(\mathrm{d}q;z) &= \mathrm{e}^{-A(q;z)}z(\mathrm{d}q) = \mathrm{e}^{-A(q;\zeta[\nu])}\zeta(\mathrm{d}q;\nu)\\ &= \mathrm{e}^{-A(q;\zeta[\nu])}T_q^\circ(\nu)\nu(\mathrm{d}q) = \nu(\mathrm{d}q).\end{aligned}$$

For the last identity we have used the fixed point equation (FP). Thus we have checked that if $z = \zeta[\nu]$, with $\nu \in \mathcal{V}_b$, then $\rho[z] = \nu$. Conversely, if $\nu = \rho[z]$ with $z \in \mathcal{U}_b$, then by definition of $\mathcal{U}_b$ there exists $\mu \in \mathcal{V}_b$ such that $z = \zeta[\mu]$, hence $\nu = \rho[z] = \rho[\zeta[\mu]] = \mu \in \mathcal{V}_b$ and $z = \zeta[\mu] = \zeta[\nu]$. □

Finally we provide a combinatorial formula for the function $T_q^\circ(\nu)$ appearing in the inverse $\zeta[\nu]$. Consider a genealogical tree that keeps track not only of mother-child relations, but also of groups of siblings born at the same time. This results in a tree for which children of a vertex are partitioned into cliques (singletons, twins, triplets, etc.). Accordingly for $n \in \mathbb{N}$ we define the set of enriched trees, denoted by $\mathscr{T}\mathscr{P}_n^\circ$, as the set of pairs $\big(T,(P_i)_{0\le i\le n}\big)$ consisting of:

- ◇ A tree T with vertex set $[n] := \{0,1,\dots,n\}$. The tree is considered rooted in 0 (the ancestor).

- ◇ For each vertex $i \in \{0,1,\dots,n\}$, a set partition P_i of the set of children[1] of i. If i is a leaf (has no children), then we set $P_i = \varnothing$.

For $x_0,\dots,x_n \in \mathbb{X}$, we define the weight of an enriched tree $\big(T,(P_i)_{0\le i\le n}\big) \in \mathscr{T}\mathscr{P}^\circ_n$ as

$$w\big(T,(P_i)_{0\le i\le n};x_0,x_1,\dots,x_n\big) := \prod_{i=0}^{n}\prod_{J\in P_i} A_{\#J+1}\big(x_i;(x_j)_{j\in J}\big) \tag{13.14}$$

with $\prod_{J\in\varnothing} = 1$. So the weight of an enriched tree is a product over all cliques of twins, triplets, etc., contributing each a weight that depends on the variables x_j of the clique members and the variable x_i of the parent.

Proposition 13.4 The family of power series $(T^\circ_q)_{q\in\mathbb{X}}$ from Lemma 13.1 is given by

$$T^\circ_q(z) = 1 + \sum_{n=1}^{\infty}\frac{1}{n!}\int_{\mathbb{X}^n}\sum_{(T,(P_i)_{i=0,\dots,n})\in\mathscr{T}\mathscr{P}^\circ_n} w\big(T,(P_i)_{i=0,\dots,n};q,x_1,\dots,x_n\big)z^n(\mathrm{d}\boldsymbol{x}).$$

Proof. We check that the generating function of the weighted enriched trees satisfies (FP). Functional equations for generating functions of labeled trees are standard knowledge [1], we provide a self-contained proof for the reader's convenience. Define

$$\tilde{t}_n(q;x_1,\dots,x_n) := \sum_{(T,(\mathscr{P}_i)_{i=0,\dots,n})\in\mathscr{T}\mathscr{P}^\circ_n} w\big(T,(P_i)_{0\le i\le n};q,x_1,\dots,x_n\big).$$

Further define $\tilde{B}_n(q;x_1,\dots,x_n)$ but restricting the sum to enriched trees for which $\#P_0 = 1$ (all children of the root belong to the same clique). Further set $t_0 = 1$ and $\tilde{B}_0 = 0$. For $V \subset \mathbb{N}$ a finite non-empty set, define $\mathscr{T}\mathscr{P}^\circ(V)$ in the same way as $\mathscr{T}\mathscr{P}^\circ_n$ but with $\{0,1,\dots,n\}$ replaced by $\{0\}\cup V$. For $V = \varnothing$ we define $\mathscr{T}\mathscr{P}^\circ(V) = \varnothing$ and assign the empty tree the weight 1. For non-empty trees, weights $w\big(R;(x_j)_{j\in V\cup\{0\}}\big)$ are defined in complete analogy with (13.14).

Clearly there is a bijection between enriched trees $R \in \mathscr{T}\mathscr{P}^\circ_n$ and set partitions $\{J_1,\dots,J_m\}$ of $[n] := \{1,\dots,n\}$ together with enriched trees $R_i \in \mathscr{T}\mathscr{P}^\circ(J_i)$, $i = 1,\dots,m$ for which all children of the root are in the same clique. Indeed, the number m corresponds to the number of cliques in which the children of the root are divided and the blocks $J_1,\dots,J_m$ group descendants of the root, where J_k contains the children of the root

[1] The members of the partition are assumed to be non-empty, except we consider the partition of the empty set.

which are in the k-th clique and all their descendants. The weight of an enriched tree R is equal to the product of the weights of the subtrees R_i. Therefore

$$\tilde{t}_n(q;x_1,\dots,x_n) = \sum_{m=1}^{n} \sum_{\{J_1,\dots,J_m\}\in\mathscr{P}_n} \prod_{\ell=1}^{m} \tilde{B}_{\#J_\ell}\big(q;(x_j)_{j\in J_\ell}\big). \tag{13.15}$$

Furthermore there is a one-to-one correspondence between, on the one hand, enriched trees where all the children of the root are in the same clique and, on the other hand, tuples $\big(J,(V_j)_{j\in J},(R_j)_{j\in J}\big)$ consisting of non-empty set $J\subset[n]$, an ordered partition $(V_j)_{j\in J}$ of $[n]\setminus J$ (with $V_j=\varnothing$ allowed), and a collection of enriched trees $R_j\in\mathscr{T}\mathscr{P}^\circ(V_j)$. Overall, J and $(V_j)_{j\in J}$ give a partition of $[n]$. The set J consists of the labels of the children of the root, that is the one clique which all these children form and for each $j\in J$, the set V_j consists of the labels of the descendants of j. ($V_j=\varnothing$ means that j is a leaf of the tree) It follows that

$$\tilde{B}_n(q;x_1,\dots,x_n) = \sum_{m=1}^{n} \sum_{\substack{J\subset[n]\\ \#J=m}} A_m\big(q;(x_j)_{j\in J}\big) \sum_{\substack{(V_j)_{j\in J}:\\ \dot\cup_{j\in J}V_j=[n]\setminus J}} \prod_{j\in J} \tilde{t}_{\#V_j}\big(x_j;(x_v)_{v\in V_j}\big). \tag{13.16}$$

It follows from Eqs. (13.15) and (13.16) that the formal power series with coefficients $\tilde{t}_n$ solves (FP), therefore Lemma 13.1 yields $\tilde{t}_n = t_n$. □

Bibliography

[1] Bergeron, F., Labelle, G., Leroux, P.: *Combinatorial species and tree-like structures*, volume **67** of Encyclopedia of mathematics and its applications, Cambridge University Press (1998).

[2] Gessel, I. M.: *A combinatorial proof of the multivariable Lagrange inversion formula*, J. Combin. Theory Ser. A **45**(2), 178–195 (1987).

[3] Jansen, S.: *Cluster and virial expansions for the multi-species Tonks gas*, J. Stat. Phys. **161**(5), 1299–1323 (2015).

[4] Jansen, S., Kuna, T., Tsagkarogiannis, D.: *Virial inversion and density functionals*, preprint arXiv:1906.02322 [math-ph] (2019).

[5] Jansen, S, Tate, S. J., Tsagkarogiannis, D., Ueltschi, D.: *Multispecies virial expansions*, Commun. Math. Phys. **330**(2), 801–817 (2014).

[6] Lebowitz, J. L., Penrose, O.: *Convergence of virial expansions*, J. Math. Phys. **5**(7), 841–847 (1964).

[7] Poghosyan, S., Ueltschi, D.: *Abstract cluster expansion with applications to statistical mechanical systems*, J. Math. Phys. **50**(5), 053509 (2009).

[8] Ueltschi, D.: *Cluster expansions and correlation functions*, Mosc. Math. J. **4**(2), 511–522 (2004).

14

Activity expansions for Gibbs correlation functions

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Abstract. *We consider Gibbs point processes with non-negative pair potentials. For small activities, a cluster expansion allows us to express the corresponding correlation functions by (multivariate) power series in the activity around zero. We characterise the domain of absolute convergence of those series and derive from this characterisation a new sufficient condition in the setting of abstract polymers improving the known bounds for the convergence radii.*

1 Introduction

Proving convergence conditions for cluster expansions is a classical problem with a long history – see [1, 6] and the references therein. Recent developments include a novel convergence condition by Fernández-Procacci [3] that improves the classical Kotecký-Preiss criterion [5] as well as Dobrushin's criterion [2]. We present a new necessary and sufficient convergence condition that improves on the above-mentioned criteria. The criterion applies to non-negative pair potentials for systems both continuous and discrete.

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After describing the general setting in Section 2, we proceed to introduce a system of integral equations satisfied by the activity expansions ρ, the so-called Kirkwood-Salsburg equations, in Section 3. In Section 4, we consider a sign-flipped version of those equations to prove our main result – Theorem 14.7 – characterising the domain of absolute convergence of ρ; moreover, we are able to use Theorem 14.7 to prove a new sufficient condition for systems of abstract polymers (Proposition 14.8).

2 The setting: Definitions and notations

Let $(\mathbb{X}, \mathscr{X})$ be a measurable space, λ a σ-finite reference measure, and v a non-negative pair potential, i. e., $v : \mathbb{X} \times \mathbb{X} \to \mathbb{R}_+ \cup \{\infty\}$ is measurable and symmetric (in the sense that $v(x,y) = v(y,x)$ for all $x, y \in \mathbb{X}$). Mayer's f function associated with the potential v is given by

$$f(x,y) := \mathrm{e}^{-v(x,y)} - 1.$$

An activity function is a measurable map $z : \mathbb{X} \to \mathbb{R}$. We define the measure λ_z on $\mathscr{X}$ by

$$\lambda_z(B) := \int_B z(x)\lambda(\mathrm{d}x), \qquad B \in \mathscr{X}.$$

The weight of a graph G with vertex set $[n] = \{1, \ldots, n\}$ and edge set $E(G)$ is

$$w(G; x_1, \ldots, x_n) := \prod_{\{i,j\} \in E(G)} f(x_i, x_j), \qquad x_1, \ldots, x_n \in \mathbb{X}.$$

Let $\mathscr{G}_n$ be the set of all graphs with vertex set $[n]$, $\mathscr{C}_n \subset \mathscr{G}_n$ the set of connected graphs and

$$\varphi_n^{\mathsf{T}}(x_1, \ldots x_n) := \sum_{G \in \mathscr{C}_n} w(G; x_1, \ldots, x_n)$$

the n-th Ursell function. For $k \in \mathbb{N}$ and $1 \le k \le n$, let $\mathscr{D}_{k,n} \subset \mathscr{G}_n$ the collection of all graphs G such that every vertex $j \in \{k+1, \ldots, n\}$ connects to at least one of the vertices $i \in \{1, \ldots, k\}$. We call such graphs multi-rooted graphs on $[n]$ with k roots. Consider the functions

$$\psi_{k,n}(x_1, \ldots, x_n) := \sum_{G \in \mathscr{D}_{k,n}} w(G; x_1, \ldots, x_n).$$

For $k = 1$, the functions coincide with the standard Ursell functions, i. e., $\psi_{1,n} = \varphi_n^{\mathsf{T}}$. We are interested in the associated series

$$\rho_k(x_1,\dots,x_k;z) \coloneqq z(x_1)\cdots z(x_k)\Bigg(\psi_{k,k}(x_1,\dots,x_k) + \sum_{n=1}^{\infty}\frac{1}{n!}\int_{\mathbb{X}^n}\psi_{k,k+n}(x_1,\dots,x_k,y_1,\dots,y_n)\lambda_z^{\otimes n}(\mathrm{d}\mathbf{y})\Bigg).$$

The series ρ_k corresponds to the k-point correlation function of a grand-canonical Gibbs measure [8, Eq. (4-7)], see also [4] – it is precisely the expansion of the correlation function in the activity z around zero. Proposition 14.1 provides some intuition for why $\rho = (\rho_k)_{k\in\mathbb{N}}$ is the right candidate for those activity expansions.

We say that the series $\rho_k(x_1,\dots,x_k;z)$ is absolutely convergent if

$$\sum_{n=1}^{\infty}\frac{1}{n!}\int_{\mathbb{X}^n}\Big|\psi_{k,k+n}(x_1,\dots,x_k,y_1,\dots,y_n)z(x_1)\cdots z(x_k)z(y_1)\cdots z(y_n)\Big|\boldsymbol{\lambda}^{\otimes n}(\mathrm{d}\mathbf{y}) < \infty.$$

Our main goal is to provide necessary and sufficient conditions on z ensuring that ρ converges absolutely, i. e., that the series ρ_k converge absolutely on $\mathbb{X}^k$ for all $k \in \mathbb{N}$.

3 Preparations

Some preparations are required before we can state our main results. The following representation of the activity expansions ρ – in the spirit of Equation (2.11) in [1] – turns out to be quite useful for deriving properties of interest (e. g., the signs of the series ρ_k alternating in $k \in \mathbb{N}$ (see Proposition 14.3) or their connection to the k-correlation functions of the corresponding Gibbs point process mentioned in the introduction).

Proposition 14.1 (Exponential representation of ρ) Suppose that all series $\rho_k(z)$ are absolutely convergent on $\mathbb{X}^k$ for some activity function z. Then

$$\rho_k(x_1,\dots,x_k;z) = z(x_1)\cdots z(x_k)\prod_{1\le i<j\le k}\big(1+f(x_i,x_j)\big) \times \exp\Bigg(\sum_{n=1}^{\infty}\frac{1}{n!}\int_{\mathbb{X}^n}\Bigg(\prod_{\substack{1\le i\le k\\ 1\le j\le n}}\big(1+f(x_i,y_j)\big)-1\Bigg)\varphi_n^{\mathsf{T}}(y_1,\dots,y_n)\lambda_z^{\otimes n}(\mathrm{d}\mathbf{y})\Bigg),$$

for all $k \in \mathbb{N}$ and $(x_1,\dots,x_k) \in \mathbb{X}^k$.

Sketch of proof. Under the assumption of the proposition this identity on the level of generating functions can be reduced to the following identity on the level of coefficients given by sums over weighted graphs:

$$\psi_{k,n}(x_1,\dots,x_n) = \prod_{1\le i<j\le k}\big(1+f(x_i,x_j)\big) \times \sum_{\{V_1,\dots,V_r\}}\prod_{\ell=1}^{r}\Bigg(\prod_{\substack{1\le i\le k,\\ j\in V_\ell}}\big(1+f(x_i,x_j)\big)-1\Bigg)\varphi^{\mathsf{T}}_{|V_\ell|}\big((x_j)_{j\in V_\ell}\big) \quad (14.1)$$

where the sum runs over all set partitions $\{V_1,\dots,V_r\}$ of non-root vertices $\{k+1,\dots,n\}$.

The latter identity (on the combinatorial level) can be shown simply by exploiting the structure of multi-rooted graphs and their relation to connected graphs. □

Corollary 14.2 (Alternating sign property) We have

$$\psi_{k,n}(x_1,\dots,x_n) = (-1)^{n-k}\big|\psi_{k,n}(x_1,\dots,x_n)\big|$$

for all $n\in\mathbb{N}$, all $k\in\{1,\dots,n\}$, and all $(x_1,\dots,x_n)\in\mathbb{X}^n$.

Sketch of proof. The statement follows directly from the identity (14.1) and the well-known alternating sign property of the Ursell functions φ_n, which holds by a tree-graph equation à la Penrose (e. g., see [3]). □

We use the observation captured by Corollary 14.2 to introduce the sign-flipped version of the activity expansions ρ.

Corollary 14.3 (Introducing $\tilde{\rho}$) Let z be a non-negative activity function. Then, the series $\rho_k(-z)$ converge for all $k\in\mathbb{N}$ if and only if the series $\rho_k(z)$ converge absolutely for all $k\in\mathbb{N}$. Moreover, define $\tilde{\rho}(z)$ by setting

$$\tilde{\rho}_k(x_1,\dots,x_k;z) \coloneqq (-1)^k\rho_k(x_1,\dots,x_k;-z)$$

for all $k\in\mathbb{N}$ and $(x_1,\dots,x_k)\in\mathbb{N}$. Then

$$\tilde{\rho}_k(x_1,\dots,x_k;z) = \prod_{i=1}^{k} z(x_i)\sum_{n\ge 0}\frac{1}{n!}\int_{\mathbb{X}^n}\big|\psi_{k,k+n}(x_1,\dots,x_k,y_1,\dots,y_n)\big|\,\lambda_z^{\otimes n}(\mathrm{d}\mathbf{y})$$

holds for all $k \in \mathbb{N}$ and $(x_1, \dots, x_k) \in \mathbb{N}$.

