

MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

Report No. 22/2005

**Mini-Workshop: Particle Systems with Several  
Conservation Laws: Fluctuations and Hydrodynamic Limit**

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May 1st – May 7th, 2005

ABSTRACT. The Mini-Workshop is concerned with the large-scale description of microscopic many-particle systems with two or more conservation laws. This is topic of common interest for statistical mechanics, probability theory and PDE theory. The main difficulty lies in the proof of the hydrodynamic limit in terms of a system of (generally hyperbolic) PDE's which includes a proper treatment of shock and boundary discontinuities that result from the microscopic dynamics. Moreover, fundamental properties of current-carrying stationary states of such systems (which are not Gibbs states) are studied in terms of fluctuations of macroscopic quantities. Many powerful tools developed for particle systems (or PDE's respectively) with one conservation law have no obvious generalization to systems with two or more conservation laws and hence new mathematical ideas need to be developed.

*Mathematics Subject Classification (2000):* 35L65, 60K35, 82C22.

**Introduction by the Organisers**

“Particle Systems with Several Conservation Laws: Fluctuations and Hydrodynamic Limit” connects different fields where intimate connections are just emerging. In many applications (like traffic flow, dust models in astrophysics, compressible fluid models) very natural microscopic descriptions of the stochastic dynamics of interacting particles can often be related to macroscopic continuum descriptions using nonlinear evolutionary PDEs. It is hard to rigorously relate these two levels of modelling of the same physical or biological phenomena, though.

Scientific progress in the area of hyperbolic conservation laws for systems of one and two equations has been used in rigorously proving the hydrodynamic limit of corresponding interacting particle systems. Techniques like the theory of compensated compactness in PDEs are emerging as powerful tools in the interacting particle system community. Many other original ideas were and are currently being developed within this second context for systems with two and more conservation laws. This had lead the organizers to believe that time has come to devote a high profile meeting to this subject which is situated at the intersection between non-linear hyperbolic pde theory, probability theory of interacting particle systems, nonequilibrium statistical physics.

More specifically, the choice of the topic was motivated by the following closely related issues: As it is well-known solutions of systems of hyperbolic PDEs develop shocks and this fact causes major difficulties in the mathematical analysis as well as in the physical interpretation of the microscopic particle structure of a shock. Moreover, in the presence of macroscopic currents, boundary conditions in finite systems determine the bulk behaviour of stationary solutions both of PDEs and particle systems. This has been shown to lead to boundary-induced nonequilibrium analogs of phase transitions which are novel phenomena of particular importance in applications which usually deal with effectively finite systems. It raises the question how microscopic laws of interaction find an appropriate description in terms of boundary conditions of an associated hyperbolic PDE. In our current but not fully developed understanding, the hydrodynamic limit, existence of shocks, and the nature of boundary conditions appear to be very intricately linked problems which require investigation within a common framework. In this context the workshop was concerned with the following problems:

- Derivation of hydrodynamic limit
- Microscopic structure of the shocks
- Open boundary problems
- Dynamical phase transitions
- Large deviations
- Treatment of the theory of conservation laws with entropies coming from microscopic models

The participants, coming from the US, France, Hungary and Germany, were mathematicians from PDE theory and probability theory and physicists working in the field of nonequilibrium statistical mechanics. With all of them being specialists coming from different fields, but sharing a common research interest, this miniworkshop turned out to be a highly fruitful “joint venture”. A number of very successful expository lectures on recent progress in the field helped to bridge the gaps between the different communities. More specialized talks, partly on open problems, led the participants to leave the confines of their respective communities and to interact with each other. All of us enjoyed enormously the externally tranquil, but scientifically vivid and stimulating atmosphere of Oberwolfach.

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## Abstracts

### **Hyperbolic models for chemosensitive movement in interacting cell systems**

ANGELA STEVENS

(joint work with Hyung Ju Hwang, Kyungkeun Kang, Frithjof Lutscher)

Morphogenetic processes in biology such as neurulation and gastrulation involve coordinated movement of cells. It is assumed that these processes happen due to long-range signaling, although the detailed mechanisms are not completely understood. Therefore, one is interested in biological model-systems where self-organization of cells and in particular the mechanisms of signaling can be analyzed in greater detail. A major question is whether or not short-range signaling or local interaction of cells can also be the cause of coordinated movement and morphogenetic processes.

In the talk two one-dimensional models of hyperbolic type for structure formation in interacting cell systems were presented. The first model is dealing with reorientation and motion of cells due to cell surface bound signals and describes ripple formation of myxobacteria. The second model describes chemotactic movement of cells due to a diffusive signal.

In the biological literature it is discussed, that ripple formation of myxobacteria happens due to purely local interaction. These ripples - countermigrating periodic travelling pulses - can be observed before the final aggregation of the bacteria and fruiting body formation take place. Our basic mathematical model is a one-dimensional hyperbolic system of Goldstein-Kac type with density-dependent coefficients. Conditions for the existence of travelling patterns are discussed by means of linear analysis and the construction of invariant domains. This gives rise to a certain class of turning rates which are then simulated numerically. Countermigrating oscillatory patterns can be observed. In case the conditions on the turning rates are not fulfilled the simulations show the early development of one single peak for the population density.

The second model is a one dimensional hyperbolic system for chemotactic movement of cells. The model consists of two hyperbolic differential equations for the chemotactic species and is coupled with either a parabolic or an elliptic equation for the dynamics of the external chemical signal. The speed of the chemotactic species is allowed to depend on the external signal and the turning rates may depend on the signal and its gradients in space and time, as observed in experiments. Global classical solutions are established for regular initial data and a parabolic limit is proved. This limit compares to Keller-Segel type models for chemotaxis. Thus the so-called chemotactic sensitivity in the parabolic model can be explained in terms of the parameters of the hyperbolic model, e.g. the turning frequency.

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**Exact shock measures and steady-state selection in a driven diffusive system with two conserved densities**

ATTILA RÁKOS

(joint work with Gunter M. Schütz)

Recently much attention was paid to the investigation of the stationary microscopic structure [1, 2, 3] and the microscopic dynamics [4, 5, 6, 7, 8] of shock discontinuities in driven diffusive systems. It was pointed out in [7] (and for infinite systems in [6]) that in the asymmetric simple exclusion process (ASEP) for special tuning of densities and microscopic hopping rates there exists a travelling shock with a step-like density profile even on the microscopic scale, which behaves like a collective one-particle excitation. However, little is known about the microscopic structure and dynamics of shocks in systems with two conservation laws [9, 10, 11, 12], which recently have become a focus of attention (for a review see [13] and [14, 15] for more recent work).

The talk is based on a work [16] in which we show that a shock measure with single-particle dynamics can describe also systems with two conserved densities. We also study the hydrodynamic limit of the model (under Eulerian scaling) which shows a larger class of stable shock solutions. The hierarchical structure of the hydrodynamic equations for this system allows us to deduct the steady state selection in an open system connected to particle reservoirs at its boundaries.

We study a model which is defined on an open lattice of size  $L$  with two types of particles ( $A$  and  $B$ ). These particles interact with exclusion and are subject to biased diffusion: they can hop stochastically onto nearest neighbour vacant sites and exchange position (provided they are nearest neighbours) at given rates. At the boundaries the particles can enter and leave the lattice.

Let  $P^{(k)}$  be defined as a product measure state with particle densities  $(\rho_l^A, \rho_l^B)$  on the left of site  $k$  and  $(\rho_r^A, \rho_r^B)$  on the right. These shock measures with  $k = 0 \dots L$  form a family within which the only parameter is the position of the shock. We aim at finding the most general case when this family of shock measures closes under the time evolution of the model.

Using the quantum Hamiltonian formalism [17] we find a set of conditions which are necessary and sufficient for having such an invariant family of shock measures. These are the following: (1) The left and right hopping rates of the  $A$  particles have to be equal to these rates of the  $B$  particles respectively. (2) The exchange rates of  $A$  and  $B$  have to be the same in both directions. (3) The densities have to satisfy  $\rho_l^A / \rho_l^B = \rho_r^A / \rho_r^B$  and (4)  $\rho_r(1 - \rho_l)q = \rho_l(1 - \rho_r)p$ , where  $p$  and  $q$  are the

hopping rates of both species to the right and left, and  $\rho = \rho^A + \rho^B$ . (5) There are some extra conditions for the boundary rates [16].

If the above conditions are satisfied than an initial shock measure  $P^{(k)}$  evolves into linear combinations of shock measures of this family in such a way that the shock position  $k$  performs a biased random walk with nearest neighbour jumps at rates  $p\rho_l/\rho_r$  and  $q\rho_r/\rho_l$  to the right and left respectively with reflecting boundaries.

Conditions (1-2) tell us that the species  $A$  and  $B$  have the same dynamics. Not distinguishing between them would lead to the pure ASEP. Therefore it is not surprising that condition (4) is in full agreement with the corresponding formula for the ASEP [6, 7]. The novelty is that *a*) the family of product measures remains invariant even if one distinguishes between  $A$  and  $B$  particles, *b*) there is no other possibility for having such an invariant family of shock measures up to relabelling the local states  $A$ ,  $B$  and  $0$  (empty site).

