INTERNATIONAL CENTER FOR MATHEMATICS

#32

Bulletin

Jully 2012

Editorial

Dear CIM Colleagues,

First, we are pleased to announce the launch of the new *CIM Series in Mathematical Sciences* to be published by Springer-Verlag. The birth of the CIM Series occurred during a meeting between the Executive Board of CIM and the Springer-Verlag Executive Editor Mathematics Martin Peters who honored us with a visit to CIM.

The CIM Series will contain proceedings of CIM events, consisting of expository articles, research monographs and lecture course notes, among others. Springer will develop a special book design for the CIM Series in close collaboration with CIM and will publish, distribute and sell the books in the CIM series worldwide in any medium, in particular, in electronic form. The president of the Executive Board of CIM and the president of the Scientific Council of CIM will be the editors of the CIM Series. The first book to be published will be a book arising from the conference Mathematics of Planet Earth. The authors and editors of CIM volumes should have an international recognized scientific impact in their research area. CIM invites you to propose volumes for the CIM series by sending an email to CIM and to the editors.

Also, I would like to remind you of CIM's upcoming contribution to the international program Mathematics of Planet Earth (MPE 2013). To support this global effort, CIM is organizing two international conferences and corresponding advanced schools: Planet Earth, Mathematics of Energy and Climate Change, 25–27 March 2013, with the Advanced School Planet Earth, Mathematics of Energy and Climate Change, 18–23 March and 27–28 March 2013; and Planet Earth, Dynamics, Games and Science, 2–4 September 2013, with the Advanced School Planet Earth, Dynamics, Games and Science, 26–31 August and 5-7 September 2013. The Portuguese Society of Mathematics (SPM), the Portuguese Society of Statistics (SPE) and the Portuguese Society of Operational Research (APDIO) enthusiastically support the conferences and advanced schools we are organizing for MPE-2013. The two international conferences will be hosted in Calouste Gulbenkian Foundation. Further information is already available at http://sqig.math.ist.utl.pt/cim/mpe2013/ and the registration will open soon.

On behalf of the CIM Board, thank you for your continued support and interest.

Alberto Adrego Pinto
President of CIM

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Coming Events

Statue of Prometheus (Universidade do Minho, Campus de Gualtar)

Particle systems and PDE's
Braga, Portugal
December 05–07, 2012
[https://sites.google.com/site/meetingpspde/]

This is a first meeting on particle systems and PDE's to be held at the Centre of Mathematics (CMAT) of the University of Minho at 5,6 and 7 of December of 2012. The idea of the meeting is to get together researchers from two different areas of mathematics, namely Particle Systems and Partial Differential Equations and to present recent scientific results in both areas. The goal of the meeting is to present to a vast and varied public and even to young researchers, the subject of Interacting Particle Systems, its motivation from Physics and the impact of its results in the area of Physics and its relation with the subjects of PDE's. This will elucidate and highlight the interdisciplinary nature of mathematics and bring us the possibility to attract young students to dedicate to a scientific career on these subjects.

It is our pleasure to announce that there will be Proceedings of the event to be published by Springer. You can find more information here:
https://sites.google.com/site/meetingpspde/home/proceedings

Date: December 5-7, 2012.
Place: Universidade do Minho, Campus de Gualtar, Braga, Portugal.

Contacts: please send an e-mail to the address
meetingpspde@gmail.com
or contact the organizing committee.
Financial Support: provided by FCT through the research project "Non-equilibrium statistical physics" PTDC/MAT/109844/2009 and CMAT through the project PEst-C/MAT/UI0013/2011.

Attendance is free but needs registration

Scientific committee:
Pablo Ferrari (UBA, Argentina)
Felipe Linares (IMPA, Brazil)
Maria Conceição Carvalho (FCUL, Portugal)

Organizing committee:
Patricia Gonçalves (CMAT) patg@math.uminho.pt
Mahendra Panthee (CMAT) mpanthee@math.uminho.pt
Ana Jacinta Soares (CMAT) ajsoares@math.uminho.pt

Invited speakers:
Adriana Neumann* (UFRGS, Brazil)
Cedric Bernardin (ENS Lyon, France)
Claudio Landim (IMPA)
Cristina Toninelli (CNRS Paris 6 and 7, France)
Diogo Gomes (IST, Portugal)
François Golse (École Polytechnique France)
Gideon Amir (Bar- Ilan University)
M. Conceição Carvalho (Lisbon University, Portugal)
M. João Oliveira (CMAF, Portugal)
Marielle Simon (UMPA, Lyon, France)
Marton Balazs (Budapest University, Hungary)
Milton Jara (IMPA, Brazil)
Patrik Ferrari (Bonn University, Germany)
Simone Calogero (Granada University)
Stefano Olla (University Paris-Dauphine, France)
Sunder Sethuraman (Arizona University, USA)
Tertuliano Franco (University of Bahia, Brazil)
Valeria Ricci (University of Palermo, Italy)

* To be confirmed

An Interview

with Peter Jephson Cameron

by **Gracinda M . S. Gomes** [CAUL and DM-FCUL, Universidade de Lisboa]

Peter Cameron received a B.Sc. from the University of Queensland and a D.Phil. in 1971 from the University of Oxford, with Peter M. Neumann as his supervisor. Subsequently he was a Junior Research Fellow and then a Tutorial fellow at Merton College, Oxford. He was awarded the London Mathematical Society's Whitehead Prize in 1979 and is joint winner of the 2003 Euler Medal of the Institute of Combinatorics and its Applications, http://www.lms.ac.uk/content/list-lms-prize-winners and http://en.wikipedia.org/wiki/Euler_Medal.

Peter Cameron is the author of over 300 papers and has written 7 books as well as various lecture notes, with more than 130 collaborators; counts with 34 Ph.D. students, and 9 "honorary" students, as well as many more Master's students, http://www.ams.org/mathscinet/search/author.html?mrauthid=44560.

Tell me about your way into Mathematics. Did you always want to be a mathematician?

I never seriously wanted to be anything else! But I didn't realise that you could be a mathematician as a job until I went to University for an interview for admission as a student. Before that I thought I would have to work in some field like Engineering or Physics that contained some mathematics. But I saw the people on the other side of the desk and thought, they are mathematicians, I could be one too!

Some of my early childhood memories are mathematical. I grew up on a dairy farm, and we took the milk to the cheese factory on a horse-drawn cart. I remember sitting on the back of the cart counting to a thousand. A bit later I discovered how to sum geometric progressions while chasing the cows in to be milked. This was a job that didn't need much concentration: just sit on a horse and follow the cows. So I could let my mind wander and think about adding up powers of 2, and 3, and so on.

How did you get interested in Algebra?

I think I have always been better at the discrete than the continuous. If combinatorics had been a university subject when I was a student, I may have been seduced by that! As it was, algebra suited me very well; I liked the way it was highly structured. I did my undergraduate honours project on the simplicity of the groups PSL(2,q) (though I took this from Dickson's book, he calls these groups LF(2,q), which was a bit confusing to me later).

The purpose of a group is to act on something, and it is always interesting to play off the group and the structure it acts on against one another; one learns interesting things in this way.

A couple of years ago I had a student who did a project on Sylow's proofs of his theorems. Sylow's original proof of his first theorem was phrased in terms of double cosets; now we would write it in terms of group actions. That was a stunningly beautiful proof, and is now my favourite of all the many proofs of that theorem. Very briefly, you show that if a group G has an overgroup which has a Sylow p-subgroup, then G also has one. By Cayley's theorem, every group of order n can be embedded in the symmetric group S_n, and S_n can be embedded in GL(n,p), which obviously has a Sylow subgroup (the upper triangular matrices).

In which way is your recent research going?

As usual, in many different directions. I have never been good at concentrating hard on one problem until I solve it; someone comes along with another interesting problem, and I can't resist having a go.

There are several big things going on at the moment, all in the area between algebra and combinatorics. One project is to understand the algebraic properties of roots of the chromatic polynomials of graphs. Partly as a result of the connection with statistical mechanics, we know a lot about the location of these roots in the complex plane, but much less about, say, the degrees of the splitting fields, and their Galois groups.

Another is the work that brings me to Lisbon, my joint work with João Araújo and others on connections between semigroups, permutation groups, and various parts of combinatorics. João believes that, as a result of improvements in our understanding of groups, it is time to revisit the study of semigroups through their groups of units. The connection between transformation semigroups and permutation groups is especially close.

It turns out, too, that various concepts of optimality of block designs in the theory of experimental design in statistics can be expressed in terms of Laplacian eigenvalues of graphs. This is an area which also connects with random walks, electrical networks, isoperimetric problems, and other hot topics in network theory.

Between your many results, do you have a particular dear theorem?

There are two theorems of mine that I particularly like. One, with Jean-Marie Goethals, Jaap Seidel and Ernie Shult, was not a new theorem (Alan Hoffman had essentially the same result but with a very complicated proof which was never published), but our proof was new. The theorem describes all graphs for which the least eigenvalue of the adjacency matrix is -2 or greater. The novelty in our proof was to use the classification of the finite-dimensional root systems, from the theory of simple Lie algebras.

The second was my first venture into the realm of infinite permutation groups. John McDermott asked for an analogue of the Livingstone-Wagner theorem, about groups which act transitively on the set of k-subsets for all k, but are not k-transitive for some k. I was able to give a complete description of these groups: they preserve or reverse a linear or circular order on the underlying set. My proof was a typical finite group theorist's proof; immediately afterwards, Graham Higman came up with a proof using ideas from model theory and compactness. He called the lectures he gave about it "a Cameronian commentary".

I am also proud to have a constant named after me, from my work on sum-free sets, which also gave me Erdős number 1 (*see* Fig. 1).

And how do you see the importance of algebra in mathematics and in other fields of knowledge?

Algebra is the best example of how the abstract method has revolutionised mathematics and its applications.

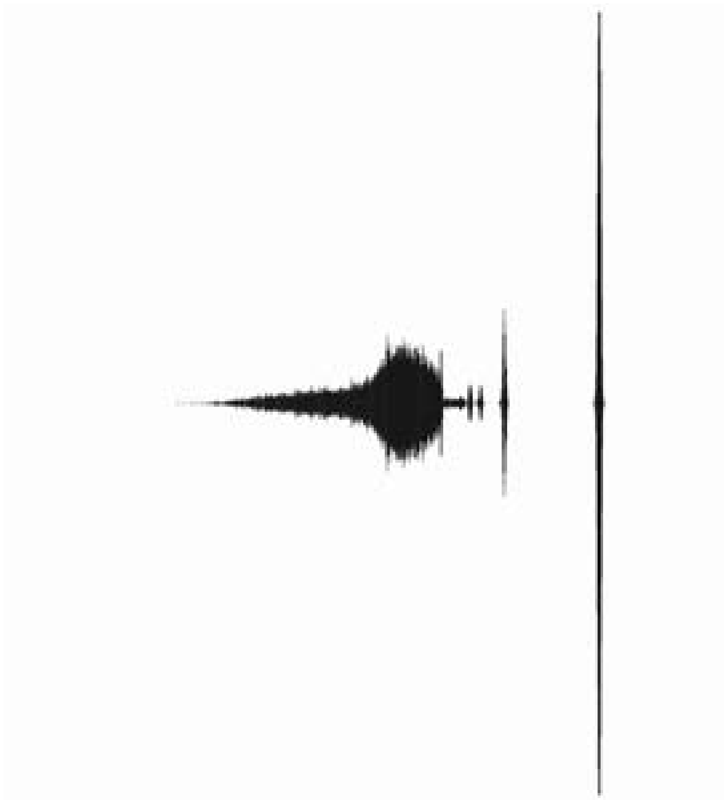


Figure. 1.—An approximation to the density spectrum of a random sum-free set. We choose a sum-free set of natural numbers in order: if n is the sum of two numbers in the set, then n is excluded, otherwise we toss a fair coin to decide whether to include n. The spikes on the right of the picture can be explained; for example, the biggest spike corresponds to sets of odd numbers, which occur with probability about 0.218 ("Cameron's constant"). The shape on the left, however, is still a mystery.

Douglas Adams, one of my favourite authors (who wrote "Hitch-Hikers' Guide to the Galaxy"), said "Algebra, for instance (and hence the whole of computer programming), derives from the realisation that you can leave out all the messy, intractable numbers." Numbers, matrices, permutations, symmetries, all obey a few simple laws; anything we can deduce from those laws (which is an impressive amount) will hold in all of these structures.

A few years ago, my department went back to doing something we had not done for a very long time: teaching abstract algebra to first-year students. I was given the job of designing and presenting the course. The students found it hard going, but worked very hard, and the results were good.

I am a Professor of Mathematics, and proud of that title. My work has taken me from model theory (in logic) to measurement theory (in mathematical psychology). A thread of algebra runs through all of these things.

I probably don't have to tell your readers about the importance of, and impact of, mathematics in our life today. Angus Macintyre, the immediate past president of the London Mathematical Society, argues that the economic impact of elliptic curve cryptography (which is responsible for the security of cash dispensers, among other things) far outweighs anything most disciplines have to offer. This is an important issue now, when the paymasters are interested in the economic impact of our research. But there are many other mathematical top-

Figure 2.—A Latin square, used in agricultural research at Rothamsted Experimental Station. Latin squares are the Cayley tables of quasigroups. This picture was provided by Sue Welham.

ics which also have practical importance, such as Latin squares (see Fig. 2).

Some interesting directions of research in algebra?

I am glad to see that various generalizations of groups, whose theories grew up more or less independent of group theory, are now moving together again. A very good example was the talk by Michael Kinyon, in July 2011 in Lisbon, which I talk about later, combining semigroups and quasigroups.

As well, there is a lot of Algebra underlying developments in mathematical physics, such as conformal field theory. But to my mind, the most interesting thing that has happened to Algebra during my career is the re-focusing of group theory following the Classification of Finite Simple Groups. Some people thought that finite group theory would fade away; this hasn't happened, since we have found so many interesting things about the subgroup structure and representation theory of the almost simple groups. Also, some areas of infinite group theory, notably locally finite groups and profinite groups, have been re-fashioned by our new knowledge of finite groups.

How do you expect the interplay of semigroups and groups to develop further?

It is probably unwise of me to make predictions about semigroups; I don't know so much about them. But the work I am doing suggests that it is time to look again at the group of units of a semigroup, or at its automorphism group, and to use the much stronger information we have about finite groups in order to make progress.

A longer term goal would be to do something similar with infinite transformation semigroups. Infinite permutation groups are a particular love of mine, and I would like to see some of the recent work in this area put to use. In a different area, I have seen that the relationship between the semigroup and the group given by the same (inverse-free) presentation is being studied. I have a recent paper on set-theoretic solutions of the Yang-Baxter equation from statistical physics, in which this situation arises naturally (and the group given by the presentation has a natural homomorphism to a permutation group).

You are a very popular lecture and supervisor, how important is for you to teach?

I very much enjoy teaching. In some ways it is a greater challenge than research. Rather than just finding an argument that convinces me, I have to convince many people with different backgrounds and expectations. It is very useful that some theorems have many different proofs: some students get the hang of one, others catch on to a different one.

I have learned a lot from my students, probably far more than they have learned from me. It is always better when students are involved in the decision about what to work on; I prefer not just to lay down the law on this. It does become more difficult, as funders now prefer us to have specific projects laid out, and give grants to students to work on these.

Your many research students, are they all academics? Or have they opted for other kind of jobs?

Not all of them have become academics, though some have very successful careers in the academy. Some of my students have done their PhDs part-time, which is much more difficult but means that they don't have to look for a job at the end. Some have gone into commerce, or the civil service, others (I am happy to say) into schoolteaching and curriculum development.

When I was a student, the assumption was that a PhD always led to an academic job. But this is no longer true. I meet many people in the research council who have PhDs http://www.epsrc.ac.uk/

Do you have an advice for the students who are finishing their PhD? With nowadays job situation some feel rather concerned.

It is not an easy time to be finishing a PhD! In the longer term, things are likely to get better; a pendulum will always swing back eventually. But if you are starting out on your career, this is not comforting advice.

In my own case, a post-doctoral fellowship was a wonderful opportunity to do whatever I wanted, to learn new things, and to start really enjoying doing mathematics. Not all post-doc positions give as much freedom as this, but most supervisors understand that a young mathematician needs to spread her/his wings, and most people judging the outcome of a research grant also realise this and are not too strict if the original objectives haven't been met, as long as some good work has been done. I encouraged my most recent post-doc to broaden his interests, and now he has a lecturing job in a good department. So I think the advice is: if you can get a post-doc position, make the most of it!

