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About the cover: the picture is a density plot of data from computer simulation of the Symmetric Inclusion Process with 20000 particles on 2000 horizontal sites with periodic boundary conditions. The parameter m in the model is dynamically changed during the simulation starting from m=100, corresponding to almost pure diffusion and reduced to m=0.3 at the end, corresponding to a significant increase in inclusion moves versus diffusion. The time on the vertical axis runs from 0 to 116 on a linear scale from up to down.

Duality, Bosonic Particle Systems and Some Exactly Solvable Models of Non-Equilibrium

Proefschrift

ter verkrijging van
de graad van Doctor aan de Universiteit Leiden,
op gezag van Rector Magnificus prof.mr. P.F. van der Heijden,
volgens besluit van het College voor Promoties
te verdedigen op dinsdag 13 december 2011
klokke 16.15 uur

door

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geboren te Iran

in 1981

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copromotor: prof. dr. Frank den Hollander (Universiteit Leiden)

Contents

0 Introduction

The fundamental quest of statistical mechanics is to understand the macroscopic laws of thermodynamics from the microscopic world of interacting particles. In equilibrium statistical mechanics, the transition from the microworld to the macroworld is conceptually well understood. The macroscopic equilibrium properties can be obtained by studying the Boltzmann-Gibbs distribution as a function of temperature and other parameters such as external fields.

The Gibbs formalism, i.e., the study of Boltzmann-Gibbs distributions in the thermodynamic limit has been rigorously formulated in the so-called DLR (Dobrushin-Lanford-Ruelle) formalism. Within this framework, one can rigorously understand macroscopic equilibrium phenomena such as phase transitions and the laws of equilibrium thermodynamics. Even if the equilibrium formalism is well-established, it is still rarely the case that models in this framework are exactly solvable, i.e., that one has e.g. explicit expressions for the free energy. Exactly solvable models such as the Ising model serve as paradigmatic examples where fine details such as correlation functions even at the critical point can be computed.

In non-equilibrium statistical mechanics, there is no analogue of the Gibbs formalism, i.e., there is no general formalism that gives the distribution of microstates even for a "simple" non-equilibrium scenario such as a system in contact with two heat reservoirs at different temperatures or with two particle reservoirs with different chemical potentials. Only close to equilibrium there is the general theory of linear response that relates currents to equilibrium correlation functions.

One problem with the theory of non-equilibrium is the diversity of phenomena it is supposed to describe, as John Von Neumann once put it: "theory of non-elephants". In this work, we therefore want to focus on the simplest possible non-equilibrium systems, which are systems in contact with two different reservoirs. The aim is to derive rigorous and exact properties of the so-called non-equilibrium steady state (NESS). This is the stationary measure of such a system, which, although stationary, is non-equilibrium because of the non-equilibrium constraints imposed by the reservoirs. In other words, the stationary measure will be non-reversible, and the system will have a strictly positive stationary entropy production. Typically the non-reversible character is clearly visible in the presence of a stationary current.

The nature of NESS is quite different from that of an equilibrium measure. E.g. quite generically long-range correlations are expected (see [4],[7]), whereas in equilibrium systems, they usually appear only at the critical point. These long-range correlations are also manifest in the large deviations from the NESS temperature or density profile. Generically, the associated free energy is a non-local function [4]. From a macroscopic point of view, i.e., starting from the hydrodynamic limit and associated large deviations, Bertini, Jona-Lasinio, Landim et al [1, 2, 3, 4] developed a quite general theory predicting the non-equilibrium density or temperature profile, as well as large deviations, i.e., the leading order of the exponentially small probability of deviations from this profile.

Our aim is to study models where in the NESS the profile can be computed exactly, as well as correlation functions, such as the two-point function. The obtained expressions can then be used to test general non-equilibrium theories, such as the formalism developed in [1], or the theory of McLennan ensembles [18]. The models studied in this thesis belong to the class of interacting particle systems, or systems of interacting diffusions. Interacting particle systems (IPS) are systems of particles moving on a lattice and interacting with each other according to stochastic rules. Their study started in the early seventies in papers by Spitzer [25] and Dobrushin [5]. A standard reference is Liggett [15]. A famous and thoroughly studied example of IPS is the exclusion process (EP) where particles move on a lattice according to independent random walks with the additional constraint that each lattice site is occupied by at most one particle. Interacting diffusion models come up naturally if one wants to model heat conduction, or energy transport.