It is also of interest to drop the conditions (3-4) and see how this model behaves on the macroscopic scale. The hydrodynamic limit of the model (under Eulerian scaling) is described by a set of partial differential equations for the time evolution of the particle densities, in which one equation (for the total density  $\rho(x, t)$ ) is decoupled and takes the form of the well-known Burgers equation which can be solved exactly [18]. The second equation than gives  $\rho^A/\rho^B = \text{const.}$  along the curves  $x(t)$  satisfying  $\dot{x}(t) = 1 - \rho(x, t)$ .

A general feature of driven systems with two conservation laws is that an initial sharp discontinuity develops two shocks (or rarefaction waves) of different type. The shock measures discussed before are pure shocks of one type so they don't split further. In our model, due to its degeneracy, the other type of shocks are microscopically not sharp: their width scales with  $\sqrt{t}$  because of the diffusive dynamics of the  $A$  and  $B$  particles. However, this broadening remains invisible on Euler-scale.

In a finite system with open boundaries coupled to particle reservoirs one is left with the question of steady state selection. In case of one conserved density the current-density relation already determines the phase diagram in terms of the boundary densities [19, 20] but in case of more conservation laws the question turns out to be much more intricate and no general rule is known to apply [10]. However, in our model, due to the special hierarchical structure of the hydrodynamic equations, it is possible to determine the resulting steady state for any given boundary densities. So our model, even though degenerate, may serve as a testing ground for any general theory.

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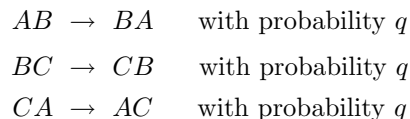
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### Exact steady state of exclusion processes with several species of particles

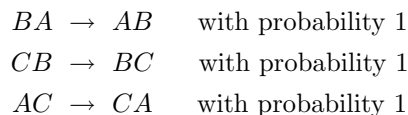
BERNARD DERRIDA

Second class particles were introduced in one dimensional exclusion processes to locate shocks [1]. It was shown that for the asymmetric exclusion process, when the asymptotic densities are  $\rho_L$  and  $\rho_R$  (with  $\rho_L < \rho_R$  when the asymmetry favors jumps to the right), if one introduces a second class particle, this second class particle is attracted by the shock, and there is an invariant measure [2], seen from the second class particle, which can be calculated explicitly in terms of the matrix ansatz [3, 4]. Second class particles are not the only way to locate a shock at a microscopic scale, and the invariant measure seen from the shock depends on how the location of the shock is defined. There exist however invariants [5] which characterize the shock at the microscopic scale, and which do not depend on the definition used to locate the shock.

Another aspect described in the talk is the *ABC* model [6] on a ring of  $L$  sites. In the *ABC* model, each site is occupied by either a *A* particle, a *B* particle or a *C* particle. The exchange rates are given by



and



When  $q < 1$  there are in the steady state 3 macroscopic domains: all the *A* are grouped together with on their right all the *B*'s and on their left all the *C*'s except



for fluctuations at the microscopic scale near the domain boundaries. On the other hand, when  $q = 1$ , all configurations are equally likely and all the three species are totally mixed. It is possible to show that the system undergoes a phase transition [7] for a weakly asymmetric case, that is when

$$q = \exp\left(-\frac{\beta}{L}\right)$$

where the value  $\beta_c$  of  $\beta$  at the transition depends on the densities  $\rho_A, \rho_B, \rho_C$  (with  $\rho_a + \rho_b + \rho_c = 1$ ). For equal densities of the three species, one can show that

$$\beta_c = 2\pi\sqrt{3}$$

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### Hyperbolic systems: Hydrodynamic limits via PDE methods

JÓZSEF FRITZ

(joint work with Bálint Tóth)

The main purpose of this talk is to point out some similarities and differences of the *microscopic theory of hydrodynamics* and *numerical schemes for solving hyperbolic equations and systems of conservation laws*. Let  $\zeta = (\zeta_k(t) : k \in \mathbb{Z})$  denote the *conserved quantities* at time  $t \geq 0$  of a one-dimensional lattice model. The associated *empirical process* is defined for  $\epsilon > 0$ ,  $t \geq 0$  and  $x \in \mathbb{R}$  as  $z_\epsilon(t, x) := \zeta_k(t\epsilon^\alpha)$  if  $|\epsilon k - x| < \epsilon/2$ , where  $\epsilon \rightarrow 0$  is the *scaling parameter* interpreted as the macroscopic size of the lattice, and  $\alpha = -2$  for diffusive,  $\alpha = -1$  for hyperbolic systems. In the examples below,  $\zeta$  is a scalar, or it is a vector of two components. The *hydrodynamic law of large numbers* means that the empirical process converges to a deterministic limit,  $z(t, x)$  that solves the *macroscopic equation*. In the diffusive case we get  $\partial_t z = \partial_x^2 f(z)$ ; the number of conservation laws is irrelevant, and a well developed theory is available, see [6] for the first basic results.

Hyperbolic problems are more difficult because of several reasons. Relative entropy is the only general tool, but it works only in a regime of smooth macroscopic solutions [13]. *Attractive models* result in a single conservation law,  $\partial_t z + \partial_x f(z) = 0$ , see [10,9]. Treatment of less specific systems requires an intensive application of PDE techniques, namely *entropy-flux pairs* and *the method of compensated compactness* [7,8,11,1]. The *asymmetric Ginzburg-Landau model* is perhaps the most transparent example to demonstrate some basic notions, it is given by a system of stochastic differential equations:

$$d\omega_k = (a/2)(V'(\omega_{k+1}) - V'(\omega_{k-1})) dt + \sigma \Gamma(\omega) dt + \sqrt{2\sigma T}(d\omega_{k-1} - d\omega_k),$$

where  $\Gamma := V'(\omega_{k+1}) + V'(\omega_{k-1}) - 2V'(\omega_k)$ ,  $V \in C^2(\mathbb{R})$  is convex at infinity,  $\omega_k \in \mathbb{R}$ , and  $w_k$  is a family of independent standard Wiener processes; the noise maintains *temperature*  $T > 0$ . Total spin,  $\sum \omega_k$  is the only conservative quantity, and we have a one-parameter family,  $\lambda_q$  of stationary product measures if  $\sigma, T > 0$ ; its marginal densities are specified as  $f(\omega_k) := \exp(q\omega_k - T^{-1}V(\omega_k) - F(q, T))$ ,  $F$  is the normalization. The equilibrium mean of  $V'(\omega_k)$  is just  $Tq$ ,  $\rho := \lambda_q(\omega_k) = F'_q(q, T)$ , thus  $q = S'_\rho(\rho, T)$ , where  $S$  is the convex conjugate of  $F$  at a fixed value of  $T > 0$ . This is a diffusive system if  $a = 0$ , and its hydrodynamic limit reads as  $\partial_t \rho = \sigma T \partial_x^2 S'_\rho(\rho, T)$ . In the hyperbolic case of  $a \neq 0$  the presence of  $\Gamma$  is very important even if  $T = 0$ . The numerical procedure, when  $T = 0$ , certainly converges if  $V$  is convex,  $\partial_t \rho = a \partial_x V'(\rho)$  is the macroscopic equation. There are many other possibilities to choose the regularization  $\Gamma$ , its present form is dictated by a general principle of statistical physics: *the microscopic system must have a family of stationary states associated to the conservation laws*. At positive temperatures the macroscopic equation is modified by large deviation effects due to the noise, it turns into  $\partial_t \rho = aT \partial_x S'_\rho(\rho, T)$ , see [3]. If  $V$  is convex (attractive case), then uniqueness of the limit is also known, the general case is problematic.

Systems with two conservation laws are not attractive, interacting exclusion processes constitute a nice example [4]. We consider particles with  $\pm 1$  velocities on  $\mathbb{Z}$  with full exclusion, thus  $\omega_k = 0, \pm 1$  is the configuration at site  $k \in \mathbb{Z}$ . The microscopic evolution is generated by  $\mathcal{L} = \mathcal{L}_0 + \sigma \mathcal{S}$ , the dynamics consists of independent exchanges at neighboring sites. The asymmetric component,  $\mathcal{L}_0$  sends  $(1, 0)$  to  $(0, 1)$  and  $(0, -1)$  to  $(-1, 0)$  at a unit rate, interaction means that  $(1, -1)$  turns into  $(-1, 1)$  at rate two; any other action is banned. Finally,  $\sigma = \sigma(\epsilon) > 0$ , and the symmetric  $\mathcal{S}$  exchanges  $\omega_k$  and  $\omega_{k+1}$  at rate 1. The conserved quantities are chosen as  $\eta_k := 1 - \omega_k^2$  and  $\xi_k := -\omega_k$ , then  $\mathcal{L}_0 \eta_k = \phi_{k+1} - \phi_k$ ,  $\mathcal{L}_0 \xi_k = \psi_{k+1} - \psi_k$ ,

$$\begin{aligned} \phi_k &= \frac{1}{2}(\eta_k \xi_{k+1} + \eta_{k+1} \xi_k) + \frac{1}{2}(\eta_k - \eta_{k+1}), \\ \psi_k &= \frac{1}{2}(\eta_k + \eta_{k+1} + 2\xi_k \xi_{k+1} - 2) + \frac{1}{2}(\eta_k \xi_{k+1} - \eta_{k+1} \xi_k) + \xi_k - \xi_{k+1} \end{aligned}$$

are the fluxes. The symmetric component,  $\mathcal{S}$  is acting as a discrete Laplacean; it plays the role of the elliptic stabilization what we need even for numerical procedures. Since all stationary states are superpositions of Bernoulli measures,

the familiar Leroux system,

$$\partial_t \rho + \partial_x(\rho u) = 0, \quad \partial_t u + \partial_x(\rho + u^2) = 0$$

is expected as the result of HDL;  $\rho$  and  $u$  are the asymptotic densities of  $\eta$  and  $\xi$ , respectively.