Sketch of proof. The statement follows directly from the alternating sign property given by Corollary 14.2. □

Now we are ready to introduce systems of integral equations satisfied by the activity expansions – the so-called Kirkwood-Salsburg equations. Notice the close relation between those and the GNZ equations (named after Georgii, Nguyen and Zessin; e. g., see [4]), which can serve to define grand-canonical Gibbs measures. In general, the Kirkwood-Salsburg relations for the correlation functions follow from the GNZ equations and even the equivalence holds under additional assumtions (e. g., see [4, Lemma 3.1] and the discussion thereafter.)

Definition 14.4 (Kirkwood-Salsburg operators) Given a fix activity function z, define K_z by the following formal expressions: For $a = (a_p)_{p\in\mathbb{N}}$ such that $a_p : \mathbb{X}^p \to \mathbb{R}$ is measurable for all $p \in \mathbb{N}$, set

$$\begin{aligned}\big(K_z a\big)_{p+1}(x_0, x_1, \dots, x_p) &:= z(x_0) \prod_{i=1}^{p} \big(1 + f(x_0, x_i)\big) \\ &\times \left(a_p(x_1, \dots, x_p) + \sum_{k=1}^{\infty} \frac{1}{k!} \int_{\mathbb{X}^k} \prod_{j=1}^{k} f(x_0, y_j) a_{p+k}(x_1, \dots, x_p, y_1, \dots, y_k) \lambda^{\otimes k}(\mathrm{d}\mathbf{y}) \right),\end{aligned}$$

where we use the natural convention $a_0 := 0$ for the case $p = 0$.

Similarly, define $\tilde{K}_z$ by

$$\begin{aligned}\big(\tilde{K}_z a\big)_{p+1}(x_0, x_1, \dots, x_p) &:= z(x_0) \prod_{i=1}^{p} \big(1 + f(x_0, x_i)\big) \\ &\times \left(a_p(x_1, \dots, x_p) + \sum_{k=1}^{\infty} \frac{1}{k!} \int_{\mathbb{X}^k} \prod_{j=1}^{k} \big|f(x_0, y_j)\big| a_{p+k}(x_1, \dots, x_p, y_1, \dots, y_k) \lambda^{\otimes k}(\mathrm{d}\mathbf{y}) \right).\end{aligned}$$

Furthermore, for all $(x_1, \dots, x_p) \in \mathbb{X}^p$ set $\big(e_z\big)_1(x_1) := z(x_1)$ and $\big(e_z\big)_p(x_1, \dots, x_p) := 0$ for $p \geq 2$.

Proposition 14.5 (Kirkwood-Salsburg equations for ρ) Assume that $\rho(z)$ converges absolutely for some activity function z (i. e., the series $\rho_p(x_1,\ldots,x_p;z)$ are absolutely convergent for all $p \in \mathbb{N}$ and all $(x_1,\ldots,x_p) \in \mathbb{X}^p$), then

$$\rho(z) = K_z\rho(z) + e_z, \tag{14.2}$$

in the sense that $\rho_p(x_1,\ldots,x_p;z) = \big(K_z\rho(z) + e_z\big)_p(x_1,\ldots,x_p)$ for all $p \in \mathbb{N}$ and all $(x_1,\ldots,x_p) \in \mathbb{X}^p$.

Sketch of proof. Following the proof by Jansen in [4], one uses the structure of multi-rooted graphs to show that $\rho(z)$ is given (pointwise) by the limit of the Picard iterates of the map $a \mapsto K_z a + e_z$, which by a slight abuse of notation we denote $K_z + e_z$, starting in e_z (i. e. $\rho(z) = \lim_{n\to\infty}(K_z + e_z)^n e_z$, where $(K_z + e_z)^n$ denotes the n-fold composition of $K_z + e_z$ with itself). □

Furthermore, for the sign-flipped functions $\tilde{\rho}_k(z)$, a system of integral equations in terms of the sign-flipped operator $\tilde{K}_z$ can be derived from the original Kirkwood-Salsburg equations for $\rho_k(z)$.

Proposition 14.6 (Kirkwood-Salsburg equations for $\tilde{\rho}$) Assume that $\tilde{\rho}(z)$ converges for some non-negative activity function z (i. e., the series $\tilde{\rho}_p(x_1,\ldots,x_p;z)$ are convergent for all $p \in \mathbb{N}$ and all $(x_1,\ldots,x_p) \in \mathbb{X}^p$), then

$$\tilde{\rho}(z) = \tilde{K}_z\tilde{\rho}(z) + e_z, \tag{14.3}$$

in the sense that $\tilde{\rho}_p(x_1,\ldots,x_p;z) = \big(\tilde{K}_z\tilde{\rho}(z) + e_z\big)_p(x_1,\ldots,x_p)$ for all $p \in \mathbb{N}$ and all $(x_1,\ldots,x_p) \in \mathbb{X}^p$.

Sketch of proof. The statement follows directly from Proposition 14.5 by the definition of $\tilde{\rho}(z)$ and the alternating sign property from Corollary 14.2. □

4 Main results

Now we are ready to state our main result – a condition both necessary and sufficient for absolute convergence of $\rho(z)$ – inspired by the extended Gruber-Kunz approach as introduced by Bissacot et al. in [1].

Theorem 14.7 Let z be a non-negative activity function. Then the following statements are equivalent:

1) $\tilde{\rho}(z)$ converges.

2) There exists a sequence of non-negative measurable functions a, such that

$$\tilde{K}_z a + e_z \leq a. \tag{14.4}$$

Sketch of proof. The implication 1) $\Rightarrow$ 2) is given by Proposition 14.6. For the converse, we notice that $\tilde{\rho}(z)$ is – if convergent – equal to the Neumann series $\sum_{n=0}^{\infty} \tilde{K}_z^n e_z$, since the latter is also given by the unique limit of the Picard iterates of $\tilde{K}_z + e_z$ starting in e_z, i. e., $\sum_{n=0}^{\infty} \tilde{K}_z^n e_z = \lim_{n\to\infty} (\tilde{K}_z + e_z)^n e_z = \tilde{\rho}(z)$. Following a proof by Fernández and Procacci (see [1]) one can exploit certain positivity and monotonicity properties of $\tilde{K}_z$ to show that 2) implies the convergence of the Neumann series $\sum_{n=0}^{\infty} \tilde{K}_z^n e_z$. □

Given Theorem 14.7, proving sufficient conditions for absolute convergence of the activity expansions can be reduced to finding appropriate ansatz functions a satisfying the system of Kirkwood-Salsburg inequalities (14.4). We demonstrate how this can be done by considering the classical criteria:

1) Kotecký-Preiss criterion: First introduced by Kotecký and Preiss in [5] for abstract polymers, the criterion was generalised for the setup of repulsive pair interactions by Ueltschi in [9]; its generalised version can be formulated as: If there exists $\mu : \mathbb{X} \to [0,\infty)$, such that for all $x_0 \in \mathbb{X}$

$$z(x_0) e^{\int |f(x_0,y)| \mu(y) \lambda(\mathrm{d}y)} \leq \mu(x_0), \tag{14.5}$$

then the activity expansions $\rho(z)$ converge absolutely.

In this case, choose $a = (a_p)_{p\in\mathbb{N}}$ to be given by $a_p(x_1,\ldots,x_p) := \prod_{i=1}^{p} \mu(x_i)$ for some $\mu \geq 0$ satisfying condition (14.5). Just by using the uniform bound $|1+f| \leq 1$ (repulsive interactions) one immediately confirms that this choice of a satisfies the inequalities (14.4).

2) Fernández-Procacci criterion: First introduced by Fernández and Procacci in [3] for abstract polymers, the criterion was generalised for the setup of repulsive pair

interactions by Jansen in [4]; its generalised version can be formulated as: If there exists $\mu : \mathbb{X} \to [0,\infty)$, such that for all $x_0 \in \mathbb{X}$

$$z(x_0)\left(1+\sum_{k=1}^{\infty}\frac{1}{k!}\int_{\mathbb{X}^k}\prod_{j=1}^{k}\left|f(x_0,y_j)\right|\prod_{1\le i<j\le k}\big(1+f(y_i,y_j)\big)\prod_{j=1}^{k}\mu(y_j)\lambda^{\otimes k}(\mathrm{d}\mathbf{y})\right) \le \mu(x_0), \quad (14.6)$$

then the activity expansions $\rho(z)$ converge absolutely.

Here we define $a=(a_p)_{p\in\mathbb{N}}$ by $a_p(x_1,\dots,x_p) \coloneqq \prod_{1\le i<j\le p}\big(1+f(x_i,x_j)\big)\prod_{i=1}^{p}\mu(x_i)$ for some $\mu \ge 0$ satisfying condition (14.6). Again, the uniform bound $|1+f| \le 1$ immediately yields the inequalities (14.4) for our choice of a.

But not only can the classical convergence criteria be reconstructed by the approach given by Theorem 14.7, also new results improving on the known bounds for the convergence radii can be proven by choosing "less multiplicative" ansatz functions (notice that all the ansatz functions a considered are submultiplicative – in the sense that $a_{p+k}(x_1,\dots,x_p,x_{p+1},\dots,x_{p+k}) \le a_p(x_1,\dots,x_p)\,a_k(x_{p+1},\dots,x_{p+k})$ for all $p,k\in\mathbb{N}$ and all $(x_1,\dots,x_p,x_{p+1},\dots,x_{p+k}) \in \mathbb{X}^{p+k}$). In the following we consider the setup of abstract polymers, in which the two classical conditions above were first introduced.

Let $\mathbb{X}$ be a countable set (the set of polymers), let $\mathscr{X}$ be the powerset of $\mathbb{X}$ and let λ simply be given by the counting measure. Moreover, let $R \subset \mathbb{X}\times\mathbb{X}$ be a symmetric and reflexive relation. We write $x \nsim y$ for $(x,y)\in R$ and $x \sim y$ for $(x,y)\notin R$. We set $\Gamma(x) \coloneqq \{y\in\mathbb{X}|\ y\nsim x\}$ for any $x\in\mathbb{X}$ and extend this notation to $\Gamma(X) \coloneqq \cup_{x\in X}\{y\in\mathbb{X}|\ y\nsim x\}$ for any $X\subset\mathbb{X}$. Notice that we do not require $\Gamma(x)$ to be finite sets and that $x\in\Gamma(x)$ for every $x\in\mathbb{X}$. Finally, we consider hard-core interactions given by $f(x,y) \coloneqq -\mathbb{1}_{\{x\nsim y\}}$.

In this setting we prove the following new sufficient condition:

Proposition 14.8 Let z be a non-negative activity function. If there exists $\mu : \mathbb{X} \to [0,\infty)$, such that for all $x_0 \in \mathbb{X}$

$$z(x_0)\left(1+\sum_{k\ge1}\sum_{\substack{Y=\{y_1,\dots,y_k\}\\ y_i\nsim x_0,\ y_i\sim y_j}}\prod_{i=1}^{k}\mu(y_i)\prod_{w\in\Gamma(Y)}e^{\mu(w)}\right) \le \mu(x_0)\prod_{w\in\Gamma(x_0)}e^{\mu(w)}, \quad (14.7)$$

then the activity expansions $\rho(z)$ converge absolutely.

Sketch of proof. One shows that – under the assumption of the the proposition – the ansatz functions $a = (a_p)_{p\in\mathbb{N}}$, $a_p : \mathbb{X} \to [0,\infty)$, given by setting

$$a_p(x_1,\dots,x_p) := \prod_{1\le i<j\le p} \mathbb{1}_{\{x_i\sim x_j\}} \prod_{i=1}^{p} \mu(x_i) \prod_{w\in\Gamma(X)} e^{\mu(w)}$$

for some μ satisfying (14.7), any $p \in \mathbb{N}$ and every $(x_1,\dots,x_p) \in \mathbb{X}^p$, satisfy the system of Kirkwood-Salsburg inequalities (14.4). □

Notice how the sufficient conditions are successively improved by having the corresponding ansatz functions a capture more of the structure of the expansion from Proposition 14.1 (for a modified activity $\mu \ge z$, where the inequality is understood to hold pointwise). To illustrate the improvement we consider the following somewhat typical case of an abstract polymer model given by subset polymers, i. e. the polymers are given by finite subsets of the regular lattice $\mathbb{Z}^d$ and the relation R on the set of polymers is given by having non-empty intersection.

Example 14.9 Consider non-overlapping (hard-core-interactions) cubes on $\mathbb{Z}^2$ of side-length 2 with translation-invariant activity z. The sufficient condition on z for the absolute convergence of $\rho(z)$ given by the Fernández-Procacci criterion provides the bound

$$z \le \max_{\mu\ge 0} \frac{\mu}{1+9\mu+16\mu^2+8\mu^3+\mu^4} \approx 0.057271,$$

while our condition from Proposition 14.8 provides

$$z \le \max_{\mu\ge 0} \frac{\mu e^{9\mu}}{1+9e^{9\mu}\mu+(6e^{15\mu}+8e^{16\mu}+2e^{17\mu})\mu^2+8e^{21\mu}\mu^3+e^{25\mu}\mu^4} \approx 0.060833.$$

This corresponds to an improvement of approximately 6 percent.

Bibliography

[1] Bissacot, R., Fernández, R. and Procacci, A.: *On the convergence of cluster expansions for polymer gases*, J. Stat. Phys. **139**(4), 598–617 (2010).

[2] Dobrushin, R.: *Estimates of semi-invariants for the Ising model at low temperatures*, in "Topics in statistical and theoretical physics", Amer. Math. Soc. Transl. **177**(2), 59–81 (1996).

[3] Fernández, R., Procacci, A.: *Cluster expansion for abstract polymer models. New bounds from an old approach*, Commun. Math. Phys. **274**(1), 123–140 (2007).

[4] Jansen, S.: *Cluster expansions for Gibbs point processes*, Adv. Appl. Prob. **51**(4), 1129–1178 (2019).

[5] Kotecký, R., Preiss, D.: *Cluster expansion for abstract polymer models*, Commun. Math. Phys. **103**(3), 491–498 (1986).

[6] Poghosyan, S., Ueltschi, D.: *Abstract cluster expansion with applications to statistical mechanical systems*, J. Math. Phys. **50**(5), 053509 (2009).

[7] Ruelle, D.: *Statistical mechanics: Rigorous results*, W. A. Benjamin (1969).

[8] Stell, G.: *Cluster expansions for classical systems in equilibrium*, The equilibrium theory of classical fluids (H. L. Frisch and J. L. Lebowitz, eds.), W. A. Benjamin, 171–261 (1964).

[9] Ueltschi, D.: *Cluster expansions and correlation functions*, Mosc. Math. J. **4**(2), 511–522 (2004).

15

Phase separation and sharp large deviations

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Abstract. *Using a refined analysis of phase boundaries, we derive sharp asymptotics of the large deviation probabilities for the total magnetisation of a low-temperature Ising model in two dimensions.*

1 Introduction

The phenomenon of "phase separation" has been at the heart of the theory of phase transitions in low-temperature lattice systems since its discovery by Minlos and Sinai [3, 4] in the late 1960s. Under suitable conditions, it allows the description of the canonical ensembles of such models in terms of (families of) large contours, or "phase boundaries", and, as a result, enables the study the limiting behaviour of the corresponding probability distributions and their partition functions. This approach is especially successful in two dimensions, as the resulting phase boundaries are one-dimensional contours, whose statistical behaviour is well understood.

When combined with a careful analysis of the related variational problem, these results can provide a detailed description of the typical configurations in such ensembles.

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supported by EPSRC studentship EP/M507854/1

In the setting of the low-temperature Ising model on a two-dimensional torus, the famous Dobrushin-Kotecký-Shlosman theorem [2] rigorously justifies the so-called Wulff construction and approximates the rescaled phase boundary by that of the Wulff shape, a two-dimensional region enclosed by a curve with the smallest surface energy. In turn, this determines the asymptotics of the logarithm of large deviation probabilities for the total magnetisation of the model.

To derive a sharp large deviation principle for the total spin, one needs to carefully analyse the shape dependence of the corresponding distribution. We illustrate the approach in the case of a low-temperature Ising model in two dimensions.

2 Model

For integer $N, M \geq 1$ consider a finite box

$$V_{NM} := \big\{x = (x_1, x_2) \in (\mathbb{Z}^2)^* : |x_1| \leq N, |x_2| \leq M\big\}$$

of the (dual) two-dimensional integer lattice $(\mathbb{Z}^2)^* := \{x = (x_1, x_2) : x_1 + 1/2, x_2 + 1/2 \in \mathbb{Z}\}$. To each site $x \in V_{NM}$ associate a spin $\sigma_x \in \{-1, +1\}$ and write $\sigma = (\sigma_x, x \in V_{NM})$ for a configuration in $\Omega_{NM} := \{-1, +1\}^{V_{NM}}$. Write $x \sim y$ if sites x and y are neighbours in $(\mathbb{Z}^2)^*$, i. e., $|x - y| := |x_1 - y_1| + |x_2 - y_2| = 1$. For a subset $V \subset (\mathbb{Z}^2)^*$, use ∂V to denote the external boundary of V, namely, the set $\{y \in (\mathbb{Z}^2)^* \setminus V : \exists x \in V \text{ with } x \sim y\}$.