And what about the ones who are dueling between their wish of taking a PhD and looking for a job immediately?

I would never take on a PhD student without giving a couple of warnings; in particular, there is no promise that it will lead to a successful career, and certainly not to a big salary! I think that someone who does not feel the inner compulsion to do mathematics is almost certainly better off looking for a job. But if the candidates decides that they are committed, I will do the best I can to help turn their dream into reality.

Have you been the head of a research group? What are your thoughts about running a group?

I was director of pure mathematics at Queen Mary for several years, but I have never officially run a research group. What happened was that people came to work with me, or to study, and a strong group of researchers just happened without any bureaucratic interventions. In particular, starting from almost nothing, a very active group in combinatorics now exists in my department.

Now it is difficult to run a group in this "hands-off" way, as universities introduce performance management and group leaders are expected to use the stick as well as the carrot. I am happy that I don't have to do this.

Keeping the blog http://cameroncounts.wordpress.com/ brought the students even closer to you and to mathematics?

Not so much students as ordinary people. I have discovered a large number of acquaintances, some of whom I have met, some are just pen-names, who respond to exposition of mathematics, or who ask me questions.

A lot of what I blog about is expository: I have a long series about the symmetric groups, for example. These are the posts that keep up their popularity after months and years when other more topical posts have faded into obscurity. I used to get this kind of satisfaction from writing books, but blogging is so much easier, and the responses come much quicker.

At the university, some defend that the number of just research places should be increased, how do you feel about this? Teaching and research can be dissociated in a good university?

I feel very strongly that dissociating teaching and research would be a bad mistake. There are a very few brilliant researchers who I would be reluctant to put in front of a large first-year class, but for the most part, the same people are good at both teaching and research.

Everybody benefits from this arrangement. In preparing teaching, or in questions from students, I get a supply of

Figure 3.—With my supervisor, Peter Neumann, and some of my students, at my 60th birthday conference in Ambleside.
Standing: **Michael Giudici, Pablo Spiga, Dugald Macpherson, Eric Lander, Cheng Ku, Fuad Shareef, Sarah Rees, David Cohen, Colva Roney-Dougal, Robert Bailey, Carrie Rutherford, Thomas Bending, Fatma Al-Kharoosi, Thomas Britz, Francesca Merola, Emil Vaughan.**
Seated: **Julian Gilbey, Taoyang Wu, Debbie Lockett, Josephine Kusuma, Sam Tarzi.**

research problems. If I find a new piece of mathematics and I am bursting to tell people about it, it often finds its way into my teaching. And I don't think students will ever understand what mathematics is really about unless they come into close contact with the best researchers.

In your page http://www.maths.qmul.ac.uk/~pjc/MTH6128/study.pdf there is a "letter" of advice to the students that come to the university. Do you feel that the students find adjusting to the university harder nowadays?

Yes. I think there are several reasons for this, but let me say to start that it is not true that students are less talented these days. An important factor is that schools do not prepare students for independent thought. The pressures on schools to achieve good exam results are so strong now that it is in everyone's interest, pupils and teachers alike, to be able to respond mechanically to exam questions without stopping to think for too long. Besides, this has the effect that pupils believe that the teacher's job is to help them get good exam results, not to make them think. So students arriving at university need to have their expectations changed.

The number of students going to university has greatly increased, while the proportion of the population with the ability and interest to do a mathematics degree probably has not. At some point ten years or so ago, word got around that a mathematics degree was the best way into a well-paid job in the finance industry. Not even the economic crisis has destroyed this expectation.

How did your connection to Portugal start? And how do you do see its development?

It started without warning in a talk by my PhD supervisor Peter M. Neumann, who discussed a question sent to him by João Araújo, and his answer to it. At almost the

Figure 4.—With João Araújo at CAUL

same time, I was working with a former student Cristy Kazanidis on highly symmetric cores (graphs with no proper endomorphisms), and also I was visited by another former student Robert Bailey who reported to me a conversation he had had with Ben Steinberg at a bus stop in Ottawa (interrupted by the arrival of Ben's bus) about a related topic. The upshot is that a group of us, with João as the driving force, began working on a connection between synchronizing automata and permutation groups, which rapidly grew almost beyond control!
Amazingly enough, at that point I had never been to Portugal. Since then I have been three times and plan to return soon, and this last one has been particularly fruitful with three papers about to be finished!
Who can say how it will develop? It seems that interesting things will continue to happen; and now I have discovered for myself what a beautiful city Lisbon is, I will certainly be coming back whenever I can!

Last year CAUL and CIM, in collaboration, organized the conference "Groups and Semigroups: interactions and computations" in which you were one of the main speakers, what did you think of the impact of this meeting in the field?

I mentioned above how good it is that groups and semigroups are coming together again at last.
There were two particular interactions that made the meeting very worthwhile for me. One was meeting John Meakin again. John and I were students together at the University of Queensland, and then went different ways, and our paths didn't cross until 2005, when we were both invited speakers at Groups St Andrews. This time John had a whole raft of questions which he thought would catch my interest. He was right, though I haven't got very far with them yet.
The other was Michael Kinyon, who works on the other kind of generalisation of groups (that is, quasigroups

and loops), and might have been expected to be at the conference on those which was happening in Prague at the same time. But he came to Lisbon and told us about a very interesting cross-fertilisation between semigroups and loops. Just as a loop has a multiplication group, so Michael's more general structures (which he called "semi-loops") have a multiplication semigroup.

It was also very interesting to see that even people who work at the most theoretical end of group theory are turning to computation in their research, to make and test conjectures and even to help prove theorems. This is a trend which will continue!

You are a traveler; would you like to tell us about a special trip/episode?

There are so many stories I could tell, and some of the best are possibly embarrassing or dangerous to tell. Mathematicians form a universal fellowship, and wherever I go, even in places with authoritarian regimes, the mathematicians treat me like one of them, and I see the place from the inside. Seeing places as different as Iran and Japan from the inside is an amazing experience: skimming stones on the Caspian Sea at sunset as the night fishermen were setting out, and the tea ceremony in Tokyo escorted by the partner of a colleague.

One thing that remains with me happened on my visit to India in 1988. I was staying at the University of Bombay, and they arranged for me to make a visit to Poona to give a talk. I went up and back by train. While I was there, the algebraist Devadatta Kulkarni took me round the city on the back of his scooter. One of the days of my visit happened to be Christmas Day, but it was a busy day at the mathematics department, since a big conference was beginning the next day. So, two students were given the job of looking after me and taking me round the town, to temples, markets, and so on. I found out on talking to them that, as well as studying for their PhDs, they were both teachers at the local high school, doing something like 20 contact hours a week! I tried to repay my debt to them by talking about mathematics, going through a paper they were reading and helping them with some of their difficulties.

I keep travel diaries on many of my trips, and put them on my web page if they are not too scurrilous! The story of my Indian trip, and a later trip to India, are both there. http://www.maths.qmul.ac.uk/~pjc/travel/

Along the years, you have been seriously interested in sport, music, literature, painting, which are your hobbies nowadays?

Sport was probably my most serious interest — I was Australian Universities champion at cross-country running when I was a student — but, as I get older, I find that injuries take longer to heal, so I do more walking than running now. I try to go for a long walk at least once a week (anything from 15 to 50 kilometres). London is a good city for walking, since the transport system is centralized, so it is easy to escape in any direction. Also, I have rediscovered photography. Digital compact cameras now are probably as good as the SLR I had when I was a student, and I am building up a good collection of photographs of places where I walk.

I play the guitar (I learned this at university where I played in a band). Since I play by ear, I am not restricted in what I can play. The guitar is a good barometer of my stress levels; if I go for months without picking it up, I am in a bad way! London is also a good city for music since every great musician (like every great mathematician) comes to visit.

I didn't read much at school, but discovered literature at university, and now I am an avid reader; maybe I am addicted to print.

An e-reader fan or do you prefer the "real thing", the paper book?

For me, a real book is better. Maybe you like what you grow up with! When I first had an e-reader, I tried using it for keeping slides of my talks, so I would know what was coming next; but I found I was never using it. The advantage of an e-reader is that you can get classics free or very cheaply. I am currently reading Gibbon's "Decline and Fall of the Roman Empire".

I would say that you are a free spirit; would that have its deep roots in your upbringing in Australia?

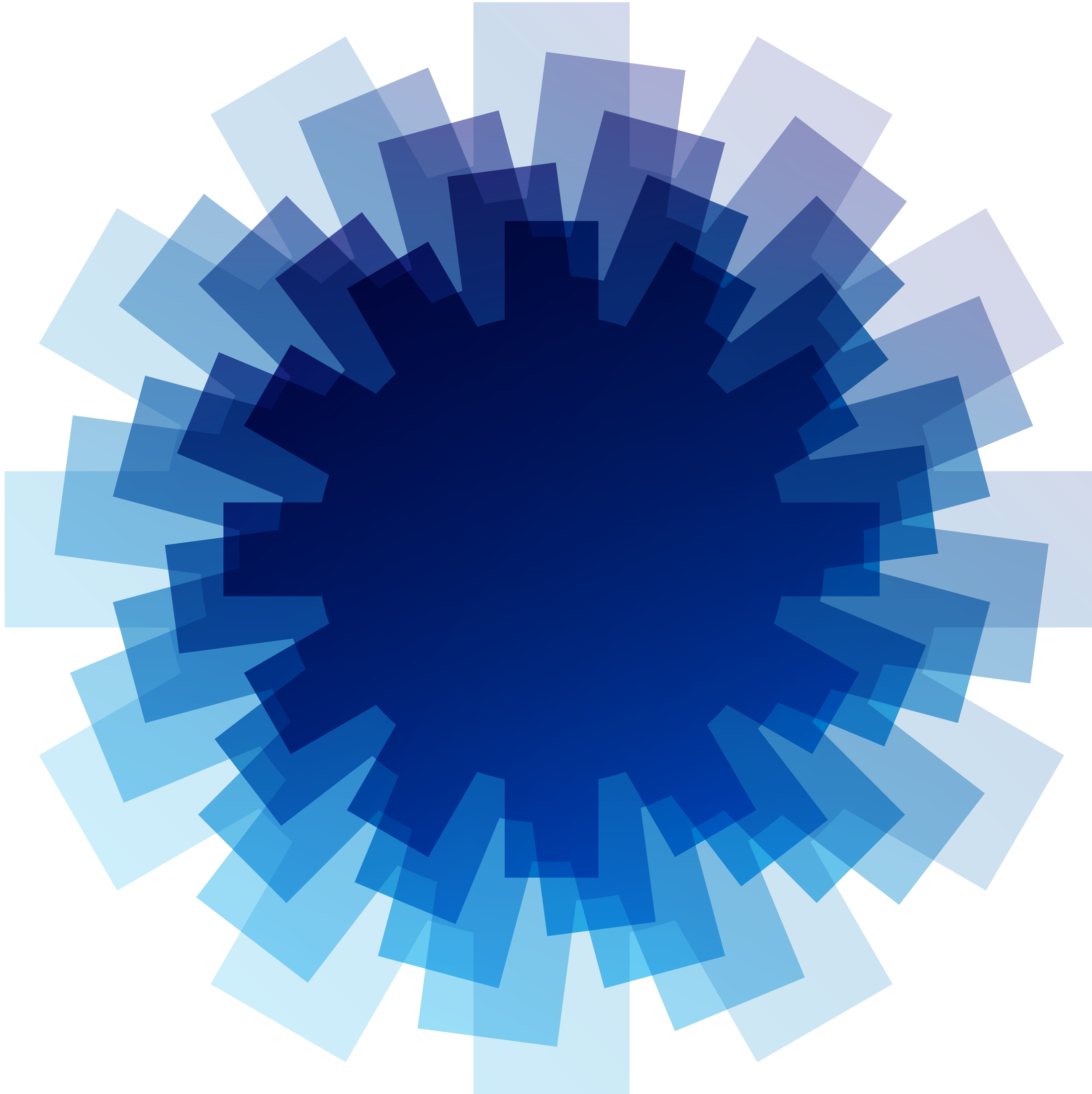
A hard question. Australians are, in fact, very conventional people. We introduced the term "tall poppy", meaning someone who is better than others at something and has to be cut down to size. I suppose this means that I learned to do what I wanted to do without making a song and dance about it. But it was also true that, growing up in the country, I learned that if nobody else could be found to do something, I could always simply do it myself. Travelling to the other side of the world to study and making a new life there must also have helped make me more independent.

Thank you Peter, it was a pleasure to interview you.

Lisboa, April 18, 2012

The 86th European Study Group with Industry

by Manuel B. Cruz [LEMA, Laboratory of Engineering Mathematics, School of Engineering of Porto's Polytechnic]



7 - 11 May, 2012
ISEP - School of Engineering | Polytechnic of Porto

The 86th European Study Group with Industry took place from May 7 to May 11, 2012 at ISEP, the School of Engineering of Porto's Polytechnic, organized by the Laboratory of Engineering Mathematics (LEMA) (*see*: http://www.lema.isep.ipp.pt/esgi86/). This meeting has counted with the participation of several experts with a large experience in this type of events. By the 5th consecutive year, Portuguese researchers and academics tried to strength the links between Mathematics and Industry by using Mathematics to tackle industrial problems that were proposed by industrial partners (*see*: http://www.ciul.ul.pt/~freitas/esgip.html).

In this edition there were selected 5 problems proposed by different companies namely, Neoturf (http://www.neoturf.pt/en), TAP Maintenance and Engineering (http://www.staralliance.com/en/ about/airlines/tap-Portugal_airlines/#), INESC (http://www2.inescporto.pt/ip-en/), Sonae Indústria – Produção e Comercialização de Derivados de Madeira, S.A and Euroresinas – Indústrias Quimicas Euroresinas, S.A., also a Sonae Group company (http://www.sonaeindustria.com/). For us, these problems were mathematically interesting challenges. For the companies, those were open-problems that had not been solved with their own (and/or consulting) resources, some of them for several years. This *bouquet* of problems was "multicharacteristic" in several ways. First of all due to different origin companies, second, due to the "multi-scope" of the problems. And last, the multitude of mathematical subjects used during the event which comprehended statistics, classification, optimization, numerical analysis or partial differential equations, just to name a few.

In this year's Portuguese ESGI, the results overwhelmed the organizers (and the companies') best expectations. For the organizers, some of them involved since 2007 when the first Portuguese ESGI edition took place, the objective is to spread mathematical knowledge and use it to help the industrial tissue. According to them, the success of ESGI's in Portugal may be measured by the growing number of participants, proposed problems, and by the fact that some companies are submitting new problems after their first participation. The comments from the companies' representatives were very positive. Pedro Mena and Fernando Guimarães (Euroresinas representatives), told at the end of the Study Group: "ESGI'86 was the first Sonae Industria participation on ESGI events. This format and analysis is, as such, newer to the company and is being addressed with great expectation and curiosity. After this initial experience, we consider of great significance this Mathematics-Industry partnership in the approach of subjects with most relevance to the national industry."

Telmo Rodrigues, from Sonae Indústria, said in the last day: "This meeting was very important, as it allows us to understand some phenomena of processes that weren't perfectly characterized". Neoturf CEO, Paulo Palha, went a little bit further in a post-ESGI interview. In the context of the workshop when asked about if the workshop fulfilled Neoturf expectations, he stated: "Undoubtedly! It certainly exceeded our best expectations as the problem proposed was identified more than 10 years ago but remained unsolved since then. We had consulted several software companies, tried some of their proposals, but nothing got even closer to the result achieved by the ESGI study group." The organizers, as mathematicians who care about the relation between academia and industry, also asked him how this format could be improved. His answer enclosed an important clue: "I think it would be very important to spread extensively this event, as most of the Small and Medium Companies aren't aware of the huge arsenal of techniques and resources that mathematicians have to solve our problems. Another idea is to have workgroups that can be hired by industry."

Kinetic approach to reactive mixtures: theory, modelling and applications

by Ana Jacinta Soares*

Abstract.—Some recent studies arising in the kinetic theory of chemically reactive mixtures will be revisited here, with the aim of describing some methods and tools of the kinetic theory used to model reactive mixtures and investigate some mathematical and physical problems.

Keywords.—Mathematical modelling; Kinetic theory; Chemically reactive systems.

1. Introduction

The kinetic theory of gases is a branch of statistical mechanics which deals with non-equilibrium dilute gases, i.e. gas systems slightly removed from equilibrium. Instead of following the dynamics of each particle, the kinetic theory approach describes the evolution of the gas system in terms of certain statistical quantities, namely velocity distribution functions, which give information about the distribution of particles in the system as well as the distribution of particle's velocities. One of the main tasks is then to deduce the macroscopic properties of the gas system from the knowledge of the molecular dynamics in terms of the distribution functions and, at the same time, to derive governing equations for these macroscopic properties in the hydrodinamic limits.

