数理解析研究所講究録
第 1658 巻 2009 年 161-172

Free Kawasaki Dynamics in the Continuum

L. Streit

June 2, 2009

CCM, Univ. da Madeira and BiBoS, Univ. Bielefeld

1 Introduction

The Ising model with spins ± 1 on the sites of a lattice, in its interpretation as a "lattice gas" is paradigmatic for models of discrete configurations where a particle is present resp. absent at the site. Sin flips are interpreted as birth resp. death of a particle at the site. Processes with independent births and deaths are called "Glauber dynamics", while "Kawasaki dynamics" involve simultaneous death and birth at a pair of sites: particles hop from one site to the other, the particle number is conserved.

For the dynamics of particles in discrete configuration spaces - lattice gases - there exists a vast literature [16]. For configurations in the continuum much less is known. Recent results can e.g. be found

- for Glauber dynamics in [1]
- for Kawasaki in [12]-[15],

and in the literature cited there.

Relevant methods are those of Markov processes, with the complications that for infinite configurations infinitely many jumps may occur in any finite time interval, and that - even without interactions - jumps can produce infinite local densities in finite times.

Hilbert space methods include Dirichlet forms, evolution operators, etc., and are in particular suitable to describe the (approach to) equilibrium states.

In this paper our intention is to present some - and by far not all! - of the Hilbert space methods which can be used for the study of such infinite particle systems, and to illustrate them with the example of free Kawasaki dynamics which was recently elaborated in [12].

2 Configuration Space, Poisson Measures [19]

2.1 Configuration Space

We want to describe infinite systems of particles: "configurations" of indistinguishable point particles in R^d or in some subset $X \subseteq R^d$.

The *configuration space* $\Gamma := \Gamma_X$ is the set of all **locally finite subsets** of X, *i.e.*,

$$\Gamma := \{\gamma \subset X : \#(\gamma \cap K) < \infty \text{ for bounded } K \subset X\}.$$

For a given configuration $\gamma = \{x_1, x_2, \ldots\}$ we denote

$$\langle \gamma, f \rangle = \sum_{x \in \gamma} f(x) = \sum_{x \in \gamma} \int \delta(x - x') f(x') dx'.$$

This is well defined if f is continuous and zero outside a finite volume: the sum is then finite - no problem of convergence arises.

2.2 Dynamics on Configurations

Kawasaki dynamics would then be described by

$$\partial_t F(\gamma) \quad = \quad \sum_{x \in \gamma} \int_{\mathbb{R}^d} dy\, g\, (F(\gamma \backslash x \cup y) - F(\gamma)).$$

Particles are hopping from x to y with rate g , which might depend on x, y, γ.If the jump rate does not depend on the configuration, we shall speak of free Kawasaki dynamics, with $g = g(x - y)$.

Glauber "Birth and Death" with birth rate b and death rate d would be described by

$$\begin{aligned} \partial_t F(\gamma) \quad &= \quad \int_{\mathbb{R}^d} dy\, b(y)\, (F(\gamma \cup y) - F(\gamma)) \\ &\quad + \sum_{x \in \gamma} d(x)\, (F(\gamma \backslash x) - F(\gamma)) \end{aligned}$$

2.3 Poisson Measures

We begin by considering configurations in a finite volume:

$$|X| = V < \infty$$

For configurations of only one point $x \in R^d$ the obvious choice will be a probability proportional to the volume element dv.

For n-point configurations, elements of $\Gamma_X^{(n)}$ we shall use

$$dm_n = \frac{1}{n!} (dv)^n$$

the combinatorial 1/n! factor for the indistinguishability of the n particles. - But we are interested in configurations of arbitrary many particles, i.e. we want a probability measure on

$$\Gamma_X = \bigsqcup_{n=0}^{\infty} \Gamma_X^{(n)}.$$

We first extend the measures m_n to a measure m on Γ_X, simply by setting

$$m|_{\Gamma_X^{(n)}} = m_n.$$

This is not a probability:

$$\begin{aligned} m(\Gamma_X) &= m\left(\bigsqcup_{n=0}^{\infty} \Gamma_X^{(n)}\right) = \sum_n m\left(\Gamma_X^{(n)}\right) \\ &= \sum_n \frac{1}{n!}\left(\int_X dv\right)^n = \exp(V). \end{aligned}$$