The hydrodynamic law of large numbers is materialized at a level of block averages. For any  $\epsilon > 0$ ,  $l = l(\epsilon) \in \mathbb{N}$  and space-time process  $\zeta$  let

$$\hat{\zeta}_\epsilon(t, x) := \frac{1}{l} \sum_{k \in \mathbb{Z}} a \left( \frac{x - k\epsilon}{l\epsilon} \right) \zeta_k(t/\epsilon)$$

where  $a \geq 0$  is a smooth density of compact support. For example, if  $\zeta := (\eta, \xi)$  then  $\hat{\zeta}_\epsilon$  denotes the empirical process, and  $\hat{J}_\epsilon$  corresponds to the microscopic flux  $J_k := (\phi_k, \psi_k)$ . Suppose that  $\sigma(\epsilon) \approx \log(1/\epsilon)\sqrt{1/\epsilon}$ ,  $l(\epsilon) \approx \sqrt{(1/\epsilon)\log(1/\epsilon)}$ , and let  $P_\epsilon$  denote the distribution of  $\hat{\zeta}_\epsilon$ . We prove that  $P_\epsilon$  is tight in the strong topology of  $L^1_{\text{loc}}(\mathbb{R}_+^2)$ , and all limit points are concentrated on weak entropy solutions of the Leroux system. There is no result on uniqueness of the limit.

The first step of the proof is the replacement of  $\hat{J}_\epsilon$  with  $f(\hat{\zeta}_\epsilon)$ , where  $f(z)$ ,  $z := (\rho, u)$  is the macroscopic current. This follows by LSI for  $\mathcal{S}$ , and it is remarkable that, in contrast to diffusive systems, there is no transition from large microscopic block averages to small macroscopic ones: we have to start with blocks of size  $l \approx \epsilon^{-1/2}$ . This step is not present in numerical procedures where block averages do not play any role. Having now the right macroscopic flux, an easy compactness argument shows that all limit distributions of the empirical process are concentrated on a set of *measure solutions*.

The method of compensated compactness is used to prove the Dirac property of the limit distributions. We consider *Lax entropy pairs*  $(S, F)$  and the related *entropy production*  $X_\epsilon := \partial_t S(\hat{\zeta}_\epsilon) + \partial_x F(\hat{\zeta}_\epsilon)$ . It is a rapidly oscillating quantity because the microscopic system can not have nontrivial entropy pairs, the crucial point of the proof is to establish tightness of its distribution in  $H^{-1}$ . In this way the *div-curl lemma* [8,11] and the *Lax entropy condition* are verified at the level of limit distributions of the Young measure of the empirical process. Now we are in a position to prove the Dirac property of the limiting Young measure, this is not difficult in the case of single conservation laws. The Leroux system is of Temple class, it has such a nice family of entropy pairs that the div-curl lemma yields the Dirac property by convexity.

The probabilistic part of the argument above extends to several two-component models, but the last step is restricted to the Leroux system. Indeed, most physical systems of conservation laws have singular points where the conditions of strict hyperbolicity and genuine nonlinearity break down, therefore the general results of DiPerna [1] and others do not apply. To exclude singularities from the phase space, a Conley- Chueh - Smoller type maximum principle would be needed for the Riemann invariants of the macroscopic equations. Unfortunately, this is not available for microscopic stochastic models, but there is a minor hope to prove it.

In the case of one-component systems the Lax entropy condition is sufficient for uniqueness of HDL, [4] discusses some one-component models of this kind.

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### Hydrodynamic limit for the Fourier’s law

STEFANO OLLA

Hamiltonian models perturbed with stochastic dynamics have been proven useful as microscopic dynamics for the hydrodynamic limit for the Euler equations for compressible gas, at least in the smooth regime (cf. [4]). We expose here some recent attempt to use these type of models in order to obtain Fourier law of diffusion of heat and compressible Navier-Stokes equations. Atoms are labelled by  $x \in \{1, \dots, N-1\}$ . Atom 1 and  $N-1$  are in contact with two separate heat reservoirs at two different temperatures  $T_l$  and  $T_r$ . The interaction between the reservoirs is modelled by two Ornstein-Uhlenbeck processes at the corresponding temperatures. The moments of the atoms are denoted by  $p_1, \dots, p_{N-1}$  and the positions by  $q_1, \dots, q_{N-1}$ . The distances between the positions are denoted by

$r_1, \dots, r_{N-2}$ , where  $r_x = q_{x+1} - q_x$ . The Hamiltonian of the system that represents the total energy inside the system is given by

$$\mathcal{H}_N = \sum_{x=1}^{N-1} e_x, \quad e_x = \frac{(p_x^2 + (r_x - \rho)^2)}{2} \quad x = 1, \dots, N-2; \quad e_{N-1} = \frac{p_{N-1}^2}{2}.$$

The dynamics is described by the following system of stochastic differential equations:

$$\begin{aligned} dr_x &= (p_{x+1} - p_x)dt, & x = 1, \dots, N-2 \\ dp_x &= (r_x - r_{x-1})dt - \gamma p_x dt + \sqrt{\gamma}(p_{x-1}dw_{x-1,x} - p_{x+1}dw_{x,x+1}), \\ & & x = 2, \dots, N-2 \\ dp_1 &= (r_1 - \rho)dt - \frac{1+\gamma}{2}p_1 dt - \sqrt{\gamma}p_2 dw_{1,2} + \sqrt{T_l}dw_{0,1}, \\ dp_{N-1} &= -(r_{N-2} - \rho)dt - \frac{1+\gamma}{2}p_{N-1}dt + \sqrt{\gamma}p_{N-2}dw_{N-2,N-1} + \sqrt{T_r}dw_{N-1,N}, \end{aligned}$$

Here  $w_{x,x+1}(t), x = 0, \dots, N-1$ , are independent standard Brownian motions (with 0 average and diffusion equal to 1). The parameter  $\gamma > 0$  regulates the strength of the random exchange of momenta between the nearest neighbor particles. Observe that by translating  $r_x$  in  $r_x - \rho$  one has the same equations for the new coordinate but with  $\rho = 0$ . So we set  $\rho = 0$  without any loss of generality. The generator of the evolution has the form

$$\begin{aligned} L_N &= \sum_{x=1}^{N-2} (p_{x+1} - p_x)\partial_{r_x} + \sum_{x=2}^{N-2} (r_x - r_{x-1})\partial_{p_x} + r_1\partial_{p_1} - r_{N-2}\partial_{p_{N-1}} \\ &+ \frac{\gamma}{2} \sum_{x=1}^{N-2} X_{x,x+1}^2 + \frac{1}{2} (T_l\partial_{p_1}^2 - p_1\partial_{p_1}) + \frac{1}{2} (T_r\partial_{p_{N-1}}^2 - p_{N-1}\partial_{p_{N-1}}) \end{aligned}$$

where

$$X_{x,x+1} = p_{x+1}\partial_{p_x} - p_x\partial_{p_{x+1}}$$

One can check easily that the Lie algebra generated by these fields and the Hamiltonian part of  $L_N$  has full rank at every point of the state space  $\mathbb{R}^{N-1} \times \mathbb{R}^{N-2}$ . By Hörmander theorem it follows that this operator is hypoelliptic (cf. thm 22.2.1 in [3]), so the stationary measure has a smooth density. We denote with  $\langle \cdot \rangle$  the expectation with respect to the stationary measure. In [2] the existence and uniqueness of this stationary measure is proven. If  $T_l = T_r = T$  this stationary measure is identified as the product gaussian measure of variance  $T$ . If  $T_l \neq T_r$  the stationary state is not Gaussian neither product. Energy is conserved by the bulk part of the dynamics and we have

$$L_N e_x = j_{x-1,x} - j_{x,x+1}$$

with

$$j_{x,x+1} = -r_x p_{x+1} - \frac{\gamma}{2}(p_{x+1}^2 - p_x^2), \quad x = 1, \dots, N-2$$

$$j_{0,1} = \frac{1}{2}(T_l - p_1^2), \quad j_{N-1,N} = -\frac{1}{2}(T_r - p_{N-1}^2)$$

Consequently  $j_{x,x+1}$  is called instantaneous current of energy. Because of stationarity, for any  $x = 1, N-1$  we have

$$\langle j_{x,x+1} \rangle = \langle j_{0,1} \rangle = \langle j_{N-1,N} \rangle$$

Observe that this model does not conserve momentum. This is in fact dissipated and in a Euler scaling hydrodynamic limit there will be no transport of energy. A diffusion of energy is present in the diffusive scaling of space and time, and the corresponding conductivity coefficient can be studied by the transport properties of the stationary state. The following theorems are proven in [2].