Historically, the modern kinetic theory starts with the contributions from August Krönig (1822–1879), Rudolf Clausius (1822–1888), James Maxwell (1831–1879) and Ludwig Boltzmann (1844–1906) and the central result of this theory is attributed to the celebrated Boltzmann equation (BE), derived in 1872, see Ref. [1]. This is an integro-differential equation that describes the evolution of a gas as a system of particles (atoms or molecules) interacting through brief collisions in which momentum and kinetic energy of each particle are modified but the states of intramolecular excitation are not affected.

The Boltzmann equation arises in the description of a wide range of physical problems in Fluid Mechanics, Aerospace Engineering, Plasma Physics, Neutron Transport as well as other problems where chemical reactions, relativistic or quantum effects are relevant. From the mathematical point of view, the Boltzmann equation presents several difficulties, mainly associated to the integral form of the collisional term describing the molecular interactions. In particular a general method for solving the Boltzmann equation does not exist, and only equilibrium (exact) solutions are know. Thus the mathematical analysis of the Boltzmann equation, in particular the properties of the collisonal terms, existence theory and approximate methods of solutions, constitute an interesting research topic in Mathematical Physics.

Available techniques for solving the Boltzmann equation and its variants are based on the approximate methods proposed by David Hilbert (1862–1943) in 1912 and by Sidney Chapman (1888–1970) and David Enskog (1884–1947) around 1916–17. The Hilbert method is a formal tool that obtains approximate solutions of the Boltzmann equation in the form of a power series of a small parameter inversely proportional to the gas density (the Knudsen number). Enskog generalized the Hilbert's idea and introduced a systematic formalism for solving the Boltzmann equation by successive approximations, and Chapmann followed the method of Maxwell to determine the transport coefficients of diffusion, viscosity and thermal conductivity. The ideas of Enskog combined with the method of Chapman led to the so called

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Chapman-Enskog method described in Ref. [2] and then followed by several authors and extended to more general gas systems.

In this paper, we present a general review of some recent studies arising in the kinetic theory of chemically reactive mixtures, mainly oriented to the modelling of reactive systems, mathematical structure and properties of the governing equations, application to detonation dynamics and existence results.

The studies presented in this paper have been obtained in collaboration with several researchers, cited here in chronological order, Miriam Pandolfi Bianchi (Politecnico di Torino, Italy), Gilberto Medeiros Kremer (Universidade Federal do Paraná, Curitiba, Brazil), Filipe Carvalho (CMAT-UM, Ph.D. Student), Jacek Polewczak (California State University, Northridge, LA, USA).

The paper is organized as follows. The main basic aspects of the kinetic theory are introduced in Section 2, with emphasis on the mathematical modelling, consistency properties of the kinetic modelling and connection to hydrodynamics. A particular model for symmetric chemical reaction is introduced in Section 3 and then used in Section 4 to mimic detonation problems. The simple reacting spheres (SRS) model is briefly described in Section 5 and an existence result about the solution of the partial differential equations of the model is presented in Section 6.

2. Kinetic theory background

In kinetic theory of gases, the state of a chemically reactive mixture can be described by the Boltzmann equation. There exist several references on this topic and we quote here the relevant contributions presented in the books [3,4,5,6].

In this section, we introduce the background of the kinetic theory of chemically reactive mixtures necessary to follow the general ideas and results presented in the following sections. We have tried to be as concise as possible in this presentation and do not use so much specialized formalisms. However some notations and nomenclature are needed to introduce the topic and the results.

2.1 *Mathematical modelling*

The present work is restricted to a dilute reactive mixture consisting of *four* constituents, say A_α, $\alpha = 1,2,3,4$, with molecular masses m_α, diameter d_α and chemical binding energies ε_α. Internal degrees of freedom, like translational, rotational and vibrational molecular motions, are not taken into account. Besides elastic scattering, particles undergo reactive collisions with a reversible bimolecular chemical reaction which can be represented schematically by

$$A_1 + A_2 \rightleftharpoons A_3 + A_4. \qquad (1)$$

The mass conservation associated to the chemical reaction results in $m_1 + m_2 = m_3 + m_4$. We assume that collisions take place when the particles are separated by a distance $\mathrm{d}_{12} = (\mathrm{d}_1 + \mathrm{d}_2)/2$ or $d_{34} = (\mathrm{d}_3 + \mathrm{d}_4)/2$.

A parameter of interest for the present modelling is the heat of the chemical reaction defined as $Q_R = \varepsilon_3 + \varepsilon_4 - \varepsilon_2 - \varepsilon_1$. The chemical reaction is endothermic when $Q_R > 0$ and it is exothermic when $Q_R < 0$.

At the molecular level, the thermodynamic state of the mixture can be described by the constituent distribution functions $f_\alpha(\boldsymbol{x}, \boldsymbol{c}_\alpha, t)$, $\alpha = 1, \dots, 4$, that represent, at time $t \in \mathbb{R}_0^+$, the number of particles of constituent α with velocity $\boldsymbol{c}_\alpha \in \mathbb{R}^3$ in the point $\boldsymbol{x} \in \mathbb{R}^3$. Function f_α, $\alpha = 1, \dots, 4$, are governed, in the phase space, by generalized Boltzmann equations of type

$$\frac{\partial f_\alpha}{\partial t} + \sum_{i=1}^{3} c_i^\alpha \frac{\partial f_\alpha}{\partial x_i} = \mathcal{Q}_\alpha^E + \mathcal{Q}_\alpha^R \qquad (2)$$

where the differential term in the left-hand side represents the streaming operator that describes the motion of particles along their trajectories in the phase space, and the term in the right-hand side represents the collision part that describes the changes of particles resulting from collisions. More in detail, $\mathcal{Q}_\alpha^E = \sum_{\beta=1}^4 \mathcal{Q}_{\alpha\beta}^E$ is the elastic collision term describing the dynamics of inert molecular collisions among constituent α and all other constituents $\beta = 1, \dots, 4$, and $\mathcal{Q}_\alpha^R$ is the reactive collision term describing the dynamics of chemical interactions. Terms $\mathcal{Q}_\alpha^E$ and $\mathcal{Q}_\alpha^R$ can be written in the following form, see Ref. [6],

$$\mathcal{Q}_\alpha^E = \sum_{\beta=1}^{4} \int_{\mathcal{D}\times\mathbb{R}^3} \left(f'_\alpha f'_\beta - f_\alpha f_\beta\right) g_{\beta\alpha}\sigma_{\beta\alpha} d\Omega_{\beta\alpha} d\mathbf{c}_\beta \qquad (3)$$

$$\mathcal{Q}_\alpha^R = \int_{\mathcal{D}^*\times\mathbb{R}^3} \left[f_\beta f_\delta \left(\frac{m_\alpha m_\gamma}{m_\beta m_\delta}\right)^3 - f_\alpha f_\gamma\right] \sigma_{\alpha\gamma}^\star g_{\gamma\alpha} d\Omega^* dc_\gamma \qquad (4)$$

where the primes denote post-collisional states, $g_{\beta\alpha}$ is the relative velocity between the α and β particles, $d\Omega_{\beta\alpha}$ and $d\Omega^*$ are elements of solid angles for elastic and reactive collisional processes, $\mathcal{D}$ and $\mathcal{D}^*$ the corresponding domains of integration, $\sigma_{\beta\alpha}$ the elastic cross section and $\sigma_{\alpha\gamma}^*$ the reactive cross section. For what concerns the reactive terms, the indices $(\alpha, \gamma, \beta, \delta)$ are from the set

$$\{(1,2,3,4), (2,1,4,3), (3,4,1,2), (4,3,2,1)\}.$$

The specification of the cross sections $\sigma_{\beta\alpha}$ and $\sigma_{\alpha\gamma}^*$ complete the definition of the kinetic model at the molecular level. In general, they satisfy symmetrical relations as those assumed here, of type

$$\sigma_{\beta\alpha} = \sigma_{\alpha\beta}, \quad (m_1 m_2 g_{21})^2 \sigma_{12}^* = (m_3 m_4 g_{43})^2 \sigma_{34}^*.$$

In many kinetic theories, $\sigma_{\beta\alpha}$ follows a hard-spheres model, which means that during elastic collisions, the particles behave as if they are rigid spheres, and $\sigma_{\alpha\gamma}^*$ is defined in terms of the activation energy of the chemical reaction, which means that only those particles such that the kinetic energy of the relative motion is greater than the activation energy can collide with chemical reaction.

A kinetic theory based on the statistical description in terms of Eqs.(2) and (3–4) can be of great importance in obtaining a detailed understanding of several processes involving chemically reactive mixtures. The investigation of transport properties and evaluation of transport coefficients is a valuable example. In fact, the transport coefficients of viscosity, diffusion, thermal conductivity and others can not be obtained from macroscopic theories; they have been supplied by experiments and phenomenological considerations. However the kinetic theory can provide these coefficients from the knowledge of the solution of the Boltzmann equation, even if only approximate soloutions are available in general.

2.2 *Consistency properties of the kinetic modelling*

The kinetic modelling defined in terms of Eqs. (2) and (3–4) possesses the following properties consistent with the chemical kinetics of the reaction, macroscopic laws and equilibrium state.

2.2.1 Proposition [Elastic terms].—The elastic collision terms are such that

$$\int_{\mathbb{R}^3} \mathcal{Q}_\alpha^E \, d\boldsymbol{c}_\alpha = 0, \quad \alpha = 1, \dots, 4 \qquad (5)$$

that is, elastic collisions do not modify the number of particles of each constituent.

2.2.2 Proposition [Reactive terms].—The reactive collision terms are such that

$$\int_{\mathbb{R}^3} \mathcal{Q}_1^R \, d\boldsymbol{c}_\alpha = \int_{\mathbb{R}^3} \mathcal{Q}_2^R \, d\boldsymbol{c}_\alpha \qquad (6)$$

$$= -\int_{\mathbb{R}^3} \mathcal{Q}_3^R \, d\boldsymbol{c}_\alpha = -\int_{\mathbb{R}^3} \mathcal{Q}_4^R \, d\boldsymbol{c}_\alpha.$$

that is, reactive collisions assure the correct chemical exchange rates for the chemical reaction (1).

Motivated by the above Proposition 2.2.2, the *reaction rate* of the α-constituent, that gives the production rate of α-particles, is defined by

$$\tau_\alpha = \int_{\mathbb{R}^3} \mathcal{Q}_\alpha^R \, d\boldsymbol{c}_\alpha, \quad \text{with} \quad \tau_1 = \tau_2 = -\tau_3 = -\tau_4. \qquad (7)$$

2.2.3 Proposition [Conservation laws].—Elastic and reactive collision terms are such that

$$\sum_{\alpha=1}^{4} \int_{\mathbb{R}^3} \Psi_\alpha \mathcal{Q}_\alpha^E \, d\boldsymbol{c}_\alpha = 0 \qquad (8)$$

$$\sum_{\alpha=1}^{4} \int_{\mathbb{R}^3} \Psi_\alpha \mathcal{Q}_\alpha^R \, d\boldsymbol{c}_\alpha = 0 \qquad (9)$$

where $(\Psi_1, \Psi_2, \Psi_3, \Psi_4)$ is a function of the molecular velocities $\boldsymbol{c}_\alpha$ whose components are given alternatively by

$$\Psi_\alpha = m_\alpha$$

$$\Psi_\alpha = m_\alpha c_{\alpha x}, \; \Psi_\alpha = m_\alpha c_{\alpha y}, \; \Psi_\alpha = m_\alpha c_{\alpha z} \qquad (10)$$

$$\Psi_\alpha = \frac{1}{2} m_\alpha c_\alpha^2 + \varepsilon_\alpha$$

Therefore elastic and reactive collision terms are consistent with the physical conservation laws for mass, momentum components and total energy of the whole mixture.

2.2.4 Proposition [Equilibrium].—The following conditions are equivalent

(a) $\mathcal{Q}_\alpha^E = 0$ and $\mathcal{Q}_\alpha^R = 0$, $\alpha = 1, \dots, 4$

(b) $\displaystyle\sum_{\alpha=1}^{4} \int_{\mathbb{R}^3} \left(\mathcal{Q}_\alpha^E + \mathcal{Q}_\alpha^R\right) \log\left(\frac{f_\alpha}{m_\alpha^3}\right) d\boldsymbol{c}_\alpha = 0$

(c) f_α is Maxwellian, $f_\alpha = f_\alpha^M$, given by

$$f_\alpha^M = n_\alpha \left(\frac{m_\alpha}{2\pi kT}\right)^{3/2} \exp\left(-\frac{m_\alpha(\boldsymbol{c}_\alpha - \boldsymbol{u})^2}{2kT}\right) \qquad (11)$$

for $\alpha = 1, \dots, 4$, where k is the Boltzmann constant, and n_α, $\boldsymbol{u}$, T are functions of $(\boldsymbol{x}, t)$, see Subsection 2.3, with

$$\frac{n_1 n_2}{n_3 n_4} = \exp\left(\frac{Q_R}{kT}\right) \left(\frac{m_1 m_2}{m_3 m_4}\right)^{3/2}. \qquad (12)$$

Proposition 2.2.4 characterizes Maxwellian distributions defining an equilibrium solution of the Boltzmann Eqs. (2). More in detail, Maxwellian distributions (11) with uncorrelated number densities n_α characterize a mechanical equilibrium only, in the sense that $\mathcal{Q}_\alpha^E = 0$ but $\mathcal{Q}_\alpha^R \neq 0$ in general. Conversely, Maxwellian distributions (11) with the number densities constrained to the mass action law (12) characterize a complete thermodynamical equilibrium state (mechanical and chemical), since $\mathcal{Q}_\alpha^E = 0$ and $\mathcal{Q}_\alpha^R = 0$.

2.2.5 Proposition [Entropy production].—Elastic and reactive collision terms are such that

$$-\sum_{\alpha=1}^{4} \int_{\mathbb{R}^3} \log\left(\frac{f_\alpha}{m_\alpha^3}\right) \mathcal{Q}_\alpha^E \, d\boldsymbol{c}_\alpha \geq 0.$$

$$-\sum_{\alpha=1}^{4}\int_{\mathbb{R}^3}\log\left(\frac{f_\alpha}{m_\alpha^3}\right)\mathcal{Q}_\alpha^R\,dc_\alpha \geq 0.$$

Moreover, the convex function

$$\mathcal{H}(t)=\sum_{\alpha=1}^{4}\int_{\mathcal{S}}\int_{\mathbb{R}^3} f_\alpha\log\left(\frac{f_\alpha}{m_\alpha^3}\right)dc_\alpha dx$$

with $\mathcal{S}$ being a closed domain in $\mathbb{R}^3$ where the mixture evolves, is a Liapunov functional for the extended Boltzmann equations (2), that is

$$\frac{d\mathcal{H}}{dt}(t)\leq 0, \quad \text{for } t\geq 0,$$

$$\frac{d\mathcal{H}}{dt}(t)=0, \quad \text{iff the distribution functions are Maxwellian characterized by Eqs. (11–12).}$$

The first part of Proposition 2.2.5 means that both elastic and reactive collisions contribute to increase the entropy of the mixture. The second part indicates that the $\mathcal{H}$-function drives the reactive mixture from the initial distribution to an equilibrium state.

The proof of the second part of the proposition, see Ref. [7], indicates that function $\mathcal{H}$ splits into a *mechanical* part and a *reactive* part, $\mathcal{H}^E+\mathcal{H}^R$, such that both $\mathcal{H}^E$ and $\mathcal{H}^R$ show a time decreasing behaviour and that $d\mathcal{H}^E/dt=0$ iff f_α are Maxwellian given by (11), whereas $d\mathcal{H}^R/dt=0$ iff f_α are Maxwellian constrained by (12).

2.3 *Connection to hydrodynamics*

The kinetic model previously introduced provides a consistent macroscopic theory in the hydrodynamic limit of Euler or Navier-Stokes level.