Must normalize to get a probability measure on Γ

$$\pi \equiv \exp(-V) \cdot m$$

2.4 The Characteristic Function

For the measure πit is now straightforward to calculate the characteristic function

$$\begin{aligned} E(\exp(i\langle\gamma, f\rangle)) &= \int_\Gamma \exp(i\langle\gamma, f\rangle) d\pi(\gamma) \\ &= \sum_n \int_{\Gamma^{(n)}} \exp(i\langle\gamma, f\rangle) d\pi(\gamma) \end{aligned}$$

$$\begin{aligned} &= \exp(-V)\sum_n \frac{1}{n!}\left(\int_{X^n} \exp(i\sum_{k=1}^{n} f(x_k)) \prod{}_k (dx_k)\right) \\ &= e^{-V}\sum_n \frac{1}{n!}\left(\int_X \exp(if(x))dx\right)^n = e^{-V}\left(\int_X \exp(if(x))dx\right) \\ &= \exp\left(\int_X (\exp(if(x) - 1)\, dx\right). \end{aligned}$$

We have (re)discovered the characteristic function or Fourier transform, of the Poisson White Noise probability measure:

$$\begin{aligned} E(\exp(i\langle\gamma, f\rangle)) &= \exp\left(\int_X (\exp(if(x) - 1)\, dx\right) \\ &= C_\pi(f) = \int e^{i\langle\omega, f\rangle} d\pi(\omega) \end{aligned}$$

Note: No need to restrict ourselves to a space of finite volume, since

$$C_\pi(f) = \left(\int_{R^d} (\exp(if(x) - 1)\, dx\right)$$

is well defined even in the limit where $X = R^d$, and we have a limiting measure

$$\pi = \lim_{X \to R^d} \pi|_{\Gamma_X}$$

Likewise for more general densities, with

$$dv = z(x)dx$$

where z is a non-negative "intensity":

$$C_{\pi_z}(f) = \exp\left(\int_{R^d} (\exp(if(x) - 1)\, z(x)dx\right)$$

Recall that the Bochner-Minlos theorem guarantees the existence of a probability measure on the space of distributions such that

$$C_{\pi_z}(f) = \int_{D^*} e^{i\langle\gamma, f\rangle} d\pi_z(\gamma)$$

see e.g. [3]. - In our explicit construction we have used the formula

$$\langle\gamma, f\rangle = \sum_{x\in\gamma} f(x) = \sum_{x\in\gamma} \int \delta(x - x')f(x')dx'.$$

We see from this that the measure is concentrated on only those distributions which are sums of Dirac δ-functions

$$\gamma = \sum_{x\in\gamma} \delta_x.$$

2.5 Charlier Polynomials

In $L^2(d\pi_z)$ consider functions

$$e(f, \gamma) = \exp\left(\langle\gamma, \ln(1 + f)\rangle - \langle f\rangle\right) = \exp\left(-\langle f\rangle\right) \prod_{x\in\gamma} (1 + f(x)), \tag{1}$$

with

$$\langle f\rangle = \int f(x)z(x)dx.$$

Their scalar product is computed straightforwardly from the characteristic function:

$$\left(e\left(f\right), e\left(g\right)\right)_{L^2(d\pi_z)} = e^{(f,g)_{L^2(dv)}}.$$

Note that this is exactly the scalar product of two coherent states in Fock space!

$e(f,\gamma)$ is generating function of orthogonal polynomials ("*Charlier polynomials*") in ω. Expanding $e(f)$ in orders of f

$$e(f,\gamma)=\sum_{n=0}^{\infty}\frac{1}{n!}\langle C_n(\gamma),f^{\otimes n}\rangle,$$

we get the orthogonality relation

$$\left(\langle C_n(\gamma),f^{\otimes n}\rangle,\langle C_m(\gamma),g^{\otimes m}\rangle\right)_{L^2(d\pi)}=\delta_{mn}n!\left(f^{\otimes n},g^{\otimes n}\right)_{L^2}$$

Extending from

$$f^{\otimes n}=f(x_1)\dots f(x_n)$$

to symmetric functions

$$f_n=f_n(x_1,\dots,x_n)$$

we can express any square integrable F as

$$F(\gamma)=\sum_{n=0}^{\infty}\langle C_n(\gamma),f_n\rangle$$

and obtain an isomorphism of Hilbert spaces $L^2(\Gamma,d\pi(\gamma))\simeq\mathcal{F}$:

$$\int F(\gamma)\,G(\gamma)\,d\pi(\gamma)\quad=\quad\sum_{n=0}^{\infty}n!\int f_n(x_1,\dots,x_n)g_n(x_1,\dots,x_n)d^nv.$$

2.6 Annihilation and creation operators in Poisson space

Recall that in Fock space coherent states are eigenstates of annihilation operators. What is their image in the Poisson L^2 space?

$$a(h)\,e(f)=(h,f)e(f).$$

For

$$F(\gamma)=e(f,\gamma)=\exp\left(\langle\gamma,\ln(1+f)\rangle-\langle f\rangle\right)$$

one verifies

$$(a(h)\,F)(\gamma)\quad=\quad\int_X(F(\gamma\cup\{x\})-F(\gamma))\,h(x)\,dv$$

and hence by linear extension for all F$\in D(a(h))$.