Given an angle $\varphi \in (-\pi/2, \pi/2)$, let $\bar\sigma = \big(\bar\sigma_x, x \in (\mathbb{Z}^2)^*\big)$ be the two-component boundary conditions, where $\bar\sigma_x = +1$ iff $x = (x_1, x_2)$ satisfies $x_2 \geq x_1 \tan\varphi$ for $x_1 > 0$ or $x_2 > x_1 \tan\varphi$ for $x_1 < 0$; otherwise, put $\bar\sigma_x = -1$. Notice that in $\bar\sigma$ the pairs of sites which are centrally symmetric with respect to the origin $(0,0)$ have spins of the opposite sign, $\bar\sigma_{-x} \equiv -\bar\sigma_x$ for all x.

The Gibbs distribution in Ω_{NM} with boundary conditions $\bar\sigma$ is defined via

$$\mathsf{P}^{\bar\sigma}_{V_{NM}}(\sigma) := \big(Z(V_{NM}, \bar\sigma)\big)^{-1} \exp\big\{-\beta \mathscr{H}(\sigma|\bar\sigma)\big\}, \qquad \sigma \in \Omega_{NM}, \tag{15.1}$$

where the partition function is

$$Z(V_{NM}, \bar\sigma) = \sum_{\sigma \in \Omega_{NM}} \exp\big\{-\beta \mathscr{H}(\sigma|\bar\sigma)\big\} \tag{15.2}$$

and the (joint) energy is given by

$$\mathscr{H}(\sigma|\bar{\sigma}) = -\frac{1}{2}\sum_{\{x\sim y\}\subset V_{NM}} \sigma_x\sigma_y - \sum_{x\sim y; x\in V_{NM}, y\in\partial V_{NM}} \sigma_x\bar{\sigma}_y\,, \tag{15.3}$$

where the first sum runs over all pairs of neighbouring sites in V_{NM}, while the second sum is restricted to boundary pairs (x,y) of neighbouring sites with $x \in V_{NM}$ and $y \in \partial V_{NM}$. In what follows we always assume that the temperature $1/\beta > 0$ is sufficiently low.

Of key interest is the distribution of the total magnetisation $S_{V_{NM}} := \sum_{x\in V_{NM}} \sigma_x$ in large volumes, namely, the limiting behaviour of the probability

$$\mathsf{P}^{\bar{\sigma}}_{V_{NM}}(b_N) := \mathsf{P}^{\bar{\sigma}}_{V_{NM}}\big(\{\sigma \in \Omega_{NM} : S_{V_{NM}} = b_N\}\big)$$

as $N \to \infty$, for a suitable sequence of integer values b_N; of course, for the last probability to be positive b_N must be of the same parity as the number $|V_{NM}|$ of sites in V_{NM}, i. e., even, and satisfy the *a priori* bound $|b_N| \le |V_{NM}|$. In what follows we assume that b_N satisfies these constraints.

For a given $\varphi \in (-\pi/2, \pi/2)$, assume additionally that $(2N)^{-2}b_N \to b$ as $N \to \infty$ with the limiting value satisfying $|b| < b(\varphi)$, for a suitably chosen constant $b(\varphi) > 0$, see below. Then the Dobrushin-Kotecký-Shlosman theory [2] implies that for some $\alpha \in (0,1)$

$$\ln \mathsf{P}^{\bar{\sigma}}_{V_{NM}}(b_N) = -2\beta N\mathscr{W}(\varphi,b) + O(N^\alpha) \qquad \text{as } N\to\infty\,, \tag{15.4}$$

provided $\beta \ge \beta_0$ with suitably chosen $\beta_0 > 0$, and the aspect ratio M/N is uniformly bounded from below by a positive constant depending on φ. Here ln denotes the natural logarithm, and the rate functional $\mathscr{W}(\varphi,b)$ can be expressed in terms of the surface energy of the Wulff profile, a unique solution to the related variational problem, see below.

Our aim here is to derive a sharp asymptotic of the probability $\mathsf{P}^{\bar{\sigma}}_{V_{NM}}(b_N)$, equivalently, to improve the expansion in (15.4) up to the zero order term. To state our main result, we need to introduce some additional concepts.

Similarly to the Gibbs distribution (15.1)–(15.3) with two-component boundary conditions $\bar{\sigma}$, consider its analogue $\mathsf{P}^{+}_{V_{NM}}(\sigma)$, $\sigma \in \Omega_{NM}$, where $\bar{\sigma}$ is replaced by the constant "plus" configuration $\sigma^+ = \big(\sigma^+_x, x \in (\mathbb{Z}^2)^*\big)$ with $\sigma^+_x = 1$ for all x. The corresponding

energy is defined via

$$\mathscr{H}(\sigma|+) = -\frac{1}{2}\sum_{\{x\sim y\}\subset V_{NM}} \sigma_x\sigma_y - \sum_{x\sim y; x\in V_{NM}, y\in\partial V_{NM}} \sigma_x\sigma_y^+, \tag{15.5}$$

and the partition function is

$$Z(V_{NM},+) = \sum_{\sigma\in\Omega_{NM}} \exp\bigl\{-\beta\mathscr{H}(\sigma|+)\bigr\}.$$

Then the *surface tension* in direction of the normal n_φ to the line $x_2 = x_1\tan\varphi$ is

$$\tau(n_\varphi) := -\lim_{N\to\infty}\lim_{M\to\infty} \frac{\cos\varphi}{2\beta N}\ln\frac{Z(V_{NM},\bar\sigma)}{Z(V_{NM},+)}. \tag{15.6}$$

Informally, $\tau(n_\varphi)$ is the price (per unit length) of the presence of the phase boundary induced by the two-component boundary conditions $\bar\sigma$, relative to the constant "plus" boundary conditions σ^+. As shown in [2], $\tau(n_\varphi)$ also arises in the simultaneous limit $N\to\infty$ and $M\to\infty$ in (15.6) along a sequence of suitably shaped volumes; in particular, this holds for rectangular volumes V_{NM} with uniform condition $M \ge (1+|\tan\varphi|)N$.

The related Wulff variational problem is to minimise the value of the Wulff functional,

$$\mathscr{W}(\gamma) := \int_\gamma \tau(n_s)\,\mathrm{d}s, \tag{15.7}$$

in the class of all rectifiable curves γ enclosing area $|V(\gamma)| \ge 1$. Its solution $W = W_\beta$, known as the *Wulff shape*, is unique (up to translations), and can be constructed by a simple geometric procedure [2, 5]. The boundary of the Wulff shape W is strictly convex for all $\beta \ge \beta_0$ [2].

The rate functional $\mathscr{W}(\varphi, b)$ in (15.4) can be defined in terms of the surface energy of a suitable part of the Wulff shape boundary [1]. Without loss of generality, let $b < 0$. By strict convexity of the Wulff shape W_β there is a unique position of a straight line at angle φ to the horizontal intersecting W_β, such that the area a of the top part and the horizontal projection w of its straight boundary, see Figure 15.1, satisfy the relation

$$a = w^2|b|/\bigl(2m(\beta)\bigr), \tag{15.8}$$

where the spontaneous magnetisation $m(\beta)$ is positive for all β large enough. Then, rescaling the resulting shape (see the right part of Fig. 15.1) so that the horizontal projec-

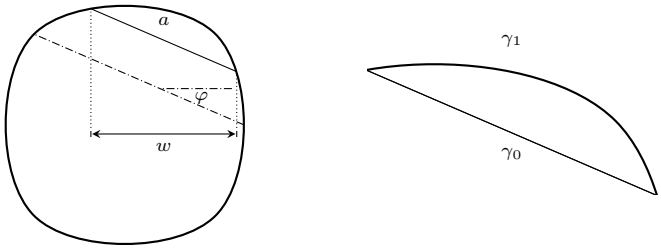

Figure 15.1: Construction of the Wulff profile corresponding to $\mathscr{W}(\varphi,b)$.

tion of γ_0 equals one, we have

$$\mathscr{W}(\varphi,b) = \mathscr{W}(\gamma_1) - \mathscr{W}(\gamma_0)\,,$$

recall (15.7). The strict convexity of the surface tension $\tau(n_\varphi)$ implies that $\mathscr{W}(\varphi,b) \geq 0$.

Let $a(\varphi)$ be the value of the area corresponding to the straight line at angle φ to the horizontal passing through the right-most point of W_β (the dashed line on the left of Fig. 15.1); write $w(\varphi)$ for the horizontal projection of the resulting shape. If $|a| < a(\varphi)$, the tangent at every point of the boundary γ_1 is non-vertical. As shown in [1], for such a the fluctuations of the phase boundary of the Ising model (15.1)–(15.3) around the suitably scaled curve γ_1 are asymptotically Gaussian.

The maximal value $b(\varphi)$, determining the validity of (15.4), is linked to $a(\varphi)$ via (15.8) with $w = w(\varphi)$. In what follows we assume that the sequence b_N of even numbers is φ-admissible in that there is $\varepsilon > 0$ such that for all N we have $(2N)^{-2}|b_N| < b(\varphi) - \varepsilon$.

Theorem 15.1 Let $|\varphi| < \pi/2$ and consider a φ-admissible sequence b_N with $b = \lim_{N\to\infty}(2N)^{-2}b_N$. Fix a sequence of volumes V_{NM} such that $M = M_N$ with $M/N \to c > 0$ as $N \to \infty$, for large enough $c = c(\varphi) > 0$. Then there exist $\beta_0 > 0$ and a positive constant $C = C(\varphi,b)$ such that for $\beta \geq \beta_0$,

$$\mathsf{P}^{\bar\sigma}_{V_{NM}}(b_N) = \frac{C(\varphi,b)}{\sqrt{2\pi N^3}}\exp\bigl\{-2\beta N\mathscr{W}(\varphi,b)\bigr\}\bigl(1+o(1)\bigr) \qquad \text{as } N\to\infty\,. \tag{15.9}$$

Remark 15.2 The asymptotic (15.9) improves the error in (15.4) to $\frac{3}{2}\ln N + \text{const}$. The constant $C(\varphi,b)$ can be expressed in terms of the covariances of the related tilted distributions.

3 Sketch of the proof

It is convenient to represent each configuration $\sigma \in \Omega_{NM}$ in terms of contours, the connected components of edges of $\mathbb{Z}^2$ separating neighbouring spins of different values, see Figure 15.2. By the choice of the values N and M, one of the contours of $\sigma \in \Omega_{NM}$ is an open polygon S connecting the vertical sides of V_{NM} (and called the *phase boundary*), while all other contours, if any, are closed polygons. Let $\mathscr{G}_{NM}$ be the collection of all possible phase boundaries of configurations $\sigma \in \Omega_{NM}$; write $\mathsf{S} \sim \sigma$ (or $\sigma \sim \mathsf{S}$) if S is the phase boundary of σ. For $\mathsf{S} \in \mathscr{G}_{NM}$, write $\{\mathsf{S}\}$ for the event $\{\sigma \in \Omega_{NM} : \sigma \sim \mathsf{S}\}$.

To derive the sharp asymptotics (15.9), we first use the formula of total probability,

$$\mathsf{P}^{\bar\sigma}_{V_{NM}}(S_{V_{NM}} = b_N) = \sum_{\mathsf{S}\in\mathscr{G}_{NM}} \mathsf{P}^{\bar\sigma}_{V_{NM}}\big(S_{V_{NM}} = b_N \big| \{\mathsf{S}\}\big)\, \mathsf{P}^{\bar\sigma}_{V_{NM}}\big(\{\mathsf{S}\}\big), \tag{15.10}$$

study the S-dependence of the conditional probability in (15.10) and then re-sum. It is crucial that for typical phase boundaries S decomposing V_{NM} into two parts with fixed cardinality ratio, the conditional probability in (15.10) regularly depends on S. In the remainder of this section we present the main ingredients of the proof; the complete argument will appear elsewhere.

Step I. For $\sigma \in \Omega_{NM}$ with phase boundary $\mathsf{S} = \mathsf{S}(\sigma) \in \mathscr{G}_{NM}$ write $\mathscr{G}(\sigma)$ for the collection of all other (closed, if any) contours in σ. Then the probabilities $\mathsf{P}^{\bar\sigma}_{V_{NM}}(\sigma)$ in (15.1) are proportional to $\exp\big\{-2\beta\big(|\mathsf{S}| + \sum_{\Gamma\in\mathscr{G}(\sigma)}|\Gamma|\big)\big\}$, where $|\Gamma|$ denotes the length (number of edges) of polygon Γ.

To study the behaviour of the total magnetisation one uses the tilted distribution

$$\mathsf{P}^{\bar\sigma}_{V_{NM},h}(\sigma) = \big(Z(V_{NM},h,\bar\sigma)\big)^{-1} \exp\Big\{-\beta\big(2|\mathsf{S}| + 2\sum_{\Gamma\in\mathscr{G}(\sigma)}|\Gamma| - hS_{V_{NM}}(\sigma)\big)\Big\}, \tag{15.11}$$

with suitably defined normalisation $Z(V_{NM},h,\bar\sigma)$. This distribution, however, lacks the necessary analyticity properties, and, as in [2], one needs to restrict attention to configurations with cutoffs; subsequently, following the approach of [2, Chap. 3], one can relax the cutoff constraint for the events of interest.

As in [2], for $\omega_N > 0$ we let

$$\Omega^{\omega_N}_{NM} := \big\{\sigma \in \Omega_{NM} : \forall \Gamma \in \mathscr{G}(\sigma), \operatorname{diam}\Gamma \le \omega_N\big\}$$

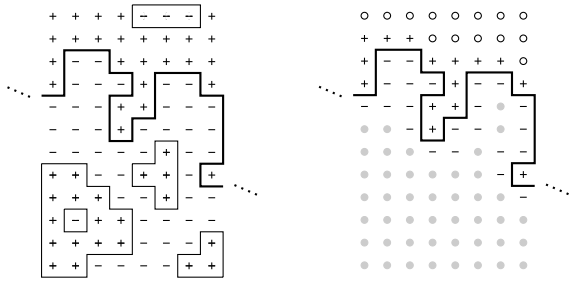

Figure 15.2: Contour representation of the Ising model: the open contour is the phase boundary S corresponding to the bounday conditions along the dotted line. Left picture: a configuration with its contours. Right picture: $\Delta^+(\mathsf{S})$ is the collection of plus spins along S, $\Delta^-(\mathsf{S})$ is the collection of minus spins, open circles form $V_+(\mathsf{S})$ and filled circles form $V_-(\mathsf{S})$.

be the configurations with cutoff ω_N, and for each $\sigma \in \Omega_{NM}^{\omega_N}$ put

$$\mathsf{P}^{\bar\sigma}_{V_{NM},h,\omega_N}(\sigma) = \big(Z(V_{NM},h,\bar\sigma,\omega_N)\big)^{-1} \exp\Big\{-\beta\Big(2|\mathsf{S}| + 2\sum_{\Gamma\in\mathscr{G}(\sigma)}|\Gamma| - hS_{V_{NM}}(\sigma)\Big)\Big\}, \tag{15.12}$$

with suitably defined normalisation $Z(V_{NM},h,\bar\sigma,\omega_N)$. As shown in [2, Chap. 3], if $\omega_N \geq K\ln|V_{NM}|$ with sufficiently large constant K, and if $|h|\omega_N < c < 1$, the limiting properties of the probability distributions (15.11) and (15.12) are similar. At the same time, for the partition function $Z(V_{NM},h,\bar\sigma,\omega_N)$ the usual low-temperature cluster expansion holds, provided complex h satisfies $|h|\omega_N < c < 1$.

Step II. We then adapt the argument of [2, Chap. 3] to study the conditional distribution $\mathsf{P}^{\bar\sigma}_{V_{NM},h,\omega_N}\big(\sigma\big|\{\mathsf{S}\}\big)$, generated by (15.12). Let

$$M(\mathsf{S}) \equiv M^{\bar\sigma}_{V_{NM},h,\omega_N}(\mathsf{S}) := \mathsf{E}^{\bar\sigma}_{V_{NM},h,\omega_N}\big(S_{V_{NM}}\big|\{\mathsf{S}\}\big) \tag{15.13}$$

be the expectation of the total spin $S_{V_{NM}}$ with respect to $\mathsf{P}^{\bar\sigma}_{V_{NM},h,\omega_N}\big(\sigma\big|\{\mathsf{S}\}\big)$. For (even) integer b denote

$$q^{\mathsf{S}}_{NM}(b) := \frac{2}{\big(2\pi|V_{NM}|d(\beta)\big)^{1/2}} \exp\left\{-\frac{\big(b-M(\mathsf{S})\big)^2}{2|V_{NM}|d(\beta)}\right\}, \tag{15.14}$$

where $d(\beta) > 0$ is the specific variance of a single spin in the pure plus phase, i. e., the limit of the Gibbs distribution $\mathsf{P}^+_{V_{NM}}(\sigma)$ with plus boundary conditions.

The following analogue of Theorem 3.18 in [2] holds.

Proposition 15.3 Fix a sequence of volumes V_{NM} as in Theorem 15.1. Let $h = h_N$ and $\omega_N \geq K \ln |V_{NM}|$, with $K = K(\beta) > 0$ large enough, be such that $|h|\omega_N < c < 1$. Then there exists $\beta_0 > 0$ such that for all $\beta \geq \beta_0$ we have

$$\lim_{N\to\infty} \frac{\mathsf{P}^{\bar\sigma}_{V_{NM},h_N,\omega_N}\big(S_{V_{NM}} = b \big| \{\mathsf{S}\}\big)}{q^{\mathsf{S}}_{NM}(b)} = 1 \tag{15.15}$$

for all even b satisfying $|b - M(\mathsf{S})| \leq K'\big(|V_{NM}|d(\beta)\big)^{1/2}$ with some $K' < \infty$.

