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Classical and Quantum Mechanical Models of Many-Particle Systems

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Abstract. The topic of this meeting were non-linear partial differential and integro-differential equations (in particular kinetic equations and their macroscopic/fluid-dynamical limits) modeling the dynamics of many-particle systems with applications in physics, engineering, and mathematical biology. Typical questions of interest were the derivation of macro-models from micro-models, the mathematical analysis (well-posedness, stability, asymptotic behavior of solutions), and –to a lesser extend– numerical aspects of such equations.

Mathematics Subject Classification (2000): 35Qxx, 82Cxx, 82B40, 81S30.

Introduction by the Organisers

The Oberwolfach meeting described here aimed at presenting the latest mathematical results in the field of kinetic theory (both classical and quantum).

There were 50 participants, among which 15 young participants (PhD students, post-docs or young assistant professors). Two of them (M.-P. Gualdani and R. Strain) were invited within the program "US Junior Oberwolfach Fellows" : they are promising young researchers working in the US.

The program of the meeting was made in such a way that a lot of time remained for people to meet informally and discuss about scientific issues. It also ensured that almost everybody attended all (or most of) the scheduled talks .

The program was structured in the following way : three subtopics were defined (relationships between micro/meso/macroscopic models ; kinetic theory for complex particles : granular media, coagulation/fragmentation, chemotaxis and sprays ; quantum mechanical kinetic theory). For each subtopic, there were a few (2 or 3) longer talks (about 40 minutes) by senior participants. For those talks,

a specific effort of clarity was asked to the speakers, and the subject had to be rather broad.

Then, shorter talks of about 20 minutes were planned , on more specialized issues. Finally, a special (much longer) talk in two parts was presented by one of the participants (C. Villani), in order to describe in a very didactical way an emerging link between kinetic theory, optimal transport, and Riemannian geometry.

Some participants did not give a talk within this program, but organized an informal discussion around a poster, with an audience composed of specially interested people.

Here is a brief description of each of the subtopics.

(1) Much attention has been given to the passage from microscopic to mesoscopic models, and the latest breakthroughs in this subdomain have been described. The talks by R. Esposito, F. Golse and P.-E. Jabin are representative of this line of ideas. The question related to the Boltzmann equation and its macroscopic limit have also been presented, like for example in the works by A. Bobylev and H. S. Yu. This last talk is typical of the new and brilliant ideas recently introduced by the Asiatic research groups on kinetic equations.

(2) Many talks have been devoted to the study of kinetic equations for complex particles, showing the interest of the mesoscopic description in many models. The use of entropy methods in these new fields of application has led to interesting and unexpected results, as shown in the talks by J. Carrillo or K. Fellner.

(3) Finally, the asymptotics of quantum mechanical models has played a central role in this meeting, and in particular the rigorous derivation of (simplified) one-particle models from many-particle systems. A typical example of this research line was presented in the talk of L. Erdös on the derivation of the Gross-Pitaevskii equation for Bose-Einstein condensates.

We finally would like to emphasize the ideas and trends which have emerged within the two or three last years and which have been present in this Oberwolfach meeting : a new approach of the relations between the hydrodynamic and non hydrodynamic part of the Boltzmann equation; explicit estimates for the spectrum of the linearized Boltzmann equation when the kernel is singular; the treatment of coagulation/fragmentation equations as infinite-dimensional reaction-diffusion equations with the help of entropy methods; the use of the ideas of kinetic theory in fields coming out from the industry rather than from theoretical physics (supply chains, industrial sprays, etc.).

Workshop: Classical and Quantum Mechanical Models of Many-Particle Systems

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Abstracts

The Spatially Inhomogeneous Aizenman-Bak model: Convergence to Equilibrium and Fast-Reaction Limit

Klemens Fellner
(joint work with Jose A. Carrillo, Laurent Desvillettes)

The Aizenman-Bak model for reacting polymers is considered for spatially inhomogeneous situations in which polymers diffuse in space with a non-degenerate size-dependent coefficient. Denoting $f = f(t,x,y)$ the concentration of polymers/clusters with length/size $y \geq 0$ at time $t \geq 0$ and point $x \in \Omega \subset \mathbb{R}^d$, $d \geq 1$, we consider

$$\partial_t f - a(y) \triangle_x f = Q(f,f)\,. \tag{1}$$

The polymers/clusters are confined in a smoothly bounded domain Ω (with normalized volume $|\Omega| = 1$) satisfying homogeneous Neumann boundary conditions. We assume the diffusion coefficient $a(y)$ to be non-degenerate in the sense that there exist $a_*, a^* \in \mathbb{R}^+$ such that

$$0 < a_* \leq a(y) \leq a^*. \tag{2}$$

The reaction term $Q(f,f)$ of (1) models chemical degradation – break-up or fragmentation – and polymerization – coalescence or coagulation – of polymers or clusters, respectively. More precisely, the full collision operator reads as

$$Q(f,f) = Q_c^+(f,f) - Q_c^-(f,f) + Q_b^+(f,f) - Q_b^-(f,f)$$

where we have

- Coalescence of clusters of size $y' \leq y$ and $y - y'$ results into clusters of size y:
$$Q_c^+(f,f) := \int_0^y f(t,x,y-y')f(t,x,y')\,dy'.$$
- Polymerization of clusters of size y with other clusters of size y' produces a loss in its concentration:
$$Q_c^-(f,f) := 2f(t,x,y)\int_0^\infty f(t,x,y')\,dy'.$$
- Break-up of clusters of size y' larger than y contributes to create clusters of size y:
$$Q_b^+(f,f) := 2\int_y^\infty f(t,x,y')\,dy'.$$
- Break-up of polymers of size y reduces its concentration:
$$Q_b^-(f,f) := y\,f(t,x,y).$$

This kind of models finds its application not only in polymers and cluster aggregation in aerosols [9, 10, 1, 2, 4] but also in cell physiology [7], population dynamics [6] and astrophysics [8]. Here, fragmentation and coagulation kernels are all set up to constants as in the original Aizenman-Bak model [1].

We demonstrate that the entropy-entropy dissipation method applies directly in this inhomogeneous setting giving not only the necessary basic a priori estimates to start the smoothness and size decay analysis in one dimension, but also (for constant diffusion coefficient in any spatial dimension or for non-degenerate diffusion in dimension one) the exponential convergence towards global equilibria

$$f_\infty = e^{-\frac{y}{\sqrt{N_\infty}}}\,, \tag{3}$$

uniquely determined due to the conservation of the total number of monomers

$$\int_\Omega \int_0^\infty y\, f(t,x,y)\, dy\, dx = \int_\Omega N(t,x)\, dx = \int_\Omega N(t=0,x)\, dx := N_\infty > 0\,. \tag{4}$$

Theorem 1 ([3])**.** *Let Ω be $(0,1)$ with diffusion coefficients satisfying* (2) *or let $\Omega \subset \mathbb{R}^d$, $d \geq 1$ with $a(y) = a > 0$ being constant. Assume nonnegative initial data $f_0 \neq 0$ such that $(1 + y + \ln f_0) f_0 \in L^1((0,1) \times (0,\infty))$.*

Then, the global weak solutions (see [5]*) $f(t,x,y)$ of* (1) *decay exponentially to the global equilibrium state* (3) *with explicitly computable constants C_1, C_2 and rate α, both in global relative entropy and in the $L^1_{x,y}$ sense :*

$$\|f(t,\cdot,\cdot) - f_\infty\|_{L^1_{x,y}} \leq C_2\, e^{-\frac{\alpha}{2}\, t} \tag{5}$$

for all $t \geq 0$, where f_∞ is defined by (3) and $N_\infty > 0$ is determined by the conservation of mass (4)*.*

Up to our knowledge, this is the first result of explicit equilibration rates for spatially inhomogeneous coagulation-fragmentation models.

We show further that solutions in the one dimensional case are immediately smooth in time and space while in size distribution solutions are decaying faster than any polynomial, i.e.

$$\int_0^\infty (1+y)^q\, \|f(t,\cdot,y) - f_\infty(y)\|_{L^\infty_x}\, dy \leq C_3\, e^{-\alpha\, t}\,,$$

for all $t \geq t_*$, $t_* > 0$ and $q \geq 0$, and explicitly computable constants $C_3, \alpha > 0$.

Secondly, in a work in progress, we consider the inhomogeneous Aizenman-Bak model rescaled for fast reactions

$$\partial_t f^\varepsilon - a(y)\, \partial_{xx} f^\varepsilon \;=\; \frac{1}{\varepsilon} Q(f^\varepsilon, f^\varepsilon)\,.$$

Letting formally $\varepsilon \to 0$ we expect $f^\varepsilon \to f^0$ satisfying $Q(f^0, f^0) = 0$, i.e. $f^\varepsilon \to e^{-y/\sqrt{N^0}}$, where the limiting density $N^0(t,x)$ satisfies a nonlinear non-degenerate diffusion equation being the limit of the conservation law of the mass density :

$$\partial_t N^0 - \partial_{xx}\, n(N^0) = 0\,,$$

where $n(N)$ denotes the function $n(N) = \int_0^\infty a(z\sqrt{N}) z e^{-z}\, dz$.

In making the limit rigorous, we exploit the entropy dissipation as well as the properties of the limiting equation. So far, to prove convergence, we have to assume a uniform lower and upper bound on the number density of the polymer distribution.

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Reaction–diffusion equations for gas mixtures in a host medium

Marzia Bisi

There exists an ample literature about the uneasy problem of a consistent quantitative description of chemically reacting rarefied flows starting from a kinetic approach. By extending usual methods of kinetic theory, it is possible to write down integro-differential Boltzmann-like equations for the evolution of the distribution functions for each participating species. In some recent papers on the subject [1, 2], we assume that the rarefied reacting mixture is not an isolated system, but it is diffusing in a much denser medium, considered as a fixed background, whose evolution is not influenced by collisions with atoms/molecules, and that is taken to be in local thermodynamic equilibrium, with prescribed density, mass velocity, and temperature. First of all we have considered a mixture of four species, undergoing a bimolecular reversible chemical reaction, and elastic collisions both with field particles and between the species themselves. After deriving kinetic equations for the distribution functions, we analyze the hydrodynamic limit in the collision dominated regime. To this aim, as usual in kinetic theory, we analyze the reactive Boltzmann equations in dimensionless form: the main effect of the

adimensionalization is the appearance of some ratios involving the different scales that measure the relative importance of each operator during the evolution of the mixture. Such ratios can be expressed in terms of a small parameter, typically a proper Knudsen number, and the sought hydrodynamic closure can be achieved by a suitable asymptotic procedure with respect to such parameter. We assume that the elastic scattering with the background medium, much denser than the other species, plays a crucial role, so that the linear elastic operators are taken as dominant in driving the process. Reactive processes are assumed less frequent than elastic scattering, since reactions involve more complicated microscopic effects such as change of chemical nature and mutual exchange of internal energy. A formal asymptotic analysis of this system leads, at the macroscopic level, to a closed set of reaction–diffusion equations for number densities of single species, with diffusion coefficients depending on elastic collision frequencies and background temperature. The passage from the kinetic level to the macroscopic equations may be proved in a mathematically rigorous way in a special (linear) case in which the existence of solutions to the kinetic equations is known [1].

The whole procedure may then be extended to more involved chemical frameworks, including very important and common reactive processes, like reactions of dissociation and recombination, one of the essential ingredients characterizing diatomic gases in the air. According to the model proposed in [3], a diatomic gas is described as a mixture of three interacting species: atoms, stable diatomic molecules, and unstable molecules, the latter playing the role of a transition state. Stable and unstable molecules are endowed with their own internal energies. Both atoms and stable molecules undergo binary reversible elastic collisions with other atoms, stable molecules and background particles, whereas unstable molecules are not involved in elastic scattering, since they are characterized by a very small mean lifetime and rapidly disappear through a (fast) chemical reaction. In this model one assumes that two atoms can form a stable molecule passing through the transition state, whose de-excitation occurs via an inelastic scattering process. Conversely, both stable and unstable diatomic molecules may dissociate into two atoms. All encounters fulfill conservation of mass, momentum, and internal (thermal plus chemical) energy. Reactive collisions are described in terms of the so-called scattering kernel formulation of the Boltzmann equation, involving collision frequencies and transition probabilities. In the dimensionless kinetic equations, chemical operators involving the unstable molecules are supposed significantly faster than other chemical processes, consistently with the role played by transition state molecules in the present physical model. At the macroscopic level we get again a closed set of reaction-diffusion equations for the densities of the two stable species [2], of course more complicated than the ones derived in [1], with reactive contributions involving also rational functions of the densities themselves. Analysis of other meaningful scalings, as well as some rigorous investigation, are scheduled as future work.

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Optimal transport in non-smooth Riemannian geometry

Cédric Villani

This talk was concerned with the connection between kinetic theory, optimal transport, and Riemannian geometry from a geometric perspective. In the joint work with Otto [3], we had given heuristic arguments in favor of the following conjecture. Take a smooth Riemannian manifold, and for any probability density on it, define the H-functional, or (negative) entropy, with the usual Boltzmann-Shannon formula. Then this functional is displacement convex, in the sense that it is convex along geodesics of optimal transport, as soon as the Ricci curvature is nonnegative everywhere. This conjecture was rigorously proven by Cordero-Erausquin, McCann and Schmuckenschläger in a very interesting paper ([1]). Then Sturm and von Renesse ([4]) noticed that there is actually equivalence between that displacement convexity property, and the nonnegativity of the Ricci curvature (there is a more general statement: K-displacement convexity is equivalent to Ricci being bounded below by K). This simple remark was of great conceptual importance because it opened the door to a possible synthetic treatment of Ricci curvature bounds in terms of optimal transport tools, that are very robust. In a joint work with John Lott [2], we explored these connections in the setting of length spaces, defining what it means for a measured length space to have Ricci curvature bounded below by K, and showing that this concept is stable under measured Gromov-Hausdorff convergence. There is another criterion saying that, in some sense, "dimension is less than N and Ricci curvature is nonnegative". Our generalized notions are also strong enough to imply several famous inequalities such as generalized spectral gap, Sobolev, logarithmic Sobolev, Bishop-Gromov, or a weak form of the Bonnet-Myers theorem. For details cf. [2].

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Asymptotic analysis of the strongly confined, nonlinear, Schrödinger equation

François Castella
(joint work with N. Ben Abdallah and F. Méhats)

We consider a gas of quantum particles described by a nonlinear Schrödinger equation. The gas is assumed confined both in the horizontal, x direction ($x = (x_1, x_2) \in \mathbb{R}^2$) and in the vertical z direction ($z \in \mathbb{R}$), the latter confinement being much stronger than the former. In the idealized limit when the vertical confinement becomes infinitely strong, the goal of this work is to find a reduced dynamics for the electronic gas in the horizontal x plane, upon averaging out the strong oscillations of the wave function induced by the confinement in z.

The key point is, we perform the averaging procedure upon observing that the induced oscillations naturally occur in an *almost-periodic* fashion in time: this allows us, amongst others, to average out the oscillations *without* dealing with any small denominator difficulties. In this way we extend to the general case previous studies that were restricted to the case of only *one* oscillation.

Let us come to some technical details.

Let $V_c(z)$ and $V(x)$ be two smooth, confining potentials, and $F \in C^\infty(\mathbb{R}, \mathbb{R})$ be a given nonlinearity. Define the two Hamiltonians $H_z = -\Delta_z + V_c(z)$ and $H_x = -\Delta_x + V(x)$, and consider the scaled nonlinear Schrödinger equation

$$i\partial_t \psi_\epsilon(t,x,z) = H_x \psi_\epsilon + \frac{1}{\epsilon} H_z \psi_\epsilon + F\left(|\psi_\epsilon|^2\right)\, \psi_\epsilon, \tag{1}$$

supplemented with a smooth initial datum. Here, ϵ is a small parameter measuring the relative strength of the confinement in the z direction, and we wish to perform the limit $\epsilon \to 0$ in (1).

The first, naive, idea, to perform the desired limit, lies in projecting (1) over the eigenbasis of H_z, i.e. over the $\chi_p(z)$'s solution to $H_z\chi_p(z) = E_p\chi_p(z)$ (the E_p's are the eigenenergies of H_z). Upon defining the projected quantities $\psi_p^\epsilon(t,x) := \langle \psi_\epsilon\,,\, \chi_p\rangle$ where $\langle u\,,v\rangle := \int u\,\overline{v}\,dz$, and upon filtering out the time oscillations of the $\psi_p^\epsilon(t,x)$'s through the introduction of $\phi_p^\epsilon(t,x) := \exp(+itH_z/\epsilon)\,\psi_p^\epsilon(t,x)$, it is readily seen that the ϕ_p^ϵ's satisfy the following system of nonlinear, coupled PDE's

$$\begin{aligned} &i\partial_t \phi_p^\epsilon(t,x) = \\ &H_x\phi_p^\epsilon + \sum_{r\geq 0} \phi_r^\epsilon \times \mathrm{e}^{-it\frac{E_r-E_p}{\epsilon}} \left\langle F\left(\left|\sum_{q\geq 0} \phi_q^\epsilon(t,x)\chi_q(z)\mathrm{e}^{-it\frac{E_q}{\epsilon}}\right|^2\right)\,,\, \overline{\chi_r}\chi_p\right\rangle. \end{aligned} \tag{2}$$

Passing to the limit directly in equation (2) causes two types of difficulties. On the one hand, it leads to obvious *small denominator* difficulties. In the case when $F(u) = u$ for instance, it leads to the necessity of controlling terms of the form $1/(Eq - E_s + E_r - E_p)$ on the set $Eq - E_s + E_r - E_p \neq 0$, for large values of the integers (r,s,q,p). This task is not to be completed in general (*i.e.* for a general

confining Hamiltonian H_z). On the other hand, it also leads to controlling the decay, as (r, s, q, p) go to infinity, of terms of the form $\langle \chi_q \chi_r \, , \, \chi_s \chi_p \rangle$, say, and the analysis requires such terms be reasonably summable at infinity. In order obtain such estimates, the natural orthogonality of the eigenfunctions χ_p turn out not to be enough to obtain any reasonable decay estimate at infinity.