The basic technical tool developed to study the models in this thesis is *duality*. Via duality, we connect models of interacting diffusions to simpler interacting particle systems, both in equilibrium and non-equilibrium setting. Because duality is such a powerful method, part of the thesis is also devoted to develop a general formalism that can be used to produce dual processes and associated duality functions or self-duality functions. In the following we give an overview of the results and models introduced and studied in this thesis. In the first section we define and shortly review the Brownian Momentum Process (aka BMP) and its dual, the Symmetric Inclusion Process (aka SIP, which is a new interacting particle system). Although we also consider several other models in detail in later chapters and give many statements and theorems that are equally applicable to a wider class of models, these two models and their generalizations are an essential starting point in our work and are used extensively as illustrating examples. After that we give a review of the chapters in the thesis in a way to emphasize the link between the different chapters rather than the details. Finally we give some future research directions.

0.1 BMP and its relation with SIP

Heat conduction is an example of a non-equilibrium phenomenon closely related to mass transport. In a given microscopic model, it is of interest to know the temperature profile in the non-equilibrium steady state (NESS) for specific boundary conditions. One aim is to derive the Fourier's law from the microscopic model. Fourier's law is a macroscopic phenomenological law which tells that the heat current is proportional to the temperature difference across the boundaries and the proportionality constant is independent of the temperature. Besides showing the Fourier's law one wants to understand better the correlation structure of the microscopic degrees of freedom in the NESS. It is expected that non-equilibrium systems exhibit generically long range correlations in the steady state, related to the inverse of the Laplacian (Dirichlet Green's function), see [4], [7] and [17]. Therefore it is important to have microscopic models where the two-point function and possibly higher order correlation functions can be computed explicitly.

The Brownian Momentum Process (aka BMP) is a model of heat conduction with stochastic diffusion of energy analyzed in [8]. To each site i of a lattice we associate a continuous degree of freedom x_i which has to be thought of as momentum. Between every two adjacent sites $(i, i+1)$ and for every small time interval there is a random exchange of momentum that leaves the total energy of the two sites $\{x_i^2 + x_{i+1}^2\}$ invariant.

More precisely, the model is defined as a Markov diffusion process on the configuration space of N-dimensional vectors $(x_1, \ldots, x_N) \in \mathbb{R}^N$, interpreted as the momenta associated to the lattice sites $\{1, \ldots, N\}$. The boundary sites 1 and N are in contact with heat baths at temperatures T_L and T_R respectively.

The generator of BMP working on the core of smooth functions is:

$$L = B_1 + B_N + \sum_{i=1}^{N-1} L_{i,i+1}. \tag{0.1.1}$$

Here

$$L_{i,j} = (x_i \partial_j - x_j \partial_i)^2$$

represents the exchange of momentum in the bulk part of the system. The operators B_1 and B_N are the generator of the Ornstein-Uhlenbeck processes representing the coupling to the heat baths at temperatures T_L and T_R and are given by

$$B_1 = T_L \partial_1^2 - x_1 \partial_1$$

$$B_N = T_R \partial_N^2 - x_N \partial_N .$$

One way to intuitively understand the effect of the bulk part of the generator is to consider the operator

$$\mathscr{A} = \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)^2 \tag{0.1.2}$$

In the polar coordinates where $x = r \cos\theta$ and $y = r \sin\theta$, this operator reduces to

$$\mathscr{A} = \frac{\partial^2}{\partial \theta^2}$$

which is the generator of a Brownian process for the variable θ. This means that in the process $(x(t), y(t))$ with generator (0.1.2) we will have $r(t) = r(0)$ unchanged and $\theta(t)$ will be a Brownian motion on the interval $[0, 2\pi]$. This provides for the mixing of the values of the $(x(t), y(t))$ while the value of $r(t)^2$ (total energy) remains preserved, thus providing an energy-conserving mechanism for the transport of momentum in the model.

This diffusive exchange of momentum between adjacent sites is different from the energy transport mechanism in the well known KMP model [6]. The later is a model of *energy* transport where energy is exchanged randomly at discrete random times. The two models are however closely related. One can obtain KMP via the 'instantaneous thermalization' limit [9] of the Brownian Energy Process which is directly related to BMP (see chapter 1 for more details).

0.2 Duality

Duality is a powerful tool in the study of Markov processes. It has played a fundamental role in the study of interacting particle systems and in models of population dynamics [19]. For example in the context of the Symmetric Exclusion Process (aka

SEP) it has been the crucial tool in order to obtain the complete ergodic theory of this process (see [15], chapters 2 and 8).