We intend to also determine the action of the adjoint operator $a^*(g)$. To do so we use the "Mecke Identity"

$$\int_\Gamma\sum_{x\in\gamma}H(\gamma,x)d\pi(\gamma)\quad=\quad\int_X\int_\Gamma H(\gamma\cup\{x\},x)d\pi(\gamma)dx$$

(see, *e.g.*, [17]).

The action of $a^*(g)$ turns out to be

$$(a^*(g)F)(\gamma) := \sum_{x\in\gamma} F(\gamma\backslash\{x\})g(x) - \langle g\rangle\, F(\gamma).$$

For later reference we finally introduce

$$e_B(f,\omega_\gamma) = \exp\langle f\rangle\, e_B(f,\omega_\gamma) = \prod_{x\in\gamma}(1+f(x)).$$

Their expectations w.r. suitable measures μon configuration space

$$E\left(e_B\left(f\right)\right) \;=\; \int_\Gamma e_B(f,\omega_\gamma)d\mu\left(\gamma\right) = \sum_n \frac{1}{n!}\left\langle k_n^\mu, f^{\otimes n}\right\rangle$$

are called Bogoliubov functionals and are the generators of the nthorder correlation functions for the distribution μ.

3 Return to Kawasaki

Recall the free Kawasaki dynamics:

$$\partial_t F(\gamma) \;=\; HF(\gamma) = \sum_{x\in\gamma}\int_{\mathbb{R}^d} dy\, g(x-y)\left(F(\gamma\backslash x\cup y) - F(\gamma)\right)$$

In terms of creation and annihilation operators one finds

$$H = \int dx\, z(x)\int dy\left(g(x-y) - g_0\delta(x-y)\right)\left(a^*(x)a(y) - a(y)\right),$$

Clearly, in Fock space language this corresponds to a quadratic Hamiltonian and time development can be calculated in closed form.

Time evolution of Bogoliubov exponentials takes on a particularly simple form:

$$e^{Ht}e_B(f) = e_B(e^{tA}f)$$

$$Af(x) := \int_{\mathbb{R}^d} dy\, g(x-y)\left(f(y) - f(x)\right).$$

Evolution of the initial (Poisson) distribution

$$\pi_z \longrightarrow P_{\pi_z,t}$$

under the adjoint of e^{Ht} is characterized by

$$\int e_B(\varphi,\gamma)P_{\pi_z,t}(d\gamma) = \int e_B(e^{tA}\varphi,\gamma)\pi_z(d\gamma) = \exp\left(\int_{\mathbb{R}^d} e^{tA}\varphi(x)z(x)dx\right).$$

A Markov process $\mathbf{X}_t$ on Γ, associated with the Kawasaki dynamics, requires a technical restriction [12]: the process may not start at any arbitrary initial configuration $\gamma \in \Gamma$. Consider the set Θ of all $\gamma \in \Gamma$ such that, for some $m \in \mathbb{N}$ (depending on γ),

$$|\gamma_{B(n)}| \leq m \operatorname{vol}(B(n)), \quad \forall n \in \mathbb{N}.$$

Have $\mu(\Theta) = 1$ for every probability measure μ on Γ whose correlation functions $k_\mu^{(n)}$, $n \in \mathbb{N}$, fulfill the Ruelle bound

$$k_\mu^{(n)} \leq C^n$$

i.e. for Poisson measures with bounded intensity, and for Gibbs measures with suitable potentials, cf. [Ruelle; 1970].

Below we shall use the so-called empirical field corresponding to a $\varphi \in \mathcal{D}(\mathbb{R}^d)$,

$$n_t(\varphi,\mathbf{X}) := \langle\varphi,\mathbf{X}_t\rangle = \sum_{x\in\mathbf{X}_t}\varphi(x).$$

3.1 Evolution of Distributions

The distribution at time t, $P_{\pi_z,t}(d\gamma)$ is again Poissonian, with intensity $z_t \in L^\infty(\mathbb{R}^d,dx)$, given by

$$\int_{\mathbb{R}^d} dx\, e^{tA}f(x)z(x) = \int_{\mathbb{R}^d} dx\, f(x)z_t(x), \tag{2}$$

for all $f \in L^1(\mathbb{R}^d,dx)$. Since e^{tA} is positivity preserving in $L^1(\mathbb{R}^d,dx)$, it follows from (2) that $z_t \geq 0$.