2.3.1 *Macroscopic variables*

The starting point foi the macroscopic description is the definition of certain average quantities, called macroscopic variables, taken over the distributions f_α by integrating with respect to the velocities $\boldsymbol{c}_\alpha$. The number density of each constituent and the one of the mixture are given by

$$n_\alpha(\boldsymbol{x},t)=\int_{\mathbb{R}^3} f_\alpha(\boldsymbol{x},\boldsymbol{c}_\alpha,t)\,d\boldsymbol{c}_\alpha, \qquad n=\sum_{\alpha=1}^{4} n_\alpha$$

and the corresponding mass densities are defined as

$$\varrho_\alpha(\boldsymbol{x},t)=m_\alpha n_\alpha(\boldsymbol{x},t), \qquad \varrho=\sum_{\alpha=1}^{4}\varrho_\alpha.$$

The mean velocity of the mixture is given by

$$\boldsymbol{u}(\boldsymbol{x},t)=\frac{1}{\varrho(\boldsymbol{x},t)}\sum_{\alpha=1}^{4}\int_{\mathbb{R}^3} m_\alpha \boldsymbol{c}_\alpha f_\alpha(\boldsymbol{x},\boldsymbol{c}_\alpha,t)\,d\boldsymbol{c}_\alpha$$

and the diffusion velocity of each constituent is

$$\boldsymbol{u}_\alpha(\boldsymbol{x},t)=\frac{1}{\varrho_\alpha(\boldsymbol{x},t)}\int_{\mathbb{R}^3} m_\alpha(\boldsymbol{c}_\alpha-\boldsymbol{u})f_\alpha(\boldsymbol{x},\boldsymbol{c}_\alpha,t)\,d\boldsymbol{c}_\alpha.$$

The components of the mixture stress tensor are

$$p_{ij}(\boldsymbol{x},t)=\sum_{\alpha=1}^{4}\int_{\mathbb{R}^3} m_\alpha(\boldsymbol{c}_{\alpha i}-\boldsymbol{u}_i)(\boldsymbol{c}_{\alpha j}-\boldsymbol{u}_j)\times f_\alpha(\boldsymbol{x},\boldsymbol{c}_\alpha,t)\,d\boldsymbol{c}_\alpha.$$

The pressure of the mixture is defined by

$$p(\boldsymbol{x},t)=\frac{1}{3}\sum_{\alpha=1}^{4}\int_{\mathbb{R}^3} m_\alpha(\boldsymbol{c}_\alpha-\boldsymbol{u})^2 f_\alpha(\boldsymbol{x},\boldsymbol{c}_\alpha,t)\,d\boldsymbol{c}_\alpha$$

so that the temperature is assumed as

$$T(\boldsymbol{x},t)=\frac{p(\boldsymbol{x},t)}{kn(\boldsymbol{x},t)}.$$

The components of the heat flux of the mixture are

$$q_i(\boldsymbol{x},t)=\sum_{\alpha=1}^{4}\left(\int_{\mathbb{R}^3}\frac{1}{2}m_\alpha(\boldsymbol{c}_\alpha-\boldsymbol{u})^2(\boldsymbol{c}_{\alpha i}-\boldsymbol{u}_i)\times f_\alpha(\boldsymbol{x},\boldsymbol{c}_\alpha,t)\,d\boldsymbol{c}_\alpha+n_\alpha\varepsilon_\alpha\boldsymbol{u}_{\alpha i}\right).$$

2.3.2 *Balance equations*

To complete the connection, one can derive the balance equations and the conservation laws describing the balance of the constituent number densities, and conservation of both momentum components and total energy of the whole mixture. It is enough to consider the Boltzmann Eqs. (2), then multiply both sides by the elementary function Φ_α whose components are $\Phi_{\alpha\beta}=\delta_{\alpha\beta}$ and functions (10) of Proposition 2.2.3, and finally integrate with respect to $\boldsymbol{c}_\alpha$. The resulting equations are

$$\frac{\partial n_\alpha}{\partial t}+\sum_{i=1}^{3}\frac{\partial}{\partial x_i}\left(n_\alpha\boldsymbol{u}_{\alpha i}+n_\alpha\boldsymbol{u}_i\right)=\tau_\alpha \qquad (16)$$

$$\frac{\partial}{\partial t}(\varrho\boldsymbol{u}_i)+\sum_{j=1}^{3}\frac{\partial}{\partial x_j}\left(p_{ij}+\varrho\boldsymbol{u}_i\boldsymbol{u}_j\right)=0,\ i=1,2,3 \qquad (17)$$

$$\frac{\partial}{\partial t}\left(\frac{3}{2}nkT+\sum_{\alpha=1}^{4}n_\alpha\varepsilon_\alpha+\frac{1}{2}\varrho\boldsymbol{u}^2\right)+\sum_{i=1}^{3}\frac{\partial}{\partial x_i}\left[q_i+\sum_{j=1}^{3}p_{ij}\boldsymbol{u}_j+\left(\frac{3}{2}nkT+\sum_{\alpha=1}^{4}n_\alpha\varepsilon_\alpha+\frac{1}{2}\varrho\boldsymbol{u}^2\right)\boldsymbol{u}_i\right]=0. \qquad (18)$$

Macroscopic Eqs. (16–18) constitute a system of 8 equations in 36 uknowns, namely n_α, τ_α, $\boldsymbol{u}_{\alpha i}$, $\boldsymbol{u}_i$, p_{ij}, T and q_i, where $\alpha=1,2,3,4$ and $i,j=1,2,3$. To close the system one passes to the hydrodynamic limit and deduces the constitutive equations for the 28 unknowns τ_α, $\boldsymbol{u}_{\alpha i}$, p_{ij} and q_i.

2.3.3 *Hydrodynamic limit*

The passage of the kinetic level of Eqs. (2) to the hydrodynamic limit requires the solution of the Boltzmann Eqs. (2), that can be obtained resorting to a systematic expansion technique, see Refs. [2,5,6,8] for a detailed description of the Chapaman-Enskog method, Hilbert method and moment method.

In particular, concerning the Chapaman-Enskog (CE) method, one starts with an appropriate scalling of Eqs. (2) in terms of the so called elastic and reactive Knudsen numbers [3], consistent with the chemical regime of validity of the resulting macroscopic equations. This scalling defines a clear separation of the effects of the *fast* and *slow* processes, the former being some collisonal processes (elastic or reactive) that drive the distribution function towards a local equilibrium state, and the latter being the other processes that contribute to disturb the distribution function. Then one assumes that the thermodynamical state of the reactive mixture is close to the equilibrium and looks for a solution of Eqs. (2) of type

$$\tilde{f}_\alpha=f_\alpha^{(0)}\left[1+\sum_{n=1}^{+\infty}\varepsilon^n\phi_\alpha^{(n)}\right] \qquad (19)$$

where $f_\alpha^{(0)}$ is a quasi-equilibrium distribution function, ε represents a formal expansion parameter related to the Knudsen numbers (then it is settled equal to one) and $\sum_{n=1}^{+\infty}\varepsilon^n\phi_\alpha^{(n)}f_\alpha^{(0)}$ is the disturbance induced by the slow processes, that is assumed to be small.

Introducing expansion (19) into Eqs. (2), neglecting non-linear terms in the disturbances and equating equal terms in ε^n, one obtains linear integral equations for the zero-order term $f_\alpha^{(0)}$ as well as for the disturbances $\phi^{(1)}$, $\phi^{(2)}$, etc. The consistency properties introduced in Subsection 2.2 are fundamental to obtain the solution of these integral equations. After an involved analysis of the equations, the disturbances are obtained as functions of n_α, $\boldsymbol{u}$, T and both transport fluxes and transport coefficients. Inserting the considered approximate solution into the definitions of the reaction rate τ_α, diffusion velocities $\boldsymbol{u}_{\alpha i}$, stress tensor p_{ij} and heat flux q_i, one obtains the constitutive equations that allow to close the macroscopic Eqs. (16–18).

In particular, it comes out that the zero-order approximation $f_\alpha^{(0)}$ is the Maxwellian distribution (11) that leads to the reactive Euler equations without transport effects; the first-order perturbed distributions, $f_\alpha^{(0)}(1+\phi_\alpha^{(1)})$, are governed by linearized Boltzmann equations and lead to the Navier-Stokes equations involving the transport effects of diffusion, viscosity, thermal conductivity and maybe others; successive approximations lead to the Burnett and super Burnett complicated equations.

According to Propositions 2.2.4 and 2.2.5, one concludes that in a hydrodynamic limit of an Eulerian regime, the *mechanical* entropy of the mixture remains constant and slow reactive processes contribute to drive the mixture from a mechanical to a complete thermodynamical equilibrium state. Conversely, in the hydrodynamic limit associated to the Navier-Stokes equations, both elastic and reactive collisions contribute to increase the entropy of the mixture, and the entropy flux is also due to diffusion, heat transfer and sheat viscosity phenomenon.

The Chapman-Enskog method converges asymptotically for small Knudsen number, and the Euler and Navier-Stokes equations have a good accuracy.

3 Model for symmetric reaction

A very simple model corresponds to a binary mixture of constituents A and B undergoing the symmetric reaction $A+A\rightleftharpoons B+B$. In this particular case, one has $A_2=A_1=A$, $A_4=A_3=B$, so that $m_B=m_A=m$, $\mathrm{d}_\alpha=\mathrm{d}$, $\varepsilon_2=\varepsilon_1=\varepsilon_A$, $\varepsilon_4=\varepsilon_3=\varepsilon_B$, $Q_R=2(\varepsilon_B-\varepsilon_A)$. Assuming hard sphere cross sections for elastic collisions and step cross sections with activation energy for reactive interactions, the collision terms are (see Ref. [9] for a complete description of the model)

$$\mathcal{Q}_\alpha^E=\sum_{\beta=A}^{B}\int\left(f'_\alpha f'_\beta-f_\alpha f_\beta\right)\mathrm{d}^2 g_{\beta\alpha}\cdot\mathbf{k}_{\beta\alpha}\,d\mathbf{k}_{\beta\alpha}d\mathbf{c}_\beta \qquad (20)$$

$$\mathcal{Q}_\alpha^R=\int\left(f_\beta f'_\beta-f_\alpha f'_\alpha\right)\sigma_\alpha^\star g_\alpha\cdot\mathbf{k}_\alpha\,d\mathbf{k}_\alpha d\mathbf{c}'_\alpha\,. \qquad (21)$$

In expression (21), the primes are used to distinguish two identical particles that participate in the reactive event, and $\sigma_\alpha^\star$ is given by

$$\sigma_\alpha^\star=\begin{cases} s^2\mathrm{d}^2 & \text{if} \quad \gamma_\alpha>\varepsilon_\alpha^\star\\ 0 & \text{if} \quad \gamma_\alpha<\varepsilon_\alpha^\star\end{cases} \qquad (22)$$

where s represents the steric factor, γ_α is the relative translational energy, $\varepsilon_\alpha^\star$ the forward $(\alpha=A)$ and backward $(\alpha=B)$ activation energy, both expressed in units of the thermal energy of the mixture, kT,

$$\gamma_\alpha=\frac{mg_\alpha^2}{4kT}, \qquad \varepsilon_\alpha^\star=\frac{\varepsilon_\alpha}{kT}.$$

At the macroscopic scale, the mixture is described by the variables n_A, n_B, $\boldsymbol{u}$, T, that are governed by balance equations and conservation laws of type (16) and (17–18). At the hydrodynamic Euler level, and for a chemical regime in which elastic collisions are more frequent than reactive encounters, the Chapman-Enskog method has been used in [9] to obtain the following approximate solution for the distribution function

$$\tilde{f}_\alpha=f_\alpha^M\left[1+\phi_\alpha\right], \qquad (23)$$

where f_α^M is a Maxwellian distribution and

$$\phi_\alpha = \left(\frac{15}{8} - \frac{5m(c_\alpha - v)^2}{4kT} + \frac{m^2(c_\alpha - v)^4}{8k^2T^2}\right) \tag{24}$$
$$\times x_A^2 \frac{\mathrm{d}^2}{\mathrm{d}_r^2} \frac{Q_R^\star}{8}\left(Q_R^\star + Q_R^\star \varepsilon_A^\star - \varepsilon^\star + 2\varepsilon_A^{\star 2} - 1\right) e^{-\varepsilon_A^\star}$$

with $x_A = n_A/n$ being the concentration of constituent A, d_r the reactive molecular diameter and $Q_R^* = Q_R/kT$. Expression (23) indicates that this solution characterizes a non-equilibrium state and expression (24) specifies the deviation from the equilibrium in terms of the activation energy ε_A^* and reaction heat Q_R^*. The macroscopic equations associated to this hydrodynamic limit characterizes a non-difusive, non-heat conducting and non-viscous reactive mixture, that is

$$\boldsymbol{u}_{\alpha i} = 0, \qquad q_i = 0, \qquad p_{ij} = p\delta_{ij}$$

and the reaction rate is explicitly given by

$$\tau_B = -\tau_A, \quad \tau_A = -4n_A^2 \mathrm{d}_r^2 \sqrt{\frac{\pi kT}{m}}\, e^{-\varepsilon_A^\star} \Theta \tag{25}$$

$$\Theta = \Big[1 + \varepsilon_A^\star + \frac{x_A^2}{128}\left(\frac{\mathrm{d}}{\mathrm{d}_r}\right)^2 Q_R^\star\Big(1 + Q_R^\star + Q_R^\star \varepsilon_A^\star$$
$$+ \varepsilon_A^\star - 2\varepsilon_A^{\star 2}\Big)\left(4\varepsilon_A^{\star 3} - 8\varepsilon_A^{\star 2} - \varepsilon_A^\star - 1\right) e^{-\varepsilon_A^\star}\Big].$$

The hydrodynamic equations are the reactive Euler equations corrected with the effects of the reaction heat. In one space dimension, they are given by

$$\frac{\partial n_\alpha}{\partial t} + \frac{\partial}{\partial x}\left(n_\alpha u\right) = \tau_\alpha, \quad \alpha = A, B \tag{26}$$

$$\frac{\partial u}{\partial t} + \frac{1}{\varrho}\frac{\partial p}{\partial x} + u\frac{\partial u}{\partial x} = 0 \tag{27}$$

$$\frac{\partial p}{\partial t} + u\frac{\partial p}{\partial x} + \frac{5}{3}p\frac{\partial u}{\partial x} + \frac{2}{3}\sum_{\alpha=A}^{B} \varepsilon_\alpha \tau_\alpha = 0 \tag{28}$$

where u is now the x-component of the mixture velocity.

4 Application to detonation phenomenon

Detonation is a rapid and violent form of combustion accompanied by an important energy release. The propagation of detonation waves in gaseous explosives is a problem of great practical importance, due to the economic impact as well as several engineering applications, such as safety and military issues, propulsion devices and hard rock mining.

A detonation is essentially a reacting wave consisting in a leading shock that propagates into the explosive, followed by a reaction zone where the reactants transform into products. The shock heats the material by compressing it so that a rapid and violent chemical reaction is triggered.

On the other hand, experimental and computational investigations show that the detonation wave, specially in gaseous mixtures, tends to be unstable to small perturbations and exhibit a significant unsteady structure. The first step of a formal study of the detonation instability is the analysis of the hydrodynamical stability, which consists in imposing small deviations in the steady solution and studying the evolution of the state variables perturbations. The assumption of small deviations allows to linearize the equations and determine the instability modes and growth rate perturbations.

The kinetic theory of chemically reactive mixtures can be used to study the detonation phenomenon and describe some of the physical and chemical aspects observed in experiments. In particular the kinetic modelling of Section 3 has been used in Ref. [10] to investigate the propagation and hydrodynamic stability of a steady detonation wave in a binary reactive mixture with a symmetric chemical reaction. In this section we present the main aspects of this study, with emphasis on the spatial structure of the steady detonation wave and the response of the steady solution to one-dimensional disturbances.