Two Markov processes $\{x_t : t \geq 0\}$ and $\{\xi_t : t \geq 0\}$ with state spaces Ω, resp. Ω' and with generators L, resp. $\mathscr{L}$ are called dual to each other if there exist a duality function $D : \Omega' \times \Omega \to \mathbb{R}$ such that

$$LD(\xi, \vec{x}) = \mathscr{L}D(\xi, \vec{x}) \tag{0.2.1}$$

where in the lhs of (0.2.1) the operator L is working on the $\vec{x}$ variable, and in the rhs the operator $\mathscr{L}$ is working on the ξ variable (here we implicitly assume that $D(\xi, .)$ is in the domain of L and $D(., \vec{x})$ is in domain of $\mathscr{L}$). This relation then lifts to the semigroups (which arise by exponentiation of the generator) and to the processes. This then yields the duality relation between the processes:

$$\mathbb{E}_{\vec{x}}[D(\xi, \vec{x}(t))] = \hat{\mathbb{E}}_{\xi}[D(\xi(t), \vec{x})]. \tag{0.2.2}$$

This relation is useful in the case that the $\{x_t : t \geq 0\}$ is ‘complicated’ and the $\{\xi_t : t \geq 0\}$ is ‘easy’ and the set of dual functions is sufficiently rich. For instance one can think of ξ being discrete objects indexing polynomials in $\vec{x}$.

In case that $\Omega = \mathbb{R}^N$, if the equations for the evolution of correlation functions of degree n for the x process are closed (i.e. there is no polynomial of higher order than n involved), that can be a hint to the existence of the duality property where the dual process will then be a particle system where the number of particles is not increasing.

0.3 Duality between BMP and SIP

In the study of BMP, a crucial ingredient is that it is dual to a discrete particle system with absorbing left and right boundaries. The configuration space of this particle system is $\Omega = \mathbb{N}^{N+2}$. We interpret $\xi \in \Omega = \mathbb{N}^{N+2}$ as prescribing the number of particles in each lattice site $i \in \{0, \dots, N+1\}$.

The dual process is as follows. A configuration $\xi = (\xi_0, \dots, \xi_{N+1})$ represents K particles (or walkers) on $\{0, 1, \dots, N+1\}$ with $K = \sum_{i=0}^{N+1} \xi_i$. The walkers can only jump to neighboring sites and are stuck when arriving to sites 0 or $N+1$. The rate at which there is a jump of a walker depends on how many walkers there are at neighboring sites. If we have ξ_i walkers at site i, ξ_{i-1} walkers at site $i-1$ and ξ_{i+1}

walkers at site $i+1$ (for $i = 2, \dots N-1$) then each of the walkers at site i jumps to site $i-1$ at rate $2(2\xi_{i-1}+1)$ and to site $i+1$ at rate $2(2\xi_{i+1}+1)$.

The duality function relating BMP to this dual particle system is a polynomial indexed by the particle configuration $\xi = (\xi_0, \dots, \xi_{N+1})$, $\xi_i \in \mathbb{N}$ explicitly given by

$$D(\xi, \vec{x}) = T_L^{\xi_0} T_R^{\xi_{N+1}} \prod_{i=1}^{N} \frac{x^{2\xi_i}}{(2\xi_i - 1)!!} \tag{0.3.1}$$

where $k!! = \prod_{j=1}^{k}(2j-1)$. Due to the symmetry of the generator only even powers of x_i need to be considered here.

In the dual process particles tend to jump with higher rates to the neighbors which contain more particles. This causes an attractive interaction between the particles, hence we choose the name Symmetric Inclusion Process (aka SIP) for this process. This has to be seen in contrast to the repulsive interaction in the exclusion process (SEP) where there is at most one particle per site..

At the boundaries each of the ξ_1 walkers at site 1 is absorbed at site 0 at rate 2 and it jumps to site 2 at rate $2(2\xi_2+1)$; each of the ξ_N walkers at site N is absorbed at site $N+1$ at rate 2 and it jumps to site $N-1$ at rate $2(2\xi_{N-1}+1)$. So particles that are absorbed at the 0 and $N+1$ boundary sites do not interact with each other and with other particles. An important property of this process is that it conserves the total number of particles and that starting from any initial configuration, all of the particles will be ultimately absorbed at either one of the boundaries. Duality between BMP and SIP has been used to obtain the temperature profile, exact expressions for the two-point correlation functions, proofs that the equilibrium ($T_L = T_R$) is Gaussian and of the existence of a unique stationary measure in the non-equilibrium case ($T_L \neq T_R$) [8].