**Theorem 1.** For any  $\gamma > 0$

$$\lim_{N \rightarrow \infty} N \langle j_{x,x+1} \rangle = \frac{1}{2}(\gamma + \gamma^{-1})(T_l - T_r).$$

**Theorem 2.** For any  $\gamma > 0$

$$\lim_{N \rightarrow \infty} \frac{1}{N} \langle \mathcal{H}_N \rangle = \frac{1}{2}(T_l + T_r).$$

It is easy to see that the averages of the total kinetic and potential energy are equal. It follows then, as corollary of theorem 2, that the same result is valid for the kinetic and the potential energies, i.e.

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{x=1}^{N-1} \langle p_x^2 \rangle = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{x=1}^{N-2} \langle r_x^2 \rangle = \frac{1}{2}(T_l + T_r)$$

**Theorem 3.** For  $\gamma = 1$  and any bounded function  $G : [0, 1] \rightarrow \mathbb{R}$ , we have

$$\lim_{N \rightarrow \infty} \left\langle \frac{1}{N} \sum_{x=1}^{N-1} G(x/N) e_x \right\rangle = \int_0^1 G(q) T(q) dq$$

where  $T(q) = T_l + (T_r - T_l)q$  is the linear profile interpolating  $T_l$  and  $T_r$ .

Remarks:

- The case  $\gamma = 0$  is exactly the case studied in [5], where the conductivity is proven infinite because of the complete integrability of the bulk dynamics.
- The proof of the results exposed, like the existence and uniqueness of the stationary state, are based on second moment estimates that are obtainable from the conservation properties of the bulk dynamics. If one could prove some higher moment control, much stronger statement will follow, like a law of large number version for the linear profile of temperature.
- In the case  $\gamma = 1$ , a non equilibrium hydrodynamic limit for this model is proven in [1].

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**Perturbation of equilibria: a hydrodynamic limit.**

BENEDEK VALKÓ

(joint work with Bálint Tóth)

We present the results contained in [6]. We consider one-dimensional, locally finite interacting particle systems with two conservation laws which under Eulerian hydrodynamic limit lead to two-by-two systems of conservation laws:

$$\begin{cases} \partial_t \rho + \partial_x \Psi(\rho, u) = 0 \\ \partial_t u + \partial_x \Phi(\rho, u) = 0, \end{cases}$$

with  $(\rho, u) \in \mathcal{D} \subset \mathbb{R}^2$ , where  $\mathcal{D}$  is a convex compact polygon in  $\mathbb{R}^2$ . This may be showed by a standard application of Yau's relative entropy method (see [8, 1, 4] and [5]).

The system is *typically* strictly hyperbolic in the interior of  $\mathcal{D}$  with possible non-hyperbolic degeneracies on the boundary  $\partial\mathcal{D}$ . We consider the case of isolated singular (i.e. non hyperbolic) point on the interior of one of the edges of  $\mathcal{D}$ , call it  $(\rho_0, u_0) = (0, 0)$  and assume  $\mathcal{D} \subset \{\rho \geq 0\}$ . (This can be achieved by a linear transformation of the conserved quantities.) We investigate the propagation of *small nonequilibrium perturbations* of the steady state of the microscopic interacting particle system, corresponding to the densities  $(\rho_0, u_0)$  of the conserved quantities.

We prove that for a very rich class of systems, under proper hydrodynamic limit the propagation of these small perturbations are *universally* driven by the two-by-two system

$$\begin{cases} \partial_t \rho + \partial_x(\rho u) = 0 \\ \partial_t u + \partial_x(\rho + \gamma u^2) = 0 \end{cases}$$

where the parameter  $\gamma := \frac{1}{2}\Phi_{uu}(\rho_0, u_0)$  (with a proper choice of space and time scale) is the only trace of the microscopic structure. The proof is valid for the cases with  $\gamma > 1$ .

The proof relies on the relative entropy method and thus, it is valid only in the regime of smooth solutions of the pde. But there are essential new elements: in order to control the fluctuations of the terms with Poissonian (rather than Gaussian) decay coming from the low density approximations we need to rely on a fine interplay of probabilistic and pde methods. To be able to control the

large fluctuations of the asymptotically Poisson random variables, we need to use a cutoff. It turns out that this is possible by the use of martingale techniques, but only if the cutoff function is of very special form: it has to be a partial derivative of a *Lax entropy* of the pde system in question. Thus we need to construct a Lax entropy with specific properties for a given system which (in theory) is a purely pde problem: it may be solved using straightforward (although a bit lengthy) computations relying on the theory of hyperbolic pde's (see [2, 3]). It is very interesting though, that probability theory helps here as well: a suitable transformation of the thermodynamic entropy of the original microscopic system (in other words: the rate function of joint large deviations of the two conserved quantities) provides the right Lax entropy. The fact, that our proof only works in the  $\gamma \geq 1$  case, comes from this part: for  $\gamma < 1$  our constructed cutoff function is not powerful enough for the fluctuations of the Poisson tail. This can be explained by the shape of the level lines of Riemann invariants for the limiting pde: these are convex for  $\gamma < 1$ , linear for  $\gamma = 1$  and concave for  $\gamma > 1$ . This change of convexity causes a change of behavior from the pde point of view, in particular the Lax-Chuey-Conley-Smoller maximum principle is only applicable for  $\gamma \geq 1$ .

The presented results are complemented by that of [7] where it was shown that perturbations around a hyperbolic equilibrium point are driven by two decoupled Burgers-type equations.

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**Vanishing viscosity term in hydrodynamic description of multispecies driven particle systems with open boundaries**

VLADISLAV POPKOV

(joint work with Gunter M. Schütz)

We consider continuous time Markov processes describing many species particle systems out of thermodynamic equilibrium, which have Bernoulli stationary measure. Two particular examples are:

I. Multilane generalization of the Asymmetric Exclusion process [1]. In this model there are particles hopping along the  $M$  copies of one-dimensional finite lattices. The hoppings between the lattices are excluded so that there are  $M$  particle species each conserving separately.

II. Asymmetric exclusion process with two types of particles, see, e.g., [3]. There is a one-dimensional finite lattice, occupied of particles of two different species  $A, B$ , which exchange with nearest neighbours and the holes with predefined rates. Here the number of species  $M = 2$ .

In both cases, one can prove that macroscopic shocks and rarefaction waves arising in these systems due no nonlinearity, after Euler rescaling of space and time, satisfy the same conditions of stability and existence as the system of hyperbolic conservation law equations (without the right-hand side)

$$(1) \quad \frac{\partial \rho}{\partial t} + \frac{\partial \mathbf{j}(\rho)}{\partial x} = \varepsilon \frac{\partial}{\partial x} \eta(\rho, \frac{\partial \rho}{\partial x}), \quad \text{where } \varepsilon \rightarrow 0$$

according to Lax criteria [8]. The proof is based on the analysis of the local excitations evolution along the in the system within the Markov processes Hamiltonian formalism [2], along the lines of [7], [4]. In (1) we have  $\rho(x, t) = (\rho^1(x, t), \rho^2(x, t), \dots, \rho^M(x, t))$ , where  $\rho^Q(x, t)$  is a coarse-grained density of particles of specie  $Q$  as function of space and time, and  $\mathbf{j}(\rho)$  is the macroscopic flux. The particle system is coupled with boundary reservoirs of the fixed particle densities, see [3], which in hydrodynamic limit become

$$(2) \quad \rho(0, t) = \rho_-; \quad \rho(L, t) = \rho_+;$$

In order to regularize solution of the (1) in presence of the boundaries, we have added a vanishing viscosity term to the right-hand side of it. We are interested in the large time evolution of the particle system and conservation law equations of motion (1), when system reaches a steady state, and in the approach to the steady state. The asymptotic in time evolution of the steady state is governed by the motion of shocks and rarefaction waves, together with boundary layers defined implicitly by the choice of the vanishing viscosity matrix in (1). Several questions arise.

- Does the form of a viscosity term matter?
- How to choose the "physical form" of viscosity term, which selects the physical solution after the interaction with the boundary?

- How to describe an interaction of shocks with the boundary for a given viscosity matrix ?
- Which novel dynamical properties can the viscosity term choice in (1) predict for the physical system with many particle species?