4.1 *Dynamics of steady detonation waves*

We consider a detonating binary mixture undergoing a reversible reaction of symmetric type, described by the kinetic modelling of Section 3. The mathematical analogue for the detonation dynamics is the hyperbolic set of reactive Euler equations (26–28). Such equations admit steady traveling wave solutions that describe a combustion regime in which a strong planar shock wave ignites the mixture and the burning keeps the shock advancing and proceeding to equilibrium behind the shock. The Zeldovich, von Neumann and Doering (ZND) idealized model [11,12] gives a good and accepted description of the detonation wave solution. The configuration of the ZND wave consists of a leading, planar, non-reactive shock wave propagating with constant velocity D, followed by a finite reaction zone where the chemical reaction takes place. The spatial structure of the detonation wave is determined by means of the Rankine-Hugoniot conditions, connecting the fluxes of the macroscopic quantities ahead (superscrip +) and behind (plain symbols) the shock front, together with the rate equation, describing the advancement of the chemical process in the reaction zone. They can be written in the form

$$\frac{dn_A}{dx} = \frac{Dt_c \tau_A}{v - D + n_A \frac{dv}{dn_A}} \tag{29}$$

$$n_B\left(n_A\right) = \frac{\left(n_B^+ + n_A^+\right)D}{D - u} - n_A \tag{30}$$

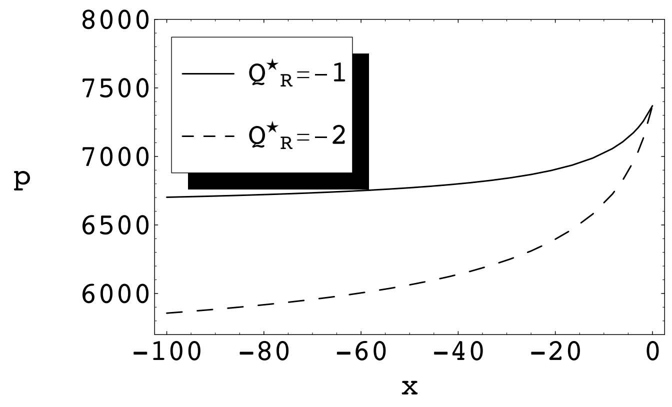

Figure 1.—Detonation wave profile (exothermic chemical reaction) for the mixture pressure *p*.

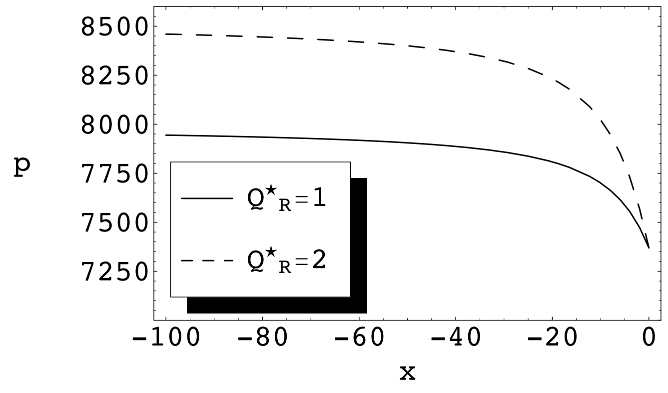

Figure 2.—Detonation wave profile (endothermic chemical reaction) for the mixture pressure *p*.

$$T\left(n_A\right) = \frac{(D - u)\left(\varrho^+ Du + n^+ kT^+\right)}{n^+ kD} \tag{31}$$

$$v\left(n_A\right) = \frac{2Q_R^* n_A + 3\varrho^+ D^2 - 5n^+ kT^+}{8\varrho^+ D} \tag{32}$$
$$+ \frac{1}{8\varrho^+ D}\Big[\left(2Q_R^* n_A + 3\varrho^+ D^2 - 5n^+ kT^+\right)^2$$
$$-32\varrho^+ Q_R^* D^2\left(n_A - n_A^+\right)\Big]^{1/2}.$$

System (29–32), with detonation velocity D, reaction heat Q_R^* and activation energy ε_A^* as parameters, characterize any arbitrary state within the reaction zone (plain symbols) in dependence of the quiescent initial state (superscrip +). This system has been solved numerically with the following input data for kinetic and thermodynamical reference parameters

$$D = 1700\, ms^{-1}, \quad m = 0.01\, Kg/mol,$$
$$E_A = 2400\, K, \quad \varepsilon_A^\star = 6$$
$$T^+ = 298.15\, K, \quad n_A^+ = 0.35\, mol/l, \quad n_B^+ = 0\, mol/l.$$

Some numerical simulations have been performed in Ref. [10] to determine the structure of the detonation wave in both cases of exothermic ($Q_R^* < 0$) and endothermic ($Q_R^* > 0$) chemical reactions. Figures 1 and 2 show representative profiles for the mixture pressure p in both cases of exothermic and endothermic chemical reactions, respectively. The configuration of the solution consists in a reactive rarefaction wave (Figure 1) when the reaction is exothermic and reproduces the typical structure of an idealized ZND wave arising in real explosive system with exothermic chemical reaction [11,12]. Conversely, the configuration of the solution consists in a reactive compression wave (Figure 2) when the reaction is endothermic and reproduces the essential features of the endothermic stage of a typical chain-branching reactive system with pathological-type detonation [11,12]. Such detonation occurs when further complexities are introduced in the reactive system and some dissipative effects are present.

Other numerical simulations have been considered in Ref. [10] to supplement the representation of the detonation dynamics.

4.2 *Linear stability of steady detonation waves*

The stability of the steady detonation solution described in Subsection 4.1 is formulated in terms of an initial-boundary value problem describing the evolution of the state variables perturbations.

We assume that a small rear boundary perturbation is assigned so that a distortion in the shock wave position is observed; such distortion induces further perturbations in the state variables and the steady detonation solution can degenerate into an oscillatory solution in the long-time limit.

From the mathematical point of view, the stability problem requires the transformation to the perturbed shock attached frame, and then the linearization of the reactive Euler equations and Rankine-Hugoniot conditions around the steady detonation solution. A normal mode approach with exponential time dependent perturbations and complex growth rate parameter is adopted and standard techniques are used to deduce the stability equations as well as initial and boundary conditions. The details are omitted here due to the space limitations. The reader is addressed to Ref. [10] and the references therein cited for the comprehensive study on the detonation satbility.

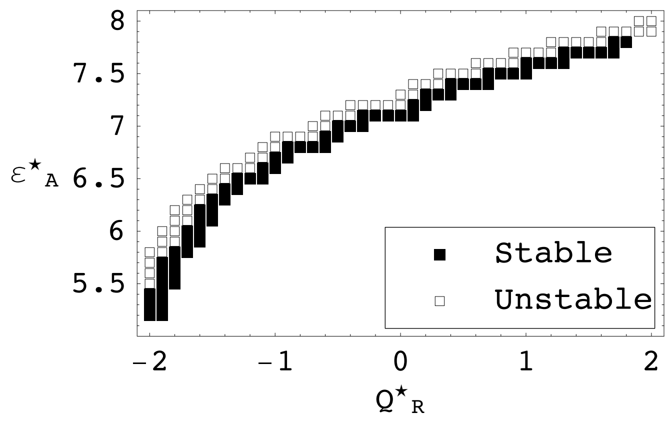

Figure 3.—Stability boundary in the Q^*_R-ϵ^*_A plane.

The initial boundary value problem describing the detonation stability has been numerically treated in Ref. [10], using a rather involved numerical scheme that combines an iterative shooting technique with the argument principle. For a given set of thermodynamical and chemical parameters describing the steady detonation solution, the disturbances of the state variables have been determined in a given rectangular domain of the growth rate parameter, and detailed information about the instability parameter regimes have been provided.

Figure 3 represents the stability boundary in the parameter plane defined by the reaction heat Q^*_R and forward activation energy $\varepsilon^\star_A$.

In this representation, a pair $(Q^*_R, \varepsilon^\star_A)$ in the stability zone indicates that for the corresponding values of the reaction heat and activation energy, no instability modes have been found. Conversely, a pair in the instability zone indicates that for the corresponding values of the reaction heat and activation energy, one instability mode, at least, has been found. Moreover, Figure 3 reveals that for a fixed value of the activation energy, the detonation becomes stable for larger values of the reaction heat, whereas for a fixed value of the reaction heat, the detonation becomes stable for smaller values of the activation energy. These results are consistent with known experimental works and numerical simulations [12], in the sense that increasing the reaction heat, or decreasing the activation energy, tends to stabilize the detonation.

5 Simple reacting spheres model

The simple reacting spheres model considers hard-sphere cross sections for elastic collisions and reactive cross sections with activation energy, of hard-spheres type. The molecules behave as if they were single mass points with two internal states of excitation. Collisions may alter the internal states and this occurs when the kinetic energy associated with the reactive motion exceeds the activation energy.

The kinetic theory of simple reacting spheres (SRS) has been developed in Ref. [13] for a quaternary mixture A, B, C, D with the assumptions of no mass exchange $(m_1 = m_3, m_2 = m_4)$ and no alteration of particle diameters $(\mathrm{d}_1 = \mathrm{d}_3, \mathrm{d}_2 = \mathrm{d}_4)$. Further advances concerning essentially physical and mathematical properties of the SRS sytem and existence theory for the partial differential equations of the model have been considered in Refs. [14,15,16,17]. The SRS theory has been extended in Ref. [18], with no restrictions on the molecular masses and diameters, and a global existence result has been stated.

The SRS modelling refers to the reactive mixture introduced in Section 2, whose particles undergo the reversible bimolecular reaction (1). The reactive Boltzmann equations for this mixture have the general form of Eqs. (2) but the collisional terms are corrected for the occurrence of reactive encounters. More specifically, the elastic operator contains a correction term which subtracts from the total number of collisions those events that lead to chemical reaction. As before, we assume that collisions take place when the particles are separated by a distance $\mathrm{d}_{12} = \frac{1}{2}(\mathrm{d}_1 + \mathrm{d}_2)$ or $\mathrm{d}_{34} = \frac{1}{2}(\mathrm{d}_3 + \mathrm{d}_4)$, but only those particles such that the kinetic energy of the relative motion is greater than the activation energy of the chemical reaction can collide with chemical reaction.

The collision terms are given by (see Ref. [18] for a detailed derivation)

$$\mathcal{Q}^E_\alpha = \sum_{\beta=1}^4 \mathrm{d}^2_{\alpha\beta} \int (f_\alpha' f_\beta' - f_\alpha f_\beta)\langle \epsilon, \boldsymbol{c}_\alpha - \boldsymbol{c}_\beta\rangle d\epsilon d\boldsymbol{c}_\beta \quad (33)$$
$$-s\mathrm{d}^2_{\alpha\gamma} \int (f_\alpha' f_\gamma' - f_\alpha f_\gamma)$$
$$\times\Theta\Big(\langle \epsilon, \boldsymbol{c}_\alpha - \boldsymbol{c}_\gamma\rangle - \Gamma_{\alpha\beta}\Big)\langle \epsilon, \boldsymbol{c}_\alpha - \boldsymbol{c}_\gamma\rangle d\epsilon d\boldsymbol{c}_\gamma$$

$$\mathcal{Q}^R_\alpha = s\mathrm{d}^2_{\alpha\gamma} \int \left[\left(\frac{\mu_{\alpha\gamma}}{\mu_{\beta\delta}}\right)^3 f_\beta' f_\delta' - f_\alpha f_\gamma\right] \quad (34)$$
$$\times\Theta\Big(\langle \epsilon, \boldsymbol{c}_\alpha - \boldsymbol{c}_\gamma\rangle - \Gamma_{\alpha\beta}\Big)\langle \epsilon, \boldsymbol{c}_\alpha - \boldsymbol{c}_\gamma\rangle d\epsilon d\boldsymbol{c}_\gamma.$$

Above, the primes indicate post collisional states, $\mu_{\alpha\beta} = m_\alpha m_\beta/(m_\alpha + m_\beta)$ is a reduced mass of the colliding pair, $\Gamma_{ij} = \sqrt{2\gamma_i/\mu_{ij}}$ is a threshold velocity for the chemical reaction, Θ the Heaviside step function, and s the steric factor. The second term in the right-hand side of Eq. (33) is the correction term that excludes from the total number of collisions those events that lead to chemical reaction when the kinetic energy of the colliding particles is greater than the activation energy.

The SRS model possesses important mathematical properties. At the microscopic level, the model incorporates the correct detailed balance and microscopic reversibility principle, that is direct and reverse collisions of both elastic and reactive types occur with the same probability. At the macroscopic level, the SRS model has good consistency properties (Subsection 2.2) concerning correct chemical exchange rates, conservation laws, entropy production, $\mathscr{H}$-function and trend to equilibrium.

Both microscopic and macroscopic properties asserting the consistency of the SRS model are crucial for the mathematical analysis of the system of partial differential equations of the SRS model. In particular, existence, uniqueness, and stability results can be investigated on the basis of such properties.

6 Existence result for the SRS model

In this section, the global existence result of Ref. [18], for the extended Boltzmann equations (2), (33) and (34) of the SRS model, is revisited. The proof of the theorem is based on the renormalized theory proposed by DiPerna and Lions in Ref. [19] for the inert one-component Boltzmann equation, and then followed in Ref. [16] for a reactive mixture such that reactive collisions do not cause neither mass transfer nor molecular diameter alteration. The general idea of the proof is here sketched.

We introduce the notation $\mathcal{Q}^{E+}_\alpha, \mathcal{Q}^{E-}_\alpha$ to represent the gain and loss terms of the elastic collision operator, and $\mathcal{Q}^{R+}_\alpha, \mathcal{Q}^{R-}_\alpha$ with analogous meaning, so that

$$\mathcal{Q}^E_\alpha = \mathcal{Q}^{E+}_\alpha - \mathcal{Q}^{E-}_\alpha, \quad \mathcal{Q}^R_\alpha = \mathcal{Q}^{R+}_\alpha - \mathcal{Q}^{R-}_\alpha.$$

6.0.1 Definition [Mild solution].—Non-negative functions $f_\alpha \in L^1_{loc}(\mathscr{S} \times \mathbb{R}^3; [0, T])$ define a mild solution of the system (2), (33–34) if, for each $T \in]0, \infty[$, the gain and loss terms $\mathcal{Q}^{E+}_\alpha, \mathcal{Q}^{E-}_\alpha, \mathcal{Q}^{R+}_\alpha, \mathcal{Q}^{R-}_\alpha$ are in $L^1(0, T)$, *a.e.* in $(\boldsymbol{x}, \boldsymbol{c}_\alpha) \in \mathscr{S} \times \mathbb{R}^3$ and

$$f^\#_\alpha(\boldsymbol{x}, \boldsymbol{c}_\alpha, t) - f^\#_\alpha(\boldsymbol{x}, \boldsymbol{c}_\alpha, s) = \int_s^t \Big[\mathcal{Q}^{E\#}_\alpha(\boldsymbol{x}, \boldsymbol{c}_\alpha, \tau)$$
$$+ Q^{R\#}_\alpha(\boldsymbol{x}, \boldsymbol{c}_\alpha, \tau)\Big] d\tau, \quad 0 < s < t < T \quad (35)$$

where $f^\#_\alpha(\boldsymbol{x}, \boldsymbol{c}_\alpha, t) = f_\alpha(\boldsymbol{x} + \boldsymbol{c}_\alpha t, \boldsymbol{c}_\alpha, t)$ and similarly for $Q^{E\#}_\alpha$ and $Q^{R\#}_\alpha$.

6.0.1 Theorem [Global existence result].—Assume that for $\alpha = 1, \dots, 4$, the initial distributions $f_{\alpha 0} \geq 0$ are such that

$$\sup_\alpha \iint_{\mathscr{S}\times\mathbb{R}^3} \left(1 + x^2 + c^2_\alpha + \log^+ f_{\alpha 0}\right) f_{\alpha 0}\, dc_\alpha dx < \infty \quad (36)$$

with $\log^+(z) = \max\{\log(z), 0\}$. Then, there exists a non-negative mild solution $\{f_1, f_2, f_3, f_4\}$ of the system (2), (33–34) with $f_\alpha \in C([0, T]; L^1(\mathbb{R}^3 \times \mathbb{R}^3))$, such that $f_\alpha(t)\big|_{t=0} = f_{\alpha 0}$, for $\alpha = 1, 2, 3, 4$.

The result expressed in Theorem 6.0.1 states the existence of a global in time, spatially inhomogeneous, and L^1 solution for the SRS model, provided that the initial mass, momentum, total energy and entropy are finite, as assumed in hypothesis (36).

Sketch of the proof of Theorem 6.0.1.—The proof of Theorem 6.0.1 follows similar arguments as in Ref. [16]. It is based on the following tools [19,16].

(i) *A priory estimations* of type

$$\sup_\alpha \sup_{t\in[0,T]} \iint_{\mathscr{S}\times\mathbb{R}^3} \left(1 + x^2 + c^2_\alpha + \log^+ f_\alpha\right) f_\alpha dc_\alpha dx < \infty \quad (37)$$

that are obtained from the conservation laws of total mass, momentum and total energy, as well as from a suitable entropy identity (see Ref. [18]). Bounds (37) assure that there is no infinite concentration of densities in the system governed by Eqs. (2), (33–34).

(ii) *Velocity averaging results* that, in some sense, transfer the regularity of functions f_α for velocity averaged quantities, such as the macroscopic variables, see Ref. [20]. Velocity averaging results compensate the lack of regularity of the non-linear collision terms.