Remark 15.4 As shown in [2, Theorem 3.19], in the case $h_N \equiv 0$ the Gaussian approximation (15.15) can be extended to all even b_N satisfying

$$\lim_{N\to\infty} \frac{|b_N - M(\mathsf{S})|}{|V_{NM}|^{2/3}} = 0,$$

where $M(\mathsf{S})$ is defined via (15.13) with $h = 0$.

The following analogue of Proposition 3.26 in [2] is also true.

Proposition 15.5 Let the cutoff levels ω_N satisfy $\lim_{N\to\infty} \omega_N/(\ln|V_{NM}|)^3 = 0$. For positive constants C and c, define

$$\alpha_{NM}(x) := \begin{cases} C\exp\{-cx^2/|V_{NM}|\}, & \text{if } |x| \leq |V_{NM}|/\omega_N, \\ C\exp\{-c|x|/\omega_N\}, & \text{if } |x| > |V_{NM}|/\omega_N. \end{cases}$$

Then there exist β_0 large enough, positive constants $C = C(\beta)$ and $c = c(\beta)$ such that

$$\mathsf{P}^{\bar\sigma}_{V_{NM},0,\omega_N}\big(S_{V_{NM}} = b \big| \{\mathsf{S}\}\big) \leq \alpha_{NM}\big(b - M(\mathsf{S})\big) \tag{15.16}$$

for all b, where $\beta > \beta_0$ and $M(\mathsf{S})$ is defined via (15.13) with $h = 0$.

As a result, the probability distribution $\mathsf{P}^{\bar\sigma}_{V_{NM},0,\omega_N}\big(S_{V_{NM}} = b \big| \{\mathsf{S}\}\big)$ is well concentrated around the corresponding average $M(\mathsf{S})$.

Step III. We next describe dependence of the average $M(\mathsf{S})$ on the shape of the phase boundary S. Let $\Delta^+(\mathsf{S})$ (respectively, $\Delta^-(\mathsf{S})$) be the set of all $x \in V_{NM}$ such that $\sigma_x \equiv 1$

(respectively, $\sigma_x \equiv -1$) for all configurations $\sigma \in \Omega_{NM}$ compatible with S, i. e., $\sigma \sim \mathsf{S}$. Then the complement $V_{NM} \setminus \big(\Delta^+(\mathsf{S}) \cup \Delta^-(\mathsf{S})\big)$ decomposes into two regions, one of which is surrounded by only plus spins for all $\sigma \sim \mathsf{S}$ (denoted $V_+ = V_+(\mathsf{S})$) while the other is surrounded by only minus spins for all $\sigma \sim \mathsf{S}$ (and denoted $V_- = V_-(\mathsf{S})$), see Fig. 15.2. Then

$$M(\mathsf{S}) = |\Delta^+(\mathsf{S})| - |\Delta^-(\mathsf{S})| + \mathsf{E}^+_{V_+,h,\omega_N}(S_{V_+}) + \mathsf{E}^-_{V_-,h,\omega_N}(S_{V_-}),$$

with obvious interpretation of the last two averages. It is natural to expect that for typical S and large V_{NM} we have

$$\mathsf{E}^+_{V_+,h,\omega_N}(S_{V_+}) \approx m(\beta)|V_+|, \qquad \mathsf{E}^-_{V_-,h,\omega_N}(S_{V_-}) \approx -m(\beta)|V_-|,$$

where $m(\beta)$ is the spontaneous magnetisation, so that

$$M(\mathsf{S}) \approx M_*(\mathsf{S}) := |\Delta^+(\mathsf{S})| - |\Delta^-(\mathsf{S})| + m(\beta)\big(|V_+| - |V_-|\big). \tag{15.17}$$

A naïve application of the shape dependence results from [2, Chap. 3] suggests that

$$|M(\mathsf{S}) - M_*(\mathsf{S})| \le K\big(|\Delta^+(\mathsf{S})| + |\Delta^-(\mathsf{S})| + N + M\big),$$

with the right-hand side value of order N for typical S. At the same time, for such S the difference $\delta_-(\mathsf{S}) := |\Delta^+(\mathsf{S})| - |\Delta^-(\mathsf{S})|$ has symmetric distribution with zero mean, and it is intuitively "obvious" that the typical values of this difference are much smaller than

$$\delta_+(\mathsf{S}) := |\Delta^+(\mathsf{S})| + |\Delta^-(\mathsf{S})| \le 4|\mathsf{S}|.$$

In fact, it is not difficult to show that for some $\alpha \in (1/2, 1)$ the rescaled difference $\delta_-(\mathsf{S})N^{-\alpha}$ has exponential tails. By applying a suitably adjusted version of the cluster expansions used in [1], one can verify that a similar property holds for $M(\mathsf{S}) - M_*(\mathsf{S})$, and therefore

$$M(\mathsf{S}) = m(\beta)\big(|V_+| - |V_-|\big) + O(N^\alpha) \tag{15.18}$$

for typical $\mathsf{S} \in \mathscr{G}_{NM}$.

Step IV. Let $q(\mathsf{S}) := (|V_+(\mathsf{S})| - |V_-(\mathsf{S})|)/2$ be the area defect created by the phase boundary S, so that (15.18) becomes $M(\mathsf{S}) \approx 2m(\beta)\, q(\mathsf{S})$. Using this approximation in (15.14), it is easy to see that the simplified version of the local CLT asymptotics (15.15) is valid for

all b satisfying $|b-2m(\beta)\,q(\mathsf{S})| \ll |V_{NM}|^{2/3}$. When combined with the uniform estimates (15.16) for the remaining values of b, one can see that the sum in (15.10) is essentially reduced to the phase boundaries S satisfying $q(\mathsf{S}) = q$ with

$$\left| q - \frac{b_N}{2m(\beta)} \right| \ll N^{4/3}\,. \tag{15.19}$$

On the other hand, the area defect $q(\mathsf{S})$ has standard deviation of order $O(N^{3/2})$ and therefore the probability of the event $\{q(\mathsf{S}) = q\}$ is almost constant for all q in (15.19). As a result, the sum in (15.10) is well approximated by the value

$$\mathsf{P}^{\bar\sigma}_{V_{NM}}\big(q(\mathsf{S}) = b_N/2m(\beta)\big)\,,$$

whose asymptotic can be derived from the results in [1]. The target relation (15.9) follows.

Bibliography

[1] Dobrushin, R., Hryniv, O.: *Fluctuations of the phase boundary in the* 2*D Ising ferromagnet*, Commun. Math. Phys. **189**(2), 395–445 (1997).

[2] Dobrushin, R., Kotecký, R., Shlosman, S.: *Wulff construction: A global shape from local interaction*, Translations of Mathematical Monographs **104**, American Mathematical Society, Providence, RI (1992).

[3] Minlos, R. A., Sinaĭ, J. G.: *The phenomenon of "separation of phases" at low temperatures in certain lattice models of a gas. I*, Mat. Sb. (N.S.) **73**(115), 375–448 (1967).

[4] Minlos, R. A., Sinaĭ, J. G.: *The phenomenon of "separation of phases" at low temperatures in certain lattice models of a gas. II*, Trudy Moskov. Mat. Obšč. **19**, 113–178 (1968).

[5] Wulff, G.: *Zur Frage der Geschwindigkeit des Wachstums und der Auflösung der Krystallflächen*, Z. Kryst. **34**, 449–530 (1901).

16

Numerical study for the phase transition of the area-interaction model

Pierre Houdebert[*]

Abstract. *In this paper we present numerical analysis of the phase transition of the area-interaction model, which is a standard model of Statistical Mechanics. The theoretical results are based on a recent paper [4] which provides a complete phase diagram except on a bounded (implicit) domain. With our numerical analysis we give an approximative explicit description of this domain. Furthermore our numerical results confirm the still unproven conjecture stating that non-uniqueness holds if and only if $z = \beta$ is large enough, with a value of the threshold obtained from the simulation of $\beta_c \simeq 1.726$.*

1 Introduction

The finite volume area-interaction measure (also called Widom-Rowlinson measure) on a bounded window $\Lambda \subset \mathbb{R}^d$ is defined as modification of the stationary Poisson Point

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This research has been partially funded by Deutsche Forschungsgemeinschaft (DFG) – SFB1294/1-318763901.

process of intensity z. Its unnormalised density is given by $\exp\big(-\beta\mathscr{L}^d\big(B_1(\omega)\big)\big)$ where $B_1(\omega)$ is the union of the unit balls centred at each point of the configuration ω and $\mathscr{L}^d$ is the Lebesgue measure on $\mathbb{R}^d$. The parameter $\beta \geq 0$ is called *inverse temperature* and the interaction is getting more and more attractive as β is large. The parameter z, called *activity*, is related to the intensity of the model.

In the infinite volume regime a global density is senseless and area-interaction measures are defined through equations specifying their conditional laws. But a solution of these equations can heuristically be seen as the limit of a finite volume area-interaction measure on increasing windows, with an additional boundary condition. In this paper we are interested in the uniqueness/non-uniqueness (called *phase transition*) of area-interaction measures for given parameters z and β. Earlier work of Ruelle [15] proved that in the symmetric case $z = \beta$, phase transition occurs when $z = \beta$ is large enough. A modern proof of this result, based on percolation tools, was done in [1]. Until recently almost nothing was proven for the case $z \neq \beta$, and it is conjectured that phase transition (i. e. non-uniqueness) occurs if and *only if* $z = \beta$ large enough. This conjecture is based on similar result for the Ising model, see [6]. But to the best of our knowledge, no numerical study has been done in order to observe if this conjecture is true.

Recently it was proven in [4] that uniqueness of the area-interaction measure is valid for $z < \widetilde{z}_c^a(\beta, 1)$, where $\beta \mapsto \widetilde{z}_c^a(\beta, 1)$ is a non-decreasing function which is the percolation threshold corresponding to the area-interaction model. Furthermore this function satisfies $\widetilde{z}_c^a(\beta, 1) \equiv \beta$ for β large enough. With some duality property of the model, it provides an almost complete picture of the phase diagram of the model. But on a bounded region of the parameters (z, β) it is still not proved whether there is phase transition or not. We refer to this region as the *unknown region*. This result is rigorously stated in Theorem 16.6 and a sketch of the proof is provided. Finally the theoretical phase transition diagram is provided in Figure 16.1.

In the present paper we provide a numerical study of the area-interaction model in order to experimentally plot the curve $\beta \mapsto \widetilde{z}_c^a(\beta, 1)$ to observe the region which is not covered by Theorem 16.6; we validate experimentally the conjecture and find an approximative value of the threshold. Our simulations are done in dimension $d = 2$ using a standard birth and death MCMC algorithm, as presented in [11]. To implement it we used the so-called *Fortuin-Kasteleyn* representation of the area-interaction model, which provides a construction of the model using the *generalised Continuum Random Cluster*

Model (gRCM), which was recently introduced in [9]. The definition of the gRCM and the Fortuin-Kasteleyn representation is done at the beginning of Section 4. From our numerical study we compute the value of the percolation threshold $\widetilde{z}_c^a(\beta,1)$ for several values β and provide a plot of the function $\beta \mapsto \widetilde{z}_c^a(\beta,1)$, see Figure 16.2 and Figure 16.3. From this we observe that the unknown region is really small. Furthermore from our simulation we can validate the conjecture, see Figure 16.4, with an approximative threshold $\beta_c \simeq 1.726$. This value matches with numerical studies that have been done in the symmetric case, see [7, 10].

2 Preliminaries

Let us consider the state space $\mathbb{R}^d$. Let Ω be the set of locally finite configurations ω on $\mathbb{R}^d$. This means that $\#(\omega \cap \Lambda) < \infty$ for every bounded Borel set Λ of $\mathbb{R}^d$, with $\#\omega$ being the cardinality of the configuration ω. We write ω_Λ as a shorthand for $\omega \cap \Lambda$. To a configuration $\omega \in \Omega$ we associate the germ-grain structure $B_r(\omega) := \bigcup_{x\in\omega} B_r(x)$, where $B_r(x)$ is the closed ball centred at x with radius $r > 0$. Let π^z be the distribution on Ω of the standard homogeneous Poisson point process with intensity $z > 0$. For $\Lambda \subset \mathbb{R}^d$ bounded, we denote by π^z_Λ the restriction of π^z on Λ.

2.1 Area-interaction measures

The area-interaction measures – also called Widom-Rowlinson measures – are defined through the standard Gibbs DLR formalism prescribing the conditional probabilities. For a bounded $\Lambda \subset \mathbb{R}^d$, we define the Λ-*Hamiltonian* $H_\Lambda(\omega) := \mathscr{L}^d\big(B_1(\omega_\Lambda) \setminus B_1(\omega_{\Lambda^c})\big)$. The *area specification* on a bounded $\Lambda \subseteq \mathbb{R}^d$ with boundary condition ω_{Λ^c} is defined by

$$\mathscr{P}^{z,\beta}_{\Lambda,\omega_{\Lambda^c}}(d\omega'_\Lambda) := \frac{e^{-\beta H_\Lambda(\omega'_\Lambda \omega_{\Lambda^c})}}{Z^{\text{area}}_{z,\beta,\Lambda,\omega_{\Lambda^c}}} \pi^z_\Lambda(d\omega'_\Lambda)$$

with the standard *partition function* $Z^{\text{area}}_{z,\beta,\Lambda,\omega_{\Lambda^c}} := \int_\Omega e^{-\beta H_\Lambda(\omega'_\Lambda \omega_{\Lambda^c})} \pi^z_\Lambda(d\omega'_\Lambda)$ which is always non-degenerate (i. e. $0 < Z^{\text{area}}_{z,\beta,\Lambda,\omega_{\Lambda^c}} < +\infty$). Let us point out that for $\beta = 0$, we have $\mathscr{P}^{z,\beta}_{\Lambda,\omega_{\Lambda^c}} \equiv \pi^z_\Lambda$.

Definition 16.1 A probability measure P on Ω is an *area-interaction measure* of activity z and inverse temperature β, written $P \in \mathscr{G}^{\text{area}}_{z,\beta}$, if for every bounded Borel set $\Lambda \subset \mathbb{R}^d$ and every bounded measurable function f,

$$\int_\Omega f\, dP = \int_\Omega \int_\Omega f(\omega'_\Lambda \omega_{\Lambda^c}) \mathscr{P}^{z,\beta}_{\Lambda,\omega_{\Lambda^c}}(d\omega'_\Lambda) P(d\omega). \tag{16.1}$$

Equations (16.1), for all bounded Λ, are called *DLR equations*, after Dobrushin, Lanford and Ruelle. Those equations prescribe the conditional probabilities of a Gibbs measure.

Heuristically a solution of the DLR equations can be seen as the limit of $\mathscr{P}^{z,\beta}_{\Lambda_n,\omega_{\Lambda_n^c}}$ for an increasing sequence Λ_n and some boundary condition ω. There is *phase transition*, i. e. non-uniqueness, if the limit depends on the boundary condition ω.

2.2 Percolation

The theory of percolation studies the connectivity in random structures and is a crucial tool to prove phase transition of the area-interaction measure.

Definition 16.2 Let $r > 0$. A configuration ω is said to r-percolate if the germ-grain structure $B_r(\omega)$ has at least one unbounded connected component. Furthermore a probability measure P on Ω is said to *r-percolate* (resp. *to not percolate*) if $P\big(\{\omega\ r\text{-percolates}\}\big) = 1$ (resp. $P\big(\{\omega\ r\text{-percolates}\}\big) = 0$).

Thanks to standard monotonicity arguments applied to the Gibbs specification we have:

Proposition 16.3 For all $\beta > 0$ and $r > 0$, there exists $0 < \bar{z}^a_c(\beta, r) < \infty$ such that

- ◇ for all $z < \bar{z}^a_c(\beta, r)$, every area-interaction measure $P \in \mathscr{G}^{\text{area}}_{z,\beta}$ almost never r-percolates, i.e $P\big(\{\omega\ r\text{-percolates}\}\big) = 0$;
- ◇ for all $z > \bar{z}^a_c(\beta, r)$, every area-interaction measures $P \in \mathscr{G}^{\text{area}}_{z,\beta}$ almost surely r-percolates, i.e $P\big(\{\omega\ r\text{-percolates}\}\big) = 1$.

A proof of this result is provided in [4, Prop. 2.7]. In the general case the only information known about $\bar{z}^a_c(\beta, r)$ is the following bound coming from stochastic domination:

$$\bar{z}^a_c(0, r) \leq \bar{z}^a_c(\beta, r) \leq \bar{z}^a_c(0, r) \exp(\beta v_d),$$

where $\widetilde{z}_c^a(0,r)$ is the percolation threshold of the Poisson Boolean model of constant radii r. Experimental studies showed that in dimension $d=2$ we have $\widetilde{z}_c^a(0,r) \simeq 0.359072 \cdot r^2$, see [12]. To the best of our knowledge there exists no approximation for cases $\beta \neq 0$.