**The form of viscosity matter does matter.** It was demonstrated in [1] by comparing numerical solution of the multilane ASEP model and corresponding conservation law equation that the choice of the vanishing viscosity term is crucial. E.g., a "naive" choice of diagonal unit matrix

$$(3) \quad \varepsilon \frac{\partial^2 \rho}{\partial x^2}$$

used widely in the literature, in the right-hand side of (1) leads to huge inconsistencies, e.g., false phase transitions are predicted. At the same time the "physical" choice, to be discussed later, leads to perfect agreement between the particle model and PDE evolution on Euler scale, as far as numerics can tell.

**How to obtain the "physical" viscosity term.** Our heuristic approach uses averaging, and then mean-field like treatment, of the exact operator equations of motion for particle number operator in the Markov process, explained in [4] for model II, and in [5],[1], for the model I. For example, for the model II it takes the form

$$(4) \quad \begin{aligned} \frac{\partial \rho^A}{\partial t} + \frac{\partial}{\partial x} (j^A(\rho^A, \rho^B)) &= \varepsilon \frac{\partial}{\partial x} \left( \frac{\partial \rho^A}{\partial x} + \left( \frac{\partial \rho^A}{\partial x} \rho^B - \frac{\partial \rho^B}{\partial x} \rho^A \right) \right) \\ \frac{\partial \rho^B}{\partial t} + \frac{\partial}{\partial x} (j^B(\rho^A, \rho^B)) &= \varepsilon \frac{\partial}{\partial x} \left( \frac{\partial \rho^B}{\partial x} + \left( \frac{\partial \rho^B}{\partial x} \rho^A - \frac{\partial \rho^A}{\partial x} \rho^B \right) \right), \end{aligned}$$

where  $j^A(\rho^A, \rho^B) = \rho^A(1 - \rho^A + \rho^B)$ ,  $j^B(\rho^A, \rho^B) = -\rho^B(1 - \rho^B + \rho^A)$ .

#### Boundary eigenvalue equation

Let us determine under which conditions an infinitely small boundary layer at, say, left boundary, will be stationary, for the model II (4). To do this, consider the system of equations (4) on a half-axis  $[0, +\infty)$  with a boundary condition

$$\rho^A(0, t) = \rho_-^A, \quad \rho^B(0, t) = \rho_-^B.$$

We assume that (a) stationary solution has been reached (b) the density profiles are constant with the densities  $r^A, r^B$  except in the  $\varepsilon$ -vicinity of the boundary, where they decay exponentially:  $\rho^A(x) - r^A \sim \exp(-\lambda x/\varepsilon)$ ,  $\rho^B(x) - r^B \sim \exp(-\lambda x/\varepsilon)$ . (c) for all  $x$ ,  $\|\rho^A(x) - r^A\| \ll 1$ ,  $\|\rho^B(x) - r^B\| \ll 1$ . All our assumptions can be justified microscopically for a shock wave which is glued to the boundary. Demanding stationarity  $\partial \rho^A/\partial t = \partial \rho^B/\partial t = 0$ , we get from (4) integrating once:  $j^A(\rho^A(x), \rho^B(x)) = j^A(r^A, r^B) + \varepsilon \frac{\partial \rho^A}{\partial x} + \left( \frac{\partial \rho^A}{\partial x} \rho^B - \frac{\partial \rho^B}{\partial x} \rho^A \right)$ . The Taylor expansion of around the  $\rho_-^A, \rho_-^B$  gives in the first order approximation  $\left( \frac{\partial j^A}{\partial \rho^A} \right)_- \delta \rho^A + \left( \frac{\partial j^A}{\partial \rho^B} \right)_- \delta \rho^B = -\lambda (\delta \rho^A + \rho_-^B \delta \rho^A - \rho_-^A \delta \rho^B)$ , where we denoted  $\delta \rho^A = \rho^A(x) - r^A$ ,  $\delta \rho^B = \rho^B(x) - r^B$ . Here and below the subscript "-" denotes the substitution

$\rho^A, \rho^B \rightarrow \rho_-^A, \rho_-^B$ . Doing the same procedure with the second equation in (4), we obtain

$$(5) \quad (\mathcal{D}\mathbf{j})_- \Psi = \lambda B \Psi = \lambda \begin{pmatrix} 1 + \rho^B & -\rho^A \\ -\rho^B & 1 - \rho^A \end{pmatrix}_- \Psi; \quad \Psi = \begin{pmatrix} \delta\rho^A \\ \delta\rho^B \end{pmatrix}$$

where  $(\mathcal{D}\mathbf{j})$  denotes the Jacobian of the flux  $(\mathcal{D}\mathbf{j})_{kl} = \partial j_k / \partial \rho_l$ .

Note that the system of equations (4), after the substitutions  $\rho = 1 - \rho^A - \rho^B, u = \rho^B - \rho^A$ , becomes **Leroux system**

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) &= \varepsilon \frac{\partial^2 \rho}{\partial x^2}; \quad \frac{\partial u}{\partial t} + \frac{\partial}{\partial x}(\rho + u^2) \\ &= \varepsilon \frac{\partial}{\partial x} \left( \frac{\partial u}{\partial x} + \left( u \frac{\partial \rho}{\partial x} - \rho \frac{\partial u}{\partial x} \right) \right). \end{aligned}$$

The **boundary eigenvalue equation (5) for Leroux system** will correspondingly take the form

$$(6) \quad (\mathcal{D}j)_- \begin{pmatrix} \delta\rho \\ \delta u \end{pmatrix} = \lambda B \begin{pmatrix} \delta\rho \\ \delta u \end{pmatrix}; \quad B = \begin{pmatrix} 1 & 0 \\ u & 1 - \rho \end{pmatrix}_-$$

**Infinite reflections of shock waves from the boundaries.** The eigenvalues  $\Psi$  of the boundary eigenvalue equation (6) determine allowable infinitesimal shifts  $\delta\rho^A$  and  $\delta\rho^B$  away from a fixed boundary values  $\rho_-^A, \rho_-^B$ . The argument can be repeated for the right boundary, leading to the same equations (5) where the substitutions  $\rho^A, \rho^B \rightarrow \rho_+^A, \rho_+^B$  now have to be made. On the other hand, we have an equation for infinitesimal shocks coexistence  $(\mathcal{D}j)\Phi = \mu\Phi$  for the domain away from the boundary layer region. The lines of characteristics defined by the eigenvalues  $\Phi$ , being different from the "boundary" characteristics, defined by the eigenvalues  $\Psi$  of (5), produce an effect of infinite (although converging) reflections of a shock between the boundaries of the system, explained in details in [5], [3] for the models I and II respectively. This phenomenon is generic for the many particle species: in one-species case it never occurs.

The last remark is that with the usual choice of the viscosity term (3) to regularize conservation law equations with the boundaries, the matrices  $B$  from (5),(6) reduce to unit matrix  $B \equiv I$ . In this case, no infinite shocks reflections will be observed.

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### Equivalence of ensembles for two-component zero-range invariant measures

STEFAN GROSSKINSKY

Consider a finite lattice  $\Lambda_L$  of size  $L$ . We are interested in distributions of particles on  $\Lambda_L$  that arise naturally as stationary measures of interacting particle systems. In this area of research systems with several species of conserved interacting components are currently of particular interest [9]. Although our results apply to more general situations, we fix ideas and consider a system with two species of particles, where  $\eta_i(x) \in \mathbb{N} = \{0, 1, \dots\}$  denotes the number of particles of species  $i$  at site  $x$ . The state space of the process  $X_L = (\mathbb{N}^2)^{\Lambda_L}$  is the set of all configurations  $\boldsymbol{\eta} = (\boldsymbol{\eta}(x))_{x \in \Lambda_L}$ , where  $\boldsymbol{\eta}(x) = (\eta_1(x), \eta_2(x))$ .

Suppose that the process has a stationary weight  $w^L \in \mathcal{M}(X_L)$  of product form, that the dynamics conserves the number of particles  $\Sigma_L^i(\boldsymbol{\eta}) \in \mathbb{N}$  and that these are the only conserved quantities. Due to the conservation laws there exists a family of stationary measures for the process which are absolutely continuous w.r.t. the weight  $w^L$  with a density that depends only on the conserved quantities. The set of all stationary measures is convex and the extremal measures are given by choosing the density  $\delta_{\Sigma_L^1, N_1} \delta_{\Sigma_L^2, N_2}$ . This corresponds to fixing the number of particles to  $\mathbf{N} = (N_1, N_2)$ , yielding the canonical ensemble

$$(1) \quad \pi_{L, \mathbf{N}}(\boldsymbol{\eta}) := \frac{1}{Z_{L, \mathbf{N}}} \prod_{x \in \Lambda_L} w(\boldsymbol{\eta}(x)) \delta_{\Sigma_L^1(\boldsymbol{\eta}), N_1} \delta_{\Sigma_L^2(\boldsymbol{\eta}), N_2} .$$

The measures are well defined for each  $\mathbf{N} \in \mathbb{N}^2$  and concentrate on the finite set  $X_{L, \mathbf{N}} \subset X_L$  with (finite) normalization  $Z(L, \mathbf{N})$ . By assumption the process is irreducible on  $X_{L, \mathbf{N}}$  and the canonical measures are unique.