(iii) *Renormalized theory* [19], that considers a suitable notion of mild solution, see Definition 6.0.2 below. The method of renormalization introduces a nonlinear change of variable that reformulates the Boltzmann equations (2), (33–34) to an equivalent form, provided that certain bounds are satisfied, see Lemma 6.0.1.

6.0.2 Definition [Renormalized solution].—Non-negative functions $f_\alpha \in L^1_{loc}(\mathscr{S} \times \mathbb{R}^3; [0, T])$ are renormalized solutions of the system (2), (33–34) if

$$\frac{1}{1 + f_\alpha}\mathcal{Q}^{E\pm}_\alpha, \ \frac{1}{1 + f_\alpha}\mathcal{Q}^{R\pm}_\alpha \in L^1_{loc}(\mathscr{S} \times \mathbb{R}^3; [0, T])$$

$$\frac{\partial}{\partial t}\log(1 + f_\alpha) + c_\alpha \frac{\partial}{\partial \boldsymbol{x}}\log(1 + f_\alpha) = \frac{\mathcal{Q}^{E\pm} + \mathcal{Q}^{R\pm}}{1 + f_\alpha}$$

in the sense of distributions on $[0, T] \times \mathscr{S} \times \mathbb{R}^3$.

6.0.1 Lemma.—
Non-negative functions $f_\alpha \in L^1_{loc}(\mathscr{S} \times \mathbb{R}^3; [0, T])$ are renormalized solutions of the system (2), (33–34) if and only if they are mild solutions and

$$\frac{1}{1 + f_\alpha}\mathcal{Q}^{E\pm}_\alpha, \ \frac{1}{1 + f_\alpha}\mathcal{Q}^{R\pm}_\alpha \in L^1_{loc}(\mathscr{S} \times \mathbb{R}^3; [0, T]).$$

Then the central idea of the proof is to define suitable approximate collision terms $\mathcal{Q}^E_{\alpha n}$ and $\mathcal{Q}^R_{\alpha n}$, with $n = 1, 2, \dots$, satisfying the main consistency properties of $\mathcal{Q}^E_\alpha$ and $\mathcal{Q}^R_\alpha$, such that the approximate problems

$$\frac{\partial f^n_\alpha}{\partial t} + \sum_{i=1}^3 c^\alpha_i \frac{\partial f^n_\alpha}{\partial x_i} = \mathcal{Q}^E_{\alpha n} + \mathcal{Q}^R_{\alpha n}$$
$$f^n_\alpha(x, c_\alpha, 0) = f^n_{\alpha 0}(x, c_\alpha), \quad \alpha = 1, 2, 3, 4$$

can be studied with known methods for PDE's (semi-group techniques have been used, see [16] for details). Then one takes the weak limit $f_\alpha^n \longrightarrow f_\alpha$ and uses stability results to show that the sequence $\{f_1^n, f_2^n, f_3^n, f_4^n\}$ converges to a renormalized solution of the system (2), (33–34). A crucial part in this passage to the limit is the estimation of the renormalized collision terms, for which the velocity averaging results provide an important tool.

6.0.1 Remark [Relevance of Theorem 6.0.1].—The existence result stated in Theorem 6.0.1 has important implications at the level of approximation questions.

6.0.2 Remark [Future perspectives].—The spatially homogeneous theory of the SRS model, in which the distribution functions do not depend on the x variable, is a topic of great interest. Some advances have been made in view of studying existence of solutions, uniqueness and stability results for the homogeneous reactive equations.

Another regime of interest corresponds to the case in which the distribution functions are assumed very close to the equilibrium. In this case, one considers the linearized version of the SRS model around an equilibrium solution and uses the spectral properties of the linearized collision operators to prove existence and stability of close to equilibrium solutions for the SRS system. Some studies have been developed also in this direction.

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On the Fourier-Stieltjes transform of Minkowski's question mark function and the Riemann hypothesis: Salem's type equivalences

by Semyon Yakubovich*

1 Introduction and auxiliary results

In this presentation we pay tribute to the work in analysis and analytic number theory of the famous mathematician Raphaël Salem (1898–1963). Precisely, we will extend his approach to study Fourier-Stieltjes coefficients behavior at infinity with singular measures. In particular, we will prove an equivalent proposition related to the known and still unsolved question posed by Salem in [8], p. 439 whether Fourier-Stieltjes coefficients of the *Minkowski's question mark function* vanish at infinity. Furthermore, we establish a class of Salem's type equivalences to the Riemann hypothesis, which is based on Wiener's *closure of translates* problem.

It is well known in the elementary theory of the Fourier-Stieltjes integrals that if $h(x)$ is absolutely continuous then

$$g(t) = \int_\Omega e^{ixt} dh(x), \quad \Omega \subset \mathbb{R},\ t \in \mathbb{R} \qquad (1)$$

tends to zero as $|t| \to \infty$, because in this case the Fourier-Stieltjes transform $g(t)$ is an ordinary Fourier transform of an integrable function. Thus $h(x)$ supports a measure whose Fourier transform vanishes at infinity. Such measures are called *Rajchman measures* (see details, for instance, in [4]). However, when h is continuous, the situation is quite different and the classical Riemann-Lebesgue lemma for the class L_1, in general, cannot be applied. The question is quite delicate when it concerns singular monotone functions (see [11], Ch. IV). For such singular measures there are various examples and the Fourier-Stieltjes transform need not tend to zero, although there do exist measures for which it goes to zero. For instance, Salem [8,10] gave examples of singular functions, which are strictly increasing and whose Fourier coefficients still do not vanish at infinity. On the other hand, Menchoff in 1916 [5] gave a first example of a singular distribution whose coefficients vanish at infinity. Wiener and Wintner [17] (see also [2]) proved in 1938 that for every $\varepsilon > 0$ there exists a singular monotone function such that its Fourier coefficients behave as $n^{-1/2+\varepsilon}$, $n \to \infty$.

Our goal here is to construct some Rajchman's measures, which are associated with continuous functions of bounded variation. In particular, we will prove that the famous Minkowski' s question mark function $?(x)$ [1] is a Rajchman measure if and only if its Fourier-Stieltjes transform has a limit at infinity, and then, of course, the limit should be zero. This probably can give an affirmative answer on the question posed by Salem in 1943 [8}.

The *Minkowski question mark function* $?(x) : [0, 1] \mapsto [0, 1]$ is defined by [1]

$$?([0, a_1, a_2, a_3, \ldots]) = 2 \sum_{i=1}^{\infty} (-1)^{i+1} 2^{-\sum_{j=1}^{i} a_j}, \qquad (2)$$

where $x = [0, a_1, a_2, a_3, \ldots]$ stands for the representation of x by a regular continued fraction. We will keep the notation $?(x)$, which was used in the original Salem's paper [8], mildly resisting the temptation of changing it and despite this symbol is quite odd to denote a function in such a way. It is well known that $?(x)$ is continuous,

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strictly increasing and singular with respect to Lebesgue measure. It can be extended on $[0,\infty]$ by using the following functional equations

$$?(x) = 1 - ?(1-x), \quad (3)$$

$$?(x) = 2?\left(\frac{x}{x+1}\right), \quad (4)$$

$$?(x) + ?\left(\frac{1}{x}\right) = 2, \quad x > 0. \quad (5)$$

When $x \to 0$, it decreases exponentially $?(x) = O\left(2^{-1/x}\right)$. Key values are $?(0) = 0$, $?(1) = 1$, $?(\infty) = 2$. For instance, from (3) and asymptotic behavior of the Minkowski function $?(x)$ near zero one can easily get the finiteness of the following integrals

$$\int_0^1 x^{\lambda}\, d?(x) < \infty, \ \lambda \in \mathbb{R}, \quad (6)$$

$$\int_0^1 (1-x)^{\lambda}\, d?(x) < \infty, \ \lambda \in \mathbb{R}. \quad (7)$$

Further, as was proved by Salem [8], the Minkowski question mark function satisfies the Hölder condition

$$\left|?(x) - ?(y)\right| < C|x-y|^{\alpha}, \quad (8)$$

of order

$$\alpha = \frac{\log 2}{2\log\frac{\sqrt{5}+1}{2}}, \quad (9)$$

where $C > 0$ is an absolute constant. We will deal in the sequel with the following Fourier-Stieltjes transforms of the Minkowski question mark function

$$f(t) = \int_0^1 e^{ixt} d?(x), \qquad F(t) = \int_0^{\infty} e^{ixt} d?(x), \ t \in \mathbb{R}, \quad (10)$$

$$f_c(t) = \int_0^1 \cos xt\, d?(x), \qquad F_c(t) = \int_0^{\infty} \cos xt\, d?(x), \ t \in \mathbb{R}_+, \quad (11)$$

$$f_s(t) = \int_0^1 \sin xt\, d?(x), \qquad F_s(t) = \int_0^{\infty} \sin xt\, d?(x), \ t \in \mathbb{R}_+, \quad (12)$$

where all integrals converge absolutely and uniformly with respect to t because of straightforward estimates

$$|f(t)| \le \int_0^1 d?(x) = 1, \quad |F(t)| \le \int_0^{\infty} d?(x) = 2,$$

$$|f_c(t)| \le 1, \quad |F_c(t)| \le 2,$$

$$|f_s(t)| \le 1, \quad |F_s(t)| \le 2.$$

Further we observe that functional equation (3) easily implies $f(t) = e^{it} f(-t)$ and therefore $e^{-it/2} f(t) \in \mathbb{R}$. So, taking the imaginary part we obtain the equality

$$\cos\left(\frac{t}{2}\right) f_s(t) = \sin\left(\frac{t}{2}\right) f_c(t). \quad (13)$$

Hence, for instance, letting $t = 2\pi n$, $n \in \mathbb{N}_0$ it gives $f_s(2\pi n) = 0$ and $f_c(2\pi n) = d_n$. In 1943 Salem asked [8] whether $d_n \to 0$, as $n \to \infty$.

Further, by using functional equations (4), (5) for the Minkowski function we derive the following useful relations

$$\int_0^1 e^{ixt}\, d?(x) = \int_0^{\infty} e^{ixt}\, d?(x) - \int_1^{\infty} e^{ixt}\, d?(x)$$

$$= \int_0^{\infty} e^{ixt}\, d?(x) + e^{it}\int_0^{\infty} e^{ixt}\, d?\left(\frac{1}{x+1}\right)$$

$$= \int_0^{\infty} e^{ixt}\, d?(x) + \frac{e^{it}}{2}\int_0^{\infty} e^{ixt}\, d?\left(\frac{1}{x}\right)$$

$$= \left(1 - \frac{e^{it}}{2}\right)\int_0^{\infty} e^{ixt}\, d?(x),$$

which imply the functional equation

$$F(t) = \frac{2f(t)}{2 - e^{it}}. \quad (14)$$

Taking real and imaginary parts in (14) and employing functional equation (3) it is not difficult to deduce the following important equalities for the Fourier-Stieltjes transforms (11), (12)

$$F_c(t) = \frac{2}{5 - 4\cos t} f_c(t), \quad (15)$$

$$F_s(t) = \frac{6}{5 - 4\cos t} f_s(t). \quad (16)$$

Indeed, we have, for instance

$$\int_0^{\infty} \cos xt\, d?(x) = \frac{2}{5 - 4\cos t}$$

$$\times\left[(2 - \cos t)\int_0^1 \cos xt\, d?(x) - \sin t\int_0^1 \sin xt\, d?(x)\right]$$

$$= \frac{2}{5 - 4\cos t}\left[2\int_0^1 \cos xt\, d?(x) - \int_0^1 \cos t(1-x)\, d?(x)\right]$$

$$= \frac{2}{5 - 4\cos t}\int_0^1 \cos xt\, d?(x)$$

and this yields relation (15). Analogously we get (16). In particular, letting $t = 2\pi n, n \in \mathbb{N}_0$ in (15), (16) we find accordingly

$$\int_1^{\infty} \cos(2\pi n x)\, d?(x) = \int_0^1 \cos(2\pi n x)\, d?(x),$$

$$\int_1^{\infty} \sin(2\pi n x)\, d?(x) = 5\int_0^1 \sin(2\pi n x)\, d?(x) = 0$$

via (13). Generally, equalities (15), (16) yield

$$\int_1^{\infty} \cos xt\, d?(x) = \frac{1 - 8\sin^2(t/2)}{1 + 8\sin^2(t/2)}\int_0^1 \cos xt\, d?(x),$$

$$\int_1^{\infty} \sin xt\, d?(x) = \frac{5 - 8\sin^2(t/2)}{1 + 8\sin^2(t/2)}\int_0^1 \sin xt\, d?(x).$$

respectively. For instance,

$$\int_1^{\infty} \cos(xt_m)\, d?(x) = 0,$$

$$\int_1^{\infty} \sin(xt_k)\, d?(x) = 0$$

for any t_m, t_k, which are roots of the corresponding equations

$$\sin(t_m/2) = \pm 1/(2\sqrt{2}),$$

$$\sin(t_k/2) = \pm\sqrt{5/8}, \quad m, k \in \mathbb{N}.$$

Further, since (see (14), (15), (16))

$$\frac{1}{2}|F(t)| \le |f(t)| \le \frac{3}{2}|F(t)|, \quad (17)$$

$$\frac{1}{2}|F_c(t)| \le |f_c(t)| \le \frac{9}{2}|F_c(t)|, \quad (18)$$

$$\frac{1}{6}|F_s(t)| \le |f_s(t)| \le \frac{3}{2}|F_s(t)|, \quad (19)$$

then Fourier-Stieltjes transforms of the Minkowski question mark function over $(0,1)$ tend to zero when $|t| \to \infty$ if and only if the same property is guaranteed by Fourier-Stieltjes transforms over $(0,\infty)$.

2 Some Rajchman measures

In this section we prove several theorems, characterizing Rajchman measures, which are associated with Fourier-Stieltjes integrals over finite and infinite intervals.

We begin with the following general result.

Theorem 1.—Let φ be a real-valued continuous integrable function of bounded variation on $(0,\infty)$ vanishing at infinity. Then φ supports a Rajchman measure relatively its Fourier-Stieltjes transform

$$\Phi(t) = \int_0^{\infty} e^{ixt}\, d\varphi(x), \quad (20)$$

if and only if it has a limit at infinity ($|t| \to \infty$).