3 Theoretical results

The first fundamental question in Gibbs point process theory is the existence of at least one probability measure satisfying the DLR equations (16.1). This is an interesting and non-trivial question treated for several kinds of interactions, see e. g. [3, 2, 5, 13]. Since the area-interaction process has a finite-range interaction, existence is long proved, see [14].

Proposition 16.4 For all $z, \beta \geq 0$, the set $\mathscr{G}_{z,\beta}^{\text{area}}$ of area-interaction measures is non-empty.

The second question concerning the area-interaction process is its uniqueness/non-uniqueness, known as *phase transition*. It is conjectured that non-uniqueness happens if and only if $z = \beta$ is large enough.

Conjecture 16.5 There exists $0 < \beta_c < \infty$ such that phase transition occurs for the area-interaction model if and only if $z = \beta > \beta_c$.

This conjecture is motivated by a similar result proved for the lattice Ising model, see for instance [6, Thm. 3.28 & Thm. 3.46]. Although this conjecture is still open, the following theorem based on our recent work [4] provides an almost complete picture of the phase diagram, see Figure 16.1.

Theorem 16.6

1) There exists $\beta_1 < \infty$ such that for $z = \beta > \beta_1$, there is non-uniqueness of the area-interaction measure;

2) for z, β such that $z < \widetilde{z}_c^a(\beta, 1)$, there is uniqueness of the area-interaction measure. Using a duality property, we obtain the same for $\beta < \widetilde{z}_c^a(z, 1)$;

3) there exists $\beta_2 \in [\beta_1, \infty[$ such that $\widetilde{z}_c^a(\beta, 1) = \beta$ for $\beta > \beta_2$. This partially proves the conjecture.

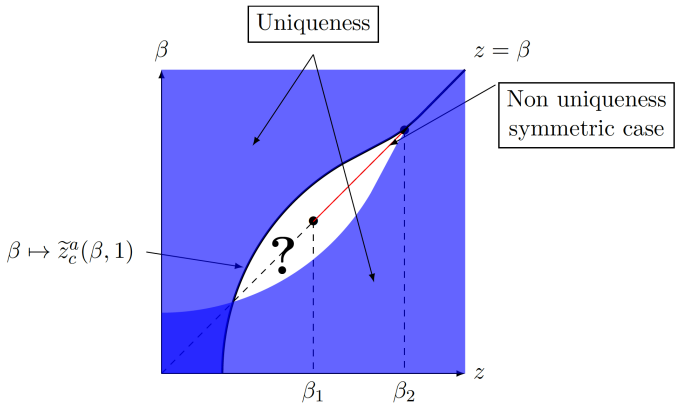


Figure 16.1: Theoretical uniqueness/non-uniqueness regimes for the area-interaction measures with parameters z, β.

Sketch of the proof. The first point was initially proved in 1971 by Ruelle (see [15]) using Peierls argument. Then a modern proof based on a Fortuin-Kasteleyn representation satisfied by the area-interaction model was provided in [1]. As a byproduct of their construction, the authors proved that $\widetilde{z}_c^a(\beta, 1/2) = \beta$ for $\beta > \beta_1$. The second point is a generalisation of the disagreement percolation construction introduced in [8]. The idea of disagreement percolation is to compare the Gibbs specification $\mathscr{P}^{z,\beta}_{\Lambda,\omega_{\Lambda^c}}$ with the same parameters z, β but with two different boundary conditions $\omega^1_{\Lambda^c}, \omega^2_{\Lambda^c}$, using percolation ideas. The duality property is a consequence of the representation using the Widom-Rowlinson model, and is stated in [4, Proposition 2.5]. The third point is proved in [4, Section 4.4.1] using the Fortuin-Kasteleyn representation introduced in [1] and an elegant stochastic domination argument which, using the fact that as soon as $\widetilde{z}_c^a(\beta, 1/2) = \beta$ for β large, one gets that $\widetilde{z}_c^a(\beta, 1) = \beta$ for β even larger. □

4 Numerical study of the phase diagram

In this section we will use numerical approximation, in dimension $d = 2$, in order to

1) experimentally plot the curve $\beta \mapsto \widetilde{z}_c^a(\beta, 1)$ to see the region which is not covered by Theorem 16.6;

2) validate experimentally the conjecture and find an approximative value of the threshold β_1.

To do our numerical study we will use a birth and death MCMC algorithm to sample the area-interaction process. The general algorithm we used for birth and death MCMC can be found in [11]. One could have considered using an *exact simulation* technique, as implemented in [7], but the computation of the percolation threshold requires to sample the model in a large window, which would be extremely time consuming using exact simulation techniques. We chose to sample the area-interaction model from the Fortuin-Kasteleyn representation using the gRCM, introduced in [9].

Definition 16.7 On a bounded window Λ, the generalised Continuum Random Cluster Model with activity parameter $\rho \geq 0$ and $\alpha_1, \alpha_2 \geq 0$ such that $\alpha_1 + \alpha_2 = 1$ is defined as $P_\Lambda^{gRCM}(d\omega) \sim \prod_C \left(\alpha_1^{\#C} + \alpha_2^{\#C}\right) \pi_\Lambda^\rho(d\omega)$, where the product is over the clusters of $B_{1/2}(\omega)$.

Proposition 16.8 Considering a configuration $\omega \sim P_\Lambda^{gRCM}$ and removing each cluster C of $B_{1/2}(\omega)$ with probability $\alpha_2^{\#C}/(\alpha_1^{\#C} + \alpha_2^{\#C})$, one obtains a configuration sampled from the area-interaction measure $P_\Lambda^{area}(d\omega) \sim \exp(-\beta|B_1(\omega) \cap \Lambda|)\pi_\Lambda^z(d\omega)$ with parameters $z = \alpha_1\rho$ and $\beta = \alpha_2\rho$.

This representation gives a good feeling for the third point of Theorem 16.6. Indeed, a large cluster will be removed (resp. kept) with very high probability when $\alpha_1 < \alpha_2$ (resp. $\alpha_1 > \alpha_2$). But percolation is highly dependent of the status of the large clusters.

In our numerical study we sample area-interaction measures in a window $\Lambda = [0,100]^2$, using a MCMC algorithm sampling the gRCM and then thinning the configuration according to the previous proposition. We observe the experimental intensity and whereas the center of the window is connected to its boundary in $B_1(\omega)$. For each pair of parameters (z,β), we sampled the model 1000 times in order to obtain an experimental intensity and an experimental probability of percolation. The C++ code used is accessible on GitHub.[1]

In order to determine $\widetilde{z}_c^{\alpha}(\beta,1)$, the percolation threshold of the model for a given β, we arbitrarily decide that the percolation threshold is the first observed value of z such that the probability of the center of the box $[0,100]^2$ to be connected to the boundary is larger than 0.01. Indeed, theoretically, for the infinite volume model the threshold is the first value of z such that the probability of the origin (or any given point) belongs to the

[1] https://github.com/PierreHoudebert/area_perco_multithread

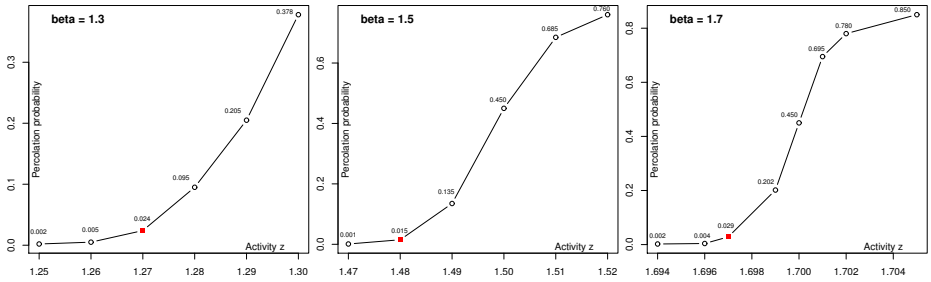
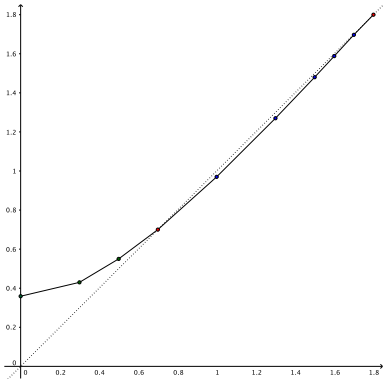


Figure 16.2: Percolation probability as a function of the activity z. The value corresponding to the percolation threshold $\widetilde{z}_c^a(\beta,1)$ is the plain square.

infinite connected component is positive. But for the finite volume model this probability is always positive.

For some values of β the percolation probability, as a function of z, is displayed in Figure 16.2. The obtained values of the percolation threshold $\widetilde{z}_c^a(\beta,1)$ and the corresponding graph is displayed in Figure 16.3.

Considering the conjecture, it is known that phase transition occurs at a given pair (z_0,β_0) if the intensity, as a function of z for β_0 fixed, is discontinuous in z_0. This is



β	$\widetilde{z}_c^a(\beta,1)$
0.3	0.43
0.5	0.55
0.7	0.7
1.0	0.97
1.3	1.27
1.5	1.48
1.6	1.588
1.7	1.697
1.8	1.8
2.0	2

Figure 16.3: Obtained values of the percolation threshold, and corresponding approximation curve.

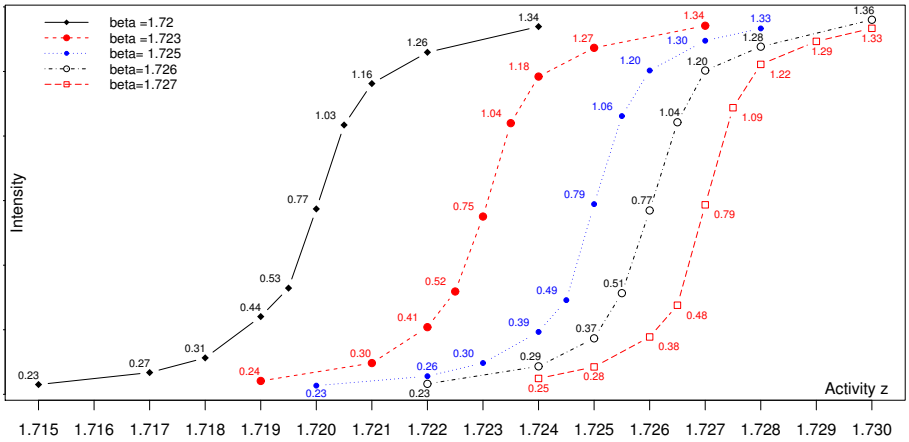


Figure 16.4: Experimental intensity as a function of z, for several values of β.

proven for the Ising model, see for instance [6], and could be proven similarly for the area-interaction model.

As before for a given pair of parameters (z, β), we sample the model 1000 times on the bounded window $\Lambda = [0, 100]^2$, and observed the experimental intensity obtained. For given values of β, we provide the graph of the intensity as a function of z in Figure 16.4. We observe from Figure 16.4 that the experimental intensity is indeed discontinuous only for $z = \beta$ larger than some value β_c. This amounts to saying that phase transition occurs only for $z = \beta$, as conjectured. However from the figure it is not clear what is the exact value of the threshold β_c, but it seems to be approximately $\beta_c \simeq 1.726$, which is coherent with the value obtained in [10] where the authors considered only the symmetric case.

Bibliography

[1] Chayes, J. T., Chayes, L., Kotecký, R.: *The analysis of the Widom-Rowlinson model by stochastic geometric methods*, Commun. Math. Phys. **172**(3), 551–569 (1995).

[2] Dereudre, D., Drouilhet, R., Georgii, H.-O.: *Existence of Gibbsian point processes with geometry-dependent interactions*, Prob. Theory Rel. Fields **153**(3–4), 643–670 (2012).

[3] Dereudre, D., Houdebert, P.: *Infinite volume continuum random cluster model*, Electron. J. Probab. **20**(125) (2015).

[4] Dereudre, D., Houdebert, P.: *Sharp phase transition for the continuum Widom-Rowlinson model*, arXiv e-prints (2018).

[5] Dereudre, D., Vasseur, T.: *Existence of Gibbs point processes with stable infinite range interaction*, arXiv e-prints (2019).

[6] Friedli, S., Velenik, Y.: *Statistical mechanics of lattice systems: A concrete mathematical introduction*, Cambridge University Press, Cambridge (2018).

[7] Häggström, O., van Lieshout, M.-C. N. M., Møller, J.: *Characterization results and Markov chain Monte Carlo algorithms including exact simulation for some spatial point processes*, Bernoulli **5**(4), 641–658 (1999).

[8] Hofer-Temmel, C., Houdebert, P.: *Disagreement percolation for Gibbs ball models*, Stoch. Proc. Appl. **129**(10), 3922–3940 (2019).

[9] Houdebert, P.: *Phase transition of the non-symmetric continuum Potts model*, arXiv e-prints (2019).

[10] Johnson, G., Gould, H., Machta, J., Chayes, L. K.: *Monte Carlo study of the Widom-Rowlinson fluid using cluster methods*, Phys. Rev. Lett. **79**, 2612–2615 (1997).

[11] Møller, J., Waagepetersen, R. P.: *Statistical inference and simulation for spatial point processes*, volume 100 of Monographs on Statistics and Applied Probability, Chapman & Hall/CRC (2004).

[12] Quintanilla, J., Torquato, S., Ziff, R. M.: *Efficient measurement of the percolation threshold for fully penetrable discs*, J. Phys. A **33**(42), 399–407 (2000).

[13] Roelly, S., Zass, A.: *Marked Gibbs point processes with unbounded interaction: an existence result*, arXiv e-prints, (2019).

[14] Ruelle, D.: *Statistical mechanics: Rigorous results*, W. A. Benjamin (1969).

[15] Ruelle, D.: *Existence of a phase transition in a continuous classical system*, Phys. Rev. Lett. **27**, 1040–1041 (1971).

17

Zero-range hamiltonians for three quantum particles

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Abstract. *Characterisation of the confined states of quantum systems made of many particles interacting via short range forces was the main goal for theoretical physicists investigating the structure of nuclei in the early years of Quantum Mechanics. A rigorous formulation of the problem was given at the beginning of the sixties by the Russian school of mathematical physics. The analysis of the three-body problem already revealed intriguing pathologies opening at the same time promising prospects for the future. We summarise the history and recent attempts of this line of research.*

1 Introduction

The three quantum particle problem is a line of research that Robert A. Minlos has been following for most of his scientific career. Together with Berezin and Faddeev he framed the problem of zero-range interactions in Quantum Mechanics inside the theory of self-adjoint extensions of symmetric operators. He was able to formulate in a rigorous way the

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unboundedness problem for three-particle zero-range Hamiltonians and he also suggested possible ways out of such a difficulty.

Following his suggestions, resumed later by Albeverio, Hoegh-Krohn and Wu [2], we attempted to work out partial solutions to the problem. It is worth mentioning that nowadays the interest in the problem has shifted toward many other research fields, e. g. it is actively investigated by physicists and applied mathematicians working in low temperature physics of quantum many particle systems (see e. g. [7] and reference therein). We want first to give an outline of the way zero-range interactions and the quantum three-body problem appeared in the physical literature.

Heuristically, point interactions are quantum interactions supported on points or "thin sets" (e. g. low dimensional hypersurfaces). They are also called zero-range interactions or contact interactions. They are used whenever the range of interparticle interactions is much shorter than other relevant length scales. They have the advantage of permitting better insight allowing for "explicit computations": for this reason they are used in the mathematical modeling of many natural phenomena.

Let $\mathscr{M}$ be a submanifold of $\mathbb{R}^d$ of dimension $s < d$. Consider the operator

$$H_{0,0} := -\Delta \restriction C_0^\infty\left(\mathbb{R}^d \setminus \mathscr{M}\right)$$

As a restriction of a self-adjoint operator $H_{0,0}$ is symmetric but not self-adjoint. In fact, denoting with $(\cdot,\cdot)$ the inner product in $L^2(\mathbb{R}^d)$,

$$D(H_{0,0}^*) = \left\{ \psi \in L^2(\mathbb{R}^d) \,\middle|\, |(\psi, -\Delta\phi)| < C\|\phi\| \ \forall \phi \in C_0^\infty(\mathbb{R}^d \setminus \mathscr{M}) \right\}$$

includes any function in $D(-\Delta) = H^2(\mathbb{R}^d)$ as well as any function $\psi \in L^2(\mathbb{R}^d)$ such that

$$-\Delta\psi = \xi + T, \qquad \xi \in L^2(\mathbb{R}^d), T \in D'(\mathbb{R}^d) \text{ with } \operatorname{supp} T \subseteq \mathscr{M}$$

where $D'(\mathbb{R}^d)$ is the vector space of distributions in $\mathbb{R}^d$.

Definition 17.1 Any (non-trivial) self-adjoint extension of $H_{0,0}$ (if any) will be denoted as a Hamiltonian with zero-range interaction on $\mathscr{M}$.

The simplest case is when $\mathscr{M} = \underline{y} \equiv \{y_1, \ldots, y_N\} \in \mathbb{R}^{Nd}$, i. e. a discrete set of points of $\mathbb{R}^d$.