3.1.1 Invariant Distributions

Poisson distributions are invariant under free Kawasaki dynamics iff their intensity

$$z(x) = const.$$

$H^*1 = 0$ iff the linear annihilation term in H vanishes:

$$\int dya(y)\left(\int dxz\,(x)\,(g\,(x-y) - g\,(x))\right) \stackrel{!}{=} 0$$

Using Fourier transforms one sees that this requires z=const.

In the symmetric case, for g even and constant $z > 0$, H gives rise to a symmetric Dirichlet form on $L^2(\Gamma,\pi_z)$,

$$(F, HF) = -\frac{1}{2}\int_{\Gamma} \pi_z(d\gamma) \sum_{x\in\gamma} \int_{\mathbb{R}^d} dy\, g(x-y)\, |F(\gamma)|^2 .$$

This allows to derive a Markov process on Γ with *cadlag* paths and having π_z as an invariant measure . In this setting H is a negative essentially self-adjoint operator on $L^2(\Gamma, \pi_z)$, and the generator of a contraction semi-group on $L^2(\Gamma, \pi_z)$.

4 Asymptotics

4.1 Large Time Asymptotics

Asymptotics t$\rightarrow \infty$

We have seen that any Poisson state of constant intensity is invariant under the evolution (equilibrium). Now we consider "local equilibria": Poisson states with non-constant intensity z=z(x).

Recall that the state at t$\geq$0 is again Poissonian, with intensity $z_t \in L^\infty(\mathbb{R}^d, dx)$, given by

$$\int_{\mathbb{R}^d} dx\, e^{tA} f(x) z(x) = \int_{\mathbb{R}^d} dx\, f(x) z_t(x).$$

4.1.1 Convergence to the Arithmetic Mean

One says that a function $z \in L^1_{\text{loc}}(\mathbb{R}^d, dx)$ has arithmetic mean whenever

$$\lim_{R\rightarrow+\infty} \frac{1}{\text{vol}(B(R))} \int_{B(R)} dx\, z(x) \equiv mean(z) \tag{3}$$

exists.

Theorem. Let $z \geq 0$ be a bounded measurable function whose Fourier transform $\widetilde{z}$ is a signed measure. Then z has arithmetic mean and the one-dimensional distribution $P_{\pi_z, t}$ converges weakly to $\pi_{\text{mean}(z)}$ as t goes to infinity.

Proof (Outline):

In this case $mean(z) = \widetilde{z}(\{0\})$,

$$\int_{\mathbb{R}^d} dx\, f(x) z_t(x) = \int_{\mathbb{R}^d} dx\, e^{tA} f(x) z(x) \rightarrow mean(z) \int_{\mathbb{R}^d} dx\, f(x),$$

and

$$\pi_{z_t} \longrightarrow \pi_{mean(z)}$$

weakly, because of convergence of characteristic functions.

Remark:

1. the same conclusion holds e.g. for

$$z(x) = \begin{cases} z_1 & \text{if } x_1 \geq 0 \\ z_0 & \text{otherwise} \end{cases} .$$

with mean$(z) = \frac{z_0+z_1}{2}$, by explicit calculation although in this case $\hat{z}$ is not a signed measure. It seems natural to expect that the large time asymptotic exists for all bounded intensities which have arithmetic mean.

2. On the other hand, not all measurable bounded non-negative functions z have an arithmetic mean. Counterexamples are slowly oscillating functions such as

$$z(x) = c + \cos(\ln(1 + |x|)), \quad x \in \mathbb{R}^d,$$

where c> 1. Then for large R

$$\frac{1}{\mathrm{vol}(B(R))} \int_{B(R)} z(x)\, dx \sim c + \frac{1}{\sqrt{1+d^2}} \sin\Big(\ln(R) + \arctan(d)\Big).$$

3. The non-ergodicity of the infinite particle processes is reflected in the non ergodicity of the one particle processes in this class of initial intensities.