Proof.—Without loss of generality we prove the theorem for positive t. Evidently, the necessity is trivial and we will prove the sufficiency. Suppose that the limit of $\Phi(t)$ when $t \to +\infty$ exists. Since $\Phi(t) = \Phi_c(t) + i\Phi_s(t)$, where

$$\Phi_c(t) = \int_0^{\infty} \cos xt\, d\varphi(x), \quad (21)$$

$$\Phi_s(t) = \int_0^{\infty} \sin xt\, d\varphi(x), \quad (22)$$

we will treat these transforms separately. Taking (21) and integrating by parts we get

$$\Phi_c(t) = -\varphi(0) + t\int_0^{\infty} \varphi(x)\sin xt\, dx. \quad (23)$$

However, since $\varphi \in L_1(\mathbb{R}_+)$, we appeal to the integrated form of the Fourier formula (cf. [12], Th. 22) to write for all $x \ge 0$

$$\int_0^x \varphi(y)\, dy = \frac{2}{\pi}\int_0^{\infty}\frac{1 - \cos yx}{y}\int_0^{\infty}\varphi(u)\sin uy\, du.$$

But taking into account the previous equality after simple change of variable we come out with the relation

$$\frac{1}{x}\int_0^x \varphi(y)\, dy$$

$$= \frac{2}{\pi}\int_0^{\infty}\frac{1 - \cos y}{y^2}\left[\varphi(0) + \Phi_c\left(\frac{y}{x}\right)\right] dy, \ x > 0.$$

Minding the value of elementary Feijer type integral

$$\frac{2}{\pi}\int_0^{\infty}\frac{1 - \cos y}{y^2} dy = 1,$$

we establish an important equality

$$\frac{1}{x}\int_0^x [\varphi(y) - \varphi(0)]\, dy \quad (24)$$

$$= \frac{2}{\pi}\int_0^{\infty}\Phi_c\left(\frac{y}{x}\right)\frac{1 - \cos y}{y^2} dy, \ x > 0.$$

Meanwhile, the left-hand side of (53) is evidently goes to zero when $x \to 0^+$ via the continuity of φ on $[0,\infty)$. Further, since φ is of bounded variation on $(0,\infty)$ we obtain the uniform estimate

$$|\Phi_c(t)| \le \int_0^{\infty} dV_{\varphi}(x) = \Phi_0,$$

where $V_{\varphi}(x)$ is a variation of φ on $[0,x]$ and $\Phi_0 > 0$ is a total variation of φ. This means that $\Phi_c(t)$ is continuous and bounded on $\mathbb{R}_+$. Furthermore, the integral with respect to x in the right-hand side of (53) converges absolutely and uniformly by virtue of the Weierstrass test. Consequently, since $\Phi_c(t)$ has a limit at infinity, which is finite, say a, one can pass to the limit through equality (53) when $x \to 0^+$. Hence we find

$$\lim_{x\to 0+}\frac{1}{x}\int_0^x [\varphi(y) - \varphi(0)]\, dy$$

$$= \frac{2a}{\pi}\int_0^{\infty}\frac{1 - \cos y}{y^2} dy = a = 0.$$

In order to complete the proof, we need to verify whether the Fourier sine transform (22) tends to zero as well. To do this, we appeal to the corresponding integrated form of the Fourier formula for the Fourier cosine transform

$$-\int_0^x \varphi(y)\,dy = \frac{2}{\pi}\int_0^\infty \frac{\sin yx}{y^2}\Phi_s(y)\,dy,\ x>0, \qquad (25)$$

where after integration by parts $\Phi_s(t)$ turns to be represented as follows

$$\Phi_s(t) = -t\int_0^\infty \varphi(u)\cos ut\,du,\ t>0. \qquad (26)$$

Hence it is easily seen that $\Phi_s(t) = O(t),\ t\to 0^+$ and since $|\Phi_s(t)|\le\Phi_0$ we have that $\Phi_s(t)/t\in L_2(\mathbb{R}_+)$. This means that the integral in the right-hand side of (25) converges absolutely and uniformly by $x\ge 0$. After simple change of variable we split the integral in the right-hand side of (25) on two integrals to obtain

$$-\frac{1}{x}\int_0^x \varphi(y)\,dy = \frac{2}{\pi}\int_0^1 \frac{\sin y}{y^2}\Phi_s\left(\frac{y}{x}\right)dy + \frac{2}{\pi}\int_1^\infty \frac{\sin y}{y^2}\Phi_s\left(\frac{y}{x}\right)dy.$$

Considering again $x>0$ sufficiently small and splitting the integral over $(0,1)$ on two more integrals over $(0, x\log^\gamma(1/x))$ and $(x\log^\gamma(1/x), 1)$, where $0<\gamma<1$, we derive the equality

$$\frac{2}{\pi}\int_{x\log^\gamma(1/x)}^1 \frac{\sin y}{y^2}\Phi_s\left(\frac{y}{x}\right)dy = -\frac{1}{x}\int_0^x\varphi(y)\,dy - \frac{2}{\pi}\int_1^\infty \frac{\sin y}{y^2}\Phi_s\left(\frac{y}{x}\right)dy - \frac{2}{\pi}\int_0^{x\log^\gamma(1/x)} \frac{\sin y}{y^2}\Phi_s\left(\frac{y}{x}\right)dy.$$

Minding the inequality (see (26)) $|\Phi_s(t)|\le t\|\varphi\|_{L_1(\mathbb{R}_+)}$, $t\ge 0$, the right-hand side of the latter equality has the straightforward estimate

$$\left|\frac{1}{x}\int_0^x\varphi(y)\,dy + \frac{2}{\pi}\int_1^\infty \frac{\sin y}{y^2}\Phi_s\left(\frac{y}{x}\right)dy + \frac{2}{\pi}\int_0^{x\log^\gamma(1/x)} \frac{\sin y}{y^2}\Phi_s\left(\frac{y}{x}\right)dy\right| \qquad (27)$$

$$\le \sup_{y\ge 0}|\varphi(y)| + \frac{2}{\pi}\left[\Phi_0 + \|\varphi\|_{L_1(\mathbb{R}_+)}\log^\gamma(1/x)\right].$$

On the other hand, via the first mean value theorem

$$\frac{2}{\pi}\left|\int_{x\log^\gamma(1/x)}^1 \frac{\sin y}{y^2}\Phi_s\left(\frac{y}{x}\right)dy\right| = \frac{2}{\pi}|\Phi_s(\xi(x))| \times \int_{x\log^\gamma(1/x)}^1 \frac{\sin y}{y^2}\,dy,$$

where

$$\log^\gamma\left(\frac{1}{x}\right)\le \xi(x)\le \frac{1}{x}.$$

Meanwhile, we have

$$\frac{2}{\pi}\int_{x\log^\gamma(1/x)}^1 \frac{\sin y}{y^2}\,dy > \frac{2\sin 1}{\pi}\int_{x\log^\gamma(1/x)}^1 \frac{dy}{y} = \frac{2\sin 1}{\pi}\log\left(\frac{1}{x\log^\gamma(1/x)}\right).$$

Consequently, combining with (27) we find

$$|\Phi_s(\xi(x))| < \frac{1}{\sin 1}\left[\frac{\pi}{2}\sup_{y\ge 0}|\varphi(y)| + \Phi_0 + \|\varphi\|_{L_1(\mathbb{R}_+)}\log^\gamma(1/x)\right]\log^{-1}\left(\frac{1}{x\log^\gamma(1/x)}\right) = o(1),\ x\to 0^+. \qquad (28)$$

Thus making $x\to 0^+$ we get $\xi(x)\to+\infty$ and therefore there is a subsequence $t_n=\xi(x_n)\to\infty$ such that $\lim_{n\to+\infty}|\Phi_s(t_n)| = 0$. But since the limit of $\Phi_s(t)$ exists, when $t\to+\infty$ it will be zero. So φ supports a Rajchman measure and the theorem is proved. ∎

Corollary 1.—Under conditions of Theorem 1 φ supports a Rajchman measure if and only if two limits

$$\lim_{t\to+\infty} t\int_0^\infty \varphi(x)\sin xt\,dx,$$

$$\lim_{t\to+\infty} t\int_0^\infty \varphi(x)\cos xt\,dx$$

exist simultaneously (if so, they equal to $\varphi(0)$ and 0, respectively).

More general result deals with the smoothness of the Fourier-Stieltjes transform and a behavior at infinity of its derivatives.

We have

Corollary 2.—Let $n\in\mathbb{N}_0$, $\varphi(x)$, $x\ge 0$ be a real-valued continuous function such that $x^m\varphi(x)$ is of bounded variation on $[0,\infty)$ for each $m=0,1,\dots,n$. If $\varphi(x)=o(x^{-n})$, $x\to\infty$ and $x^n\varphi(x)\in L_1(\mathbb{R}_+)$, then the corresponding Fourier-Stieltjes transform (20) $\Phi(t)$ is n times differentiable on $\mathbb{R}_+$, its n-th order derivative is equal to

$$\Phi^{(n)}(t) = \int_0^\infty (ix)^n e^{itx}\,d\varphi(x) \qquad (29)$$

and vanishes at infinity if and only if there exists a limit of the integral

$$\Psi_n(t) = \int_0^\infty e^{itx}\,d\left(x^n\varphi(x)\right)$$

when $|t|\to\infty$.

Proof—In fact, under conditions of the corollary one can differentiate n times under the integral sign in the Fourier-Stieltjes transform (20)) via the absolute and uniform convergence. Precisely, this circumstance is guaranteed by the estimate

$$\left|\int_0^\infty (ix)^m e^{itx}\,d\varphi(x)\right| = \left|\int_0^\infty e^{itx}\,d\left((ix)^m\varphi(x)\right) - m\,i^m\int_0^\infty x^{m-1}\varphi(x)e^{itx}\,dx\right| \le Var_{[0,\infty)}\left(x^m\varphi(x)\right) + m\int_0^\infty x^{m-1}|\varphi(x)|\,dx = \Phi_m<\infty,\ m=0,1,\dots,n,$$

where the latter integral is finite since $x^n\psi(x)\in L_1(\mathbb{R}_+)$ and φ is continuous. Thus (29) holds and in order to complete the proof we write it as

$$\Phi^{(n)}(t) = i^n\left[\int_0^\infty e^{itx}\,d\left(x^n\varphi(x)\right) - n\int_0^\infty x^{n-1}\varphi(x)e^{itx}dx\right].$$

The second integral of this equality tends to zero when $t\to\infty$ via the Riemann-Lebesgue lemma. Therefore, $t\Phi^{(n)}(t)=o(1)$, $t\to\infty$, $n\in\mathbb{N}_0$ if and only if the first integral has a limit at infinity and this limit is certainly zero. ∎

3 An equivalent Salem's problem

In this section we will formulate a problem, which is equivalent to Salem's question [8], having

Corollary 3.—The Fourier-Stieltjes transform

$$f(t) = \int_0^1 e^{ixt}\,d?(x)$$

of the Minkowski question mark function vanishes at infinity, i.e. an answer on Salem's question is affirmative, if and only if two limit equalities

$$\lim_{t\to+\infty} t\int_0^\infty ?\left(\frac{1}{x}\right)\sin xt\,dx = 2,$$

$$\lim_{t\to+\infty} t\int_0^\infty ?\left(\frac{1}{x}\right)\cos xt\,dx = 0$$

take place simultaneously.

Proof.—It follows immediately from double inequality (17), simple equality due to functional equation (5)

$$\int_0^\infty e^{ixt}\,d?(x) = -\int_0^\infty e^{ixt}\,d?\left(\frac{1}{x}\right)$$

and Corollary 1, where we put
$\varphi(x) = ?(1/x),\ x>0,\ \varphi(0)=2.$ ∎

Finally, we generalize Salem's problem, proving

Theorem 2.—Let $k\in\mathbb{N}_0$. If an answer on Salem's question is affirmative, then

$$f^{(k)}(t) = \int_0^1 (ix)^k e^{itx}\,d?(x) = o(1),\ |t|\to\infty. \qquad (30)$$

Proof.—It is easily seen that the Fourier-Stieltjes transform of the Minkowski question mark function over $(0,1)$ is infinitely differentiable and so for any $k\in\mathbb{N}_0$ we have (30). Suppose that $f^{(k)}$ does not tend to zero as $|t|\to\infty$. Then we can find a sequene $\{t_m\}_{m=1}^\infty$, $|t_m|\to\infty$ such that

$$\left|\int_0^1 x^k e^{it_m x}\,d?(x)\right|\ge\delta>0.$$

Let $t_m/(2\pi) = n_m+\beta_m$, where n_m is an integer and $0\le\beta_m<1$. One can suppose that β_m tends to a limit β, we can always do it choosing again subsequence from $\{t_m\}$ if necessary. Hence

$$|f^{(k)}(t_m)| = \left|\int_0^1 e^{2\pi i\beta x}x^k e^{2\pi i n_m x}\,d?(x)\right|\ge\delta>0.$$

But this contradicts to Salem's lemma [11], p. 38, because $f(2\pi n)\to 0$, $n\to\infty$ via assumption of the theorem and the Riemann-Stieltjes integral

$$\int_0^1 e^{2\pi i\beta x}x^k\,d?(x)$$

converges for any $k\in\mathbb{N}_0$. ∎

4—A class of Salem's type equivalences to the Riemann hypothesis

As it is widely known, *Riemann zeta function* $\zeta(s)$ [13] satisfies the functional equation

$$\zeta(s) = 2^s\pi^{s-1}\sin\left(\frac{\pi s}{2}\right)\Gamma(1-s)\zeta(1-s),$$

where $\Gamma(z)$ is *Euler's gamma-function*. Moreover, in the half-plane $\mathrm{Re}\,s = c_0>1$ it is represented by the absolutely and uniformly convergent series with respect to $t\in\mathbb{R}$, $s=c_0+it$

$$\zeta(s) = \sum_{n=1}^\infty \frac{1}{n^s} \qquad (31)$$

and by the uniformly convergent series

$$(1-2^{1-s})\zeta(s) = \sum_{n=1}^\infty \frac{(-1)^{n-1}}{n^s} \qquad (32)$$

in the half-plane $\mathrm{Re}\,s>0$. We also note the useful formula

$$\frac{1}{\zeta(s)} = \sum_{n=1}^\infty \frac{\mu(n)}{n^s},\quad \mathrm{Re}\,s>1, \qquad (33)$$

where $\mu(n)$ is *the Möbius function* [7].

In 1953 Salem [9] proved that the Riemann hypothesis is true, i.e. the Riemann zeta-function $\zeta(s)$ is free of zeros in the strip $1/2<\mathrm{Re}\,s<1$ is equivalent to the fact, that the homogeneous integral equation

$$\int_0^\infty \frac{y^{\sigma-1}}{e^{xy}+1}\varphi(y)dy = 0,\ x>0,\ \frac{1}{2}<\sigma<1 \qquad (34)$$

has no nontrivial solutions in the space of bounded measurable functions on $\mathbb{R}_+$. Our goal is to extend this fact to the entire class of equivalent propositions, involving integral equations with the *Widder-Lambert type kernels* (cf. [3], [15]). However, our starting point will be a characterization of mapping properties of the corresponding integral transformations in a special functional space $\mathscr{M}^{-1}(L_c)$ (see in [14]).

Definition 1.—Denote by $\mathscr{M}^{-1}(L_c)$ the space of functions $f(x), x \in \mathbb{R}_+$, representable by inverse *Mellin transform* of integrable functions $f^*(s) \in L_1(c)$ on the vertical line $c = \{s \in \mathbb{C} : \mathrm{Re}\, s = c_0 > 1\}$:

$$f(x) = \frac{1}{2\pi i}\int_c f^*(s)x^{-s}ds. \qquad (35)$$

The space $\mathscr{M}^{-1}(L_c)$ with the usual operations of addition and multiplication by scalar is a linear vector space. If the norm in $\mathscr{M}^{-1}(L_c)$ is introduced by the formula

$$\|f\|_{M^{-1}(L_c)} = \frac{1}{2\pi}\int_{-\infty}^{+\infty}|f^*(c_0+it)|dt,$$

then it becomes a Banach space. Simple properties of the space $\mathscr{M}^{-1}(L_c)$ follow immediately from Definition 1 and the basic properties of the Fourier and Mellin transforms of integrable functions. For instance, the Riemann-Lebesgue lemma yields that $x^{c_0}f(x)$ is uniformly bounded, continuous on $\mathbb{R}_+$ and $x^{c_0}f(x) = o(1)$, when $x \to +\infty$ and $x \to 0$. Moreover, if $f(x), g(x) \in M^{-1}(L_c)$, where $g(x)$ is the inverse Mellin transform (35) of the function $g^*(s)$, then $x^{c_0}f(x)g(x) \in \mathscr{M}^{-1}(L_c)$ because the product $x^{c_0}f(x)g(x)$ is the inverse Mellin transform of the function

$$\frac{1}{2\pi i}\int_c f^*(\tau)g^*(s-\tau+c_0)d\tau,$$

which belongs to $L_1(c)$ by Fubini's theorem. Finally we note that if $f(x) \in \mathscr{M}^{-1}(L_c)$ and $x^{c_0-1}g(x) \in L_1(\mathbb{R}_+)$, then the Mellin convolution

$$\int_0^\infty g(u)f\left(\frac{x}{u}\right)\frac{du}{u} \in M^{-1}(L_c).$$

In fact, the latter integral is an inverse Mellin transform of the function $f^*(s)g^*(s)$ and since $f^*(s) \in L_1(c)$ and $g^*(s)$ is essentially bounded on c, we have $f^*(s)g^*(s) \in L_1(c)$.

A more general space $\mathscr{M}^{-1}_{c_1,c_2}(L_c)$, which will be involved as well is defined similarly to the one in [14].

Definition 2.—Let $c_1, c_2 \in \mathbb{R}$ be such that $2\,\mathrm{sign}\, c_1 + \mathrm{sign}\, c_2 \geq 0$. By $\mathscr{M}^{-1}_{c_1,c_2}(L_c)$ we denote the space of functions $f(x), x \in \mathbb{R}_+$, representable in the form (35), where $s^{c_2}e^{\pi c_1|s|}f^*(s) \in L_1(c)$.