Take $\psi = G^z(\cdot - y_i)$ where $G^z = \mathscr{F}^{-1}(k^2 - z)^{-1}$ for any $z \in \mathbb{C} \setminus \mathbb{R}^+$. It belongs to $L^2(\mathbb{R}^d)$ for $d = 1,2,3$ and

$$\big(G^z(\cdot - y_i), -\Delta_x \phi\big) = \big([-\Delta_x - z]G^z(\cdot - y_i), \phi\big) + \big(zG^z(\cdot - y_i), \phi\big) = \big(zG^z(\cdot - y_i), \phi\big)$$

for all $\phi \in C_0^\infty\big(\mathbb{R}^d \setminus \{y_1, \dots, y_N\}\big)$, which means that $G^z \in D(H_{0,0}^*)$ (but it does not belong to $H^2(\mathbb{R}^d)$) and that $G^z(\cdot - y_i)$ is an eigenvector of $H_{0,0}^*$ relative to the eigenvalue z. The same result holds true for any partial derivative of G^z belonging to $L^2(\mathbb{R}^d)$ (which is true only for the first derivatives of G^z in $d = 1$).

It is possible to classify the entire family of self-adjoint extensions of $H_{0,0}$ for $d = 1,2$ and 3. It turns out that in each dimension the family of self-adjoint extensions shows peculiar properties. We will be interested in particular in the following operators that can be proved (see [1]) to be a subset of the family of self-adjoint extensions of $H_{0,0}$ in $L^2(\mathbb{R}^3)$.

For any $\underline{\alpha} = \{\alpha_1, \dots, \alpha_n\} \in \mathbb{R}^n$ and $\underline{y} = \{y_1, \dots, y_n\} \in \mathbb{R}^{3n}$, the operator $H_{\underline{\alpha},\underline{y}}$ defined by

$$D(H_{\underline{\alpha},\underline{y}}) = \Big\{ u \in L^2(\mathbb{R}^3) \,\Big|\, u = \phi_\lambda + \sum_{k=1}^n q_k G_\lambda(\cdot - y_k)\phi_\lambda \in H^2(\mathbb{R}^3), \\ \phi_\lambda(y_j) = \sum_{k=1}^n \big[\Gamma_{\underline{\alpha},\underline{y}}(\lambda)\big]_{jk} q_k, j = 1, \dots, n \Big\} \tag{17.1}$$

$$\big(H_{\underline{\alpha},\underline{y}} + \lambda\big)u = \big(-\Delta + \lambda\big)\phi_\lambda \tag{17.2}$$

where $G_\lambda \equiv G^z\big|_{z=-\lambda}$ and

$$\big[\Gamma_{\underline{\alpha},\underline{y}}(\lambda)\big]_{jk} = \left(\alpha_j + \frac{\sqrt{\lambda}}{4\pi}\right)\delta_{jk} - G_\lambda(y_j - y_k)(1 - \delta_{jk}) \tag{17.3}$$

vanishing at $y_1, \dots, y_n$ one has, see (17.1), $q_k = 0$, $\forall k$, and then, from (17.2), $H_{\underline{\alpha},\underline{y}}u = -\Delta u$.

At each point $y_j \in \mathbb{R}^3$ the elements of the domain satisfy a boundary condition expressed by the last equality in (17.1). If we define $r_j = |x - y_j|$ it is easy to see that the boundary condition satisfied by functions $u \in D(H_{\underline{\alpha},\underline{y}})$ can be equivalently written as

$$\lim_{r_j \to 0}\left[\frac{\partial(r_j u)}{\partial r_j} - 4\pi\alpha_j(r_j u)\right] = 0, \qquad j = 1, \dots, n. \tag{17.4}$$

This explains the term "local" given to this class of extensions.

The spectral structure of local point interaction Hamiltonians is not at all trivial and it is easily investigated. In fact, $-\lambda$ is a negative eigenvalue of the Hamiltonian $H_{\underline{\alpha},\underline{y}}$ if and only if $\det\Gamma_{\underline{\alpha},\underline{y}}(\lambda)=0$ and the generalised eigenfunctions are non-trivial and explicitly known. Details can be found in [1]. Here, we want only to point out that if two scatterer positions come close one to the other the off-diagonal terms of the matrix (17.3) become very large with respect to any value of the strength parameters $\underline{\alpha}$. It is easy to check that in the limit of zero distance the ground state eigenvalue of the Hamiltonian is approaching $-\infty$ (for details when n=2, see [1]).

Let us now consider the much more difficult case of many particles. The Hamiltonians for a system of N particles interacting via zero-range forces will be defined as any self-adjoint extension of

$$-\sum_{i=1}^{N}\Delta_{x_i}\restriction C_0^\infty\Big(\mathbb{R}^{dN}\setminus\bigcup_{i<j}\sigma_{ij}\Big)$$
$$\sigma_{ij}=\big\{x=(x_1,\ldots,x_N)\in\mathbb{R}^{dN}\big|x_i=x_j\big\}$$

acting on state vectors with symmetry properties which will depend on the type of particles under investigation.

In the following, we will consider the case of $N=3$ identical bosons in $\mathbb{R}^3$ with masses $1/2$, in the center of mass reference frame. Expressed in terms of the Jacobi coordinates (see e. g. [16])

$$\mathbf{x}=\mathbf{x}_2-\mathbf{x}_3,\quad \mathbf{y}=\frac{1}{2}(\mathbf{x}_2+\mathbf{x}_3)-\mathbf{x}_1,\qquad \mathbf{x}_i\in\mathbb{R}^3,\ i=1,2,3 \tag{17.5}$$

the space of square integrable functions completely symmetric in the exchange of particle coordinates is

$$L^2_s(\mathbb{R}^6)=\Big\{\psi\in L^2(\mathbb{R}^6)\,\Big|\,\psi(\mathbf{x},\mathbf{y})=\psi(-\mathbf{x},\mathbf{y})=\psi\Big(\tfrac{1}{2}\mathbf{x}+\mathbf{y},\tfrac{3}{4}\mathbf{x}-\tfrac{1}{2}\mathbf{y}\Big)\Big\}. \tag{17.6}$$

Zero-range interactions among particles will be confined on the three-dimensional hyperplanes

$$\Sigma=\{\mathbf{x}=0\}\cup\{\mathbf{y}-\mathbf{x}/2=0\}\cup\{\mathbf{y}+\mathbf{x}/2=0\}. \tag{17.7}$$

As we pointed out already, this means that we are looking for Hamiltonians in $L^2_s(\mathbb{R}^6)$ which are non-trivial s.a. extension of the operator

$$\tilde{H}_0 = -\Delta_{\mathbf{x}} - \frac{3}{4}\Delta_{\mathbf{y}}, \qquad D(\tilde{H}_0) = \left\{ \psi \in L^2_s(\mathbb{R}^6) \,\middle|\, \psi \in H^2(\mathbb{R}^6), \psi\big|_\Sigma = 0 \right\}. \tag{17.8}$$

The defect spaces of $\tilde{H}_0$ are now of infinite dimensions. This makes the examination of classes of self-adjoint extensions much more difficult and their physical interpretation more complicated.

Ter-Martirosian and Skorniakov [17], on the basis of the analogy with the point interaction potentials, proposed to define an operator H_α acting as the free Hamiltonian outside the hyperplanes and satisfying a boundary condition close to the hyperplanes. Specifically, they impose for the functions in the domain of the Hamiltonian the boundary condition

$$\psi(\mathbf{x},\mathbf{y}) = \frac{\xi(\mathbf{y})}{|\mathbf{x}|} + \alpha\,\xi(\mathbf{y}) + o(1), \qquad \text{for } |\mathbf{x}| \to 0 \text{ and } y \neq 0 \tag{17.9}$$

where ξ is a function depending on ψ. The same behaviour must hold close to the other coincidence hyperplanes for symmetry reasons. Being the singular part in (17.9), the behaviour of the potential of a charge ξ distributed on the hyperplane, the operators H_α and the boundary condition were expressed in terms of charge distribution potentials, i. e. imposing that functions in the domain of H_α were the sum of a regular and a singular part in the following way:

$$\psi = w^\lambda + \mathscr{G}^\lambda \xi, \qquad w^\lambda \in H^2(\mathbb{R}^6), \tag{17.10}$$

where $\lambda > 0$ and

$$\widehat{\mathscr{G}^\lambda \xi}(\varkappa,\mathbf{p}) = \sqrt{\frac{2}{\pi}} \cdot \frac{\hat{\xi}(\mathbf{p}) + \hat{\xi}(\varkappa - \frac{1}{2}\mathbf{p}) + \hat{\xi}(-\varkappa - \frac{1}{2}\mathbf{p})}{|\varkappa|^2 + \frac{3}{4}|\mathbf{p}|^2 + \lambda}. \tag{17.11}$$

is the $(\lambda-)$ potential of a charge density ξ identically distributed on each coincidence plane. The behaviour of the function $\mathscr{G}^\lambda \xi(\mathbf{x},\mathbf{y})$ close to the planes is easily computed:

$$\mathscr{G}^\lambda \xi(\mathbf{x},\mathbf{y}) = \frac{\xi(\mathbf{y})}{|\mathbf{x}|} - \frac{1}{(2\pi)^{3/2}} \int \mathrm{d}\mathbf{p}\, e^{i\mathbf{p}\cdot\mathbf{y}} \big(T^\lambda \hat{\xi}\big)(\mathbf{p}) + o(1), \tag{17.12}$$

where

$$\big(T^\lambda \hat\xi\,\big)(\mathbf{p}) := \sqrt{\frac{3}{4}|\mathbf{p}|^2+\lambda}\cdot\hat\xi(\mathbf{p}) - \frac{1}{\pi^2}\int \mathrm{d}\mathbf{p}'\,\frac{\hat\xi(\mathbf{p}')}{|\mathbf{p}|^2+|\mathbf{p}'|^2+\mathbf{p}\cdot\mathbf{p}'+\lambda}. \tag{17.13}$$

In this way the boundary condition (17.9) can be rephrased as an integral equation for the "charges" ξ (for details see [5] and references therein). As noticed by Danilov [9], the operators constructed in this way are not self-adjoint and admit a continuum set of eigenvalues tending to minus infinity.

2 Minlos and Faddeev seminal papers

In two fundamental papers [13, 14] on the subject Minlos and Faddeev succeeded, in 1962, in rigorously translating the attempts of Ter-Martirosian and Skornyakov in terms of Birman's theory of self-adjoint extensions of positive symmetric operators. They proved that the boundary condition (17.9) about the behaviour of functions in the domain of the Hamiltonians close to the coincidence planes was not enough to guarantee their self-adjointness.

The final result can be summarised in the following characterisation, written in momentum space, of a two-parameter family of self-adjoint Hamiltonians:

$$D(H_{\alpha,\beta}) = \Big\{ \psi\in L^2_s(\mathbb{R}^6)\,\Big|\,\psi = w^\lambda + \mathscr{G}^\lambda\xi,\ w^\lambda\in H^2(\mathbb{R}^6),\ \hat\xi\in D(T^\lambda_\beta),$$
$$\alpha\,\hat\xi(\mathbf{p}) + \big(T^\lambda\hat\xi\big)(\mathbf{p}) = \widehat{w^\lambda(0,\cdot)}(\mathbf{p})\Big\}, \tag{17.14}$$

$$(H_{\alpha,\beta}+\lambda)\psi = (H_0+\lambda)w^\lambda, \tag{17.15}$$

where

$$H_0 = -\Delta_{\mathbf{x}} - \frac{3}{4}\Delta_{\mathbf{y}}, \qquad D(H_0) = H^2(\mathbb{R}^6), \tag{17.16}$$

with

$$D(T^\lambda_\beta) = \Big\{ \hat\xi\in L^2(\mathbb{R}^3)\,\Big|\,\hat\xi = \hat\xi_1+\hat\xi_2,\ \hat\xi_1\in D(T^\lambda) \text{ and}$$
$$\hat\xi_2(\varkappa) = \frac{c}{|\varkappa|^2+1}\Big(\beta\sin\big(s_0\log|\varkappa|\big)+\cos\big(s_0\log|\varkappa|\big)\Big)\Big\} \tag{17.17}$$

where c is an arbitrary constant, s_0 is the positive solution of the equation

$$1 - \frac{8}{\sqrt{3}} \cdot \frac{\sinh \frac{\pi s}{6}}{s \cosh \frac{\pi s}{2}} = 0. \tag{17.18}$$

Apart from technical complications due to the self-adjointness requirement, one should notice the similarity between (17.14)–(17.15) and (17.1). Each function in the domain of the Hamiltonians is the sum of a regular part and the potential of some charge density distributed on the coincidence planes, the Hamiltonians operate as the free Hamiltonian acting on the regular part and the boundary condition can be expressed as an equation on the charges.

The Hamiltonians defined in the way described above were finally self-adjoint, but Minlos and Faddeev realised that their spectral structure made those Hamiltonians unphysical models for a three-body quantum system. In fact, the authors found that their point spectrum contains an infinite sequence of negative eigenvalues unbounded from below (see [10] for an alternative proof). The authors also suggest a possible way out of this unboudedness pathology. In short, their hint amounts to substitute the constant α in (17.14) with the operator A defined, in Fourier space, by

$$\big(A\hat{\xi}\big)(\mathbf{p}) = \alpha\hat{\xi}(\mathbf{p}) + \big(K\hat{\xi}\big)(\mathbf{p}) \tag{17.19}$$

with $\alpha \in \mathbb{R}$ and K the convolution operator with kernel $K(p)$ behaving for large $|\mathbf{p}|$ as

$$K(\mathbf{p}) \sim \frac{\gamma}{|\mathbf{p}|^2} \qquad \text{for } |\mathbf{p}| \to \infty.$$

3 On the negative eigenvalues

In a private communication happened years ago between one of us and L. D. Faddeev, he appeared absolutely confident that zero-range Hamiltonians bounded from below for the three-body quantum system would exist. He renewed the suggestion that he and Minlos gave in their 1962 papers, mentioning that, with regret, they were no longer involved. On the other hand, Minlos, in the rest of his scientific career, went back occasionally to zero-range Hamiltonians for many-particle quantum systems approaching the interesting case of N, $N \geq 2$, identical fermions interacting, via zero-range forces, with a different

particle, making important contributions to the stability problem (see e. g. [11, 12]; for more recent developments see [15] and references therein). Recently, we showed that at least in the case $\alpha = 0$ the strategy works very well. For details of the proof see [10].

Considering the Ter-Martirosian, Skorniakov boundary condition (17.9) for $\alpha = 0$ and adding the term suggested by Minlos and Faddeev, we have that $-\lambda$, $\lambda > 0$, is a negative eigenvalue of the Hamiltonian if

$$\frac{\delta}{2\pi^2}\int \mathrm{d}\mathbf{p}'\,\frac{\hat{\xi}(\mathbf{p}')}{|\mathbf{p}-\mathbf{p}'|^2}+\sqrt{\frac{3}{4}|\mathbf{p}|^2+\lambda}\cdot\hat{\xi}(\mathbf{p})-\frac{1}{\pi^2}\int \mathrm{d}\mathbf{p}'\,\frac{\hat{\xi}(\mathbf{p}')}{|\mathbf{p}|^2+|\mathbf{p}'|^2+\mathbf{p}\cdot\mathbf{p}'+\lambda}=0, \tag{17.20}$$

where δ is a real parameter.

In the rotationally invariant case $\hat{\xi} = \hat{\xi}(|\mathbf{p}|)$, integrating out the angular variables one gets

$$\frac{\delta}{\pi}\int_0^\infty \mathrm{d}p'\,p'\hat{\xi}(p')\log\frac{p+p'}{|p-p'|}+\sqrt{\frac{3}{4}p^2+\lambda}\cdot p\hat{\xi}(p) - \frac{2}{\pi}\int_0^\infty \mathrm{d}p'\,p'\hat{\xi}(p')\log\frac{p^2+p'^2+pp'+\lambda}{p^2+p'^2-pp'+\lambda}=0. \tag{17.21}$$

The following statement holds true:

Proposition 17.2 Let

$$\delta_0=\frac{\sqrt{3}}{\pi}\left(\frac{4\pi}{3\sqrt{3}}-1\right). \tag{17.22}$$

Then for $\delta > \delta_0$, Equation (17.21) has only the trivial solution.

The main technical tool used in the proof is the following change of variable (see [8])

$$p=\frac{2\sqrt{\lambda}}{\sqrt{3}}\sinh x, \qquad x=\log\left(\frac{\sqrt{3}p}{2\sqrt{\lambda}}+\sqrt{\frac{3p^2}{4\lambda}+1}\right) \tag{17.23}$$

which allows to diagonalise Equation (17.21) for the new function

$$\theta(x)=\begin{cases}\lambda\sinh x\cdot\cosh x\cdot\hat{\xi}\left(\frac{2\sqrt{\lambda}}{\sqrt{3}}\sinh x\right) & \text{for } x\geq 0\\ -\theta(-x) & \text{for } x<0\end{cases} \tag{17.24}$$

giving the following equation for the Fourier transform of the function θ

$$\left(1+2\frac{\delta\sinh\frac{\pi}{2}s-4\sinh\frac{\pi}{6}s}{\sqrt{3}s\cosh\frac{\pi}{2}s}\right)\hat{\theta}(s)=0. \tag{17.25}$$

It is then easy to conclude the proof showing that

$$1+2\frac{\delta\sinh\frac{\pi}{2}s-4\sinh\frac{\pi}{6}s}{\sqrt{3}s\cosh\frac{\pi}{2}s}>0 \qquad \text{for } \delta>\delta_0.$$

Other recent attempts to obtain zero-range three-body Hamiltonians bounded from below can be found in [3] and [4].