To overcome these difficulties, some authors restricted their study to the case where the initial datum in (1) is of the form $\psi_\epsilon(t = 0, x, z) = \phi_0^\epsilon(t = 0, x)\chi_0(z)$, *i.e.* only the *lower* energy level is switched on at the initial time. In that case indeed, it is possible to prove at once, using an energy estimate, that ψ_ϵ remains of the form $\psi_\epsilon(t, x, z) = \phi_0^\epsilon(t, x)\chi_0(z) + \text{small}$, *i.e.* ψ_ϵ remains essentially on the lower eigenstate as time evolves. Using this piece of information, it is readily seen that the full system (2) roughly reduces to one single scalar equation on $\phi_0^\epsilon(t, x)$, and the latter is easily averaged out since the above mentioned two difficulties no longer are present in that case.

In the present work, we wish to tackle the generic case where ψ_ϵ switches on *all* the eigenstates at the initial time, *i.e.* $\psi_\epsilon(t = 0, x, z) = \sum_{p \geq 0} \phi_p^\epsilon(t = 0, x)\chi_p(z)$ for genuinely non zero ϕ_p^ϵ's.

Our approach lies in observing that, *without* projecting (1) on the χ_p's, the filtered function $\phi_\epsilon(t, x, z) = \exp(+itH_z/\epsilon)\psi_\epsilon(t, x, z)$ satisfies the PDE

$$i\partial_t \phi_\epsilon(t, x, z) = H_x \phi_\epsilon + \mathrm{e}^{+it\frac{H_z}{\epsilon}} F\left(\left|\mathrm{e}^{-it\frac{H_z}{\epsilon}}\phi_\epsilon\right|^2\right)\phi_\epsilon. \tag{3}$$

Now the key observation is that, for any given ϕ lying in a reasonable Sobolev space (say lying in the domain $D(H_x^N) \cap D(H_z^N)$ for some large N), the mapping

$$\tau \in \mathbb{R} \mapsto F(\tau, \phi) := \mathrm{e}^{+i\tau H_z} F\left(\left|\mathrm{e}^{-i\tau H_z}\phi\right|^2\right)\phi \tag{4}$$

is *almost periodic* in τ. This actually is our key Theorem. The rough idea behind this Theorem is that the spectrum of H_z is discrete, hence the independent frequencies (in τ) carried by $\exp(i\tau H_z)$ are countable as well, a property that is stable upon composition by nonlinear functions. Once this is proved, it is easily deduced that the limit

$$F_{\mathrm{av}}(\phi) := \lim_{T \to \infty} \frac{1}{T} \int_0^T F(\tau, \phi)\, d\tau \tag{5}$$

exists (note that we have here overcome all the small denominator issues, as well as the convergence issues mentioned before). This being settled, one can deduce that ϕ_ϵ goes to ϕ, the solution to

$$i\partial_t \phi = H_x \phi + F_{\mathrm{av}}(\phi). \tag{6}$$

Naturally, the function F_{av} may be explicitely computed. Upon (a posteriori) projecting equation (6) onto the χ_p's, one recovers the physically natural models. In particular, one recovers the one mode analysis mentioned above.

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Infinite Time Aggregation for the Critical Patlak-Keller-Segel model

José Antonio Carrillo
(joint work with A. Blanchet, N. Masmoudi)

We analyze the two-dimensional parabolic-elliptic Patlak-Keller-Segel model in the whole Euclidean space $\mathbb{R}^2$.

$$\begin{cases} \dfrac{\partial n}{\partial t}(x,t) = \Delta n(x,t) - \chi \nabla \cdot (n(x,t) \nabla c(x,t)) & x \in \mathbb{R}^2 \,,\ t > 0 \,, \\ c(x,t) = -\frac{1}{2\pi} \int_{\mathbb{R}^2} \log|x-y|\, n(y,t)\, dy \,, & x \in \mathbb{R}^2 \,,\ t > 0 \,, \\ n(x, t=0) = n_0 \geq 0 & x \in \mathbb{R}^2 \,. \end{cases}$$

Under the hypotheses of integrable initial data with finite second moment and entropy, we first show local in time existence for any mass of "free-energy solutions", weak solutions with free energy estimates. Moreover, we characterize the maximal time of existence in terms of the blow-up of the entropy. The main result presented shows the global existence of free-energy solutions with initial data as before for the critical mass $8\,\pi/\chi$. Actually, we prove that solutions blow-up as a delta dirac at the center of mass as $t \to \infty$ keeping constant their second moment at any time. Furthermore, all moments larger than 2 blow-up as $t \to \infty$ if initially bounded.

Generalization to non-linear models of Boltzmann-Maxwell interactions

Irene M. Gamba
(joint work with Alexandre Bobylev, Carlo Cercignani; and with Sri Harsha Tharkabhushanam)

We study long time dynamics to solutions of initial value problems to a rather general multi-linear Boltzmann kinetic models of Maxwell type interactions that may describe qualitatively different processes in applications, but have many features in common. In particular we focus in the existence, uniqueness and asymptotics to dynamical scaling (self-similar) solutions and connections to convergence theorems for non-Gaussian states (see [4]).

We use a relationship of spectral properties of the generalized collisional model problem in Fourier space to study qualitative properties of the solution of the original initial value problem as well as the characterization of the domain of attraction to self-similar states. We clarify the connection with contractive measures for the probability measure solution of the kinetic problem and discuss the optimal decay rates in the context of characteristic functions, i.e. Fourier transforms of probability measures as introduced for the classical Boltzmann equation of Maxwell type by [1] and the corresponding fourier metrics introduced by [7].

Examples are models of Maxwell type in classical space homogeneous, elastic or inelastic Boltzmann equation [2, 3, 5], and the elastic Boltzmann equation in the presence of a thermostat [6], all with finite or infinite initial energy, as well as Pareto distributions models in economy (see [10])or more general Interacting Stochastic Processes. This first part of the presentation is collaborative work with A. Bobylev and C. Cercignani in [4]

We finally show an deterministic numerical implementation, developed in collaboration with Harsha Tharkabhushanam, that is based in Fast Fourier Transform methods combined with Langrange multipliers moment constrains (see [8]) based on modifications methods developed in [9] for the classical elastic conservative Boltzmann equation of Maxwell type. Our numerically solver is benchmarked with the dynamically scaled asymptotic limits in the case non-conservative energy model given by the elastic Boltzmann equation in the presence of a thermostast, for a specific model choice corresponding to a colored mixture problem with a given coupling parameter. As it was shown in [6], there are explicit self-similar solutions for finite (or infinity) energy, and this distribution measures are asymptotically characterized by local singular local behavior at the origin, with a rational blow up behavior in velocity space. On the other hand, for large energies these self-similar distribution measures asymptotically develop power like tails in velocity space. The theory developed in [4] shows these solutions are attractors to solutions of the initial value problem under suitable distribution measures. We use the knowledge of the spectral properties of the model to choose suitable initial states with finite energy and time scales based on the associated eigenvalues, so the solution to the initial value problem numerically converges to the explicit self-similar solution associated to this model.

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Particles approximation of singular Vlasov equations

Pierre-Emmanuel Jabin
(joint work with Maxime Hauray)

We prove the convergence in any time interval of a point-particle approximation of the Vlasov equation by particles initially equally separated for a force in $1/|x|^\alpha$, with $\alpha \leq 1$. We introduce discrete versions of the L^∞ norm and time averages of the force field. The core of the proof is to show that these quantities are bounded and that consequently the minimal distance between particles in the phase space is bounded from below.

More precisely, we consider the evolution of N particles, centered at $(X_1, \dots, X_N)$ in $\mathbb{R}^d$ with velocities $(V_1, \dots, V_N)$ and interacting with a central force $F(x)$. The positions and velocities satisfy the following system of ODEs

$$\dot{X}_i = V_i, \quad \dot{V}_i = E(X_i) = \sum_{j \neq i} \frac{1}{N} F(X_i - X_j), \tag{1}$$

where the initial conditions $(X_1^0, V_1^0, \dots, X_n^0, V_n^0)$ are given. The prime example for (1) consists in charged particles with charges α_i and masses m_i, in which case $F(x) = -x/|x|^3$ in dimension $d = 3$.

Assume that the particles are initially reasonnably well distributed in phase space or in other words that the minimal rescaled distance between two particles

$$\sup_{i \neq j} N^{1/6} \, |X_i(0) - X_j(0)| + |V_i(0) - V_j(0)|$$

is uniformly bounded in N and consider the case of a "not too singular force"

$$|F(x)| \leq \frac{C}{|x|^\alpha}, \quad |\nabla F(x)| \leq \frac{C}{|x|^{1+\alpha}} \quad |\nabla^2 F(x)| \leq \frac{C}{|x|^{2+\alpha}}, \quad \forall x \neq 0. \tag{2}$$

We then obtain at the limit a kinetic equation

$$\begin{aligned} &\partial_t f + v \cdot \nabla_x f + E(x) \cdot \nabla_v f = 0, \quad t \in \mathbb{R}_+, \ x \in \mathbb{R}^d, \ v \in \mathbb{R}^d, \\ &E(x) = \int_{\mathbb{R}^d} \rho(t,y) \, F(x-y) \, dy, \quad \rho(t,x) = \int_v f(t,x,v) \, dv, \end{aligned} \tag{3}$$

where f is the one particle distribution and is the weak limit in measure of $1/N \sum_i \delta(x - X_i) \, \delta(v - V_i)$.

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Recent results on existence, uniqueness and asymptotic decay rates for collisional kinetic models

Robert M. Strain

We discuss recent work proving exponential time decay rates to equilibrium for Boltzmann equations such as the soft potentials, Landau's equation and the linearized Balescu-Lenard model. We also mention a proof of existence and uniqueness of solutions near Maxwellian to the Vlasov-Maxwell-Boltzmann system in the whole space. Some of these projects are joint work with Yan Guo.

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High field asymptotics for the Fermion Boltzmann equation

Naoufel Ben Abdallah
(joint work with Hédia Chaker and Christian Schmeiser)

The high field scaling of the Boltzmann equation is written herebelow,

$$\partial_t f_\varepsilon + v \cdot \nabla_x f_\varepsilon + \frac{1}{\varepsilon} \left(E \cdot \nabla_v f_\varepsilon - Q(f_\varepsilon) \right) = 0$$

with

$$Q(f)(v) = \int_{\mathbb{R}^d} \sigma(v,v') \left\{ f(v')(1-f(v))M(v) - f(v)(1-f(v'))M(v') \right\} dv' \,,$$

where $\sigma(v,v')$ is the scattering cross section and $M(v)$ denotes the Maxwellian distribution

$$M(v) = \frac{1}{(2\pi)^{d/2}} \exp(-|v|^2/2) \,.$$

The unknown $f_\varepsilon(x,v,t)$ is the distribution of conduction electrons at time t in the position-velocity phase space $\mathbb{R}^d \times \mathbb{R}^d$. The electric field $E(x,t)$ is assumed as given, and the Knudsen number ε is a dimensionless parameter. The macroscopic limit $\varepsilon \to 0$ with the above scaling of the electric field (balancing the scattering effects) is called the high field limit. The scattering operator Q models the interaction of electrons with the semiconductor crystal lattice. The factors $(1-f)$ causing the quadratic nonlinearity are a semiclassical approximation of the Pauli exclusion principle and of the fermionic nature of electrons.

In the formal limit as ε tends to zero is a nonlinear conservation law. Indeed, we have under some positivity and regularity hypotheses on the cross section σ

Theorem 1. *i) For every $E \in \mathbb{R}^d$ and $n \in \mathbb{R}^+$, there exists a unique function $F(n,E) \in L^1(\mathbb{R}^d)$ such that $E \cdot \nabla_v F(n,E) \in L^1(\mathbb{R}^d)$, $0 \le F(n,E) \le 1$, and which satisfies*

$$E \cdot \nabla_v F(n,E) - Q(F(n,E)) = 0 \,, \qquad \int_{\mathbb{R}^d} F(n,E)(v) dv = n \,. \tag{1}$$

The limit as ε goes to zero is given by the mass conservation equation

$$\partial_t n + \nabla_x \cdot j(n) = 0.$$

where

$$j(n) = \int v F(n,E)\, dv.$$

In [2] the convergence is proven for smooth solutions of the limiting conservation law by means of a Hilbert expansion. The aim of this talk is to report on a new proof which shows the convergence of solutions towards the unique entropic solution of the limiting conservation law, regardless of its regularity. The result is however restricted to the case of constant electric fields. We shall therefore skip the dependence w.r.t. E of F. Two entropy like inequalities are the main mathematical tools :

Theorem 2. *Let for any fixed v, $\varphi(;v)$ be the inverse function of the mapping $n \mapsto F(n)(v)$ and let $f = f(v)$ satisfy $0 \le f \le F(n^*)$ and denote*

$$n_f = \int_{\mathbb{R}^d} \varphi(f(v),v) M(v) dv \le n^*.$$

Let χ be an increasing function such that $\chi' \geq \alpha > 0$ on $[0, n^*]$. Then there exists a positive constant $C = C(\alpha, n^*)$ such that

$$(2) \quad D(f) := \int_{\mathbb{R}^d} (Q(f) - E \cdot \nabla_v f)\chi(\varphi(f,v))dv \leq -C \int_{\mathbb{R}^d} (f - F(n_f))^2 M(v)\, dv\,.$$

Theorem 3. *i)* [16] *For any f, $g \in L^1(\mathbb{R}^d \times \mathbb{R}^l)$ such that $0 \leq f, g \leq 1$, we have*

$$(3) \qquad -\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} (Q(f) - Q(g))\,\mathrm{sgn}(f-g)dvdx \geq 0\,.$$

Equality holds iff $\mathrm{sgn}(f-g)$ *only depends on x.*

ii) [3] *Moreover, if $\int_{\mathbb{R}^d} (f-g)dv = 0$, we have*

$$(4) \qquad -\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} (Q(f) - Q(g))\,\mathrm{sgn}(f-g)dv \geq C(g)\int_{\mathbb{R}^d} |f-g|dv\,,$$

where $C(g) = \sigma_0 \int_{\mathbb{R}^d} (1-g)M\, dv$.

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From Mechanics to Biology via fragmentation processes: a survey and open problems

Juan Soler

The aim of this talk is to give an overview of the main models used to describe fragmentation from the discrete level towards multiphase flow, with a special attention to the fluid kinetic description. The idea is to explain the basic arguments of our aproach to the kinetic description of particle fragmentation and then how to deduce from first principles a fluid–kinetic interaction. We analyse how our approach is connected with biological models and at the same time how the foundations of this kind of problems in mechanics is far to be completely understood. Finally, in the last part we introduce the multicelular growing system as well as some macroscopic description induced by an hyperbolic limit.

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Spectral gap and coercivity estimates for linearized Boltzmann collision operators without angular cutoff

Clément Mouhot
(joint work with Robert Strain)

We prove new constructive coercivity estimates for the Boltzmann collision operator without cutoff, that is for long-range interactions. In particular we give a generalized sufficient condition for the existence of a spectral gap which involves both the growth behavior of the collision kernel at large relative velocities and its singular behavior at grazing and frontal collisions. It provides in particular existence of a spectral gap and estimates on it for interactions deriving from the hard potentials $\phi(r) = r^{-(s-1)}$, $s \geq 5$ or the so-called moderately soft potentials $\phi(r) = r^{-(s-1)}$, $3 < s < 5$, (without angular cutoff). In particular this paper recovers (by constructive means), improves and extends previous results of [2].

We also obtain constructive coercivity estimates for the Landau collision operator for the optimal coercivity norm pointed out in [3] and we formulate a conjecture about a unified necessary and sufficient condition for the existence of a spectral gap for Boltzmann and Landau linearized collision operators.

Here is a precise statement of the main theorem concerning Boltzmann's singular collision operators. Consider the collision operator

$$Q(f,f) = \int_{\mathbb{R}^N \times \mathbb{S}^{N-1}} \left[f(v')\, f(v'_*) \, - f(v)\, f(v_*) \right] B(|v - v_*|, \cos\theta)\, dv_*\, d\sigma$$

where

$$v' = \frac{v + v_*}{2} + \frac{|v - v_*|}{2}\sigma, \quad v'_* = \frac{v + v_*}{2} - \frac{|v - v_*|}{2}\sigma, \qquad \sigma \in \mathbb{S}^{N-1}$$

and $\cos\theta = (v'_* - v') \cdot (v_* - v)/|v_* - v|^2$.

The collision kernels B is of the form

$$B(|v - v_*|, \cos\theta) = |v - v_*|^\gamma\, b(\cos\theta), \quad \gamma \in (-N, +\infty) \tag{1}$$

with

$$b(\cos\theta) \sim_{\theta \sim 0} b^*(\theta)\ (\sin\theta/2)^{-(N-1)-\alpha}\,, \quad \alpha \in [0, 2), \tag{2}$$

where $b^*(\theta)$ is non-negative, bounded and non-zero near $\theta \sim 0$. When $\alpha \geq 0$ the angular singularity is not integrable, the operator is said to be *non-cutoff*.