It is a Banach space with the norm

$$\|f\|_{\mathscr{M}^{-1}_{c_1,c_2}(L_c)} = \frac{1}{2\pi}\int_c e^{\pi c_1|s|}|s^{c_2}f^*(s)ds|, \quad \mathrm{Re}\, s = c_0 > 1. \qquad (36)$$

Theorem 3.—Let $f \in M^{-1}(L_c)$. Then for all $x > 0$ reciprocal transformations

$$g(x) = \frac{1}{2\pi i}\int_c (1-2^{1-s})\zeta(s)f^*(s)x^{-s}ds = \sum_{n=1}^\infty (-1)^{n-1}f(xn) \qquad (37)$$

$$f(x) = \frac{1}{2\pi i}\int_c \frac{g^*(s)}{(1-2^{1-s})\zeta(s)}x^{-s}ds = \sum_{k=0}^\infty\sum_{n=1}^\infty 2^k\mu(n)g\left(xn2^k\right), \qquad (38)$$

where $g^*(s) = (1-2^{1-s})\zeta(s)f^*(s)$$ are automorphisms of the space $\mathscr{M}^{-1}(L_c)$ and satisfy the norm estimates

$$[\zeta(c_0)]^{-1}\|g\|_{M^{-1}(L_c)} \leq \|f\|_{\mathscr{M}^{-1}(L_c)} \leq (1-2^{1-c_0})^{-1}\zeta(c_0)\|g\|_{M^{-1}(L_c)},\ c_0 > 1. \qquad (39)$$

Proof.—In fact, since $|\mu(n)| \leq 1$ (see [7], [13]),

$$\sum_{n=1}^\infty |(-1)^{n-1}f(xn)| \leq x^{-c_0}\sum_{n=1}^\infty \frac{1}{n^{c_0}}\frac{1}{2\pi}\int_c |f^*(s)ds| = x^{-c_0}\zeta(c_0)\|f\|_{M^{-1}(L_c)},$$

$$\sum_{k=0}^\infty\sum_{n=1}^\infty 2^k|\mu(n)|\sum_{m=1}^\infty\left|f\left(xnm2^k\right)\right| \leq \frac{x^{-c_0}\zeta^2(c_0)}{2\pi(1-2^{1-c_0})}\int_c |f^*(s)ds| = \frac{x^{-c_0}\zeta^2(c_0)}{1-2^{1-c_0}}\|f\|_{M^{-1}(L_c)},$$

and $g^*(s) \in L_1(c)$, all changes of the order of integration and summation are allowed. Hence via (32), (33) and elementary sum of geometric progression we establish reciprocal relations (37), (38) involving the uniqueness theorem for the Mellin transform of integrable functions. Moreover, it guarantees the automorphism of the space $\mathscr{M}^{-1}(L_c)$ under these transformations and the equivalence of norms, which immediately follows from estimates

$$\|g\|_{M^{-1}(L_c)} = \frac{1}{2\pi}\int_c \left|(1-2^{1-s})\zeta(s)f^*(s)ds\right| \leq \zeta(c_0)\,\|f\|_{M^{-1}(L_c)},$$

$$\|f\|_{\mathscr{M}^{-1}(L_c)} = \frac{1}{2\pi}\int_c \left|g^*(s)\frac{ds}{(1-2^{1-s})\zeta(s)}\right| \leq (1-2^{1-c_0})^{-1}\zeta(c_0)\,\|g\|_{\mathscr{M}^{-1}(L_c)},$$

yielding (39). ■

Further, the Parseval equality for the Mellin transform [12] and Fubini's theorem allow to write the modified Laplace transform [3] of $f \in M^{-1}(L_c)$$ in the form

$$\int_0^\infty e^{-x/t}f(t)\frac{dt}{t} = \frac{1}{2\pi i}\int_c \Gamma(s)f^*(s)x^{-s}ds. \qquad (40)$$

Moreover, due to Definition 2 and *Stirling's asymptotic formula for gamma-functions* [12] it forms a bijective map of the space $\mathscr{M}^{-1}(L_c)$ onto its subspace $\mathscr{M}^{-1}_{1/2,1/2-c_0}(L_c)$. Thus appealing to Theorem 3 we will derive the Widder type inversion formulas [15] for the Widder-Lambert type transforms. Precisely, we prove

Theorem 4.—Let $f \in \mathscr{M}^{-1}(L_c)$ and $c_0 > 1$. Then the Widder-Lambert type transformation

$$g(x) = \int_0^\infty \frac{f(t)dt}{t(e^{x/t}+1)},\ x > 0. \qquad (41)$$

is a bijective map between spaces $\mathscr{M}^{-1}(L_c)$, $\mathscr{M}^{-1}_{1/2,1/2-c_0}(L_c)$ and for all $x > 0$ the following inversion formula takes place

$$f(x) = \lim_{k\to\infty}\left(-x\frac{d}{dx}\right)\prod_{j=1}^k\left(1-\frac{x}{j}\frac{d}{dx}\right) \times \sum_{m=0}^\infty\sum_{n=1}^\infty 2^m\mu(n)g(xkn2^m). \qquad (42)$$

Proof.—In fact, the proof is based on Theorem 3, equality (40), a familiar infinite product for the gamma-function

$$\frac{1}{\Gamma(s)} = \lim_{k\to\infty} sk^{-s}\prod_{j=1}^k\left(1+\frac{s}{j}\right), \qquad (43)$$

and the asymptotic behavior $|\Gamma(s)|^{-1} = e^{\pi|s|/2}|s|^{1/2-c_0}$, $s = c_0+it$, $|t| \to \infty$ via Stirling formula. So employing again (32), Theorem 3 and Fubini's theorem, we deduce the following representation of the Widder-Lambert type transform (see (37))

$$g(x) = \frac{1}{2\pi i}\int_c (1-2^{1-s})\zeta(s)\Gamma(s)f^*(s)x^{-s}ds = \sum_{n=1}^\infty (-1)^{n-1}\int_0^\infty e^{-xn/t}f(t)\frac{dt}{t} = \int_0^\infty \frac{f(t)dt}{t(e^{x/t}+1)},\ x > 0.$$

Finally, calling (43) and an elementary series we derive, reciprocally, the equalities

$$f(x) = \frac{1}{2\pi i}\int_c \frac{g^*(s)x^{-s}}{(1-2^{1-s})\zeta(s)\Gamma(s)}ds = \lim_{k\to\infty}\frac{1}{2\pi i}\sum_{m=0}2^m\int_c\prod_{j=1}^k\left(1+\frac{s}{j}\right) \times\frac{sg^*(s)\,(kx2^m)^{-s}}{\zeta(s)}ds = \lim_{k\to\infty}\left(-x\frac{d}{dx}\right)\prod_{j=1}^k\left(1-\frac{x}{j}\frac{d}{dx}\right) \times\sum_{m=0}^\infty\sum_{n=1}^\infty 2^m\mu(n)g\,(xkn2^m),$$

which yield (42). ■

Returning to (34) and making a simple change of variables and functions it becomes (41) with $g(x) = 0$ and $f(t) = t^{-\sigma}\varphi(1/t)$. Thus Theorem 4 leads to

Corollary 4.—Let $\varphi(y)$ be a solution of homogeneous equation (34) such that $y^{-\sigma}\varphi(1/y) \in \mathscr{M}^{-1}(L_c)$, $1/2 < \sigma < 1$. Then $\varphi(y) \equiv 0$.

Proof.—Indeed, there exists a function $h^*_\sigma(s) \in L_1(c)$ such that

$$y^{-\sigma}\varphi\left(\frac{1}{y}\right) = \frac{1}{2\pi i}\int_c \varphi^*_\sigma(s)y^{-s}ds,\ y > 0.$$

Hence

$$|\varphi(y)| \leq \frac{y^{c_0-\sigma}}{2\pi}\int_c |\varphi^*_\sigma(s)ds|$$

and since $c_0 > \sigma$, we have that $h(y)$ is continuous on $\mathbb{R}_+$ and $\varphi(y) = o(1)$, $y \to 0$. Applying inversion formula (42) with $g = 0$ we get the result. ■

Let us prove the following equivalence to the Riemann hypothesis of the Salem type.

Theorem 5.—The Riemann hypothesis is true, if and only if for any bounded measurable function $f(x)$ on $\mathbb{R}$ satisfying integral equation

$$\int_{\mathbb{R}^2}\frac{e^{-\sigma u}f(u)}{(e^{e^{x-u-t}}+1)(e^{e^t}+1)}du\,dt = 0, \quad \frac{1}{2} < \sigma < 1, \qquad (44)$$

for all $x \in \mathbb{R}$ it follows that f is zero almost everywhere.

Proof.—Calling again (32) and properties of the Mellin transform and its convolution [12] it is not difficult to derive the equality

$$[(1-2^{1-s})\zeta(s)\Gamma(s)]^2 = \int_0^\infty t^{s-1}\times\int_0^\infty\frac{du}{u(e^{t/u}+1)(e^u+1)}dt,\ \mathrm{Re}\, s > 0. \qquad (45)$$

On the other hand, the reciprocal inversion of the Mellin transform yields

$$\int_0^\infty\frac{du}{u(e^{x/u}+1)(e^u+1)} = \frac{1}{2\pi i}\int_{\mu-i\infty}^{\mu+i\infty}[(1-2^{1-s})\zeta(s)\Gamma(s)]^2x^{-s}ds. \qquad (46)$$

The left-hand side of (46) is positive and via (45)

$$\int_0^\infty\int_0^\infty\frac{t^{\sigma-1}dudt}{u(e^{t/u}+1)(e^u+1)} = [(1-2^{1-\sigma})\zeta(\sigma)\Gamma(\sigma)]^2,$$

which after a simple change of variables is equivalent to the condition

$$\int_{\mathbb{R}^2}\frac{e^{\sigma y}dudy}{(e^{e^{y-u}}+1)(e^{e^u}+1)} < \infty.$$

Hence following as in [9] Wiener's ideas [16] about an equivalence of the completeness in $L_1(\mathbb{R})$ of translations

$$e^{\sigma(x-y)} \int_{\mathbb{R}} \frac{du}{(e^{e^{x-y-u}}+1)(e^{e^u}+1)}, \; x \in \mathbb{R}$$

and the absence of zeros of $[(1-2^{1-s})\zeta(s)\Gamma(s)]^2$, i.e. zeros of $\zeta(s)$ in the critical strip $1/2 < \operatorname{Re} s < 1$, we complete the proof. ∎

Remark 1.—Reminding integral representation of the modified Bessel function in terms of the inverse Mellin transform [12]

$$K_\nu(2\sqrt{x}) = \frac{1}{4\pi i}\int_{\mu-i\infty}^{\mu+i\infty} \Gamma\left(s+\frac{\nu}{2}\right)\Gamma\left(s-\frac{\nu}{2}\right) x^{-s} ds, \quad \mu > |\operatorname{Re}\nu|,$$

invoking (31) and identity (see [13])

$$\zeta^2(s) = \sum_{n=1}^{\infty} \frac{d(n)}{n^s}, \quad \operatorname{Re} s > 1,$$

where $d(n)$ is *the divisor function*, we write equality (46) in the form

$$\frac{1}{2}\int_0^\infty \frac{du}{u(e^{x/u}+1)(e^u+1)} = \sum_{n=1}^{\infty} d(n)\Big[K_0(2\sqrt{nx}) - 4K_0(2\sqrt{2nx}) + 4K_0(4\sqrt{nx})\Big]. \tag{47}$$

Hence substituting (47) into (53) and changing the order of integration and summation via absolute and uniform convergence (we note that $d(n) = O(n^\varepsilon), \varepsilon > 0, n \to \infty$, see [13]), Theorem 5 can be reformulated as

Theorem 6.—The Riemann hypothesis is true, if and only if for any bounded measurable function $f(x)$ on $\mathbb{R}$ and all $x \in \mathbb{R}$ the equation

$$\sum_{n=1}^{\infty} d(n)\Big[(K_n f)(x) - 4(\mathscr{K}_{2n} f)(x) + 4(K_{4n} f)(x)\Big] = 0,$$

where

$$(K_n f)(x) = \int_{-\infty}^{\infty} e^{-\sigma u} K_0\left(2\sqrt{n}\, e^{(x-u)/2}\right) f(u) du, \quad \frac{1}{2} < \sigma < 1,$$

is the Meijer type convolution transform [3], has no non-trivial solutions.

Transformation (41) can be generalized considering the following two-parametric family of functions

$$U_{k,m}(x) = \frac{1}{2\pi i}\int_c [(1-2^{1-s})\zeta(s)]^{k+1}\Gamma^{m+1}(s) x^{-s} ds, \quad x > 0,\ k, m \in \mathbb{N}_0. \tag{48}$$

The case $k = m$ we denote by $U_k(x)$. The case $k = m = 0$ gives $U_0(x) = (e^x+1)^{-1}$. One can express the kernel (48) in terms of the iterated Mellin convolution. Indeed, via (32) and simple calculations we obtain

$$U_{k,m}(x) = \sum_{n_1, n_2, \dots, n_{k-m}=1}^{\infty} (-1)^{\sum_{j=1}^{k-m} n_j - k + m} \times \int_{\mathbb{R}_+^m} \prod_{j=1}^{m} (e^{u_j}+1)^{-1} \left(\exp\left(\frac{x n_1 n_2 \dots n_{k-m}}{u_1 u_2 \dots u_m}\right)+1\right)^{-1} \frac{du_1 du_2 \dots du_m}{u_1 u_2 \dots u_m}, \; k > m, \tag{49}$$

$$U_{k,m}(x) \equiv U_k(x) = \int_{\mathbb{R}_+^k} \left(\exp\left(\frac{x}{u_1 u_2 \dots u_k}\right)+1\right)^{-1} \times \prod_{j=1}^{k} (e^{u_j}+1)^{-1} \frac{du_j}{u_j}, \quad k = m, \tag{50}$$

$$U_{k,m}(x) = \int_{\mathbb{R}_+^m} \prod_{j=1}^{k+1} (e^{u_j}+1)^{-1} \exp\left[-\sum_{j=k+2}^{m} u_j\right]. \times \exp\left(-\frac{x}{u_1 u_2 \dots u_m}\right) \frac{du_1 \dots du_m}{u_1 u_2 \dots u_m}, \quad k < m. \tag{51}$$

Meanwhile, an analog of Theorem 4 will be

Theorem 7.—Let $f \in \mathscr{M}^{-1}(L_c)$ and $c_0 > 1$. Then the integral transformation

$$g(x) = \int_0^\infty U_{k,m}\left(\frac{x}{t}\right) f(t) \frac{dt}{t}, \; x > 0 \tag{52}$$

is a bijective map between the spaces $\mathscr{M}^{-1}(L_c)$ and $\mathscr{M}^{-1}_{(m+1)/2,(m+1)(1/2-c_0)}(L_c)$ and for all $x > 0$ the following inversion formula takes place

$$f(x) = \lim_{l\to\infty}\left(-x\frac{d}{dx}\right)^{m+1} \prod_{j=1}^{l}\left(1-\frac{x}{j}\frac{d}{dx}\right)^{m+1} \times \sum_{j_1,\dots,j_k=0}^{\infty} \sum_{n_1,\dots,n_k=1}^{\infty} \prod_{i=1}^{k} 2^{j_i}\mu(n_i) g\left[x l^{m+1} \prod_{i=1}^{k} 2^{j_i} n_i\right].$$

Finally, we will prove an analog of Theorem 5. In fact, we have

Theorem 8.—Let $k, m \in \mathbb{N}_0$, $k \le m$ and the kernel $U_{k,m}(x), x > 0$ is defined by formulas (50), (51), correspondingly. The Riemann hypothesis is true, if and only if for any bounded measurable function $f(x)$ on $\mathbb{R}$ satisfying integral equation

$$\int_{\mathbb{R}} e^{-\sigma u} U_{k,m}(e^{x-u}) f(u) du = 0, \quad \frac{1}{2} < \sigma < 1, \tag{53}$$

for all $x \in \mathbb{R}$ it follows that f is zero almost everywhere.

Proof.—Employing inversion formula (35) for the Mellin transform, we derive, reciprocally, from (48)

$$[(1-2^{1-s})\zeta(s)]^{k+1}\Gamma^{m+1}(s) = \int_0^\infty U_{k,m}(t) t^{s-1} dt, \quad \operatorname{Re} s > 0.$$

Moreover, $U_{k,m}(x),\ x > 0$ is positive (see (50), (51)) and for $\sigma \in (1/2, 1)$

$$\int_0^\infty U_{k,m}(t) t^{\sigma-1} dt = [(1-2^{1-\sigma})\zeta(\sigma)]^{k+1}\Gamma^{m+1}(\sigma).$$

This yields

$$\int_{\mathbb{R}} e^{\sigma y} U_{k,m}(e^y) dy < \infty.$$

Hence as in Theorem 5 the completeness in $L_1(\mathbb{R})$ of translations

$$e^{\sigma(x-y)} U_{k,m}(e^{x-y}), \; x \in \mathbb{R}$$

is equivalent to the absence of zeros of $[(1-2^{1-s})\zeta(s)]^{k+1}\Gamma^{m+1}(s)$, i.e. zeros of $\zeta(s)$ in the critical strip $1/2 < \sigma < 1$. ∎

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