Dedication. The authors want to dedicate this contribution to the memory of Robert A. Minlos, a leading mind of mathematical physics and a wonderful human being.

Bibliography

[1] Albeverio, S., Gesztesy, F., Hoegh-Krohn, R., Holden, H.: *Solvable models in quantum mechanics*, Springer-Verlag, New-York (1988).

[2] Albeverio, S., Hoegh-Krohn, R., Wu. T. T.: *A class of exactly solvable three-body quantum mechanical problems and the universal low energy behavior*, Phys. Lett. **83A**(3), 105–109 (1981).

[3] Basti, G., Cacciapuoti, C., Finco, D., Teta, A.: in preparation.

[4] Basti, G., Figari, R., Teta, A.: *Regularized quadratic forms for a three-boson system with zero-range interactions*, Rend. Mat. Appl. **39**(7), 205–216 (2018).

[5] Basti, G., Teta, A.: *On the quantum mechanical three-body problem with zero-range interactions*, in J. Dittrich, H. Kovarik, A. Laptev (Eds.) Functional Analysis and Operator Theory for Quantum Physics: The Pavel Exner Anniversary Volume, EMS Publishing House, 189–211 (2017).

[6] Birman, M. Sh.: Matem. Sborn. **38** 431, (1956); see M. Khotyakov, A. Michelangeli, Translation and adaptation of Birman's paper on the theory of self-adjoint

extensions of positive definite operators (1956), to appear in Mathematical Challenges of Zero-Range Physics, INdAM-Springer series (2019) SISSA preprint 082015MATE.

[7] Castin, Y., Werner, F.: *The unitary gas and its symmetry properties*. In Lect. Notes Phys. **836**, 127–189 (2011).

[8] Dell'Antonio, G., Figari, R., Teta, A.: *Hamiltonians for systems of N particles interacting through point interactions*, Ann. Inst. H. Poincaré Phys. Théor. **60**, 253–290 (1994).

[9] Danilov, G. S.: *On the three-body problem with short-range forces*, Soviet Phys. JETP **13**, (1961).

[10] Figari, R., Teta, A.: *On the hamiltonian for three bosons with point interactions*, in *Quantum and Stochastic Mathematical Physics – Sergio Albeverio Adventures of a Mathematician*, Springer Proceedings in Mathematics and Statistics, to be published in (2020).

[11] Minlos, R. A.: *On point-like interaction between n fermions and another particle*, Mosc. Math. J. **11**, 113–127 (2011).

[12] Minlos, R. A.: *A system of three quantum particles with point-like interactions*. Russ. Math. Surv. **69**, 539–564 (2014).

[13] Minlos, R. A., Faddeev L.: *On the point interaction for a three-particle system in quantum mechanics*, Soviet Phys. Dokl. **6**(12), 1072–1074 (1962).

[14] Minlos, R. A., Faddeev L.: *Comment on the problem of three particles with point interactions*, Soviet Phys. JETP **14**(6), 1315–1316 (1962).

[15] Moser, T., Seiringer, R.: *Energy contribution of a point-interacting impurity in a Fermi gas*, Ann. Inst. H. Poincaré **20**, 1325–1365 (2019). https://doi.org/10.1007/s00023-018-00757-0

[16] Reed, M., Simon, B.: *Methods of modern mathematical physics. Vol III: Scattering theory*, Academic Press, San Diego (1975).

[17] Ter-Martirosian, K. A., Skornyakov, G. V.: *The three-body problem with short range forces. Scattering for low energy neutrons by deuterons*, Soviet Phys. JETP **4** (1957).

18

3-D incompressible Navier-Stokes equations: Complex blow-up and related real flows

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Abstract. *In the framework of the Global Regularity Problem for the Navier-Stokes (NS) Equations in $\mathbb{R}^3$ Li and Sinai proved the existence of singular complex solutions ("blow-up"). We give an outline of their approach and discuss the perspectives of its extension to real solutions. We also illustrate, with the help of computer simulations, the behaviour of a real solution related to the complex blow-up. It does not blow up, due to its approximate axial symmetry, but it shows a remarkable tornado-like behaviour, with a rapid concentration and increase of speed and vorticity.*

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1 Introduction

The problem whether there are smooth solutions of the incompressible Navier-Stokes equations in $\mathbb{R}^3$ that become singular at a finite time ("blow-up") dates back to Jean Leray [6] who first proved a global weak existence theorem for all times and a uniqueness and regularity theorem only for finite times. It goes under the name "Global Regularity Problem" (GRP), and is still open, in spite of many brilliant contributions.

Leray thought that singularities exist and are related to turbulence. We now describe turbulence as a chaotic flow with no relation to singularities, but the singular solutions, if they exist, could provide a model for phenomena such as tornadoes, which exhibit a rapid increase of speed in a limited region of space, and for which there is at present no effective model. In fact we know [9] that a loss of smoothness for the NS equations implies divergence of the velocity at some point. Proofs of a finite-time blow-up were obtained for some variants of the dyadic model [3], a discrete model of the NS equations which preserves energy conservation. Moreover T. Tao [10] proved a finite-time blow-up for a NS system with a modified bilinear term satisfying the energy identity .

The evidence from computer simulations is inconclusive: a theoretical guideline on the behaviour of singularities is needed in order to control the difficulties arising in computing solutions of the 3-D NS equations for high values of the vorticity [4].

In 2008 Li and Sinai [7] proposed a negative answer to the GRP, i. e., a plan to construct explicit singular solutions. As a first step they proved that there are complex singular solutions following from initial data such that the support of the Fourier transform $\mathbf{v}(\mathbf{k},t)$ of the velocity field $\mathbf{u}(\mathbf{x},t)$ (see below) extends rapidly to high $|\mathbf{k}|$-values. The proof relies on Renormalisation Group methods, and their approach can be applied to other models [8] as well. The extension of their methods to real solutions requires more work. In the meantime important indications can come from computer simulations, which, as we explain below, if implemented in Fourier $\mathbf{k}$-space, are made easier for the class of initial data under consideration, by the fact that the extension of the support to the high $|\mathbf{k}|$-region is confined to a rather small region around a fixed axis.

The plan of the paper is as follows. We first describe the main features of the Li-Sinai approach, also with the help of some simple new results, and discuss its extension to real solutions. We then report results of recent simulations describing the behaviour of a real solution related to the complex blow-up in [7]. The solution behaves very much

tornado-like, but, as we discuss in the concluding remarks, does not blow up because of axial symmetry and we need to consider non-symmetric solutions.

2 The Li-Sinai approach

2.1 NS in k-space

Passing to a precise formulation, we consider the incompressible Navier-Stokes equations in the whole space $\mathbb{R}^3$ with no boundary conditions and external forces:

$$\frac{\partial \mathbf{u}}{\partial t} + \sum_{j=1}^{3} u_j \frac{\partial}{\partial x_j}\mathbf{u} = \Delta \mathbf{u} - \nabla p, \qquad \mathbf{x} = (x_1, x_2, x_3) \in \mathbb{R}^3 \tag{18.1}$$

$$\nabla \cdot \mathbf{u} = 0, \qquad \mathbf{u}(\cdot, 0) = \mathbf{u}_0.$$

Here $\mathbf{u} : \mathbb{R}^3 \times [0,\infty) \to \mathbb{R}^3$ is the velocity field, p is the pressure and we assume for the viscosity $\nu = 1$, which is always possible by rescaling. Two important physical quantities are the total energy $E(t)$ and the enstrophy $S(t)$, which is the integral of the square vorticity:

$$E(t) = \frac{1}{2}\int_{\mathbb{R}^3} |\mathbf{u}(\mathbf{x},t)|^2 d\mathbf{x}, \qquad S(t) = \int_{\mathbb{R}^3} |\omega(\mathbf{x},t)|^2 d\mathbf{x} \tag{18.2}$$

where $\omega(\mathbf{x},t) = \nabla \times \mathbf{u}(\mathbf{x},t)$ is the vorticity. They are related by the energy equality

$$E(t) + \int_0^t S(s)ds = E(0), \tag{18.3}$$

which implies that $E(t)$ cannot increase. If the enstrophy is bounded, it can be shown by an "enstrophy inequality" that global regularity holds [11], so that for a blow-up the enstrophy must diverge in an integrable way as we approach a critical time. A divergence of the enstrophy implies that the support is shifting to the high $\mathbf{k}$-region in Fourier space, i. e., to the fine scale structure in the physical space.

As we work in $\mathbf{k}$ space, we write the NS system (18.1) in terms of a modified Fourier transform of the velocity field $\mathbf{u}(\mathbf{x},t)$

$$\mathbf{v}(\mathbf{k},t) = \frac{i}{(2\pi)^3}\int_{\mathbb{R}^3} \mathbf{u}(\mathbf{x},t) e^{-i\langle \mathbf{k},\mathbf{x}\rangle} d\mathbf{x}, \qquad \mathbf{k} = (k_1, k_2, k_3) \in \mathbb{R}^3, \tag{18.4}$$

where $\langle \cdot, \cdot \rangle$ denotes the scalar product in $\mathbb{R}^3$. By a Duhamel formula the system (18.1) is written as a single integral equation:

$$\mathbf{v}(\mathbf{k},t) = e^{-t\mathbf{k}^2}\mathbf{v}_0(\mathbf{k}) + \int_0^t e^{-(t-s)|\mathbf{k}|^2} \int_{\mathbb{R}^3} \langle \mathbf{v}(k-k',s),\mathbf{k}\rangle\, P_{\mathbf{k}}\mathbf{v}(\mathbf{k}',s)\, d\mathbf{k}'\, ds, \qquad (18.5)$$

where $P_{\mathbf{k}}\mathbf{v} := \mathbf{v} - \frac{\langle \mathbf{v},\mathbf{k}\rangle}{|\mathbf{k}|^2}\mathbf{k}$ denotes the solenoidal projector and $\mathbf{v}_0$ is the transform of $\mathbf{u}_0$. In general $\mathbf{v}(\mathbf{k},t)$ is a complex function. Li and Sinai consider only real solutions of (18.5), which in general correspond to complex solutions of (18.1). However if $\mathbf{v}_0(\mathbf{k})$ (and hence $\mathbf{v}(\mathbf{k},t)$ for $t>0$) is antisymmetric, the solution $\mathbf{u}(\mathbf{x},t)$ is also real and antisymmetric in $\mathbf{x}$.

Taking $\mathbf{v}_0(\mathbf{k}) = A\bar{\mathbf{v}}(\mathbf{k})$, where A is a real parameter which controls the initial energy, and iterating the Duhamel formula, the solution of (18.5) is written as a power series:

$$\mathbf{v}_A(\mathbf{k},t) = A\mathbf{g}^{(1)}(\mathbf{k},t) + \sum_{p=2}^{\infty} A^p \int_0^t e^{-\mathbf{k}^2(t-s)}\mathbf{g}^{(p)}(\mathbf{k},s)\, ds, \qquad (18.6)$$

where $\mathbf{g}^{(1)}(\mathbf{k},s) = e^{-s\mathbf{k}^2}\bar{\mathbf{v}}(\mathbf{k})$, $\mathbf{g}^{(2)}(\mathbf{k},s) = \int_{\mathbb{R}^3} \left\langle \mathbf{g}^{(1)}(\mathbf{k}-\mathbf{k}',s),\mathbf{k}\right\rangle P_{\mathbf{k}}\mathbf{g}^{(1)}(\mathbf{k}',s)\, d\mathbf{k}'$ and

$$\mathbf{g}^{(p)}(\mathbf{k},s) = \sum_{\substack{p_1+p_2=p \\ p_1,p_2>1}} \int_0^s ds_1 \int_0^s ds_2\, \mathbf{g}^{(p_1,p_2)}(\mathbf{k},s_1,s_2) + \textbf{boundary terms}, \qquad p>2 \qquad (18.7)$$

$$\mathbf{g}^{(p_1,p_2)}(\mathbf{k},s_1,s_2) = \int_{\mathbb{R}^3} \left\langle \mathbf{g}^{(p_1)}(\mathbf{k}-\mathbf{k}',s_1),\mathbf{k}\right\rangle P_{\mathbf{k}}\mathbf{g}^{(p_2)}(\mathbf{k}',s_2)\, e^{-(s-s_1)(\mathbf{k}-\mathbf{k}')^2-(s-s_2)(\mathbf{k}')^2} d\mathbf{k}'$$

The boundary terms involve $\mathbf{g}^{(1)}$ and have a slightly different form [7]. The following lemma shows that the functions $\mathbf{g}^{(p)}$ satisfy, as $p\to\infty$, a Gaussian bound.

Lemma 18.1 If $\bar{\mathbf{v}} \in L_2(\mathbb{R}^3)$ is a bounded function, then the following inequalities hold

$$|\mathbf{g}^{(p)}(\mathbf{k},t)| \le K^{p-1}p^{1/2}t^{p-3/2}\phi_0^{(p)}(\mathbf{k}),$$
$$\phi_0^{(p)}(\mathbf{k}) = (\underbrace{\phi_0 * \ldots * \phi_0}_{p \text{ times}})(\mathbf{k}), \qquad \phi_0(\mathbf{k}) = |\bar{\mathbf{v}}(\mathbf{k})|, \qquad p\ge 2, \qquad (18.8)$$

where $*$ denotes convolution and K is a positive constant.

Proof. Let $\sup_{\alpha\ge 0}\alpha^{1/2}e^{-\alpha} = c_1 := (2e)^{-1/2}$. It follows that

$$|\mathbf{g}^{(2)}(\mathbf{k},s)| \le c_1A^2s^{-1/2}\int_{\mathbb{R}^3}\phi_0(\mathbf{k}-\mathbf{k}\mathbb{P})\phi_0(\mathbf{k}\mathbb{P})\, d\mathbf{k}' = c_1A^2s^{-1/2}\phi_0^{(2)}(\mathbf{k}).$$

For the terms of the sum in (18.7), using Inequality (18.8) as an ansatz, we have

$$\begin{aligned}\int_0^s ds_1 \int_0^s ds_2 \left|\mathbf{g}^{(p_1,p_2)}(\mathbf{k},s_1,s_2)\right| \\ &\leq c_1 \int_0^s ds_1 \int_0^s \frac{ds_2}{\sqrt{s-s_2}} \int_{\mathbb{R}^3} |\mathbf{g}^{(p_1)}(\mathbf{k}-\mathbf{k}\mathbb{P},s_1)| \cdot |\mathbf{g}^{(p_2)}(\mathbf{k}\mathbb{P},s_2)|\, d\mathbf{k}\mathbb{P} \\ &\leq c_1 K^{p-2}(p_1 p_2)^{\frac{1}{2}} \int_0^s s_1^{\frac{p_1-3}{2}} ds_1\, I_{\frac{p_2-3}{2}}(s)\, \phi_0^{(p)}(\mathbf{k}),\end{aligned}$$

where $I_\alpha(s) := \int_0^s \frac{u^\alpha}{\sqrt{s-u}} du$ satisfies for a semiinteger $\alpha \geq -\frac{1}{2}$ the inequality $I_\alpha(s) \leq D\frac{s^{\alpha+\frac{1}{2}}}{\alpha+1}$, for some constant $D > 0$. Hence we have $|\mathbf{g}^{(p_1,p_2)}(\mathbf{k},s)| \leq c_1 D \frac{K^{p-2}}{\sqrt{p_1}} s^{\frac{p-3}{2}}$. The boundary terms give a similar inequality. The conclusion now comes, for a suitable choice of K, by observing that $\sum_{n=1}^p \frac{1}{\sqrt{n}} \leq c_2\sqrt{p}$, for some constant $c_2 > 0$. □

By Lemma 18.1 the series (18.6) converges absolutely for small t. Moreover if the initial enstrophy is bounded, i. e., $\int_{\mathbb{R}^3} \mathbf{k}^2 |\mathbf{v}_0(\mathbf{k})|^2 d\mathbf{k} < \infty$, the local variant of the central limit theorem holds for the distribution with density $\widehat{\phi}_0(\mathbf{k}) = \frac{\phi_0(\mathbf{k})}{N}$, where $N = \int_{\mathbb{R}^3} \phi_0(\mathbf{k}) d\mathbf{k}$. Hence as $p \to \infty$ the convolution on the right of (18.8) tends to the Gaussian density with average $p\,\mathbf{m}$ and covariance matrix $\sqrt{p}\mathscr{C}$, where $\mathbf{m} = \int_{\mathbb{R}^3} \mathbf{k}\widehat{\phi}_0(\mathbf{k})\, d\mathbf{k}$ and $\mathscr{C} = (C_{ij})_{i,j=1,\ldots,3}$, $C_{ij} = \int_{\mathbb{R}^3} (k_i - m_i)(k_j - m_j)\widehat{\phi}_0(\mathbf{k})\, d\mathbf{k}$.