Choosing the density  $e^{\mu_1 \Sigma_L^1} e^{\mu_2 \Sigma_L^2}$  with chemical potentials  $\boldsymbol{\mu} = (\mu_1, \mu_2) \in \mathbb{R}^2$  gives rise to the grand-canonical (or tilted) measures

$$(2) \quad \nu_{\boldsymbol{\mu}}^L(\boldsymbol{\eta}) = \frac{1}{z(\boldsymbol{\mu})^L} \prod_{x \in \Lambda_L} w(\boldsymbol{\eta}(x)) e^{\boldsymbol{\mu} \cdot \boldsymbol{\eta}(x)} .$$

In our case they are of product form and easier to analyze than the canonical measures, which can also be written  $\pi_{L, \mathbf{N}} = \nu_{\boldsymbol{\mu}}^L(\cdot | \Sigma_L^i = N_i, i = 1, 2)$  as conditional measures. Note that the normalizing (site wise) partition function  $z(\boldsymbol{\mu}) = \sum_{\mathbf{k} \in \mathbb{N}^2} w(\mathbf{k}) e^{\boldsymbol{\mu} \cdot \mathbf{k}}$  is in our case an infinite sum in contrast to models with bounded local state space.

The thermodynamic relation  $\mathbf{R} : D_{\boldsymbol{\mu}} \rightarrow (0, \infty)^2$  where  $R_i(\boldsymbol{\mu}) = \langle \eta_i(x) \rangle_{\nu_{\boldsymbol{\mu}}^L}$  gives the expected particle densities as a function of the chemical potentials.  $D_{\boldsymbol{\mu}} \subset \mathbb{R}^n$  is the maximal domain of  $\mathbf{R}$  and  $D_{\rho} = \mathbf{R}(D_{\boldsymbol{\mu}})$  the range.  $\mathbf{R}$  is invertible and we denote the inverse of  $\mathbf{R}$  by  $\mathbf{M} : D_{\rho} \rightarrow D_{\boldsymbol{\mu}}$ .

The question if both ensembles are equivalent in the limit  $L \rightarrow \infty$  has been studied in great generality so far, e.g. when the stationary weight is a translation invariant Gibbs measure or only asymptotic decoupled [8] rather than a product measure. However these results only cover the case of bounded local state space or  $D_\rho = (0, \infty)^2$ . We are interested in the case  $D_\rho \subsetneq (0, \infty)^2$ , which characterizes a condensation transition and arises naturally in the study of zero-range processes (ZRP) [2, 4]. On the other hand these processes are generic realizations, since for any sufficiently regular product weight  $w^L$  there is a corresponding ZRP for which it is stationary [3, 6].

### RESULTS

Using regularity properties of  $D_\mu$  and  $\log z(\boldsymbol{\mu})$ , such as convexity, we can show the expected regularity of  $D_\rho$  and that on the level of chemical potentials a condensation transition is characterized by  $\partial D_\mu \cap D_\mu \neq \emptyset$ . In this case there exists a continuous extension  $\bar{\mathbf{M}} : (0, \infty)^2 \rightarrow D_\mu$  of the thermodynamic relation  $\mathbf{M}(\boldsymbol{\rho})$  which is given by the unique maximizer of the thermodynamic (specific) entropy

$$(3) \quad s(\boldsymbol{\rho}) = \sup_{\boldsymbol{\mu} \in D_\mu} (\boldsymbol{\rho} \cdot \boldsymbol{\mu} - \log z(\boldsymbol{\mu})) .$$

With this extension we can show the equivalence of ensembles even in the case of condensation, using a technique for permutation invariant product measures [1].

**Theorem.** *For every  $\boldsymbol{\rho} \in [0, \infty)^2$  the specific relative entropy vanishes,*

$$(4) \quad \lim_{L \rightarrow \infty} \frac{1}{L} H(\pi_{L, [\boldsymbol{\rho}L]} | \nu_{\bar{\mathbf{M}}(\boldsymbol{\rho})}^L) = 0 .$$

*Therefore the canonical distribution weakly converges to the product measure,*

$$(5) \quad \pi_{L, [\boldsymbol{\rho}L]} \xrightarrow{w} \nu_{\bar{\mathbf{M}}(\boldsymbol{\rho})} , \quad \text{for } L \rightarrow \infty ,$$

*for bounded cylinder test functions. The partition functions converge as*

$$(6) \quad \lim_{L \rightarrow \infty} \frac{1}{L} \log Z(L, [\boldsymbol{\rho}L]) = \log z(\bar{\mathbf{M}}(\boldsymbol{\rho})) - \boldsymbol{\rho} \cdot \bar{\mathbf{M}}(\boldsymbol{\rho}) = -s(\boldsymbol{\rho}) .$$

The proof requires only mild regularity assumptions on the weight  $w$  and the statement allows for the following interpretation for large  $L$ : In the case  $\boldsymbol{\rho} \notin D_\rho$  the system phase separates into a homogeneous background phase with density  $\boldsymbol{\rho}_c(\boldsymbol{\rho}) = \mathbf{R}(\bar{\mathbf{M}}(\boldsymbol{\rho})) \in \partial D_\rho$ , and a condensate of vanishing volume fraction, containing the  $(\boldsymbol{\rho} - \boldsymbol{\rho}_c)L$  excess particles. There can be a condensed phase of only one or both particle species. Under additional assumptions on the weight  $w$  we can show that each of these condensed phases typically consists of a single lattice site for large  $L$ , by showing a law of large numbers for the maximal occupation number as in the single species case [7, 5]. In case of two condensates for both species, a rigorous analysis of their relation remains an interesting open question.

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### The kinetic limit of a system of coagulating Brownian particles

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(joint work with Fraydoun Rezakhanlou)

Understanding the evolution in time of macroscopic quantities such as pressure or temperature is a central task in non-equilibrium statistical mechanics. We study this problem rigorously for a model of mass-bearing Brownian particles that are prone to coagulate when they are close, where the macroscopic quantity in this case is the density of particles of a given mass. Brownian motion arises in the particles of a colloid, due to the random agitation of the much smaller molecules that form the ambient environment. As such, our model could be considered as one of a colloid, where the dominant interaction between particles is that of coagulation. A theoretical discussion of coagulation in colloids was undertaken by Smoluchowski in [4].

In the model that we consider, a large number  $N$  of particles, each carrying some integer-valued mass, are, at some initial time, scattered in  $\mathbb{R}^d$ , whose dimension  $d$  satisfies  $d \geq 3$  for the purposes of this paper. These particles then perform Brownian motions. There is an  $N$ -dependent parameter  $\epsilon$  that specifies the range of interaction of any particle in the model: a pair of particles is liable to coagulate (to form a new particle that combines the mass of the old two) when the distance between the two is of order  $\epsilon$ . The choice of  $\epsilon$  as a function of  $N$  is dictated by insisting that the so-called mean free path is bounded away from zero and infinity in the limit  $N \rightarrow \infty$  of high particle number. (The mean free path is the mean time until the first collision of a particle drawn uniformly at random at the initial time. A scaling that produces a bounded mean free path is called a kinetic limit). Our model incorporates a significant degree of physical realism, absent from earlier work on this type of problem, in the sense that we permit the diffusion rate of the particle to depend on its mass, including the case where this rate is taken to be decreasing in the mass (it is physically reasonable to suppose that the diffusion

rate of a Brownian particle is inversely proportional to the mass). As we will later describe in precise terms, we also introduce a parameter into the mechanism of reaction which allows us to study such reactions over a natural range of their strengths.

We study the macroscopic evolution of this particle system by measuring the density of particles of a given mass  $m$  in the vicinity of a macroscopic location  $x$  and at some time  $t$ . We will prove that, when the initial number of particles is chosen to be high, this density typically evolves as the solution of the Smoluchowski system of PDE,

$$(1) \quad \frac{\partial f_n}{\partial t}(x, t) = d(n)\Delta f_n(x, t) + Q_1^n(f)(x, t) - Q_2^n(f)(x, t) \quad n = 1, 2, \dots$$

with initial data  $f_n(\cdot, 0) = h_n(\cdot)$ , to be specified in more detail shortly. The first term on the right-hand-side of (1) corresponds to the diffusion among particles of mass  $n$ , with  $d(n)$  being one-half of the diffusion rate of such particles. The terms in (1) corresponding to the interaction of pairs of particles are given by the gain term

$$(2) \quad Q_1^n(f)(x, t) = \sum_{m=1}^n \beta(m, n - m) f_m(x, t) f_{n-m}(x, t),$$

and the loss term

$$(3) \quad Q_2^n(f) = 2f_n(x, t) \sum_{m=1}^{\infty} \beta(m, n) f_m(x, t).$$

Here, the collection of constants  $\beta : \mathbb{N}^2 \rightarrow (0, \infty)$  quantify the macroscopic propensity of mass at a pair of values to combine. As well as deriving the system (1) as the typical macroscopic profile of our random model, we prove in this paper the precise relation between the macroscopic constants  $\beta$  and the microscopic mechanism of reaction.