Then denote by

$$\mu = \mu(v) := (2\pi)^{-N/2} e^{-|v|^2/2}$$

the normalized unique equilibrium with mass 1, momentum 0 and temperature 1, and consider fluctuations around this equilibrium of the form

$$f = \mu + \mu^{1/2}\, g$$

which results the following linearized collision operator (note the sign convention):

$$L(g) = -\mu^{-1/2} \left[Q(\mu, \mu^{1/2} g) + Q(\mu^{1/2} g, \mu) \right].$$

L (acting in the velocity space) is an unbounded symmetric operator on L^2, such that its Dirichlet form satisfies

$$D(g) := \langle Lg, g \rangle \geq 0.$$

Then we prove the following result:

Let B be a collision kernel satisfying (1,2). Then

- *For any $\varepsilon > 0$ there is a constant $C_{B,\varepsilon}$, constructive from our proof and depending on B and ε, such that the Dirichlet form D of the linearized Boltzmann collision operator associated to B satisfies*

$$D(g) \geq C_{B,\varepsilon} \left\| [g - \mathbf{P}g]\, (1 + |v|^2)^{(\gamma+\alpha-\varepsilon)/4} \right\|^2_{L^2(\mathbb{R}^N)}.$$

- *There is a constant $C_{B,0}$ (obtained by non-constructive means in our proof) such that*

$$D(g) \geq C_{B,0} \left\| [g - \mathbf{P}g] \left(1 + |v|^2\right)^{(\gamma+\alpha)/4} \right\|^2_{L^2(\mathbb{R}^N)}.$$

In this statement,

$$\mathbf{P}g = \left(a + b \cdot v + c|v|^2\right) \mu^{1/2}$$

(with $a, c \in \mathbb{R}$ and $b \in \mathbb{R}^N$) is the L^2 orthogonal projection onto the space of the so-called "collisional invariants"

$$Span\left\{\mu^{1/2}, v_1\mu^{1/2}, \ldots, v_N\mu^{1/2}, |v|^2\mu^{1/2}\right\}.$$

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Kinetic approach to long time behavior of linearized fast diffusion equations

María J. Cáceres

(joint work with Giuseppe Toscani)

In this talk we study the long time behavior of certain linearized versions of the Cauchy problem for the fast diffusion equation posed on the whole space $\mathbb{R}^N$

$$\frac{\partial v}{\partial \tau} = \Delta v^m, \quad y \in \mathbb{R}^N, \tau > 0, \quad \frac{N}{N+2} < m < 1, \tag{1}$$

$$v(y, 0) = v_0(y). \tag{2}$$

The long time asymptotics for equation (1) is described by the family of self similar *source type* Barenblatt–Pattle solutions

$$B_C(y, \tau) = \tau^{-\frac{1}{m+1}} \left(C + \frac{1-m}{2m} |y|^2 \tau^{-\frac{2}{m+1}} \right)^{\frac{1}{1-m}}, \tag{3}$$

where the constant C must be chosen in order to match the initial mass.

Recent results on the subject allow to assert that the rate of convergence is sensitive to the choice of the initial datum, and it is believed that the values of its moments play an important role. This phenomenon was first established by J.L. Vázquez in [7] for porous medium equations. In this talk we study the convergence towards the self–similar solution of certain linearized versions of the fast diffusion equation showing that their rate of convergence can be related to the number of moments of the initial datum that are equal to the moments of the self–similar

solution at a fixed time. As a consequence, we find an improved rate of convergence to self–similarity in terms of a Fourier based distance between two solutions.

Among others, we shall consider the linear version of the fast diffusion equation (1),

$$\frac{\partial v(y,\tau)}{\partial \tau} = \operatorname{div}\left(mB_C(y,\tau)^{m-1}\nabla v(y,\tau)\right), \quad y \in \mathbb{R}^N,\ \tau > 0, \tag{4}$$

$$v(y,0) = v_0(y), \tag{5}$$

where $B_C(y,\tau)$ is a Barenblatt solution suitably shifted in time. The rate of convergence to equilibrium for this equation will be studied in terms of the number of moments initially equal to those of the Barenblatt solution.

This linearized fast diffusion equation was deeply investigated in [4] by Denzler and McCann, who were able to analyze its spectrum extracting sharp rates of asymptotic convergence to the Barenblatt profile. Our result recovers this rate of convergence by different methods.

The convergence rates of the linearized equations will be here derived in terms of a Fourier based metric which has been proven very useful in finding rates of convergence towards equilibrium in kinetic theory of rarefied gases (see [5],[2] and [6]). These Fourier-based metrics d_s, for any $s > 0$, are defined as

$$d_s(f,g) = \sup_{\xi\in\mathbb{R}^N} \frac{|\hat{f}(\xi) - \hat{g}(\xi)|}{|\xi|^s} \tag{6}$$

for any pair of probability measures in $\mathcal{P}_s(\mathbb{R}^N)$, where $\mathcal{P}_s(\mathbb{R}^N)$ is the set of probability measures with bounded s-moment and as usual, $\hat{f}$ is the Fourier transform of the density $f(x)$.

The study of the convergence in terms of the distance (6) can be obtained through the analysis of its evolution. To this aim, the first tentative relies in the direct study of the evolution in time of the Fourier based distance using the linearized equation in Fourier transform. But, in view of its definition, the study of this evolution is a overcomplicated matter, due to the presence of a variable diffusion coefficient. To overcome this problem, instead of working on the Fokker–Planck equation directly, we will introduce a nonlinear kinetic model of Maxwell type [1] for which the recovering of the rate of decay in terms of the Fourier based distance is immediate.

Our main results [3] deal with the rate of decay to zero of solutions to different linearizations of the fast diffusion equation (1) in terms of the $d_{2+\delta}$ distance, where $\delta = \delta(m)$ is given in terms of the exponent m of the fast diffusion.

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A microscopic model of viscous friction

Silvia Caprino
(joint work with G. Cavallaro, C. Marchioro, M. Pulvirenti)

We consider a convex body moving horizontally and immersed in an infinitely extended fluid. We assume the fluid to be obtained in the mean field limit from a system of free particles, elastically interacting with the body. Calling V_0 and V_∞ the initial and limiting velocity of the body, we prove that the time-asymptotic trend of its velocity $V(t)$ is the following:

$$|V(t) - V_\infty| \approx Ct^{-(d+2)} \tag{1}$$

provided that the difference $|V_0 - V_\infty|$ is small enough, being d the dimension of the space and C a constant depending uniquely on the properties of the fluid and the shape of the body. In [1] we study the case in which a constant force is acting on the body, while in [2] various situation are discussed, without any external force (in which case $V_\infty = 0$), or with a x-depending force.

The power law approach to the limiting velocity is unexpected, as it is usually assumed to be exponential, by phenomenological considerations. We prove that it is due to the long memory of the dynamical system, which retains successive collisions between a gas particle and the body, even after a very long time. Indeed, as it can be easily seen, assuming that the body hits only once any particle, then the behavior of its velocity would be the expected one, that is exponential in time.

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The periodic Lorenz gas in the Boltzmann-Grad limit

François Golse
(joint work with J. Bourgain, B. Wennberg, E. Caglioti)

In the Euclidean plane $\mathbb{R}^2$, call Z_r the set of points whose distance to integer points (i.e. $\mathbb{Z}^2$) is larger than r ($0 < r < 1/2$). For $x \in Z_r$ and $|v| = 1$, call $\tau_r(x, v)$ the exit time from x in the direction $v \in S^1$, i.e.

$$\tau_r(x, v) = \inf\{t > 0 \,|\, x + tv \in \partial Z_r\}.$$

Call $\phi_r(t) = Prob\{\tau_r(x, v) > t/r\}$ for uniformly distributed (x, v).
Then,

(1) $\exists\, 0 < C < C'$ such that $\frac{C}{t} < \phi_r(t) < \frac{C'}{t}$, $\forall\, 0 < r < 1/2$, $\forall\, t > 1$.
(2) In some Cesaro' sense: $\phi_r(t) \to \phi(t)$ as $r \to 0^+$ and $\phi(t) \sim \frac{1}{\pi^2 t}$ as $t \to \infty$.
(3) The Boltzmann-Grad limit for a gas of particles undergoing elastic collisions with the boundary of Z_r (with particle-particle collision neglected) cannot be described by a linear Boltzmann equation in the single particle phase space $\mathbb{R}^2 \times S^1$.
(4) A model in some extended phase space $\mathbb{R}^2 \times S^1 \times (-1, 1) \times (1, +\infty)$ involving the impact parameter at the next collision and the time to the next collision is proposed, assuming some hypothesis on the dynamics that should be checkable numerically.

Hidden L^2 stability of scalar conservation laws

Yann Brenier

First order systems of conservation laws read:

$$\partial_t u + \sum_{i=1}^{d} \partial_{x_i}(Q_i(u)) = 0,$$

where $u = u(t, x) \in \mathbf{R}^m$ depends on $t \geq 0$, $x \in \mathbf{R}^d$ and the Q_i are given smooth functions. The system is called hyperbolic when, for each $\tau \in \mathbf{R}^d$ and each $U \in \mathbf{R}^m$, the $m \times m$ matrix $\sum_{i=1,d} \tau_i Q_i'(U)$ can be put in diagonal form with real eigenvalues. There is no general theory to solve globally in time the initial value problem for such systems of PDEs (cf. [10] for a general introduction to the field). Only two extreme cases are well understood. First, in one space dimension ($d = 1$), for a large class of systems, existence and uniqueness of global weak entropy solutions hold true for initial conditions of sufficiently small total variation [1]. Next, in the case of *scalar* conservation laws, i.e. when $m = 1$, there is a unique entropy (or Kruzhkov) solution for each given initial condition in L^∞ [13]. In both cases, solutions are L^p stable with respect to their initial conditions if and only if $p = 1$. This is a major obstruction to the construction of a unified theory of general multidimensional systems of hyperbolic conservation laws. Indeed, simple multidimensional linear systems, such as the wave equation (written as a first order system) or the Maxwell equations, are not well posed in any L^p but for $p = 2$ [7]. However, as explained below, there is a hidden L^2 stability behind any multidimensional scalar conservation law. Indeed, we exhibit for each of them a master equation well posed in L^2. Our approach is based on a combination of

level-set, kinetic and transport-collapse approximations, in the spirit of previous works by Giga, Miyakawa, Osher, Tsai and the author [3, 4, 5, 6, 11, 12, 15].

A master equation for multid scalar conservation laws

Consider, for simplicity, an initial condition $u_0(x)$ valued in $[0,1]$ and denote by $u(t,x)$ the corresponding Kruzhkov solution.
Introduce $Y_0(x,a) = a - u_0(x)$, for all $a \in [0,1]$, or, more generally, any function $Y_0(x,a)$ such that $\partial_a Y_0 \geq 0$, and $1\{Y_0(x,a) \leq 0\} = 1\{a \geq u_0(x)\}$, almost everywhere in (x,a), in the spirit of level set methods [12, 15].
Let us now solve the following subdifferential equation:

$$0 \in \partial_t Y + \sum_{i=1}^{d} Q_i'(a)\partial_{x_i} Y + \partial K[Y], \quad Y = Y(t,x,a),$$

with initial condition Y_0. Here ∂K denotes the subdifferential [8] of the convex functional defined by $K[Y] = 0$ whenever $\partial_a Y \geq 0$ and $K[Y] = +\infty$ otherwise. This equation turns out to be a master equation for both the Kruzhkov [13] and the Lions-Perthame-Tadmor kinetic formulation [14]. Indeed, we show (using the transport-collapse method [3, 4, 5, 12]) that the Kruzhkov solution can be recovered, in level set style, by:

$$u(t,x) = \int_0^1 1\{Y(t,x,a) \leq 0\} da$$

and the corresponding indicator function

$$1\{a \geq u(t,x)\} = 1\{Y(t,x,a) \leq 0\}$$

is nothing but the solution of the kinetic formulation [14]. The master equation is very simple: its operator is indeed maximal monotone in L^2 [8]. For all $p \in [1,+\infty]$, the solutions Y are L^p stable with respect to their initial conditions Y_0 and enjoy the regularity properties:

$$||\partial_x Y(t)||_{L^p} \leq ||\partial_x Y_0||_{L^p},$$

$$||\partial_t Y(t)||_{L^p} \leq ||Q'||_{L^\infty} ||\partial_x Y_0||_{L^p}.$$

Related works

This work (http://arxiv.org/pdf/math.AP/0609761, to appear in ARMA) follows [6] (where some models of pressureless fluids, made of sticky strings or sticky particles got reformulated in L^2, in a similar way). Let us quote recent related works by Bolley, B., Loeper [2] and by Carrillo, Di Francesco, Lattanzio [9]. In both cases, stability in Monge-Kantorovich distances are established or used for one-dimensional scalar conservation laws.

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Boltzmann Equation and Generalized Burnett Equations

Alexander V. Bobylev

In order to regularize the Burnett equations we use the approach described briefly in [1], i.e. "changes of coordinates". The first successful attempt to do this led to a version of hyperbolic Burnett equations published in [1]. These equations are, however, more complicated than original Burnett equations and do not have the standard form of equations of hydrodynamics. We present below another version of stable Burnett equations which is much more convenient for applications. Details of derivation of the Generalized Burnett Equations (GBEs) and all necessary proofs can be found in [2].

GBEs are equations for *auxiliary* variables for which we keep the initial notations $\rho(x,t)$ (density), $u(x,t)$ (bulk velocity) and $T(x,t)$ (absolute temperature). The *true* hydrodynamical variables $(\rho^{tr}, u^{tr}, T^{tr})$ are expressed through (ρ, u, T) by equalities

$$\rho^{tr} = \rho,\ u^{tr} = u,\ T^{tr} = T - \frac{\varepsilon^2}{\rho} div \frac{S}{\rho}, \tag{1}$$

where

$$S = a(T) \bigtriangledown \log \rho + b(T) \bigtriangledown \log T. \tag{2}$$

The functions a and b are expressed through Burnett coefficients A, B, C [1] and two parameters $\theta_{1,2}$ (a reason for such notation is clarified below):

$$
\begin{aligned}
a(T) &= \frac{2}{3}[-TA(T) + \theta_1 g(T)], \\
b(T) &= \frac{2}{3}T[C(T) - A(T)] + \theta_2 g(T), \\
g &= \frac{T}{3}(5A + 2B - 4C).
\end{aligned} \tag{3}
$$

Thus, the only "unusual" variable is $T(x,t)$ which does not coincide with true absolute temperature. Equations for (ρ, u, T) have the standard form of equations of hydrodynamics

$$
\begin{gathered}
\rho_t + div\, \rho u = 0,\ \rho \mathcal{D}_0 u_\alpha + \frac{\partial p}{\partial x_\alpha} + \varepsilon \frac{\partial}{\partial x_\beta}\Pi_{\alpha\beta} = 0, \\
\frac{3}{2}\rho \mathcal{D}_0 T + p\, div u + \varepsilon(\Pi_{\alpha\beta}\frac{\partial u_\alpha}{\partial x_\beta} + div Q) = 0,\ p = \rho T,\ \mathcal{D}_0 = \partial_t + u\partial_x
\end{gathered} \tag{4}
$$

with the new fluxes Π and Q given by equalities

$$
\begin{aligned}
\Pi_{\alpha\beta} &= \pi^{NS}_{\alpha\beta} + \varepsilon\pi^{B}_{\alpha\beta} - \varepsilon\delta_{\alpha\beta} div\frac{S}{\rho}, \\
Q_\alpha &= q^{NS}_\alpha + \varepsilon q^B_\alpha + \frac{\varepsilon}{\rho}\{3S_\beta\overline{\frac{\partial u_\alpha}{\partial x_\beta}} + (\frac{3}{2}a + b)\frac{\partial}{\partial x_\alpha} div u + \\
&+ (div u)[(a'T - 2a)\frac{\partial}{\partial x_\alpha}\log\rho + (b'T - 2b)\frac{\partial}{\partial x_\alpha}\log T]\},
\end{aligned} \tag{5}
$$

where primes denote differentiation with respect to T. The first two terms in both equalities are usual Navier-Stokes and Burnett fluxes discussed in detail in previous sections. Eqs.(4) can be obviously written in the form of standard conservation laws with Π and Q instead of π and q respectively. Note, however, that

$$
\Pi_{\alpha\alpha} = -3\varepsilon div\frac{S}{\rho} \neq 0. \tag{6}
$$

It can be shown that, under very general assumptions on intermolecular potential, there exists a non-empty region on the plane of parameters (θ_1, θ_2), where Eqs.(4) are stable. Exact necessary and sufficient conditions of stability can be found in [2]. The reason for the notation (3) becomes clear if we consider the matrix of third derivatives for Eqs.(4). Then we obtain (the continuity equation is omitted):

$$
\begin{aligned}
u_t &= \frac{\varepsilon^2}{\rho^2} g[\frac{2\theta_1}{3\rho} \triangle (\bigtriangledown\rho) + \frac{\theta_2}{T} \triangle (\bigtriangledown T)] + ..., \\
T_t &= \frac{2\varepsilon^2}{3\rho^2} g\theta_3 \triangle div u + ...,\ \theta_3 = 1 - (\theta_1 + \theta_2).
\end{aligned} \tag{7}
$$

Therefore we denote the generalized Burnett equations (4) , (5) (in the notation of Eqs. (1)-(3)) by a symbol GBEs $(\theta_1, \theta_2, \theta_3)$, having in mind that only two of three parameters $\{\theta_i,\ i = 1, 2, 3\}$ are independent. It follows from Eqs.(7) that GBEs $(\theta_1, \theta_2, \theta_3)$ are well-posed (hyperbolic) if $\theta_2\theta_3 \geq 0$ Conditions of stability depend, generally speaking, on the sign of $g(T)$ [2]. The usual approximation (exact for Maxwell molecules) leads to estimate

$$g(T) \approx \frac{37}{12}\mu^2(T). \tag{8}$$

Hence, for practical applications we can assume that $g(T) > 0$ for all $T > 0$. Then the simplest region of stability of GBEs $(\theta_1, \theta_2, \theta_3)$ is given by inequalities

$$\theta_{1,2,3} \geq 0,\ \theta_1 + \theta_2 + \theta_3 = 1. \tag{9}$$

Thus, we can choose any two of three real numbers (generally speaking, they can be also functions of T), satisfying the conditions (9) and obtain the above described stable GBEs $(\theta_1, \theta_2, \theta_3)$. It is easy to verify that new fluxes (5) contain, roughly speaking, the same tensor and vector terms as the original Burnett fluxes (with other coefficients). Hence, GBEs $(\theta_1, \theta_2, \theta_3)$ are not more complicated than the original equations. Moreover they can be simpler, in particular, in the following three cases: GBEs $(1, 0, 0)$, GBEs $(0, 1, 0)$, GBEs $(0, 0, 1)$ (note that the stability conditions (9) are satisfied). In other words, we can reduce a number of third derivatives. It is clear that the problem of boundary conditions should be considered separately for each of the three cases. We hope to return to this problem in another paper.