0.4 Duality and symmetry

If two Markov process are dual to each other, then the probabilistic properties of one can be obtained through the study of the other, given that the duality functions constitute a sufficiently rich (e.g. measure determining) class. This is specially useful if one of the processes is easier to study than the other.

Duality has been used in the probabilistic literature and particularly in interacting particle systems since Spitzer [25] used it to study symmetric exclusion process (SEP) and independent random walkers. Ligget [15] used duality systematically for studying the ergodic properties of spin systems, the SEP and the voter model. Duality has also been useful in the context of transport models and non-equilibrium statistical mechanics. For instance, Spohn used duality in the study of SEP in contact with particle reservoirs at different chemical potentials [26], showing the existence of long-range correlations. Further applications of duality are in models of energy transport like the Kipnis-Marchioro-Presutti (KMP) model [14] for heat conduction and also for other models like BMP and BEP [8]. Duality has also been used in the study of biological population models, see for example [19].

However, in general there has been no systematic way to show that there is a duality between two Markov processes, neither a method to construct a (new) dual process for a given Markov process. Duality between two Markov processes is usually obtained in an ad-hoc manner, i.e. by an explicit ansatz for a duality function.

We consider two different cases of duality. The duality between two different Markov processes as introduced before, but also the duality of a Markov process with itself, called self-duality. The use of self-duality comes from the fact that the dual process (which is just a copy of of the original process) is often running on a smaller portion of the state space than the original process, which means that probabilistic properties of a larger system can be obtained via study of a smaller system. This is most manifest in the case that the original state space is infinite and the dual state space is finite, which allows to fully understand the behavior of a system of possibly infinitely many particles in terms of the behavior of the same system with only finitely many particles.

In chapter one we show that self-duality is directly related to the non-abelian symmetries of the generator of the Markov process (we say that an operator S is a symmetry of the generator L if they commute $S.L = L.S$). In fact for every symmetry of the generator there is a duality function associated and for every duality function there is a corresponding symmetry of the generator. In the case of duality between two different Markov processes, duality requires a conjugacy relation between the two corresponding generators. So duality between two different processes can be viewed as a change of representation of the generator.

One way to think about duality and symmetry is to think of a generator L as being composed of 'abstract operators' (like for example creation and annihilation operators) which generate an algebra with specific commutation relations. Then for every different representation of this algebra we can obtain different time evolutions, not necessarily

Markov processes, which are dual to each other.

So it turns out that duality is directly related to different representations of an algebra. Notice however that such a change of representation of the algebra does not necessarily transform the generator to a new Markov generator. In the case of finite state spaces, one can already see that a change of basis does not necessarily preserve the fact that off-diagonal elements are non-negative which is a necessary property of a Markov generator. Only when after a change of representation the Markov generator is transformed into a Markov generator, we are in the situation of two Markov processes related by duality.

Sandow and Schutz [23] were the first to notice the relation between $SU(2)$ symmetry of the SEP and its self-duality, by rewriting its generator in terms of quantum spin operators. In chapter one we show in much greater generality the relation between self-dualities and symmetries and give several new examples. For interacting particle systems used as transport models such as BMP we show how to modify the duality functions in order to include the effect of the reservoirs at the boundaries. For energy transport models we uncover a hidden $SU(1,1)$ symmetry in a large class of models (including BMP, KMP model) which explains their duality property, as the $SU(2)$ does for the SEP process. We also show the $SU(1,1)$ symmetry of SIP and the corresponding self-duality.

0.5 SIP and its comparison to SEP; correlation inequalities

Particles in the SIP perform two distinct motions. In addition to a symmetric and independent random walk, they jump to neighboring sites with a rate which is proportional to the number of particles at that site (inclusion jumps, or jumps by 'invitation'). The jump rate for a particle from site i to $i+1$ is $2\xi_i(1+2\xi_{i+1})$ which can be interpreted as follows. Every particle at site i performs a random walk jump to site $i+1$ at rate 2 and additionally every particle at site $i+1$ invites every particle at i at rate 4 (the inclusion jumps from i to $i+1$).

These inclusion moves result in a net attractive interaction between particles. This has to be compared to SEP where particles tend to effectively repel each other (by not being allowed to be at the same site) in addition to their symmetric random walk.