We now give a precise definition of the microscopic process. We in fact define a sequence of such models, indexed according to the initial number  $N$  of particles in them. We define a range of interaction,  $\epsilon$ , according to  $N\epsilon^{d-2} = Z$ , where the exact value of the positive constant  $Z$  will shortly be given. In defining the model, the main elements to describe are the initial random choice of particle locations and masses, the diffusive dynamics, and the mechanism for coagulation.

To describe each of these, we require notation for labelling the particles in this time-dependent model. Let a countable set  $I$  of symbols be given. A configuration  $q$  of particles is an  $\mathbb{R}^d \times \mathbb{N}$ -valued function on a finite subset  $I_q$  of  $I$ . For any  $i \in I_q$ ,  $q(i)$  may be written as  $(x_i, m_i)$ . The particle labelled by  $i$  has mass  $m_i$  and location  $x_i$ . In practice, the index set  $I_q$  will be a function of time, with a change occurring only at collision events, of which there are finitely many in any given sample of one of the random models.

As for the dynamics of the process, the action on  $F$  of the infinitesimal generator  $\mathbb{L}$  is given by

$$(4) \quad (\mathbb{L}F)(q) = \mathbb{A}_0F(q) + \mathbb{A}_CF(q),$$

where  $F : \{\mathbb{R}^d \times \mathbb{N}\}^I \rightarrow [0, \infty)$  denotes a smooth function, its domain being given the product topology. In (4), the diffusion operator  $\mathbb{A}_0$  is given by

$$(5) \quad \mathbb{A}_0 F(q) = \sum_{i \in I_q} d(m_i) \Delta_{x_i} F,$$

while the collision operator  $\mathbb{A}_C$  is specified by

$$(6) \quad \mathbb{A}_C F(q) = \sum_{i,j \in I_q} \epsilon^{-2} V\left(\frac{x_i - x_j}{\epsilon}\right) \alpha(m_i, m_j) \\ \times \left[ \frac{m_i}{m_i + m_j} F(S_{i,j}^1 q) + \frac{m_j}{m_i + m_j} F(S_{i,j}^2 q) - F(q) \right].$$

Here,

- the collection of constants  $\alpha : \mathbb{N}^2 \rightarrow [0, \infty)$  are the parameters of strength of interaction between pairs of particles of given integer mass, to which we earlier alluded.
- the function  $V : \mathbb{R}^d \rightarrow [0, \infty)$  is assumed to be continuous, of compact support, and with  $\int_{\mathbb{R}^d} V(x) dx = 1$ . Its role is to include among the models we consider a rule for coagulation time that may be rather arbitrary, beyond the insistence that it be Markovian and cause reaction of a pair of particles at some time when this pair are to be found within an order of the range of interaction  $\epsilon$ .
- we denote by  $S_{i,j}^1 q$  that configuration formed from  $q$  by removing the indices  $i$  and  $j$  from  $I_q$ , and adding a new index from  $I$  to which  $S_{i,j}^1 q$  assigns the value  $(x_i, m_i + m_j)$ . The configuration  $S_{i,j}^2 q$  is defined in the same way, except that it assigns the value  $(x_j, m_i + m_j)$  to the new index. The specifics of the collision event then are that the new particle appears in one of the locations of the two particles being removed, with the choice being made randomly with weights proportional to the mass of the two colliding particles.

The choice of the value of the constants  $\alpha : \mathbb{N}^2 \rightarrow [0, \infty)$  transmits to the macroscopic reaction propensities appearing in the interaction terms (2) and (3) of the Smoluchowski PDE. The recipe for determining  $\beta$  from  $\alpha$  is as follows: there exists a solution  $u = u_{n,m} : \mathbb{R}^d \rightarrow (0, \infty)$  of the equation

$$(7) \quad \Delta u_{n,m}(x) = \frac{\alpha(n, m)}{d(n) + d(m)} V(x) [1 + u_{n,m}(x)]$$

that is unique subject to the decay condition  $u_{n,m}(x) = O(|x|^{2-d})$  as  $|x| \rightarrow \infty$ . The quantities  $\beta : \mathbb{N} \times \mathbb{N} \rightarrow (0, \infty)$  in (1) are then specified by the formula

$$(8) \quad \beta(n, m) = \alpha(n, m) \int_{\mathbb{R}^d} V(x) (1 + u_{n,m}(x)) dx.$$

Our main result is conveniently expressed in terms of the empirical measures on the locations of particles of a given mass. For each  $n \in \mathbb{N}$  and  $t \in [0, \infty)$ , we



write  $g_n(dx, t)$  for the measure on  $\mathbb{R}^d$  given by

$$g_n(dx, t) = \varepsilon^{d-2} \sum_{i \in I_q(t)} \delta_{x_i(t)}(dx) \mathbb{1}(m_i(t) = n).$$

We also require a mild hypothesis on the diffusion coefficients  $d : \mathbb{N} \rightarrow (0, \infty)$ . Namely, we suppose that there exists a function  $\gamma : \mathbb{N}^2 \rightarrow (0, \infty)$  such that  $\alpha \leq \gamma$ , with  $\gamma$  satisfying

$$(9) \quad n_2 \gamma(n_1, n_2 + n_3) \max \left\{ 1, \left[ \frac{d(n_2 + n_3)}{d(n_2)} \right]^{\frac{3d-2}{2}}, \left[ \frac{d(n_2 + n_3)}{d(n_2)} \right]^{2d-1} \right\} \\ \leq (n_2 + n_3) \gamma(n_1, n_2).$$

In addition, we need some moderate hypotheses on the way in which the particles are scattered at the initial time. See [2] for details. We now state our main result, whose proof is also presented in [2].

**Theorem 1.** *Let  $d \geq 3$ . Let  $J : \mathbb{R}^d \times [0, \infty) \rightarrow \mathbb{R}$  be a bounded and continuous test function. Then, for each  $n \in \mathbb{N}$  and  $t \in (0, \infty)$ ,*

$$(10) \quad \limsup_{N \rightarrow \infty} \mathbb{E}_N \left| \int_{\mathbb{R}^d} J(x, n, t) (g_n(dx, t) - f_n(x, t) dx) \right| = 0,$$

where we recall that  $\varepsilon$  is related to  $N$  by means of the formula  $N\varepsilon^{d-2} = Z$ , with the constant  $Z \in (0, \infty)$  being given by the expression  $Z = \sum_{n \in \mathbb{N}} \int_{\mathbb{R}^d} h_n$ . In (10),  $\{f_n : \mathbb{R}^d \times [0, \infty) \rightarrow [0, \infty), n \in \mathbb{N}\}$  denotes a weak solution to the system of partial differential equations (1), with the collection of constants  $\beta : \mathbb{N}^2 \rightarrow [0, \infty)$  being given by (8).

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### Relative entropy in hyperbolic relaxation

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Consider the system of hyperbolic equations with stiff relaxation terms

$$(1) \quad \partial_t U + \sum_{\alpha} \partial_{\alpha} F_{\alpha}(U) = \frac{1}{\varepsilon} R(U),$$

where  $R, F_{\alpha} : \mathbb{R}^N \rightarrow \mathbb{R}^N$ ,  $\alpha = 1, \dots, d$ , are smooth, defining the evolution of a state vector  $U(x, t) : \mathbb{R}^d \times \mathbb{R}^+ \rightarrow \mathbb{R}^N$ . It is assumed that (1) is equipped with a set of  $n$  conservation laws,

$$(2) \quad \partial_t \mathbb{P}U + \sum_{\alpha} \partial_{\alpha} \mathbb{P}F_{\alpha}(U) = 0,$$

for the conserved quantities  $u = \mathbb{P}U$ . Here,  $\mathbb{P} : \mathbb{R}^N \rightarrow \mathbb{R}^n$  is a projection matrix with rank  $\mathbb{P} = n$  which determines the conserved quantities and annihilates the vector field  $R$ , that is  $\mathbb{P}R(U) = 0$ . It is also assumed that the equilibrium solutions of  $R(U) = 0$  are parameterized in terms of the conserved quantities  $U_{eq} = M(u)$ ; these functions will be called Maxwellians. Under the above framework it is conceivable that the dynamics of  $u(x, t) : \mathbb{R}^d \times \mathbb{R}^+ \rightarrow \mathbb{R}^n$  in the hyperbolic limit  $\varepsilon \rightarrow 0$  is described by the system of conservation laws

$$(3) \quad \partial_t u + \sum_{\alpha} \partial_{\alpha} \mathbb{P}F_{\alpha}(M(u)) = 0$$

Motivated by the structure of models in kinetic theory, it has been postulated in [2] that relaxation systems (1) be equipped with a globally defined, convex entropy  $H(U)$  satisfying

$$(4) \quad \partial_t H(U) + \sum_{\alpha} \partial_{\alpha} Q_{\alpha}(U) - \frac{1}{\varepsilon} \frac{\partial H}{\partial U}(U) \cdot R(U) = 0$$

with positive dissipation. This amounts to the conditions

$$(5) \quad \begin{aligned} \nabla^2 H \nabla F_{\alpha} &= (\nabla F_{\alpha})^T \nabla^2 H, \quad \alpha = 1, \dots, d, \\ \frac{\partial H}{\partial U}(U) \cdot R(U) &\leq 0, \quad \forall U \in \mathbb{R}^N. \end{aligned}$$

Convex entropies play a stabilizing role in relaxation in accordance with kinetic theory and thermodynamical considerations.