We also mention that the original Burnett equations can be understood as a particular case of GBEs $(\theta_1, \theta_2, \theta_3)$ with parameters

$$\theta_1 = \frac{TA(T)}{g(T)},\ \theta_2 = \frac{2T[C(T) - A(T)]}{3g(T)},\ \theta_3 = 1 - (\theta_1 + \theta_2), \tag{10}$$

which lie (for typical molecular models) in the unstable region of the plane (θ_1, θ_2). A specific choice of parameters can be different for different problems. For example, it is known that Navier-Stokes equations give the correct (in the Hilbert class) answer for $1d$ stationary heat transfer problems in the case of Maxwell molecules. This property can be preserved if we choose $\theta_{1,2}$ in Eqs.(3) in such a way that $a = b$. It can be done without violation of conditions (9).

Thus, the whole class of stable GBEs $(\theta_1, \theta_2, \theta_3)$ seems to be a natural replacement for the classical (unstable) Burnett equations, though the problem of optimal choice of parameters for specific cases and the problem of corresponding boundary conditions need further investigation.

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Brownian approximation and DSMC for the non-cutoff Kac equation

Bernt Wennberg
(joint work with Mattias Sundén)

We consider the Kac equation with a thermostatted force field,

$$\partial_t f(v,t) + \partial_v \left((1-\zeta(t)v) f(v,t)\right) \quad = \quad Q(f,f)(v,t)\,,$$

where

$$\begin{aligned} Q(g,g)(v) &= \int_{\mathbb{R}} \int_{-\pi}^{\pi} \left(g(v')g(v'_*) - g(v)g(v_*)\right)\, b(\theta)\, d\theta\, dv_*\,, \\ \zeta(t) &= \int_{\mathbb{R}} v f(v,t)\, dv\,. \end{aligned}$$

This equation can be derived from a markovian jump-process on the sphere S^{N-1}:

- Between the jumps, a point $\mathbf{v}(t)$ evolves according to the equation

$$\frac{d}{dt} v_j(t) \quad = \quad E\left(1 - \frac{\sum v_k}{\sum v_k^2} v_j\right)\,.$$

- At random time intervals, $\mathbf{v}(t)$ makes a jump according to

$$\begin{aligned} &(v_1, ..., v_j, ..., v_k, ..., v_n) \mapsto \\ &\qquad (v_1, ..., v_j \cos\theta - v_k \sin\theta, ..., v_j \sin\theta + v_k \cos\theta, ..., v_n)\,, \\ &\qquad 1 \le j,k \le n,\ \theta \in]-\pi, \pi]\,. \end{aligned}$$

  These jumps occur independently with an exponential rate proportional to

$$n^{-1} b(\theta) d\theta\,.$$

Kac [4] constructed this model and used it to derive the Kac equation. The version with a thermostatted force field was derived in [7, 6] for the case of a constant collision rate, $b(\theta) = 1/2\pi$. The non-cutoff case is treated in [1].

The equation has interesting non-equilibrium stationary states, which can be computed almost explicitly, or computed very accurately using finite diffence methods to approximate the Fourier transform of the equation.

However, the usual Monte Carlo methods are less efficient in the case of a non-cutoff kernel, $\int_{-\pi}^{\pi} b(\theta)\, d\,\theta = \infty$, when the real jump frequency is infinite. It has been demonstrated [2, 3] that carrying out a simulations starting from the n-dimensional jumpprocess described above, but with truncated kernel, $\tilde{b}_\epsilon = \min(b(\theta), b(\epsilon)$, gives a good approximation if ϵ is very small. In this, non-equilibrium situation, the method does not give good results unless ϵ is very small.

The jump process can be described using a stochastic differential equation driven by a random Poisson measure:

$$\begin{aligned}\mathbf{v}(t) &= \mathbf{v}(0) + \int_0^t E\left(\mathbf{e} - \frac{\mathbf{e}\cdot\mathbf{v}(s)}{|\mathbf{v}(s)|^2}\mathbf{v}(s)\right) ds \\ &\quad + \sum_{1\le j<k\le N} \int_0^t \int_{-\pi}^{\pi} A_{j,k}(\theta_{j,k})\mathbf{v}(s_-)N(ds, d\theta_{j,k})\,.\end{aligned}$$

Here $A_{j,k}(\theta)$ is the $n \times n$-matrix that performs the jumps, $\mathbf{e} = (1, 1, ..., 1) \in \mathbb{R}^n$, and $N(ds, d\theta)$ is a Poisson random measure with intensity measure $n^{-1}b(\theta)d\theta\, dt$.

We show how this stochastic differential equation may be simulated efficiently by replacing $N(ds, d\theta)$ by a truncated measure $\tilde{N}_\epsilon(ds, d\theta)$ with intensity measure $n^{-1}\tilde{b}_\epsilon(\theta)d\theta\, dt$, and adding a Brownian term to compensate for the truncated part. The terms that are added to the right hand side are

$$\int_0^t r_W(\mathbf{v}(s))\, ds + \int_0^t \sigma(\mathbf{v}(s))dW(s)\,,$$

where $\sigma(\mathbf{v}(s))$ is the matrix that projects the standard Wiener process $W(t)$ onto the sphere S^{N-1}, scaled to give the correct variance, and where

$r_W(\mathbf{v}(s))$ is a drift term that must be added to compensate for the curvature of the sphere.

One can show that the generator to the truncated process without a Brownian term converges with a rate $\epsilon^{2-\alpha}$, and that the convergence rate is $\epsilon^{3-\alpha}$ when the Brownian term is added. When α is close to 2, the improvement is significant.

The complete result is presented in [5].

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The BGK model with external confining potential: Existence, long-time behaviour and time-periodic Maxwellian equilibria

Roberta Bosi
(joint work with María J. Cáceres)

We study global-in-time existence, stability and long-time behaviour for the inhomogeneous nonlinear Bhatnagar-Gross-Krook (BGK) model of the kinetic gas theory (cf. [2]), with an external potential Φ:

$$\partial_t f + v \cdot \nabla_x f - \nabla_x \Phi \cdot \nabla_v f = M[f] - f$$

with $(t, x, v) \in (0, +\infty) \times \mathbb{R}^N \times \mathbb{R}^N$, $M[f] = \frac{\rho(t,x)}{(2\pi T(t,x))^{N/2}} \exp\left(-\frac{|v-u(t,x)|^2}{2T(t,x)}\right)$, and $(\rho,\, \rho u,\, \rho|u|^2 + \rho TN) = \int_{\mathbb{R}^N} (1, v, |v|^2)\, f\, dv$.
The external potential $\Phi = \Phi(x)$ satisfies the assumptions

$$\Phi(x) \geq 0, \quad \Phi \in C^2(\mathbb{R}^N), \quad \exp(-\Phi(x)) \in L^1(\mathbb{R}^N),$$
$$|x||\nabla\Phi(x)| \leq c_1(1 + \Phi(x)), \quad |\nabla\Phi(x)|(1 + |v|^\sigma) \leq c_2(1 + |v|^2 + 2\Phi(x)),$$

for some $\sigma \in (0, 1]$ and $c_1, c_2 \in (0, +\infty)$.
The introduction of Φ has the aim of confining the particles for a long time and to generate non trivial steady states with finite mass and energy.
For an initial data $f_0 \geq 0$ with bounded mass, entropy and total energy we prove existence of L^1 mild solutions by compactness arguments and multipliers techniques. We follow the approach of Perthame [4]. The main point here is the control of some high moments of f in terms of the lower ones (also with some time-independent bounds).
As time goes to infinity we then show the relaxation of the system to a Maxwellian distribution. This behaviour has previously been demonstrated in the case of bounded domains with thermalizing boundary conditions (cf. [3]).
Applying the compactness method of the existence part, as $t_n \to +\infty$ we get convergence in $C([0, \tau]; L^1(\mathbb{R}^{2N}))$ of $f(t + t_n, x, v)$ to a Maxwellian steady state $m(t, x, v)$, with the same mass as f_0 and bounded energy and entropy.

Of particular interest is the case with isotropic harmonic potential $\Phi(x) = |x|^2/2$, in which Boltzmann himself found infinitely-many time-periodic Maxwellian equilibria, without leaving any interpretation of them (cf. [2]).
This behaviour is peculiar to the whole-space problem and it is shared with a full class of kinetic equations

$$\partial_t f + v \cdot \nabla_x f - x \cdot \nabla_v f = C(f)$$

with $C(f)$ a collision operator of Boltzmann-type (e.g. Boltzmann, BGK, ...).
The multistability of all these systems can be studied in terms of the (Lyapunov) relative entropy functional $H[f, g] = \int f \log(f/g) dx dv$ and in the L^1-norm.
In order to identify the limit, we operate a classification of the family $\mathcal{F}(|x|^2/2)$ of Maxwellian solutions with the same mass, energy and angular momentum as f_0, since the latter are the conserved quantities of the system. In this family there is a *stationary* (i.e. time-independent) Maxwellian f_s, which realizes the minimum

for the entropy and therefore it results the most probable equilibrium state for the system. However, the presence of the other elements of $\mathcal{F}(|x|^2/2)$ does not guarantee that the system relaxes to f_s. Actually, we find a necessary condition on the moments of f_0 in order to expect Lyapunov-convergence to $f_s(x,v) = (2\pi)^{-N}\exp(-\frac{|x|^2+|v|^2}{2})$.
More precisely, $H[f(t), f_s] \to 0$ as $t \to +\infty$ only if

$$\int_{\mathbb{R}^N} \rho_0|x|^2dx = N,\ \int_{\mathbb{R}^N} \rho_0 u_0 \cdot x dx = 0,\ \int_{\mathbb{R}^N} \rho_0 u_0 \cdot \mathbb{I} dx = 0,\ \int_{\mathbb{R}^N} \rho_0(\mathbb{I}\cdot x)dx = 0.$$

where ρ_0, u_0 are the density and the mean velocity of f_0, $\mathbb{I}$ is the unit vector in $\mathbb{R}^N$, and we consider the normalization $(1, 0, N)$ for mass, angular momentum and total energy. Moreover, the previous condition holds for all times and prevents the time-oscillation of the related moments of the distribution solution $f(t, x, v)$.

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A thin spray model with collisions: existence and uniqueness of local smooth solutions

Julien Mathiaud

Sprays are made of particles in an underlying gas. A coupling of the droplets and the gas was first proposed by Williams ([11]), Papanicolaou and Caflisch ([3])... The aim of this talk is a mathematical study of thin sprays with collisions. This means that we consider a gas in which collisions between droplets must be taken into account contrary to the volume fraction occupied by the particles. Our study is based on a gas-particle system used at the CEA ([2]).

The gas is generally described through Navier-Stokes or Euler equations. Here, the Euler representation is chosen because the gas evolves at high Reynolds number. The density ρ_g, the velocity u_g and the internal energy e_g characterize the behavior of the gas; the gas is considered to be perfect for mathematical purposes.

The particles are described via a particle density function f which obeys to a Vlasov-Boltzmann equation. Here the parameters of the p.d.f. are the time t, the position x, the velocity v and the internal energy e. The collision kernel corresponds to hard spheres.

We write down the full system of equations:

$$\partial_t \rho_g + \nabla_x \cdot (\rho_g u_g) = 0\,, \tag{1}$$

$$\partial_t u_g + (u_g \cdot \nabla_x) u_g + \frac{\nabla_x p}{\rho_g} = -\frac{1}{\rho_g} \iint\limits_{v,e} m_p F f \, dv de\,, \tag{2}$$

$$\partial_t e_g + u_g \cdot \nabla_x e_g + \frac{p}{\rho_g} \nabla_x \cdot u_g = \frac{1}{\rho_g} \iint\limits_{v,e} \left(m_p F \cdot (u_g - v) - m_p \phi\right) f \, dv de \tag{3}$$

$$\partial_t f + v \cdot \nabla_x f + \nabla_v \cdot (fF) + \partial_e (f\phi) = Q(f,f)\,, \tag{4}$$

$$F = D_p (u_g - v)\,, \tag{5}$$

$$\phi = \frac{4\pi r}{m_p} \lambda N u (T_g - T_p)\,, \tag{6}$$

$$p = (\gamma - 1) \rho_g e_g, \tag{7}$$

$$T_g = \frac{e_g}{C_{vg}}\,, \tag{8}$$

$$T_p = \frac{e}{C_{vp}}. \tag{9}$$

The coupling between the two phases is made through the drag force (in the momentum equation) and thermal exchanges (in the energy equation).

From a mathematical viewpoint, some results exist for both Boltzmann equation and Euler equations. Concerning the Boltzmann equation, there exists global renormalized solutions (a la Di Perna-Lions: [4]), perturbative solutions near Maxwellians ([10], [6]) or vacuum ([7]). On the Euler equations, only local smooth solutions are known ([8]) in all dimensions whereas for long time, only the 1D Glim solutions exist up to now ([9]).

Mathematical results have already been proved for sprays. For instance, Domelevo and Roquejoffre have shown the existence and uniqueness of regular solutions for non collisionnal thin sprays ([5]), considering the viscous Burgers equation for the gas. Recently Baranger and Desvillettes proved the existence and uniqueness of $\mathcal{C}^1$ solutions for an Euler-Vlasov system ([1]), locally in time.

We prove here the *existence* and *uniqueness* of smooth solutions using Sobolev spaces for the system presented above as it was done in [6]. The present work is the next step towards thick sprays, where the volume fraction occupied by the particles is explicitly appearing in the equations. As far as we know, it is also the first work which deals with the energies of the two phases.

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The Boltzmann equation in a slab

Shih-Hsien Yu

In this talk we present a probability representation for the initial boundary condition with a diffuse boundary condition. With law of large numbers and central limit theorem we are able to show the rate of convergence of a free transport equation with diffuse boundary condition. As application of this rate of convergence, one can show the existence of stationary boundary layer for the boundary layer in a slab.

MultiConfiguration Time Dependent Hartree Fock equations and analysis

Norbert Mauser
(joint work with C. Bardos, I. Catto, A. Gottlieb, S. Trabelsi)

The MultiConfiguration Time Dependent Hartree Fock system is a natural extension of the Hartree Fock equation, based on an approximation of the "exact" antisymmetrized many body ($\# = N$) wavefunction by a linear combination of Slater determinants of "one particle orbitals" ($\# = K$). We present the resulting time dependent equations, that forms a system for $\binom{K}{N}$ ODEs for the coefficients and K PDEs for the orbitals, together with the first results for unique existence we obtained in the case of Coulomb interactions.

Hamiltonian Systems and Liouville Equations with Discontinuous Hamiltonians: Computational High Frequency Waves in Heterogeneous Media

Shi Jin
(joint work with Xin Wen, Xiaomei Liao, K. Novak, Xu Yang, Dongsheng Yin)

We introduce Eulerian methods that are efficient in computing high frequency waves through heterogeneous media. The method is based on the classical Liouville equation in phase space, with discontinuous Hamiltonians (or singular coefficients) due to the barriers or material interfaces. We provide physically relevant interface conditions consistent with the correct transmissions and reflections, and then build the interface conditions into the numerical fluxes. This method allows the resolution of high frequency waves without numerically resolving the small wave lengths, and capture the correct transmissions and reflections at the interface. Moreover, we extend the method to include diffraction, and quantum barriers. Applications to semiclassical limit of linear Schrodinger equation, geometrical optics, elastic waves, and semiconductor device modeling, will be discussed.

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Bose-Einstein condensates: a quantum BGK model

Anne Nouri

The experiments realizing Bose-Einstein condensates in atomic vapors (Anderson, 1995; Bradley, 1995; Davies, 1995) ten years ago have renewed interest in the theory of dilute quantum gases at low temperature. Generalizing a work by Bose on photons (Bose, 1924), Einstein proved that a non-interacting Bose gas at sufficiently low temperature undergoes a phase transition (Einstein, 1924). A finite proportion of the particles falls into the ground state of zero momentum, to minimize the physical entropy. For a physical background of Bose-Einstein condensation, we refer to Chapman, 1970; Josserand, 2001; Lacaze, 2001.

So far, mathematical works in quantum kinetic theory have essentially focused on the time evolution of the distribution function of bosons satisfying the kinetic equation introduced by L.W. Nordheim (1928), then by Uehling and Uhlenbeck (1933). Results on the derivation of this equation from the interaction of a large system of bosons in a weak coupling regime are given in Benedetto (2005). The difficulty for solving this equation comes from the fact that the conservations of mass, momentum and energy, and the physical entropy decrease, allow bounded

measure solutions. Such solutions are even expected to describe Bose-Einstein condensation. It is then difficult to give a sense to the collision term containing cubic terms in the distribution function. Mild solutions to the Uehling-Uhlenbeck quantum equation are given by Lu (2000) in a space homogeneous, isotropic in momentum space, for a collision kernel with cut-off. Then distributional solutions for hard spheres are derived (Lu, 2004). The definition of such solutions is made possible by a Carleman representation (Carleman, 1957) and the space homogeneous isotropic assumption. Existence results and long time behaviour are also derived by Escobedo et al (2003) for space homogeneous and isotropic solutions, with a truncation assumption on the physical kernel. The same equation, linearized around a power like steady state is studied in Escobedo (2004). A coupling between condensates and non-condensates at very low temperature is studied in Nouri (2005) in an isotropic frame. Numerical methods for dealing with Bose-Einstein condensation are developed in Bao (2004). In the specific case of photons, their interactions with massive bosons or fermions are usually considered. The Boltzmann-Compton model is studied in Escobedo (2001) for a simplified physical collision kernel in a spatially homogeneous isotropic frame. A local existence theorem for the Cauchy problem of the same model, with the physical kernel, is derived in Chane-Yook (2004). Global existence results and numerical simulations showing the formation of condensates are given in Ferrari (2006).
In this talk, we address the problem of interaction between condensates and non-condensates. For a BGK quantum kinetic model, we derive an existence theorem in a space-dependent stationary frame, where condensates and non-condensates are clearly distinguished.