4.2 The hydrodynamic limit

The first correlation function $\rho_t(x)$ is the probability density for (the first moment of) the empirical field:

$$E\left(n_t(\varphi, \mathbf{X})\right) = E\left(\langle \varphi, \mathbf{X}_t \rangle\right) = \int \varphi(x) \rho_t(x) dx$$

Consider space-time scale transformation given by $\langle \varphi, \gamma \rangle \longrightarrow \varepsilon^d \langle \varphi(\varepsilon \cdot), \gamma \rangle$, $t \longrightarrow \varepsilon^{-\kappa} t$ for suitable $\kappa > 0$ (see below), $z \longrightarrow z(\varepsilon \cdot)$.

1. If

$$g_i^{(1)} := \int_{\mathbb{R}^d} dx\, x_i g(x) \neq 0,$$

then for $\kappa = 1$

$$\int_{\mathbb{R}^d} dx\, \rho_t(x) \varphi(x) = \int_{\mathbb{R}^d} dx\, z(x + t g^{(1)}) \varphi(x),$$

so that, if the intensity z is smooth enough

$$\frac{\partial}{\partial t} \rho_t(x) = g^{(1)} \cdot \nabla \rho_t(x) = \mathrm{div}(g^{(1)} \rho_t(x))$$

with the initial condition $\rho_0 = z$.

2. If $g^{(1)} = 0$, and

$$g_{ij}^{(2)} := \int_{\mathbb{R}^d} dx\, x_i x_j g(x)$$

then for $\kappa = 2$

$$\int_{\mathbb{R}^d} dx\, \rho_t(x) \varphi(x) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} dx\, z(x) \int_{\mathbb{R}^d} dk\, e^{ik \cdot x} e^{-\frac{t}{2} \langle g^{(2)} k, k \rangle} \hat{\varphi}(k),$$

solving the partial differential equation

$$\frac{\partial}{\partial t}\rho_t(x) = \frac{1}{2}\sum_{i,j=1}^{d} g_{ij}^{(2)} \frac{\partial^2}{\partial x_i \partial x_j}\rho_t(x).$$

3. Consider weak asymmetries, decomposing g into a sum of an even function p and an odd function q, and use the scaling

$$g_\varepsilon := p + \varepsilon q$$

and $\kappa = 2$. The limiting density ρ_t is then solution of the partial differential equation

$$\frac{\partial}{\partial t}\rho_t(x) = \operatorname{div}(g^{(1)}\rho_t(x)) + \frac{1}{2}\sum_{i,j=1}^{d} g_{ij}^{(2)} \frac{\partial^2}{\partial x_i \partial x_j}\rho_t(x).$$

4.3 Far from Equilibrium

The construction of the free Kawasaki process and its scaling limits are not restricted to Poissonian initial distributions. Sufficient conditions for admissible measures can be stated in terms of their correlation functions and are in particular fulfilled for Gibbs measures at high temperatures.

Gibbs Measures

A probability measure μ on Γ is called a Gibbs measure for V, intensity function $z \geq 0$, and inverse temperature β if it fulfills the Georgii-Nguyen-Zessin equation [18]

$$\int_\Gamma \mu(d\gamma) \sum_{x\in\gamma} H(x,\gamma) = \int_\Gamma \mu(d\gamma) \int_{\mathbb{R}^d} dx\, z(x) H(x, \gamma \cup \{x\}) e^{-\beta E(x,\gamma)} \tag{4}$$

with

$$E(x,\gamma) := \begin{cases} \sum_{y\in\gamma} V(x-y), & \text{if } \sum_{y\in\gamma} |V(x-y)| < \infty \\ +\infty, & \text{otherwise} \end{cases}.$$

(Equivalent to DLR-equation, see [Georgii, Nguyen-Zessin].)

The correlation functions corresponding to such measures fulfill a Ruelle bound, and thus, the measures are supported on Θ, but are neither reversible nor invariant initial distributions for the free Kawasaki dynamics.

Consider a Gibbs measure with translation invariant potential V, temperature and activity z which is in the high temperature low activity regime, and let the Fourier transform of z be a bounded signed measure. Then

1. the first correlation function has arithmetic mean, and the one-dimensional distribution $P_{\pi_z,t}$ converges weakly to $\pi_{\text{mean}(z)}$ when t goes to infinity.

2. Hydrodynamic scaling PDEs hold as before, where now the initial value $\rho_0(x)$ is a scaling limit of the first correlation function.

Specifically, because of translation invariance the 1st correlation function for a constant activity c is a constant

$$\rho^{(1)} = \rho^{(1)}(c)$$

For $z = z(x)$ have

$$\rho_0(x) = \rho^{(1)}(z(x)).$$

A proof and more details can be found in [12].

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