The objective of this work is to produce a relative entropy identity for general relaxation systems. Our work is motivated by computations at the level of specific relaxation systems [5] or kinetic BGK-system [1], and our aim is to extend in the case of relaxation system a well-known computation [3, 4] for comparing a weak solution and a smooth solution of a system of conservation laws. We note that the usual convergence framework for relaxation limits proceeds through analysis of the linearized (collision or relaxation) operator. By contrast, a relative entropy identity provides a simple and direct convergence framework in the smooth regime. The relative entropy computation hinges on entropy consistency, that is that the

restriction of  $H - Q$  on Maxwellians induces an entropy - entropy flux pair for the equilibrium system (3) in the form

$$(6) \quad \eta(u) = H(M(u)), \quad q(u) = Q(M(u)).$$

This structure is natural for models that have a thermodynamic origin, it is directly motivated by the formal Hilbert expansion for the relaxation limit (1), and has an interpretation in terms of the Gibbs principle.

In equilibrium statistical mechanics, the Gibbs principle states that equilibrium configurations achieve the maximum entropy under the existing constraints. (In statistical mechanics the entropy is the negative of the quantity considered here, and thus maxima become minima and accordingly production becomes dissipation). It suggests to define the entropy of a subsystem by the minimization procedure  $s(u) = \min_{\mathbb{P}U=u} H(U)$ . For  $H$  convex the resulting  $s$  is also convex. Moreover the orthogonality condition  $\frac{\partial H}{\partial U}(M(u)) \perp N(\mathbb{P})$ , resulting from the relaxation framework, induces that the minimizers satisfy  $s(u) = H(M(u)) = \min_{\mathbb{P}U=u} H(U)$ .

Under such framework a relative entropy identity is computed, valid between *smooth* solutions  $U$  of the relaxation system (1) and *smooth* solutions  $\hat{u}$  of the associated equilibrium dynamics (3). It has the form

$$(7) \quad \begin{aligned} \partial_t H_r + \sum_{\alpha} \partial_{\alpha} Q_{\alpha,r} - \frac{1}{\varepsilon} \left( \frac{\partial H}{\partial U}(U) - \frac{\partial H}{\partial U}(M(u)) \right) \cdot (R(U) - R(M(u))) \\ = - \sum_{\alpha} \nabla_u^2 \eta(\hat{u}) \partial_{\alpha} \hat{u} * \left( g_{\alpha}(u) - g_{\alpha}(\hat{u}) - \nabla g_{\alpha}(\hat{u})(u - \hat{u}) \right) \\ - \sum_{\alpha} \nabla_u^2 \eta(\hat{u}) \partial_{\alpha} \hat{u} * \mathbb{P}(F_{\alpha}(U) - F_{\alpha}(M(u))) \end{aligned}$$

where

$$\begin{aligned} H_r &= H(U) - H(M(\hat{u})) - \frac{\partial H}{\partial U}(M(\hat{u})) \cdot (U - M(\hat{u})) \\ Q_{\alpha,r} &= Q_{\alpha}(U) - Q_{\alpha}(M(\hat{u})) - \frac{\partial H}{\partial U}(M(\hat{u})) \cdot (F_{\alpha}(U) - F_{\alpha}(M(\hat{u}))) \end{aligned}$$

are the relative entropy and associated fluxes respectively, while

$$g_{\alpha}(u) = \mathbb{P}F_{\alpha}(M(u))$$

is the flux in (3).

The identity (7) yields convergence of (1) to (3) in the smooth regime provided that the entropy dissipation of the relaxation system satisfies the hypothesis

$$(8) \quad - \left( \frac{\partial H}{\partial U}(U) - \frac{\partial H}{\partial U}(M(u)) \right) \cdot (R(U) - R(M(u))) \geq \nu |U - M(u)|^2$$

and the entropy  $H$  is strictly convex (see [6] for the details). The hypothesis (8) is fulfilled for many relaxation and discrete BGK systems. In the case of the Boltzmann equation, the analog of (8) goes by the name Cercignani conjecture, and its validity has been extensively investigated in [7].

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**Linear transport equations with fast scales**

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(joint work with François James)

We investigate the case of models with a fast and a slow dynamics (which is found in many physical modelling). This usually leads to a differential system of the following kind

$$(1) \quad \frac{d}{dt} X_\varepsilon = \frac{1}{\varepsilon} a(X_\varepsilon(t)) + b(X_\varepsilon(t)), \quad X_\varepsilon(0) = x_0.$$

The unknown function is  $X_\varepsilon \in C^1(\mathbb{R}, \Pi^n)$  (with  $\Pi^n$  the torus in dimension  $n$ ), the parameter  $\varepsilon > 0$  is very small and  $a$  and  $b$  are given by the problem but are in general very regular (say at least Lipschitz continuous from  $\Pi^n$  to  $\Pi^n$ ). Moreover the flow is often measure preserving (because the system is hamiltonian for instance) and therefore a natural (though somewhat more demanding) condition is that

$$(2) \quad \operatorname{div} a = 0.$$

When  $\varepsilon$  is very small, computing numerically (1) is very expensive (all the more since  $n$  may be relatively large). The equation also typically exhibits many oscillations and it seems much more reasonable to try to find and solve a limiting problem with, in some sense, averaged trajectories. On the other hand, it is well known that Eq. (1) is equivalent to the following linear transport equation

$$(3) \quad \begin{aligned} \partial_t f_\varepsilon + b(x) \cdot \nabla_x f_\varepsilon + \frac{1}{\varepsilon} a(x) \cdot \nabla_x f_\varepsilon &= 0, \\ f_\varepsilon(t = 0, x) &= f^0(x). \end{aligned}$$

For instance if  $f^0$  is the indicatrix function of a set  $E$ , then  $f_\varepsilon(t, \cdot)$  is the indicatrix function of  $E_t$  where  $E_t$  is the image of  $E$  through the flow defined by (1). Moreover thanks to (2), all  $L^p$  norms of  $f_\varepsilon$  are preserved by (3). It is consequently very easy

to pass to the limit in (3). Taking  $f^0$  in  $L^2(\Pi^n)$ , we first obtain that any weak limit  $f$  of  $f_\varepsilon$  satisfies

$$(4) \quad f \in K = \{g \in L^2(\Pi^n) \mid a(x) \cdot \nabla_x g = 0\}.$$

Then there exists  $h$  in  $H^{-1}([0, T] \times \Pi^n)$  with ( $P_K$  being the orthogonal projection on  $K$  in  $L^2$ )

$$(5) \quad \begin{aligned} \partial_t f + b(x) \cdot \nabla_x f &= h, \\ f(t=0) &= P_K f^0, \end{aligned}$$

and

$$(6) \quad \forall \phi \in K \cap H^1([0, T] \times \Pi^n), \quad \int \phi(t, x) h(t, x) dx dt = 0.$$

In some cases, one may prove that the function  $f$  is uniquely defined by (4), (5) and (6). However this is not the case in general and in addition it is easy to find simple counterexamples for which the weak limit of  $f_\varepsilon$  is not unique. For instance take  $n = 3$ ,  $b = (1, 0, 0)$  and  $a = (0, 1, x_1 \mathbb{I}_{0 \leq x_1 \leq 1} + (2 - x_1) \mathbb{I}_{1 \leq x_1 \leq 2})$ . As the first coordinate ( $x_1$ ) is invariant under the fast scale, we may work in  $\mathbb{R} \times \Pi^{n-1}$ . Then if the support of  $f^0$  lies in the set  $-1 < x_1 < 0$ , we may easily compute that for  $t > 3$ ,

$$f_\varepsilon(t, x) = f^0(x_1 - t, x_2 - t/\varepsilon, x_3 - 1/\varepsilon).$$

Thus extracting subsequences  $\varepsilon_n$  such that  $1/\varepsilon_n$  converges in the torus  $[0, 1]$ , we find as many limits. As a consequence, the main issue can be formulated as whether, among all possible limits, one makes more sense (from a physical or mathematical point of view). We investigate this in a simplified situation containing the previous example, described below. First take  $b = (1, 0, \dots, 0)$ ,  $a = (a_1(x), \dots, a_n(x))$  with  $a_1 = 0$ . Then for each value of  $x_1$  (or almost each value to avoid the singular cases), we may define a kernel  $K_{x_1}$  by

$$K_{x_1} = \{g \in L^2(\Pi^{n-1}) \mid a(x_1, x') \cdot \nabla_{x'} g = 0\}.$$

Assuming that  $K_{x_1}$  is piecewise constant (not  $a$ , see the example above), the structure of all possible limits is explicit (the right hand side  $h$  being a sum of Dirac masses in  $x_1$  supported at the points where  $K_{x_1}$  changes). And it is also possible to define and select the “right” limit.

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