1. The model and the existence theorem.

Similarly to the classical kinetic theory (Cercignani, 1988), a BGK type model can be introduced in the quantum case (Khalatnikov, 1965). In the stationary case in the slab, it is the following relaxation model,

$$p_1 \frac{\partial F}{\partial x} = \tilde{P}_{N,P,E}(F) - F, \quad x \in [-\frac{\eta}{2}, \frac{\eta}{2}], \quad p \in I\!R^3, \tag{1}$$

where $\tilde{P}_{N,P,E}(F)$ is the Bose-Einstein distribution function having the same momenta (N, P, E) as F (Escobedo, 2003). It displays the right physical properties, i.e. the conservation of mass, momentum and energy, together with the decrease of the entropy. Planckian diffuse reflexion boundary conditions are considered, i.e.

$$F(-\frac{\eta}{2}, p) = P_-(p) \int_{p_1'<0} \mid p_1' \mid F(-\frac{\eta}{2}, p')dp', \quad p_1 > 0,$$
$$F(\frac{\eta}{2}, p) = P_+(p) \int_{p_1'>0} p_1' F(\frac{\eta}{2}, p')dp', \quad p_1 < 0.$$

Here, $P_-(p) = \frac{1}{e^{u_- p^2 + v_-} - 1}$ and $P_+(p) = \frac{1}{e^{u_+ p^2 + v_+ -} - 1}$ are given Planckian distribution functions, chosen so that

$$\int_{p_1>0} p_1 P_-(p)dp = \int_{p_1<0} \mid p_1 \mid P_+(p)dp = 1.$$

Moreover, F is required to have a fixed total outflow (e.g. equal to one),

$$\int_{p_1<0} \mid p_1 \mid F(-\frac{\eta}{2}, p)dp + \int_{p_1>0} p_1 F(\frac{\eta}{2}, p)dp = 1.$$

The model is further simplified by considering $F(x,p)$ such that

$$P(x) := \int pF(x,p)dp = 0, \quad x \in [-\frac{\eta}{2}, \frac{\eta}{2}].$$

The property $P_1 \equiv 0$ is justified by the integration of (1) with respect to p_1, and the boundary conditions. The property $P_i \equiv 0$, $2 \leq i \leq 3$ is justified by integration of (1) w.r.t. (p_2, p_3).

We take the zero point energy of the condensate into account by moving the Dirac part in the Planckian distribution function from $p = 0$ to $p = \pm(\frac{1}{n}, 0, 0)$, and denote it by $\mathcal{P}^{\frac{1}{n}}$.

Theorem 1. *For some n_0 and any $n > n_0$, and for η small enough, there is a distribution function $F \in \mathcal{M}([-\frac{\eta}{2}, \frac{\eta}{2}] \times I\!R^3)$ solution to*

$$p_1 \frac{\partial F}{\partial x} = \mathcal{P}^{\frac{1}{n}} - F, \quad x \in [-\frac{\eta}{2}, \frac{\eta}{2}],\ p \in I\!R^3,$$

$$F(-\frac{\eta}{2}, p) = P_-(p) \int_{p_1'<0} \mid p_1' \mid F(-\frac{\eta}{2}, p')dp', \quad p_1 > 0,$$

$$F(\frac{\eta}{2}, p) = P_+(p) \int_{p_1'>0} p_1' F(\frac{\eta}{2}, p')dp', \quad p_1 < 0,$$

$$\int_{p_1<0} \mid p_1 \mid F(-\frac{\eta}{2}, p)dp + \int_{p_1>0} p_1 F(\frac{\eta}{2}, p)dp = 1.$$

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Rigorous drift-diffusion asymptotics of a quantum transport equation in the high-field case

Chiara Manzini
(joint work with Giovanni Frosali)

We propose an asymptotic analysis of a linear Wigner-BGK equation in the d-dimensional case. This equation models time evolution of an open quantum system with d degrees of freedom: it is governed by transport, by the action of an external potential, and by the interaction with the environment, which is described via a relaxation term. We consider the case in which the effects of the potential and of the environment are comparable. Thus, the equation is appropriately rescaled with a small parameter ϵ. It reads,

$$(1) \quad \epsilon \left(\frac{\partial w}{\partial t} + v \cdot \nabla_x w \right) = \Theta[V]\, w - \nu\, (w - w_{\mathrm{eq}})\,, \quad t > 0\,, \quad w(t=0) = w_0\,,$$

with the unknown $w = w(x, v, t), (x, v) \in \mathbb{R}^{2d}$, the *strong* external potential $V = V(x)$ and the operator $\Theta[V]$ defined by

$$(\Theta[V]w)(x, v, t) \;=\; \frac{i}{(2\pi)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \delta V(x, \eta)\, w(x, v', t)\, e^{i(v-v')\cdot\eta}\, dv'\, d\eta\,,$$

$$\delta V(x, \eta) := \frac{1}{\hbar} \left[V\left(x + \frac{\hbar\eta}{2m}\right) - V\left(x - \frac{\hbar\eta}{2m}\right)\right], \quad (x, \eta) \in \mathbb{R}^6,\ t > 0\,.$$

The function $w_{\rm eq} = w_{\rm eq}(x, v, t)$ describes the local thermal equilibrium state at the temperature $1/k\beta$

$$w_{\rm eq}(x, v, t) = n(x, t)F(v)\left(1 + \hbar^2 \frac{\beta^2}{24}\left(-\frac{1}{m}\Delta V + \beta \sum_{r,s=1}^{d} v_r v_s \frac{\partial^2 V}{\partial x_r x_s}\right)\right)$$

with the position density $n = n[w](x, t) := \int w(x, v, t)\, dv$. This is the $O(\hbar^2)$-correction to the classical Maxwellian $F = F(v) := (\beta m/2\pi)^{d/2} e^{-\beta m v^2/2}$ [4]. The parameter ν is the inverse relaxation-time.

We apply to the equation (1) the modified Chapman-Enskog expansion up to the first order in ϵ [2]. It consists in writing the Wigner unknown w as the sum of a component which solves the problem (1) with $\epsilon = 0$, precisely $n[w](x, t)\, M(x, v)$ with

$$(2) \qquad M(x, v) = \nu \mathcal{F}^{-1} \left\{ \frac{\mathcal{F}F(\eta)}{\nu - i\delta V(x, \eta)} \left(1 - \frac{\beta\hbar^2}{24m^2} \sum_{r,s=1}^{d} \eta_r \eta_s \frac{\partial^2 V(x)}{\partial x_s x_s}\right)\right\}$$

($\mathcal{F}$ ia the Fourier transform from v to η), and its orthogonal component ψ. The latter addendum is expanded in terms of ϵ and, by disregarding terms of order ϵ^2 and using projection operators, approximated problems are introduced for both the components. The equation for n is the continuity equation corrected by terms of order ϵ, namely, the pressure terms (classical and quantum), the high-field drift and pressure terms, that appear by solving the equation for the orthogonal component ψ. It looks like

$$(3) \qquad \begin{aligned} &\frac{\partial n}{\partial t} - \frac{1}{\nu m}\nabla\cdot(n\nabla V) - \frac{\epsilon}{\nu\beta m}\nabla\cdot\nabla n - \frac{\epsilon\beta\hbar^2}{12\nu m^2}\nabla\cdot\nabla\cdot(n\nabla\otimes\nabla V) \\ &-\frac{\epsilon}{\nu^3 m^2}\left[\nabla\cdot(n(\nabla\otimes\nabla)V\nabla V) + \nabla\cdot\nabla\cdot(n\nabla V\otimes\nabla V)\right] = 0\,. \end{aligned}$$

The second line is in agreement with the derivation performed in the semi-classical case [1, 3]. The advantage of such procedure is that it allows to treat simultaneously the initial layer problem, by introducing time-evolution equations for the behaviour of the components $n\,M$ and ψ for times close to 0. By the analysis of the regularity and the behaviour with respect to time of the different components and of the expansion terms, we can prove rigorously with which accuracy with respect to ϵ the Wigner function w is approximated. We remark that establishing such estimate requires to study well-posedness of Eq. (3), which is a singularly perturbed parabolic PDE with non-homogeneous coefficients, and in particular, to obtain regularity estimates for its solution, uniform with respect to ϵ.

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Functional inequalities and applications to large time asymptotics of solutions to nonlinear diffusion equations

Jean Dolbeault

(joint work with Ivan Gentil, Arnaud Guillin and Feng-Yu Wang)

The goal is to obtain new estimates of entropy - entropy production type using various techniques of capacity - measure theory. As a consequence, we obtain rates of convergence in the large time regime for solutions to nonlinear diffusion equations.

Let μ and ν be respectively a Borel probability measure and a positive Borel measure on a Riemannian manifold (M,g), which are not necessarily absolutely continuous with respect to the volume measure. Typical examples are $M=\mathbb{R}^d$ and $M=\mathbb{T}^d$. Assume for simplicity that $q\in(1/2,1)$, although some of our results can be extended to other values of q, see [2]. We shall say that (μ,ν) satisfies a *L^q-Poincaré inequality* with constant $\mathrm{C_P}$ if for all non-negative functions $f\in\mathcal{C}^1(M)$ one has

$$(1)\qquad \big[\mathbf{Var}_\mu(f^q)\big]^{1/q}:=\left[\int f^{2q}\,d\mu-\left(\int f^q\,d\mu\right)^2\right]^{1/q}\le \mathrm{C_P}\int|\nabla f|^2\,d\nu\;.$$

According to Röckner and Wang, [4], we shall also say that (μ,ν) satisfies a *weak Poincaré inequality* if there exists a non-negative non increasing function on $(0,+\infty)\ni s\mapsto\beta_{\mathrm{WP}}(s)$ such that, for any bounded function $f\in\mathcal{C}^1(M)$,

$$\forall\, s>0\,,\quad \mathbf{Var}_\mu(f)\le\beta_{\mathrm{WP}}(s)\int|\nabla f|^2\,d\nu+s\,\big[\mathbf{Osc}_\mu(f)\big]^2\,.$$

Here we define the *oscillation* of a bounded function f by $\mathbf{Osc}_\mu(f):=\mathrm{supess}_\mu f-\mathrm{infess}_\mu f$. If μ is absolutely continuous with respect to the volume measure and f is continuous, we can therefore define such a quantity as $(\sup\tilde f-\inf\tilde f)$ where $\tilde f$ is the restriction of f to the support of μ.

Given measurable sets A and Ω such that $A\subset\Omega\subset M$, *the capacity* $\mathrm{Cap}_\nu(A,\Omega)$ is defined as $\mathrm{Cap}_\nu(A,\Omega):=\inf\big\{\int|\nabla f|^2\,d\nu\;:\;f\in\mathcal{C}^1(M),\,\mathbb{I}_A\le f\le\mathbb{I}_\Omega\big\}$. Define

the quantity

$$\beta_{\rm P} := \sup \left\{ \sum_{k\in\mathbb{Z}} \frac{\big[\mu(\Omega_k)\big]^{1/(1-q)}}{\big[{\rm Cap}_\nu(\Omega_k,\Omega_{k+1})\big]^{q/(1-q)}} \right\}^{(1-q)/q}$$

where the supremum is taken over all $\Omega \subset M$ with $\mu(\Omega) \le 1/2$ and all sequences $(\Omega_k)_{k\in\mathbb{Z}}$ such that for all $k \in \mathbb{Z}$, $\Omega_k \subset \Omega_{k+1} \subset \Omega$.

Theorem 1. *With the above notations, (μ,ν) satisfies a L^q-Poincaré inequality with a finite positive constant* $\mathrm{C_P}$ *if and only if $\beta_{\rm P}$ is finite.*

Let us introduce the following property: *There exists a non-negative non increasing function γ on $(0,1/2)$ such that for every measurable subsets A, B of M with $A \subset B$ and $\mu(B) \le 1/2$,*

$$\mathrm{Cap}_\nu(A,B) \ge \frac{\mu(A)}{\gamma(\mu(A))} \ . \tag{2}$$

The next result is due to Barthe, Cattiaux and Roberto, see [1], up to the adaptation to non absolutely continuous measures.

Theorem 2. *Assume that (μ,ν) satisfies a weak Poincaré inequality for some non-negative non increasing function $\beta_{\rm WP}(s)$. Then Property (2) holds with $\gamma(s) := 4\,\beta_{\rm WP}(s/4)$. Reciprocally, if Property (2) holds for some function γ, then (μ,ν) satisfies a weak Poincaré inequality with associated function $\beta_{\rm WP}(s) = \kappa_{\rm P}\,\gamma(s)/\,2$, $\kappa_{\rm P} = (11+5\sqrt{5})$.*

The proof uses the fact that for all $a \in \mathbb{R}$,

$$\mathbf{Var}_\mu(f^q) \le \int \left(f^q - a^q\right)^2 d\mu \le \int |f-a|^{2q}\, d\mu \ ,$$

and as an interesting special case, this inequality holds for $a = m(f)$, a median of f with respect to μ. We recall that $m(f)$ is a median of f if and only if $\mu(\{f \ge m\}) \ge 1/2$ and $\mu(\{f \le m\}) \ge 1/2$.

Using the criterion of Theorem 2, we can make the link with L^q-Poincaré inequalities using Theorem 2.3.6 of [3].

Theorem 3. *If (μ,ν) satisfies the L^q-Poincaré inequality, then it also satisfies a weak Poincaré inequality with $\beta_{\rm WP}(s) = \mathrm{K}\,\beta_{\rm P}\,s^{1-1/q}$. Reciprocally, if (μ,ν) satisfies a weak Poincaré inequality with function $\beta_{\rm WP}$, then it satisfies a L^q-Poincaré inequality with $\beta_{\rm P} \le \kappa_{\rm P}\,\big(\frac{4}{1-q}\big)^{(1-q)/q}\,\|\beta_{\rm WP}(\cdot/4)\|_{L^{q/(1-q)}(0,1/2)}$.*

On $M = \mathbb{R}$, to a probability measure μ and a positive measure ν with density ρ_ν with respect to Lebesgue's measure, if m_μ is a median of μ, we associate the functions

$$R(x) := \mu([x,+\infty)) \ , \quad L(x) := \mu((-\infty,x]) \ ,$$
$$r(x) := \int_{m_\mu}^{x} \frac{1}{\rho_\nu}\, dx \ , \quad \ell(x) := \int_{x}^{m_\mu} \frac{1}{\rho_\nu}\, dx \ .$$

Theorem 4. *With the above notations, (μ,ν) satisfies a L^q-Poincaré inequality if*

$$\int_{m_\mu}^{\infty} |\, R\, r\,|^{q/(1-q)}\, d\mu < \infty \quad \textit{and} \quad \int_{-\infty}^{m_\mu} |\, L\, \ell\,|^{q/(1-q)}\, d\mu < \infty\ .$$

To extend such a result to more general spaces, we can use *tensorization* properties of the L^q-Poincaré inequalities. If for any $i \in \{1,\cdots,n\}$, μ_i is a probability measure and (μ_i,μ_i) satisfies a L^q-Poincaré inequality with constant $\mathrm{C_P}_i$, then $(\otimes_{i=1}^n \mu_i,\ \otimes_{i=1}^n \mu_i)$ satisfies a L^q-Poincaré inequality on M^n with constant $n^{1/q-1}\mathrm{max}_{1\le i\le n}\,\mathrm{C_P}_i$.

As an application of L^q-Poincaré inequalities, consider a function $\psi \in \mathcal{C}^1(\mathbb{R}^d)$ such that $Z_\psi := \int e^{-\psi} dx < +\infty$ and define the probability measure

$$d\mu_\psi := \frac{e^{-\psi}\, dx}{Z_\psi}\ .$$

Let $\mathcal{L}$ be the symmetric operator on $L^2_{\mu_\psi}(\mathbb{R}^d)$ given by $\mathcal{L} f := \Delta f - \nabla\psi\cdot\nabla f$ and consider for $m > 1$ the nonlinear partial differential equation

$$\frac{\partial u}{\partial t} = \mathcal{L}\, u^m$$

for $t \ge 0$, $x \in \mathbb{R}^d$, corresponding to a non-negative initial condition $u(0,x) = u_0(x)$ for any $x \in \mathbb{R}^d$. Such an equation is known as the *weighted porous media equation*. A simple computation shows that

$$\frac{d}{dt}\,\mathbf{Var}_{\mu_\psi}(u) = -\frac{8m}{(m+1)^2}\int |\nabla u^{\frac{m+1}{2}}|^2\, d\mu_\psi\ .$$

If (μ_ψ,μ_ψ) satisfies a L^q-Poincaré inequality, then $\mathbf{Var}_{\mu_\psi}(u)$ decays with an algebraic rate and one can prove that such a rate of decay is actually equivalent to the fact that (μ_ψ,μ_ψ) satisfies a L^q-Poincaré inequality.