In physical terminology, one can therefore think of SIP as the bosonic counterpart of the fermionic SEP. Intuitively, particles in SIP starting from any configuration tend to gather and to be less spread out than independent symmetric random walks starting from the same configuration. Comparison inequalities (as introduced in Liggett [15] for SEP versus independent random walks) are a rigorous way of describing this idea.

In chapter 2 we analyze SIP in detail and prove the analogue of Liggets comparison inequality for it. From the comparison inequality, we deduce a series of correlation inequalities. As expected intuitively, the correlations turn from negative in SEP to positive in SIP. This is from another point of view quite remarkable because since the SIP is not a monotone process and positive correlations are in no way related to a FKG property, such as in the case of ferromagnetic Glauber dynamics. Since the SIP is dual to the heat conduction model it is immediate to extend those correlation inequalities to the Brownian momentum process and the Brownian energy process. We also consider the more general non-equilibrium case in which the system is in contact with boundary particle reservoirs where we use the self-duality property of SIP to obtain a correlation inequality.

0.6 Condensation in SIP and other models

Condensation phenomena in particle systems can be described as follows; in a given finite system we take the limit as the number of particles goes to infinity, if in the steady state almost all of the particles get concentrated on a finite number of sites , i.e. if all sites have a finite number of particles except a few (these few turn out to be the site(s) where the marginal of the reversible measure has the heaviest tail) , then the system exhibits condensation.

The attractive interaction between the particles in the SIP makes it a natural candidate to study for condensation phenomena. Condensation can arise due to the presence of sub-exponential tails resulting from a strong particle attraction, as has been shown in detail in the context of zero-range processes [12] .

In chapter 3 we show that SIP exhibits exponential tails, and thus the attraction between particles alone is not strong enough and a second contributing factor is required for condensation. One such factor can be spatial inhomogeneities (or also an asymmetry in a finite or semi-infinite system). Another possibility for condensation in SIP is to introduce a parameter m defined as the rate of random walks jumps while the rates of inclusion jumps are kept unchanged. Thus for example setting $m = 0$ would result in a pure inclusion process. We show that in the limit as $m \to 0$, SIP exhibits condensation. We also show parallel condensation phenomena in the Brownian Energy Process (derived from BMP and thus related to SIP), which gives an interesting example of condensation for continuous variables.

0.7 Weak coupling to the heat bath of BMP

In chapter 4 we study the BMP in close-to-equilibrium conditions. One way of achieving such conditions is to make the system in contact with two heat baths at the boundaries such that the temperatures of the two baths are different but very close. In this case we show that the distance between the local equilibrium measure and the true non- equilibrium steady state is of order at most the square of the temperature difference between the two baths, which is in agreement with the theory of McLennan ensembles [16].

An alternative way to achieve close to equilibrium conditions is to fix the temperatures of the two heat baths to arbitrary non-equal temperatures but modify and weaken the coupling of the bulk system to the heat bath with a parameter λ. We then study the behavior of the non-equilibrium steady state measure for small values of coupling constant λ. In particular we show which equilibrium measure is selected as $\lambda \to 0$.

For both cases the temperature profile turn out to be linear in the bulk system. We also give exact computations for the two-point correlation functions for some small finite size systems and discuss their generic form and we show that they are generally not multi-linear.

0.8 (Self)-dualities with $SU(3)/SU(n)$ symmetry; future plans

An interesting future line of research is to find new particle systems or Markov processes that exhibit new kinds of symmetries and corresponding (self-)duality properties. Natural examples are symmetric exclusion type processes with several types of particles. In the case of two type of particles its natural to expect $SU(3)$ symmetry for appropriate choices of jump rates. More generally if one considers $n-1$ types of particles we expect having $SU(n)$ symmetries.

It is an interesting problem to find the necessary and sufficient conditions on the rates and allowed transitions in a specific process such that it will have a particular symmetry and be thus an ‘exactly solvable’ model.

In search for new processes and their corresponding dualities, the the idea of the abstract generator we discussed earlier will be useful. One can start from an abstract generator of a Markov process that is composed of operators that obey a particular algebra. Different representations of the operators in the algebra will then yield different process interrelated via duality.

Moreover, as is the case for symmetric exclusion process, one can hope that appropriate asymmetric modifications of such processes are associated to the deformations of the corresponding algebras, as has been established in the case of the asymmetric exclusion process, [24] and [13].

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