2.2 Blow-up for complex solutions and behaviour of related real solutions

In the paper [7] Li and Sinai choose initial data with support inside a sphere K_R of radius R centered around a point $\mathbf{k}^{(0)}$ with $|\mathbf{k}^{(0)}| \gg R$. By Lemma 18.1 the support of $\mathbf{g}^{(p)}$ is centered around $p\mathbf{k}^{(0)}$ with a diameter of the order $\mathscr{O}(\sqrt{p})$, so that as terms $\mathbf{g}^{(p)}$ with growing p are excited, if $|\mathbf{k}^{(0)}|$ is large, the support of $\mathbf{v}(\mathbf{k},t)$ quickly extends to the high $|\mathbf{k}|$ region, causing a strong increase of the enstrophy. The key for the proof of a blow-up is the asymptotic behaviour of $\mathbf{g}^{(p)}$ as $p \to \infty$. In view of the Gaussian dominance, Li and Sinai introduce new functions $\tilde{\mathbf{g}}^{(p)}(\bar{Y},s) = \mathbf{g}^{(p)}(p\mathbf{k}^{(0)} + \sqrt{p}\bar{Y},s)$ of the new variables $\bar{Y} = \frac{\mathbf{k}-\mathbf{k}_0}{\sqrt{p}}$, and look for initial values $\mathbf{v}_0$ which lead to the asymptotics

$$\tilde{\mathbf{g}}^{(p)}(\bar{Y},s) \sim p(\Lambda(s))^p \prod_{i=1}^3 g(Y_i)\big(\mathbf{H}(\bar{Y}) + \delta^{(p)}(\bar{Y},s)\big). \tag{18.9}$$

Here $\mathbf{H}$ is a solution of a fixed point equation of the map $L^\infty := \lim_{p\to\infty} L^{(p)}$ where $L^{(p)}$: $\tilde{\mathbf{g}}^{(p)} \to \tilde{\mathbf{g}}^{(p+1)}$, $g(x) = \frac{e^{-x^2/2}}{\sqrt{2\pi}}$ is the standard Gaussian, Λ is a strictly increasing smooth function and $\delta^{(p)}(\bar{Y}, s) \to 0$ as $s \to \infty$. (The Gaussian can always be made standard by a change of variables.) The functions $\mathbf{H}$ and Λ control the excitation of the high $\mathbf{k}$-modes. As shown in [7], there are infinitely many solutions of the fixed point equation. Assuming $\mathbf{k}^{(0)} = (0,0,a)$, with $a > 0$, the ansatz (18.9) is proved in [7] for $\mathbf{H} = c\ (Y_1, Y_2, 0) =: \mathbf{H}^{(0)}(\bar{Y})$, with $c > 0$, and for a monotonic increasing function Λ. The linearisation of L^∞ at $\mathbf{H}^{(0)}$ has a 6-dimensional unstable subspace, a 4-dimensional neutral subspace, and an infinite-dimensional stable one.

The main result of [7] can be formulated as follows.

Theorem 18.2 Let $a > b \gg 1$, and consider, as for (18.6), initial data $\mathbf{v}_0 = A\bar{\mathbf{v}}$ with

$$\bar{\mathbf{v}}(\mathbf{k}) = \left[\left(k_1, k_2, -\frac{k_1^2 + k_2^2}{k_3}\right) + \Phi(k_1, k_2, k_3)\right] \prod_{i=1}^{2} g(k_i) g(k_3 - a)\, \chi_b(|\mathbf{k} - \mathbf{k}^{(0)}|) \quad (18.10)$$

where $\mathbf{k}^{(0)} = (0,0,a)$, $a > 0$, g is the standard Gaussian, $\chi_b(\mathbf{k})$ is a smooth function with $\chi_b(\mathbf{k}) = 0$ if $|\mathbf{k}| \geq b$, $\chi_b(\mathbf{k}) = 1$ if $|\mathbf{k}| \leq b - \varepsilon$, for ε small enough, $\Phi = \Phi^{(1)} + \Phi^{(2)}$, $\Phi^{(1)}$ is a linear combination of the unstable and neutral eigenfunctions of the linearised map at $\mathbf{H}^{(0)}$, and $\Phi^{(2)}$ is in the stable subspace. Then if $\Phi^{(2)}$ is small enough, there is a time interval $(S_- \leq s \leq S_+)$ and an open set of the parameters defining $\Phi^{(1)}$ for which the ansatz (18.9) with $\mathbf{H} = \mathbf{H}^{(0)}(\bar{Y})$ holds.

The blow-up is an easy consequence of Theorem 18.2. Taking $A = \pm\frac{1}{\Lambda(\tau)}$, $\tau \in (S_-, S_+)$, and replacing $\mathbf{g}^{(p)}$ by the asymptotics (18.9), it is easy to see that the series (18.6) diverges as $s \uparrow \tau$. As the initial data (18.10) are not antisymmetric the solution $\mathbf{u}(\mathbf{x}, t)$ in the physical $\mathbf{x}$-space is, as we said above, a complex function, and at the critical time τ the energy $E(t)$ diverges along with the enstrophy $S(t)$ (for complex solutions the energy equality holds but it is not coercive).

Coming to real solutions, it is natural to consider initial data obtained by antisymmetrising the data (18.10) associated to the solutions that blow-up, i. e., of the type $\mathbf{v}_0(\mathbf{k}) = A\big(\mathbf{v}_+(\mathbf{k}) + \mathbf{v}_-(\mathbf{k})\big)$, where $\mathbf{v}_+ = \bar{\mathbf{v}}$ and $\mathbf{v}_-(\mathbf{k}) = -\bar{\mathbf{v}}(-\mathbf{k})$. The functions $\mathbf{g}^{(p)}$ are now a sum of terms centered around the points $(0,0,\ell\,\mathbf{k}^{(0)})$, $\ell = -p, \ldots, p$. In fact, substituting in (18.7) the expressions of $\mathbf{g}^{(p_i)}, i = 1,2$, in terms of functions with lower indices, down to $\mathbf{g}^{(1)}$, we see that $\mathbf{g}^{(p)}(\mathbf{k}, s) = \mathscr{L}_s^{(p)}\big(\mathbf{v}_0, \mathbf{v}_0, \ldots, \mathbf{v}_0\big)(\mathbf{k})$, where $\mathscr{L}_s^{(p)}$ is a p-linear

functional. The expression for $\mathbf{g}^{(p)}(\mathbf{k},s)$ breaks into 2^p terms $\mathscr{L}_s^{(p)}\big(\mathbf{v}_{i_1},\mathbf{v}_{i_2},\ldots,\mathbf{v}_{i_p}\big)(\mathbf{k})$, $i_q \in \{\pm\}$, $q=1,\ldots,p$, of which $\binom{p}{\frac{p-\ell}{2}}$ are centered around the point $\ell\mathbf{k}^{(0)}$. For large p the main contributions comes from values $\ell = \mathscr{O}(\sqrt{p})$, and we again have a shift of the support to the high $|\mathbf{k}|$-modes.

The analysis of the fixed points for the real solutions is more difficult. In absence of theoretical results on the behaviour of the functions $\mathbf{g}^{(p)}$ for the real antisymmetric solutions, important information can be obtained by computer simulations, which can also reveal physically relevant details.

3 Results of computer simulations

Computer simulations, with a new program for the numerical study of solutions of the integral equation (18.5), were first performed for the complex functions proposed in [7] in order to find out explicit values of the parameters leading to the blow-up and the most relevant details of its development [1], [2]. As shown by Lemma 18.1, the solutions with initial data of the type (18.10), extend their support in $\mathbf{k}$-space inside a thin region around the direction of $\mathbf{k}^{(0)} = (0,0,a)$, which for large k_3 has a transverse diameter $\mathscr{O}(\sqrt{k_3 a^{-1}})$. We could then compute for values of $|\mathbf{k}|$ up to a few thousand, and could follow the solutions up to times close to the blow-up.

The simulations showed that if $20 \le a \le 40$ and the initial energy E_0 is of the order of 10^5, all initial values of the type (18.10) with Φ small, as prescribed in [7], lead to a blow up with a critical time t_c of the order of 10^{-4} time units. For smaller values of E_0 it is also possible that the critical time t_c is larger than the available computer time. The function Φ in (18.10) does not have much influence on the behaviour of the solution, except that it increases the critical time t_c. Therefore most simulations were done with $\Phi = 0$.

As discussed in [1, 2], there are two types of singular complex solutions, depending on the sign of the constant A. In both cases the divergence of the total energy and enstrophy goes as an inverse power of $t - t_c$, but the rate of divergence is slower for $A < 0$, as there are cancellations between neighbouring terms in the series (18.6).

The initial data for the computer simulations of the real flow are obtained by antisymmetrising the function (18.10) with $\Phi \equiv 0$. The general implementation of the numerical approach was obtained from previous simulations of the complex blow up [1, 2]. We only report results obtained for $a = 30$ and $E_0 = 62 \cdot 10^6$. Recall however

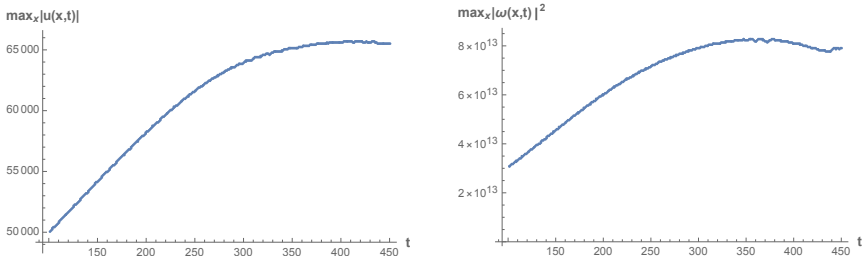

Figure 18.1: Plots of $\max_{\mathbf{x}} |\mathbf{u}(\mathbf{x},t)|$ (left) and of $\max_{\mathbf{x}} |\omega(\mathbf{x},t)|^2$ (right) as functions of time.

that the NS scaling holds: If $\mathbf{v}(\mathbf{k},t)$ is a solution of (18.5), and $\lambda > 0$ then the function $\mathbf{v}^{(\lambda)}(\mathbf{k},t) = \lambda^2 \mathbf{v}(\lambda\mathbf{k}, \lambda^{-2}t)$ is also a solution.

Simulations were performed on a mesh in $\mathbf{k}$-space which is part of a regular lattice centered at the origin with step $\delta = 1$, and maximal configuration $[-254,254] \times [-254,254] \times [-3000,3000]$. The velocity field at a given time is described by about $5 \cdot 10^9$ real numbers, close to the maximal capacity of modern supercomputers. A comparison of the accuracy of our program to that of finite-difference methods is under way.

As for the complex blow-up, the interesting phenomena take place in a very short time, and in what follows time is measured in units of $\tau = 1.5625 \times 10^{-8}$. The enstrophy $S(t)$ grows almost threefold, from $S(0) \approx 2 \times 10^8$ to $S(T_M) \approx 6 \times 10^8$, with $T_M \approx 710\tau$, after which it decreases. The maximal values of the velocity $|\mathbf{u}(\mathbf{x},t)|$ and of the vorticity $|\omega(\mathbf{x},t)|$ also grow, as shown in Figure 18.1, reaching a maximum at $t \approx 410\tau$ and $t \approx 350\tau$, respectively.

Figure 18.2 reports the behaviour in time of the marginal distributions of the square of the vorticity along the symmetry axis in the physical $\mathbf{x}$-space and in the Fourier $\mathbf{k}$-space:

$$S_3(k_3,t) = \int_{\mathbb{R}\times\mathbb{R}} |\mathbf{k}|^2 |\mathbf{v}(\mathbf{k},t)|^2 \, dk_1 \, dk_2, \qquad \tilde{S}_3(x_3,t) = \int_{\mathbb{R}\times\mathbb{R}} |\omega(\mathbf{x},t)|^2 \, dx_1 \, dx_2.$$

The behaviour of S_3 shows that, as time grows, the high $|\mathbf{k}|$ modes are enhanced and a modulated periodic pattern sets in for large k_3 with distance of the peaks close to $a = 30$. In the physical space observe that at the time $t = 400\tau$ the vorticity concentrates in sharp peaks near the planes $x_3 = \pm\bar{x}_3$ with $\bar{x}_3 \approx \frac{\pi}{a}$, corresponding to the modulated periodicity. In fact a 3-D plot would show that the high velocity and vorticity values are concentrated

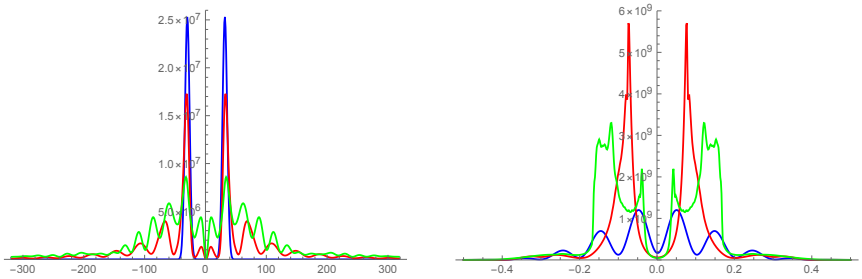

Figure 18.2: Plots of the marginal distributions $S_3(k_3,t)$ (left) and $\tilde{S}_3(x_3,t)$ (right) at the times $t = 0$ (blue), $t = 400\tau$ (red), and $t = 711\tau$ (green).

in two "doughnuts" around the x_3-axis, bisected by the planes $x_3 \approx \pm\bar{x}_3$, while elsewhere the fluid stays more or less quiet.

4 Concluding remarks

The real solution described in the previous paragraph is strongly reminiscent of tornadoes and similar phenomena, with a sharp increase and concentration of the velocity and the vorticity in an annular region around the symmetry axis. Similar solutions could be a good model of such physical phenomena, and they are likely to apply also to compressible fluids, perhaps in conditions of quasi-incompressibility.

Concerning the possibility of a blow-up, observe that our initial data are obtained by antisymmetrising the data (18.10) with $\Phi = 0$, and our solution is axially symmetric around the third axis in the physical $\mathbf{x}$-space (and also in Fourier $\mathbf{k}$-space), with no swirl (i. e., there is no rotation around the x_3-axis). This is a consequence of the choice of the fixed point $\mathbf{H}^{(0)}$, and also by taking a small $\Phi \neq 0$ we would stay close to axial symmetry with no swirl, which implies global regularity, according to a recent paper by Lei and Zang [5], in which the criticality of the axial symmetric case is also proved for the first time.

The research should be extended to real solutions related to fixed points $\mathbf{H} \neq \mathbf{H}^{(0)}$, which are not axial symmetric. The theoretical analysis requires the extension of the results of Li and Sinai to such fixed points and a deeper study of the behaviour of the series (18.6) in the real case. We also plan to obtain indications from computer simulations.

Acknowledgements. The computer simulations were performed at the Marconi Supercomputer of CINECA (Bologna, Italy), within the framework of a European PRACE Project n. 2015133169, and also of CINECA ISCRA Projects of type B and C.

Bibliography

[1] Boldrighini, C., Frigio, S., Maponi, P.: *On the blow-up of some complex solutions of the 3D Navier-Stokes equations: Theoretical predictions and computer simulation.* IMA J. Appl. Math. **83**, 697–714 (2017).

[2] Boldrighini, C., Li, D., Sinai, Ya. G.: *Complex singular solutions of the 3-d Navier-Stokes equations and related real solutions.* J. Stat. Phys. **167**(1), 1–13 (2017).

[3] Cheskidov, A.: *Blow-up in finite time for the dyadic model of the Navier-Stokes equations.* Trans. Am. Math. Soc. **10**, 5101–5120 (2008).

[4] Hou, T. Y.: *Blow-up or no blow-up? A unified computational and analytic approach to three-dimensional incompressible Euler and Navier-Stokes equations.* Acta Numer. **18**, 277–346 (2009).

[5] Lei, Z., Zang, Q.: *Criticality of the axially symmetric Navier-Stokes equations*. Pac. J. Math. **289**, 169–187 (2017).

[6] Leray, J.: *Sur le mouvement d'un liquide visqueux emplissant l'espace.* Acta Math. **63**, 193–248 (1934).

[7] Li, D., Sinai, Ya. G.: *Blowups of complex solutions of the 3D Navier-Stokes system and renormalization group method*. J. Eur. Math. Soc. **10**, 267–313 (2008).

[8] Li, D., Sinai, Ya. G.: *Blowups of complex-valued solutions for some hydrodynamic models*. Reglu. Chaot. Dyn. **15**(4–5), 521–531 (2010).

[9] Seregin, G.: *A certain necessary condition of potential blow up for Navier-Stokes equations.* Commun. Math. Phys. **312**, 833–845 (2012).

[10] Tao, T.: *Finite time blowup for an averaged three-dimensional Navier-Stokes equation.* J. Amer. Math. Soc. **29**(3), 601–674 (2016).

[11] Temam, R.: *Navier-Stokes equations: Theory and numerical analysis.* North Holland (1977).

The XI international conference Stochastic and Analytic Methods in Mathematical Physics was held in Yerevan 2–7 September 2019 and was dedicated to the memory of the great mathematician Robert Adol'fovich Minlos, who passed away in January 2018.

The present volume collects a large majority of the contributions presented at the conference on the following domains of contemporary interest: classical and quantum statistical physics, mathematical methods in quantum mechanics, stochastic analysis, applications of point processes in statistical mechanics. The authors are specialists from Armenia, Czech Republic, Denmark, France, Germany, Italy, Japan, Lithuania, Russia, UK and Uzbekistan.

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ISSN 2199-4951
ISBN 978-3-86956-485-2
9 783869 564852
Online