Our results also apply to L^q-logarithmic Sobolev inequalities

$$\mathbf{Ent}_\mu\big(f^{2q}\big)^{1/q} \le \mathrm{C_{LS}} \int |\nabla f|^2\, d\mu\ ,$$

where $\mathbf{Ent}_\mu(g) := \int g \log\big(g/\int g\, d\mu\big)\ d\mu$. See [2] for further details.

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Some progress in the Kinetic Theory

Yan Guo

In this talk, some progress in the kinetic theory is discussed. For the Boltzmann theory, It is well-known that the first-order term in the diffusive expansion of the Boltzmann equation leads to the celebrated incompressible Navier-Stokes-Fourier system in fluid dynamics. Recently, the PDE for the higher-order terms have been derived in such a diffusive expansion, and the validity of such an expansion up to any finite order has been proven. Mathematically, a new energy method is developed to uniformly control the remainder. This work opens new research line to understand the correction to the Navier-Stokes theory. See [1].

A galaxy can be modeled by the Vlasov-Poisson system, in which stars only interact with gravitational potential they create collectively. There are two important types of galaxy models: the polytropes and the King model. Over the past eight years, Rein and the author have developed a successful variational method to prove stability of the polytropes. Unfortunately, such a method fails to treat the important King model, which is almost a canonical model widely used in astrophysical literature. Recently, Rein and the author were able to prove stability of the King model among certain symmetric perturbations, via a completely new approach. This first step opens a new line of research towards the study of King model. See [2].

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Derivation of the time dependent Gross-Pitaevskii equation for the dynamics of the Bose-Einstein condensate

László Erdős

(joint work with Benjamin Schlein and Horng-Tzer Yau)

The time dependent Gross-Pitaevskii equation describes the dynamics of initially trapped Bose-Einstein condensates. In this talk we presented a rigorous proof of this fact starting from a many-body bosonic Schrödinger equation with a short scale repulsive interaction in the dilute limit. Our proof shows the persistence of an explicit short scale correlation structure in the condensate.
The Hamiltonian of N interacting bosonic particles in $\mathbf{R}^3$ is given by

$$H_N^{\mathrm{trap}} = \sum_{i=1}^{N} \big[-\Delta_{x_i} + U(x_i) \big] + \sum_{i<j} V(x_i - x_j) \tag{1}$$

where U is a trapping potential (with $U(x) \to \infty$ as $|x| \to \infty$) and V is a repulsive interaction ($V \geq 0$).
We use the scaling

$$V(x) \to V_N(x) := N^2 V(Nx)$$

that was first used for the derivation of the stationary Gross-Pitaevskii equation by [3], where it was proven that the ground state energy per particle is asymptotically given by the minimizer of the Gross-Pitaevskii functional:

$$\lim_{N\to\infty} \frac{1}{N} \inf \mathrm{Spec}\, H_N^{\mathrm{trap}} = \min\{E_{GP}(\varphi) \ : \ \|\varphi\| = 1\}$$

with

$$E_{GP}(\varphi) = \int \left(|\nabla\varphi|^2 + U|\varphi|^2 + 4\pi a_0 |\varphi|^4 \right)$$

Here the coefficient a_0 is the scattering length of the unscaled potential V and note that the scattering length of the rescaled interaction potential V_N is $a = a_0/N$. The emergence of the scattering length is due to a specific short scale correlation structure present in the ground state ψ_N of any interacting bosonic Hamiltonian. This short scale structure is characterized by a factor

$$\prod_{i<j} f(N(x_i - x_j)) \tag{2}$$

where f is the zero energy scattering solution to $(-\Delta + \frac{1}{2}V)f = 0$ with the boundary condition $f(x) \to 1$ as $|x| \to \infty$.
Morover, it was proven by Lieb and Seiringer [4] that the ground state ψ_N of the trapped Hamiltonian H_N^{trap} exhibits complete Bose-Einstein condensation, that is, the one particle density matrix,

$$\gamma_N^{(1)} := \mathrm{Tr}_{2,3,\ldots N} |\psi_N\rangle\langle\psi_N|,$$

(computed by taking the partial trace for all but one variable) satisfies

$$\lim_{N\to\infty} \gamma_N^{(1)} = |\varphi_{GP}\rangle\langle\varphi_{GP}|$$

where φ_{GP} is the minimizer of $E_{GP}(\varphi)$.
Our main theorem is the derivation of a dynamical version of the Gross-Pitaevskii theory. The initial state is assumed to be the ground state ψ_N of the trapped Hamiltonian (1) with interaction potential scaled as $V_N(x) := N^2 V(Nx)$. Then we instantenously remove the trap and observe the evolution of ψ_N, i.e. we solve the Schrödinger equation

$$i\partial_t \psi_{N,t} = H_N \psi_{N,t}$$

with a Hamiltonian without a trap,

$$H_N = \sum_{i=1}^{N} -\Delta_{x_i} + \sum_{i<j} V_N(x_i - x_j),$$

and with initial data $\psi_{N,0} = \psi_N$. Let $\gamma_{N,t}^{(1)}$ be the one particle marginal density of the time evolved wavefunction $\psi_{N,t}$. Then we have the following theorem:

Theorem 1. *For any fixed time $t \in \mathbf{R}$, $\psi_{N,t}$ exhibits complete Bose-Einstein condensation, that is*

$$\gamma_{N,t}^{(1)} \to |\varphi_t\rangle\langle\varphi_t| \qquad \text{as } N \to \infty, \tag{3}$$

where φ_t solves the Gross-Pitaevskii equation

$$i\partial_t\varphi_t = -\Delta\varphi_t + 8\pi a_0|\varphi_t|^2\varphi_t \tag{4}$$

with initial data $\varphi_{t=0} = \varphi_{GP}$. The convergence in (3) is in weak convergence of trace class operators, i.e. in the sense that Tr K $(\gamma_{N,t}^{(1)} - |\varphi_t\rangle\langle\varphi_t|) \to 0$ for any compact operator K on $L^2(\mathbf{R}^3)$.

We can also prove propagation of chaos, i.e. that higher order correlation functions factorize in the limit:

$$\gamma_{N,t}^{(k)} \to |\varphi_t\rangle\langle\varphi_t|^{\otimes k}$$

for any fixed k, where the k-point correlation function is defined as

$$\gamma_{N,t}^{(k)} = \mathrm{Tr}_{k+1,k+2,\dots N}|\psi_{N,t}\rangle\langle\psi_{N,t}|$$

The same theorem holds for a product initial data, $\psi_{N,0} = \otimes_1^N\varphi$ with $\varphi \in H^1(\mathbf{R}^3)$, despite that the corresponding energy is given by a somewhat different functional:

$$\lim_{N\to\infty}\frac{1}{N}\langle\otimes_1^N\varphi, H_N\otimes_1^N\varphi\rangle = \min_{\|\varphi\|=1}\int\left(|\nabla\varphi|^2 + U|\varphi|^2 + \frac{b_0}{2}|\varphi|^4\right)$$

where $b_0 := \int V$ and note that $b_0 > 8\pi a_0$. Thus our theorem shows that the GP energy functional does not predict the correct coupling constant in the evolution equation for a product initial data. This apparent controversy is resolved by realizing that the convergence in the theorem is only in (weak) trace sense and not in energy sense. The product initial state lacks the characteristic short scale structure (2) related to the emergence of the scattering length, but in a very short time scale this structure is dynamically formed to reduce the local energy in the regime where any two particles are at a distance $1/N$ from each other. The excess energy is presumable disperses into intermediate modes on lengthscales $\frac{1}{N} \ll \ell \ll 1$ that do not influence the dynamics of the condensate.
The proof of the main theorem can be found in [1, 2].

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An Application of Landau Zener Formula: Resolvent Estimate for Matrix-Valued Schrödinger Operator

Clotilde Fermanian Kammarer
(joint work with Vidian Rousse)

Landau-Zener formula describes quantitatively the energy transfer which may occur when there is band's crossings. We present here a joint work with V. Rousse where these formula play a crucial role.

We consider the matrix-valued Schrödinger operator acting in $L^2(\mathbf{R}^d, \mathbf{C}^2)$,

$$P(\varepsilon) = -\frac{\varepsilon^2}{2}\Delta \,\mathrm{Id} + M(x)$$

where $0 < \varepsilon \ll 1$, $M \in \mathcal{C}^\infty(\mathbf{R}^d, \mathbf{C}^{2,2})$ is self-adjoint and long-range. We write

$$M(x) = p_0(x)\,\mathrm{Id} + \begin{pmatrix} p_1(x) & p_2(x) + ip_3(x) \\ p_2(x) - ip_3(x) & -p_1(x) \end{pmatrix},\ p = (p_1, p_2, p_3),\ p_j \in \mathcal{C}^\infty(\mathbf{R}^d)$$

We aim at estimating the resolvent $R(z, \varepsilon) = (P(\varepsilon) - z)^{-1}$ on the weighted L^2-space $L^{2,s}(\mathbf{R}^d, \mathbf{C}^2)$ consisting of functions f such that $x \mapsto < x >^s f(x)$ is in $L^2(\mathbf{R}^d, \mathbf{C}^2)$, $s > \frac{1}{2}$.

In the scalar case, if $p = 0$, one considers the Hamiltonian trajectories $\rho_s = (x_s, \xi_s)$ associated with $|\xi|^2/2 + p_0(x)$. An energy $\lambda > \lambda_\infty$ is said to be non-trapping if all the trajectories of energy λ (i.e. such that $\lambda = |\xi_s|^2/2 + p_0(x_s)\ \forall s$) goes to infinity when s goes to $\pm\infty$. Then there is an equivalence between the fact that the energy λ_0 is non trapping and the existence in a neighbourhood of λ_0 of estimations of the form

$$\|R(\lambda \pm i0, \varepsilon)\|_{L^{2,s} \to L^{2,-s}} \leq \frac{C_s}{\varepsilon}. \tag{1}$$

The proof of N. Burq (see [1]) uses the invariance of semi-classical measure of solutions of a Schrödinger equation along ρ_s.

In the matrix-valued case, when the eigenvalues $v^\pm(x) = p_0(x) \pm |p(x)|$ of M are of constant multiplicity 1, i.e. when p does not vanish. T. Jecko has adapted the arguments of N. Burq to this framework: If the energy λ is non trapping for both Hamiltonian trajectories $\rho_s^\pm$ of $|\xi|^2/2 + v^\pm(x)$, then (1) holds. The key argument is that a semi-classical measure of a solution of a Schrödinger equation with such a matrix-valued potential decouples on both modes and each part is invariant along the associated Hamiltonian curves (see [4]).

Let us consider now the matrix valued case with crossings (joint work with V. Rousse). Suppose $d \in \{1, 2, 3\}$ and that $\mathrm{Rank}\,(\mathrm{d}p(x)) = d$ on the crossing points, i.e. where $p(x) = 0$. One can still define continuous Hamiltonian trajectories passing through crossing points which have non zero momentum ([2]). We call generalized trajectories the curves consisting of branches of classical trajectories with either a switch or not at each crossing time ($\mathcal{C}^0$, smooth by piece).

One can prove (see [3]) that if $\lambda_0 \geq \lambda_\infty := \mathrm{Max}\Big(\underset{\{x;\, p(x)=0\}}{\mathrm{Sup}} p_0(x),, \|M_\infty\| \Big)$ is non trapping for the generalized trajectories of energy λ_0, then, there exist $\varepsilon_0 > 0$, and a neighbourhood I of λ_0 such that (1) holds for $\lambda \in I$ and $\varepsilon \in]0, \varepsilon_0[$.
Indeed, the decoupling and propagation of semi-classical measures still hold outside the crossing points. Besides, at crossing points with non zero momentum, there is energy transfer between the modes quantified by the so-called Landau-Zener formula (see [2]).
A refined version of this result gives under more restrictive assumptions on M Strichartz estimates for the propagator and global existence of solutions of the non linear semi-classical Schrödinger equation

$$\begin{cases} \frac{\varepsilon}{i}\partial_t \psi^\varepsilon + P(\varepsilon)\psi^\varepsilon + \varepsilon^\beta |\psi^\varepsilon|^2 \psi^\varepsilon = 0, \\ \psi^\varepsilon_{t=0} = \psi^\varepsilon_0, \end{cases}$$

where $|\psi^\varepsilon|$ stands for the norm of $\psi^\varepsilon(t,x)$ in $\mathbf{C}^2$. For $\psi^\varepsilon_0 \in H^1_\varepsilon$, the solution ψ^ε belongs to $\mathcal{C}^0\left(\mathbf{R}, H^1_\varepsilon(\mathbf{R}^d, \mathbf{C}^2)\right) \cap L^p_{loc}\left(\mathbf{R}, W^{1,q}_\varepsilon(\mathbf{R}^d, \mathbf{C}^2)\right)$ with (p,q) satisfying $1/p + d/q = d/2$, $p > 2$. We emphasize that this result applies in particular when $M(x)$ is equal to a constant matrix outside a ball.

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Critical Droplet Minimizers

Rossana Marra

We are interested in the study of the form of the minimizers for a class of non local functionals, which are Liapunov functionals for kinetic models in presence of phase transition. We start by studying a similar non local functional of the form

$$(1) \qquad \mathcal{F}(m) = \int_\Omega \left[\int_\Omega \frac{1}{4}[m(x) - m(y)]^2 |J(x-y)\mathrm{d}y + f(m) - f(m_\beta) \right] \mathrm{d}x$$

where

$$(2) \quad f(m) = -\frac{1}{2}m^2 + \frac{1}{\beta}s(m); \qquad s(m) = \frac{1-m}{2}\log\frac{1-m}{2} + \frac{1+m}{2}\log\frac{1+m}{2}.$$

$J(r)$ is smooth, of range θ and monotone. The function $m(x)$, with values in $[-1,1]$, has a meaning of magnetization for a system of spins. For temperature $T = \beta^{-1}$ lesser than a critical value T_c $f(m)$ has two symmetric minima $\pm m_\beta, m_\beta > 0$, corresponding to two "phases" of the system: The minimum at $-m_\beta$ represents a

phase with negative magnetization, while the minimum at $+m_\beta$ represents phase with positive magnetization.

Since the total amount of magnetization is conserved, we are interesting in minimizing $\mathcal{F}$ under the constraint

$$\frac{1}{|\Omega|}\int_\Omega m(x)\mathrm{d}x = n \tag{3}$$

for some fixed number n.

The central problem under discussion here is this:

• *What do the minimizers of $\mathcal{F}$ under the constraint (3) look like?*

The minimizers are typically droplets whose size is determined by the total mass in the system. We exactly determine the critical mass for droplet formation. We prove the following Theorems for the *minimal free energy function* $f_L(n)$

$$f_L(n) = \inf\left\{\ \mathcal{F}(m)\ :\ \frac{1}{L^d}\int_\Omega m(x)\mathrm{d}x = n\ \right\}\ . \tag{4}$$

Theorem 1. *For all $K > 0$,*

$$\lim_{L\to\infty}\frac{f_L}{|\Gamma_0|}\left(-m_\beta + KL^{-d/(d+1)}\right) = \inf_{0\le\eta\le 1} S\left(\eta^{1-1/d} + D(K)(1-\eta)^2\right) \tag{5}$$

where

$$D(K) = C\left(-m_\beta + KL^{-d/(d+1)}\right) = \frac{2}{d\chi S}\left(\frac{\sigma_d}{d}\right)^{-1/d}\left(\frac{K}{2}\right)^{(d+1)/d}$$

and $S = 2^{3/2}/3$.

Furthermore, let $K_\star$ be defined by

$$K_\star = 2\left(\frac{d+1}{2}\right)^{d/2}\left(\frac{\sigma_d}{d}\right)^{1/(d+1)}\left(\frac{\chi S}{2}\right)^{d/(d+1)}\ . \tag{6}$$

Then for all $K < K_\star$, and all L sufficiently large, the infimum in (5) is a minimum attained uniquely at $\eta = 0$, while for all $K > K_\star$, and all L sufficiently large, the infimum in (5) is a minimum attained uniquely at $\eta = \eta_c$ where $\eta_c \ge \eta_\star$.

Theorem 2. *For all $K < K_\star$ and L sufficiently large, when*

$$-m_\beta \le n \le -m_\beta + KL^{-d/(d+1)}\ ,$$

the unique minimizer for (4) is the uniform order parameter field $m(x) = n$.

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Kinetic Limit for Wave Propagation in a Random Medium

Jani Lukkarinen
(joint work with Herbert Spohn)

In this talk we consider discrete wave-equations with a random index of refraction and in the kinetic scaling limit. Based on the results in [1, 2], we discuss how the appropriately defined lattice Wigner transform converges to a positive measure whose time-evolution satisfies a linear Boltzmann equation. This property holds for quite general initial conditions and discrete scalar wave equations. In particular, this allows solving also the time-evolution of the energy-density in the kinetic scaling limit. The proof is based on the methods developed in [3, 4], which needed to be adapted to study more general dispersion relations, and to accommodate perturbations with additional momentum dependence and matrix-structure.

More explicitly, we study the Hamiltonian system

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} q_y(t) &= v_y(t), \\ (1+\sqrt{\varepsilon}\,\xi_y)^{-2} \frac{\mathrm{d}}{\mathrm{d}t} v_y(t) &= -\sum_{y'\in\mathbb{Z}^3} \alpha(y-y') q_{y'}(t) \end{aligned} \tag{1}$$

with $y \in \mathbb{Z}^3$ and $q_y(t), v_y(t) \in \mathbb{R}$. The "mass" of the atom at site y is $(1+\sqrt{\varepsilon}\,\xi_y)^{-2}$, where $(\xi_y)_{y\in\mathbb{Z}^3}$ is a family of independent, identically distributed random variables. Their common distribution is independent of ε, has zero mean and is supported on the interval $[-\bar{\xi}, \bar{\xi}]$. Expectation with respect to ξ is denoted by $\mathbb{E}$, and we assume $\varepsilon < \bar{\xi}^{-2}$ so that $1 + \sqrt{\varepsilon}\,\xi_y > 0$ with probability one.

The coefficients $\alpha(y)$ are the elastic couplings between atoms, and we require them to be exponentially decreasing and lead to stable harmonic interactions. Let $\widehat{\alpha}(k) = \sum_{y\in\mathbb{Z}^3} \mathrm{e}^{-\mathrm{i}2\pi k\cdot y}\alpha(y)$. Then $\widehat{\alpha} : \mathbb{T}^3 \to \mathbb{R}$ is the discrete Fourier-transform of α, where $\mathbb{T}^3 = \mathbb{R}^3/\mathbb{Z}^3$ denotes the 3-torus with unit side length. Mechanical stability demands $\widehat{\alpha} \geq 0$, so that the *dispersion relation*

$$\omega(k) = \sqrt{\widehat{\alpha}(k)} \tag{2}$$

is a positive function $\omega : \mathbb{T}^3 \to \mathbb{R}$. (The name stems from the fact that, if $\varepsilon = 0$, Eqs. (1) admit plane wave solutions with wave vector $k \in \mathbb{T}^3$ and frequency $\omega(k)$.)

We solve the differential equations (1) as a Cauchy problem with initial data $q(0), v(0)$. The time-evolution (1) conserves the energy

$$E(q,v) = \frac{1}{2}\Big(\sum_{y\in\mathbb{Z}^3} (1+\sqrt{\varepsilon}\,\xi_y)^{-2} v_y^2 + \sum_{y,y'\in\mathbb{Z}^3} \alpha(y-y') q_y q_{y'} \Big), \tag{3}$$

which we assume to be finite, $E(q(0),v(0)) < \infty$. Since $\omega(k) > 0$, this implies that $q(0), v(0) \in \ell_2(\mathbb{Z}^3, \mathbb{R})$. For any realization of ξ, the generator of the time-evolution (1) is a bounded operator on $\ell_2(\mathbb{Z}^3, \mathbb{R}^2)$, and thus the Cauchy problem has a unique, norm-continuous solution in $\ell_2(\mathbb{Z}^3, \mathbb{R}^2)$.

We then switch to new variables such that the energy (3) turns into a flat ℓ_2-norm. Let Ω denote the bounded operator on $\ell_2(\mathbb{Z}^3, \mathbb{C})$ defined via

$$(\Omega\phi)_y = \sum_{y'\in\mathbb{Z}^3} \widetilde{\omega}_{y-y'} \phi_{y'}\,, \tag{4}$$

where $\widetilde{\omega}$ is the inverse Fourier-transform of the function ω. Since $q(t), v(t) \in \ell_2(\mathbb{Z}^3, \mathbb{R})$, we can introduce the vector $\psi(t) \in \ell_2(\mathbb{Z}^3, \mathbb{C}^2)$ through

$$\psi(t)_{\sigma,y} = \frac{1}{2}\left((\Omega q(t))_y + \mathrm{i}\sigma (1+\sqrt{\varepsilon}\,\xi_y)^{-1} v(t)_y \right), \tag{5}$$

where $\sigma = \pm 1$ and $y \in \mathbb{Z}^3$. Let also $\ell_2 = \ell_2(\mathbb{Z}^3, \mathbb{C})$, and $\mathcal{H} = \ell_2(\mathbb{Z}^3, \mathbb{C}^2) = \ell_2 \oplus \ell_2$.

If we regard ξ as a multiplication operator on ℓ_2, i.e., if we define $(\xi\psi)_y = \xi_y \psi_y$, then $\psi(t)$ satisfies the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\psi(t) = -\mathrm{i} H_\varepsilon \psi(t), \quad \text{with} \quad H_\varepsilon = H_0 + \sqrt{\varepsilon} V, \tag{6}$$

where

$$H_0 = \begin{pmatrix} \Omega & 0 \\ 0 & -\Omega \end{pmatrix}, \quad V = \frac{1}{2}\begin{pmatrix} \Omega\xi + \xi\Omega & -\Omega\xi + \xi\Omega \\ \Omega\xi - \xi\Omega & -\Omega\xi - \xi\Omega \end{pmatrix}. \tag{7}$$

Since H_ε is a self-adjoint operator on $\mathcal{H}$, the solution to (6) generates a unitary group on $\mathcal{H}$, and, with initial conditions ψ^ε, the solution to (6) is given by

$$\psi(t) = \mathrm{e}^{-\mathrm{i}tH_\varepsilon}\psi^\varepsilon. \tag{8}$$

Unitarity is equivalent to energy conservation, since for all t

$$\|\psi(t)\|^2 = E(q(t), p(t)). \tag{9}$$

By inspection, $\psi(t)^*_{-,y} = \psi(t)_{+,y}$ for all y and t due to $q(t), v(t) \in \mathbb{R}$. Thus we can identify the energy density at time t and site y with $2|\psi(t)_{+,y}|^2$.

To study the time-evolution of the energy density, we resort to the lattice Wigner transform of a state $\psi \in \ell_2$. Given a scale $\varepsilon > 0$, we define the Wigner transform $W^\varepsilon[\psi]$ as the tempered distribution

$$\langle J, W^\varepsilon[\psi]\rangle = \sum_{y',y\in\mathbb{Z}^3} \psi^*_{y'}\psi_y \int_{\mathbb{T}^3} \mathrm{d}k\, \mathrm{e}^{\mathrm{i}2\pi k\cdot(y'-y)} J\Big(\varepsilon\frac{y'+y}{2}, k\Big)^*. \tag{10}$$

where $x \in \mathbb{R}^3$, $k \in \mathbb{T}^3$, and J is a Schwartz function. Similarly to the usual Wigner transform of L^2-functions, the "marginals" of W^ε satisfy:

$$\int_{\mathbb{T}^3} \mathrm{d}k\, W^\varepsilon[\psi](x,k) = \sum_{y\in\mathbb{Z}^3} \delta(x-\varepsilon y)|\psi_y|^2, \qquad \int_{\mathbb{R}^3} \mathrm{d}x\, W^\varepsilon[\psi](x,k) = |\widehat{\psi}(k)|^2. \tag{11}$$

We refer to [5] for an exhaustive discussion about Wigner transforms and harmonic lattice systems in general.

We assume that the dispersion relation ω satisfies:

(DR1) ω^2 is real-analytic and $\omega(-k) = \omega(k)$.
(DR2) $\min_k \omega(k) > 0$.
(DR3, *dispersivity*) ω is a *Morse function*: it has only isolated critical points, which are non-degenerate (the Hessian is invertible at every critical point).
(DR4, *suppression of crossings*) The periodic extension of ω to $\mathbb{R}^3$ is not a constant on any affine hyperplane.

The main content of [2] is to prove that the final condition, (DR4), implies sufficient curvature of level sets of ω so that the so called crossing integrals containing three resolvent factors can be neglected in the kinetic limit.

We then study a limit where $\varepsilon \to 0^+$ via some arbitrary sequence of values. For each ε, we assume that initial conditions $\psi^\varepsilon \in \mathcal{H}$ are independent of ξ, and that the sequence $(\psi^\varepsilon)_\varepsilon$ has the following properties:

(IC1, *bounded*) $\sup_\varepsilon \|\psi^\varepsilon\| < \infty$.
(IC2, *tight*) $\lim_{R\to\infty} \limsup_{\varepsilon\to 0} \sum_{|y|>R/\varepsilon} |\psi^\varepsilon_y|^2 = 0$.
(IC3, *convergent*) The limit $\lim_{\varepsilon\to 0}\langle J, W^\varepsilon[\psi^\varepsilon_+]\rangle$ exists for all $J \in \mathcal{S}(\mathbb{R}^3\times\mathbb{T}^3)$.

Theorem 1. *Assume ω and ψ^ε satisfy the above conditions, and let $\psi(t)$ denote the random vector determined by (8). Then for all $t \geq 0$, there is a positive Radon measure μ_t such that for any $J \in \mathcal{S}(\mathbb{R}^3\times\mathbb{T}^3)$,*

$$\lim_{\varepsilon\to 0} \mathbb{E}[\langle J, W^\varepsilon[\psi(t/\varepsilon)_+]\rangle] = \int_{\mathbb{R}^3\times\mathbb{T}^3} \mu_t(\mathrm{d}x\,\mathrm{d}k)\, J(x,k)^*. \tag{12}$$

In addition, μ_t satisfies a linear Boltzmann equation, in the sense that if W denotes the formal density of μ, i.e., $\mu_t(\mathrm{d}x\,\mathrm{d}k) = W(x,k,t)\mathrm{d}x\mathrm{d}k$, then

$$\begin{aligned} &\partial_t W(x,k,t) + \frac{\nabla\omega(k)}{2\pi}\cdot\nabla_x W(x,k,t) \\ &\quad = \mathbb{E}[\xi_0^2]\, 2\pi\, \omega(k)^2 \int_{\mathbb{T}^3} \mathrm{d}k'\, \delta(\omega(k)-\omega(k'))\,(W(x,k',t) - W(x,k,t))\,. \end{aligned} \tag{13}$$

More precisely, Eq. (13) should be understood as a generator of a semi-group on bounded positive Radon measures. After solving (13), we can find the time-evolution of the kinetic limit of the energy density by integrating out the k-variable: $\mathcal{E}(x,t) = \int_{\mathbb{T}^3} \mathrm{d}k\, W(x,k,t)$.

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On the derivation of kinetic equations from macroscopic quantum mechanics

Raffaele Esposito

We consider a system of $N = \epsilon^{-3}$ quantum particles interacting via a two body potential in the weak coupling limit. We give an diagramatic expansion of the evolved j-particles Wigner functions for the full system and show that when $N \to \infty$ and the size of the potential is $\sqrt{\epsilon}$ and the initial state satisfies a suitable *molecular chaos* assumption, the expansion converges term by term to a factorized limiting sequence satisfying the Classical Boltzmann Hierarchy with a cross section computed according to the Fermi Golden Rule. Therefore the 1-particle distribution solves the Classical Boltzmann equation. The proof is achieved by a detailed analysis of the oscillating terms in the different kind of graphs. An important (technical) restriction is the assumption that the interaction potential has vanishing average.

Derivation of nonlinear Convection-Diffusion Equations from BGK Models

Christian Schmeiser

(joint work with J. Dolbeault, P. Markowich, D. Oelz)

We consider the scaled kinetic equation

$$\varepsilon^2\,\partial_t f + \varepsilon\,[v\cdot\nabla_x f - \nabla_x V(x)\cdot\nabla_v f] = Q(f)\,, \tag{1}$$

$$Q(f) := G_f - f\,, \quad G_f := \gamma\Big(\frac{1}{2}|v|^2 - \bar\mu(\rho_f(x,t))\Big)\,, \tag{2}$$

where the distribution function $f = f(x,v,t)$ depends on position $x \in \mathbb{R}^3$, velocity $v \in \mathbb{R}^3$, and time $t > 0$. The collision model is a simple relaxation kernel towards a generalized local Gibbs state G_f. The chemical potential $\bar\mu(\rho_f)$ is determined implicitly by the condition $\int_{\mathbb{R}^3} G_f\,dv = \rho_f := \int_{\mathbb{R}^3} f\,dv$, or equivalently

$$\rho = \int_{\mathbb{R}^3} \gamma\left(\frac{1}{2}\,|v|^2 - \bar\mu(\rho)\right) dv\,. \tag{3}$$

We are interested in the diffusion limit $\varepsilon \to 0$ which corresponds to a large time scale and a high collision frequency limit. In [1] we prove that in the limit $\varepsilon \to 0$, the distribution function f is a local Gibbs state: $f = G_f$, whose density is subject to a nonlinear diffusion equation

$$\partial_t \rho = \nabla_x \cdot (\nabla_x \nu(\rho) + \rho \nabla_x V) \quad \text{with } \nu'(\rho) = \rho \bar{\mu}'(\rho) \ .$$

The main modelling ingredient is the energy dependent equilibrium profile $\gamma(E) \geq 0$, which is assumed to be nonincreasing. The given external potential $V(x)$ is assumed to be 'confining'. An appropriate definition of this property depends on the profile γ. For the detailed assumptions, an exact formulation of the limit theorem, and the proof, see [1].
The most notable applications include:

(1) *Fast diffusion:* $\gamma(E) = E^{-k}$ with $k > 5/2$, giving $\nu(\rho) = c\rho^{(k-5/2)/(k-3/2)}$,
(2) *Linear diffusion:* $\gamma(E) = e^{-E}$, giving $\nu(\rho) = \rho$,
(3) *Slow diffusion:* $\gamma(E) = (E_0 - E)_+^k$ with $k > 0$, giving $\nu(\rho) = c\rho^{(k+5/2)/(k+3/2)}$.

The assumptions of the limit theorem also allow for Fermi-Dirac and Bose-Einstein equilibrium distributions.

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Rigorous analysis of a model of spray in quasi-static condition

Valeria Ricci
(joint work with Laurent Desvillettes, François Golse)

We present a rigorous derivation of Brinkman's force for a quasi-static system consisting of a cloud of spherical particles with different instantaneous velocities immersed in a Stokes (or steady Navier-Stokes) fluid in a smooth, bounded domain $\Omega \subset \mathbb{R}^3$. Equations similar to the ones we derive are sometimes used for describing the fluid phase in models of sprays or suspensions. The quasi-static assumption allows us to consider the solid particles as having fixed positions.

More precisely, we consider a system of N spheres $B_{x_k,\varepsilon}$, of radius ε and center x_k, with instantaneous velocities $v_k,$, $k = 1, \ldots, N$, sourrounded by an incompressible fluid with density $\rho = 1$, kinematic viscosity ν and velocity field u_ε, described in the domain $\Omega_\varepsilon = \Omega \setminus \bigcup_{k=1}^N B_{x_k,\varepsilon}$ by the equations

$$\left\{ \begin{array}{rcll} A(u_\varepsilon) + \nabla p_\varepsilon & = & g, & \\ \nabla \cdot u_\varepsilon & = & 0, & \text{on } \Omega_\varepsilon \end{array} \right. \tag{1}$$

with no-slip boundary conditions

$$(2)\qquad \left\{\begin{array}{rcll} u|_{\partial B_{x_k,\varepsilon}} & = & v_k, & \text{for} \quad k=1,..,N,\\ u|_{\partial\Omega} & = & 0. & \end{array}\right.$$

In (1), we consider $A(u) = -\triangle u$ (Stokes fluid) or $A(u) = u\nabla u - \nu\triangle u$ (steady Navier-Stokes fluid), p_ε is the pressure and g is the density of external force per unit of mass in the Navier–Stokes case or its ratio to the kinematic viscosity in the Stokes case.

By means of homogenization methods, following the lines in ([2]) and ([3]) (where the authors considered periodic distributions of spheres all with the same velocities resp. for the Stokes and Navier-Stokes equations and for the Laplace equation) but simplifying the computations by using solenoidal correctors for the velocity field and therefore avoiding explicit estimates of the pressure, we show that, when $g \in (L^2(\Omega))^3$, $\varepsilon = \frac{1}{N}$, $\inf_{1\le k\neq l\le N} |x_k - x_l| > 2\varepsilon^{1/3}$, $\inf_{1\le k\le N} \mathrm{dist}(x_k, \partial\Omega) > \varepsilon^{1/3}$, and the empirical measure associated to the spheres, $F_N(x,v) = \frac{1}{N}\sum_{k=1}^N \delta_{x_k,v_k}(x,v)$, is such that $\sup_{N\ge1} \iint_{\Omega\times\mathbb{R}^3} \frac{1}{2}|v|^2 F_N dxdv < \infty$, and $\rho_N = \int_{\mathbb{R}^3} F_N\, dv \rightharpoonup \rho \in C(\bar\Omega)$, $j_N = \int_{\mathbb{R}^3} F_N\, v\, dv \rightharpoonup j \in C(\bar\Omega)$ (weakly in the sense of measures), the natural extension $\bar u_\varepsilon$ of u_ε to Ω, defined by $\bar u\varepsilon(x) = u_\varepsilon(x)$ if $x \in \Omega_\varepsilon$, $\bar u\varepsilon(x) = v_k$ if $x \in B_{x_k,\varepsilon}$, converges in $(L^2(\Omega))^3$, when $N \to \infty$, to the solution U of

$$(3)\qquad \left\{\begin{array}{rcl} A(U) + \nabla\Pi & = & g + 6\,\pi\,(j - \rho\, U),\\ \nabla\cdot U & = & 0,\\ U|_{\partial\Omega} & = & 0 \end{array}\right.$$

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Some explicit expressions of the Fourier transformed Boltzmann equation

Sergej Rjasanow

(joint work with Ralf Kirsch)

The spatially homogeneous Boltzmann equation reads

$$(1)\qquad f_t(t,v) \;=\; Q(f,f)(t,v) \quad \text{for } t>0\,,\ v\in\mathbb{R}^3\,,$$

where the unknown distribution density function f depends on time $t \geq 0$ and velocity $v \in \mathbb{R}^3$. The collision operator is given by

$$Q(f,g)(v) = \int\limits_{\mathbb{R}^3} \int\limits_{S^2} B(v,w,e)\Big(f(v')g(w') - f(v)g(w)\Big)\, de\, dw\,,$$

where S^2 denotes the unit sphere and

$$v' = \frac{1}{2}\big(v + w + |v-w|\, e\big) \quad , \quad w' = \frac{1}{2}\big(v + w - |v-w|\, e\big).$$

The so-called collision kernel B describes the microscopic details of the particle interaction and is generally assumed to be of the form

$$(2) \quad B(v,w,e) = b_\lambda(\mu)\, |v-w|^\lambda\,, \qquad \mu = \frac{(v-w,e)}{|v-w|}\,, \qquad -3 < \lambda \leq 1\,,$$

where $(\cdot,\cdot)$ denotes the scalar product in $\mathbb{R}^3$. In general, the angular part b_λ contains a non-integrable singularity at $\mu = 1$. In practical applications, the so-called VHS model for hard potentials is frequently considered, i.e. the function b_λ is assumed to be constant:

$$(3) \qquad B(v,w,e) = C_\lambda\, |v-w|^\lambda\,, \qquad 0 \leq \lambda \leq 1\,.$$

1. Fourier transformed Boltzmann equation

We will denote by φ any test function in the Schwartz space $\mathbb{S}$ of infinitely smooth and rapidly decreasing functions on $\mathbb{R}^3$. The Fourier transform of φ is denoted by

$$\hat\varphi(\xi) = \mathcal{F}_{v\to\xi}(\varphi)(\xi) = \int\limits_{\mathbb{R}^3} \varphi(v)\, \mathrm{e}^{\mathrm{i}(v,\,\xi)}\, dv\,.$$

The first important step in use of the Fourier transform for the Boltzmann equation was made by Bobylev in [1], where he found that in the case of Maxwellian molecules ($\lambda = 0$ in (2)), the Fourier transform of the equation acquires the form

$$(4) \qquad \hat f_t(\xi) = \int\limits_{S^2} b_0(\mu)\left(\hat f\Big(\frac{\xi + |\xi| e}{2}\Big)\hat f\Big(\frac{\xi - |\xi| e}{2}\Big) - \hat f(\xi)\, \hat f(0)\right) de\,,$$

noting that here $\mu = (\xi, e)/|\xi|$. This remarkable result could be used to find exact solutions of the equation (1). We recall that the convolution of a tempered distribution Φ with a test function $\varphi \in \mathbb{S}$ is again a tempered distribution and that the following well-known identity holds

$$\widehat{(\Phi * \varphi)}(\xi) = \hat\Phi(\xi)\, \hat\varphi(\xi)\,.$$

For $z \in \mathbb{R}^3$, we demand that (1) is fulfilled in the sense of tempered distributions, i.e.

$$(5) \qquad \forall\, \varphi \in \mathbb{S} \,:\, \Big(f_t, \varphi(z-\cdot)\Big) = \Big(Q(f,f), \varphi(z-\cdot)\Big)\,.$$

After some manipulations we obtain that the transformed Boltzmann equation reads (cf. [2])

$$\hat{f}_t(t,\xi) = \int\limits_{\mathbb{R}^3} \hat{f}\Big(t, \frac{\xi+\eta}{2}\Big)\hat{f}\Big(t, \frac{\xi-\eta}{2}\Big)\, T_\lambda(\xi,\eta)\, d\eta\,, \tag{6}$$

where T_λ is given by

$$T_\lambda(\xi,\eta) = \frac{2^{\lambda-1}}{8\pi^3}\int\limits_{\mathbb{R}^3} |y|^\lambda \mathrm{e}^{\mathrm{i}(y,\eta)} \int\limits_{S^2} b_\lambda(\mu)\left(\mathrm{e}^{-\mathrm{i}(|y|e,\xi)} + \mathrm{e}^{\mathrm{i}(|y|e,\xi)} - \mathrm{e}^{-\mathrm{i}(y,\xi)} - \mathrm{e}^{\mathrm{i}(y,\xi)}\right) dy de\,, \tag{7}$$

which is independent of the test function φ and contains the information about the particle interaction. Recall that $y = (v-w)/2$ and, therefore, the infinitely smooth term in brackets is sufficient to cancel out the singularities in the collision kernel.

2. Examples

For the VHS model (3) the kernel (7) simplifies to

$$T_\lambda(\xi,\eta) = -C_\lambda \frac{2^\lambda}{\pi}\,\Gamma(\lambda+1)\sin\big(\frac{\pi\lambda}{2}\big)\times \left(\frac{\big||\xi|-|\eta|\big|^{-\lambda-1} - \big||\xi|+|\eta|\big|^{-\lambda-1}}{|\xi|\,|\eta|} - (\lambda+1)\Big(\frac{1}{|\xi-\eta|^{\lambda+3}} + \frac{1}{|\xi+\eta|^{\lambda+3}}\Big)\right). \tag{8}$$

For Hard spheres model ($\lambda = 1$) we get

$$T_1(\xi,\eta) = -C_1\,\frac{4}{\pi}\left(\frac{2}{\big||\xi|^2-|\eta|^2\big|^2} - \left(\frac{1}{|\xi-\eta|^4} + \frac{1}{|\xi+\eta|^4}\right)\right).$$

The kernel T_0 cannot be obtained by simply letting $\lambda \to 0$ in (8). Instead, we obtain

$$T_0(\xi,\eta) = 2C_0\left(\frac{1}{|\eta|\,|\xi|}\Big(\delta(|\xi|-|\eta|) - \delta(|\xi|+|\eta|)\Big) - 16\pi\Big(\delta(\xi-\eta)+\delta(\xi+\eta)\Big)\right)$$

The expression (8) can be used also for soft potentials, i.e. for $\lambda < 0$. Thus, letting $\lambda \to -1$ we obtain

$$T_{-1}(\xi,\eta) = -\frac{2}{\pi}\,C_{-1}\Big(\frac{1}{|\xi-\eta|^2} + \frac{1}{|\xi+\eta|^2} + \frac{\log\big||\xi|-|\eta|\big| - \log\big||\xi|+|\eta|\big|}{|\xi|\,|\eta|}\Big)$$

and, finally, for $\lambda \to -2$

$$T_{-2}(\xi,\eta) = -\frac{1}{8}\,C_{-2}\Big(\frac{2}{\min(|\xi|,|\eta|)} + \frac{1}{|\xi-\eta|} + \frac{1}{|\xi+\eta|}\Big)\,.$$

3. Conclusions

Since the operator in (6) contains only one three-dimensional integral, even the most straightforward approximation method will lead to a numerical scheme with competitive efficiency.
Moreover, the kernel T_λ in (7) is explicitly known for the practically relevant $\lambda \in (-3, 1]$ but the singularities appearing in the kernel are quite strong.

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On the blowing up of solutions to quantum hydrodynamic models on bounded domains

Maria Pia Gualdani
(joint work with Irene M. Gamba, Ping Zhang)

The evolution of a quantum fluid in a first approximation can be described by a dispersive perturbation associated to the Hamilton-Jacobi system for compressible fluid dynamics, sometimes referred as a dispersive perturbation of the Eikonal equation for the evolution of amplitude and phase velocity of quantum wave guides. This system consists in the continuity equation for the particle density ρ and for the momentum ρu

$$\rho_t + \operatorname{div}(\rho u) = 0, \qquad t > 0,\ x \in \Omega \subseteq \mathbb{R}^d, \tag{1}$$

$$(\rho u)_t + \operatorname{div}(\rho u \otimes u) + \nabla P(\rho) = \frac{\varepsilon^2}{2}\rho \nabla \left(\frac{\Delta \sqrt{\rho}}{\sqrt{\rho}} \right), \tag{2}$$

where $P(\rho) > 0$ describes a pressure function, due to the boundary or to mean field effects, and ε denotes the scaled Planck constant.
Formally equations (1), (2) can be derived through the Madelung's transform [7] from the nonlinear Schrödinger equation

$$i\varepsilon \psi_t = -\frac{\varepsilon^2}{2}\Delta \psi + h(|\psi|^2)\psi, \quad x \in \mathbb{R}^d, \tag{3}$$

for the wave function $\psi(x, t)$, where h is an integrable function such that $h'(\rho) = \frac{P'(\rho)}{\rho}$.
We show the blow-up in finite time for solutions to the multi-dimensional quantum hydrodynamic model (1), (2) in bounded domains. The proof is based on a-priori estimates for the energy functional for a new observable constructed with an auxiliary function, and it is shown that under suitable assumptions on the initial and boundary data the solution blows up after a finite time. Our method is in essence inspired in the original argument of R. Glassey [3], where he proved finite

time blow up of smooth solutions to the focusing nonlinear Schrödinger equation (3) with large initial data. Since we are dealing with a boundary value problem the weight function $a(x)$, which defines the new *observable* $I(t) = \int_\Omega a(x)\rho(x,t)\,dx$ should be chosen differently from the Cauchy-problem case. It will turn out that the function $a(x)$ must be a concave function with zero value on a part of the boundary and its form will depend on the domain and of course on the boundary conditions of the problem.

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Adiabatic approximation for quantum systems responding to laser pulses

Caroline Lasser

The response of atoms or molecules to laser pulses is described by time-dependent Schrödinger equations of the form

$$i\partial_t\psi = (H_0 + \widehat{\mu}\,F(t)\sin(\omega t))\,\psi, \qquad \psi(t_0) = \psi_0. \tag{1}$$

Typically, the envelope function $F(t)$ of the pulse's electric field varies slowly on the time-scale set by the oscillation frequency $\omega \gg 1$ of the laser. This separation of time-scales suggests the following point of view, which has been taken by several chemists and physicists, e. g. [1, 2, 3, 6]: The purely time-periodic system with frozen constant field envelope is the unperturbed problem, which is adiabatically perturbed by the slow variation of the envelope function $F(t)$. The talk explained, how for N-level systems, $H_0, \widehat{\mu} \in \mathbb{C}^{N\times N}$, the description of the unperturbed situation in terms of Floquet states shines through in an adiabatic approximation of the Schrödinger equation (1). Moreover, an outline for a mathematically rigorous

proof of this approximation was presented [4], which crucially uses ideas of Panati, Spohn, and Teufel for proving effective dynamics of Bloch electrons [5].

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Adiabatic Description of Piezoelectricity

Christof Sparber

(joint work with Gianluca Panati, Stefan Teufel)

In the year 1880 the brothers Jacques and Pierre Curie discovered that some crystalline solids (like quartz, tourmaline, topaz, ...) exhibit a relevant macroscopic property: if the sample is strained along a particular axis (called the piezoelectric axis) a macroscopic polarization at the edges of the sample appears.
Even though first technological applications already appeared only a few years later, a microscopic understanding of the phenomenon waited many decades after the appearance of quantum mechanics. Up to the mid seventies, it was common lore that the macroscopic (relative) polarization $\Delta\mathbf{P} = \mathbf{P}_{\rm fin} - \mathbf{P}_{\rm in}$ (*i.e.* the polarization in the final state with respect to the initial state of the sample) was due to the fact that, by deforming the crystal, the fundamental unit cell acquires a *non-vanishing electric dipole moment* with respect to the unperturbed state. As pointed out by Martin in 1974 [2], the previous approach was intrinsically incorrect, since the total polarization should take into account not only the sum of the dipole moments of the unit cells, but also the *transfer of charge* between unit cells. While in the ionic contribution $\Delta\mathbf{P}_{\rm ion}$ the transfer of charge is negligible, it cannot be neglected as far as the electronic contribution $\Delta\mathbf{P}_{\rm el}$ is concerned.[1] It has thus been suggested by Resta [3] to shift the attention from the charge distribution (*i.e.* the electric dipole moment) to the current, *cf.* the review papers [4, 5] and references given therein. In other words one considers

$$\Delta\mathbf{P}_{\rm el} = \int_{T_{\rm in}}^{T_{\rm fin}} {\rm d}t\ \dot{\mathbf{P}}(t),$$

[1] Thereby one clearly assumes that an approximate splitting $\Delta\mathbf{P} = \Delta\mathbf{P}_{\rm ion} + \Delta\mathbf{P}_{\rm el}$ is justified.

where $\dot{\mathbf{P}}(t)$, called the *piezoelectric current*, is the real quantity. Within this framework, Resta used linear response theory in order to conveniently re-express $\Delta\mathbf{P}_{\mathrm{el}}$ in terms of the Bloch functions [3, 4].
Elaborating on Resta's result, King-Smith and Vanderbilt [1] were able to relate the relative polarization to the Berry connection, through the formula

$$\Delta\mathbf{P}_{\mathrm{el}} = \frac{1}{(2\pi)^d} \sum_{m=0}^{M} \int_{\mathbb{T}^*} \mathrm{d}k \, \big(\mathcal{A}_m(k,T) - \mathcal{A}_m(k,0)\big), \tag{1}$$

where the sum runs over all the occupied Bloch bands, d is the space dimension, $\mathbb{T}^*$ denotes the first Brillouin zone, and $\mathcal{A}_m(k,t)$ is the Berry connection for the mth Bloch band at time $t \in \mathbb{R}$, *i.e.*

$$\mathcal{A}_m(k,t) = \mathrm{i}\,\langle \varphi_m(k,t), \nabla_k \varphi_m(k,t)\rangle_{L^2(Y)}\,. \tag{2}$$

Here φ_m is the mth eigenfunction of Bloch's spectral problem (the electronic structure problem). Thereby the deformation is supposed to take place during the time-interval $I = [0,T]$. The advantage of formula (1) is twofold: it depends only on the occupied bands, and it relates the macroscopic polarization to a geometric quantity, which, as discussed later, does not depend on the particular gauge, *i.e.* the choice of the phase of the Bloch functions.
In my talk at Oberwolfach I reported on a joint paper with the above authors [6] where we were able to provide a rigorous formula for $\Delta\mathbf{P}_{\mathrm{el}}$, which is even more general than (1), by exploiting the fact that the deformation of the crystal is an adiabatic phenomenon, *i.e.* it is extremely slow when measured on the atomic time-scale. To this end we first give a precise mathematical meaning to the Piezocurrent based on some limiting procedure which allows us to define a bulk property for particles, independent of the precise shape of the crystal. We then mainly rely on (a somewhat generalized) version of the so-called *super-adiabatic approximation* for time-dependent quantum systems in order to derive a result which is valid up to any orders in the small perturbation parameter $\varepsilon \ll 1$. A connection between the macroscopic current and the underlying geometry of the Bloch bundle is drawn and in particular the role of space-reflection symmetry is discussed. Moreover we provide an alternative derivation of (1) relying on the semiclassical dynamics of a state which is essentially concentrated on a single isolated Bloch band.

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Traffic-like models for supply chains

Pierre Degond
(joint work with D. Armbruster, C. Ringhofer)

Traffic flow type models for supply chains model the flow of items through the chain as conservation laws for an item density ρ, depending on time and a stage variable x. So, stage $x = 0$ denotes the raw material, and stage $x = 1$ denotes the finished product and the interval $[0, 1]$ models the intermediate stages of the production process, and plays the role of the 'road' in traffic flow theory. Traffic models have been used to model supply chains in [1, 2, 10, 4, 7] and, more recently to optimize them in [6, 8].
In the work [3] we have developed a traffic flow type model for a chain of suppliers with a given capacity and throughput time. It is of the form

$$\partial_t \rho(x,t) + \partial_x F(x,t) = 0, \quad F(x,t) = \min\{\mu(x), V(x)\rho\} \tag{1}$$

Here x denotes a continuous supplier index, i.e. the stage of the process. $\rho(x,t)$ denotes the density of parts in the supply chain. So, to compute the number of parts - the Work in Progress (or WIP) $W_{ab}(t)$ in a certain subset of processors, corresponding to an interval (a, b) at a given time t, we have to compute $W_{ab}(t) = \int_a^b \rho(x,t)\, dx$. As long as the processors run below capacity, the movement of parts is given by the velocity V. So $\frac{dx}{V(x)}$ is proportional to the throughput time of the processor occupying the infinitesimal interval dx. The processors are assumed to have a finite capacity, meaning that they cannot process more that $\mu(x)dt$ parts in any infinitesimal time interval dt. So the variables in (1) have units of parts / stage for ρ, parts /time for μ, and stage / time for V. We prescribe an, in general time dependent, influx of the form

$$F(0,t) = \lambda(t) \tag{2}$$

for the conservation law (1).
Equation (1) is derived rigourously in [3] from a discrete recursion for the times each part arrives at each processor, and a limiting process for the number of parts and the number of processors $M \to \infty$. However, this recursion relation is completely deterministic, and the supply chain is therefore assumed to work like an automaton.
In [5] we also discuss the inclusion of a random behavior of the processors, i.e. random breakdowns and random repair times, into the model. We model the breakdown of processors by setting the capacity $\mu(x)$ to zero. Thus, the model we consider consists of the equation (1), where $\mu = \mu(x,t)$ is a time dependent random variable. To be more precise we assume $\mu(x,t)$ to be piecewise constant in space and of the form

$$\mu(x,t) = \sum_{m=0}^{M-1} \mu_m(t) \chi_{[\gamma_m, \gamma_{m+1})}(x) \tag{3}$$

where $0 = \gamma_0 < .. < \gamma_M = 1$ denotes a partition of the stage interval $[0,1]$, corresponding to M processors, and the functions $\mu_m(t),\ m = 0,..,M-1$ take on values of either $\mu_m(t) = 0$ or $\mu_m = c_m$, where c_m denotes the capacity of the processor, in case it is running. For simplicity, we assume that the on / off switches are exponentially distributed in time. That is we assume mean up and down times τ_m^{up} and τ_m^{down}, and generate the random signal $\mu_m(t)$ by the following algorithm:

- Assuming that at time t processor m has just switched from the off state to the on state, choose Δt_{up}^m and Δt_{down}^m randomly from the distributions $d\mathcal{P}[\Delta t_{up}^m = s] = \frac{1}{\tau_m^{up}} \exp(-\frac{s}{\tau_m^{up}})ds$ and $d\mathcal{P}[\Delta t_{down}^m = s] = \frac{1}{\tau_m^{down}} \exp(-\frac{s}{\tau_m^{down}})ds$.
- Set $\mu_m(s) = c_m$ for $t < s < t + \Delta t_{up}^m$ and $\mu_m(s) = 0$ for $t + \Delta t_{up}^m < s < t + \Delta t_{up}^m + \Delta t_{down}^m$.
- At $t = t + \Delta t_{up}^m + \Delta t_{down}^m$ the processor is turned on again and we repeat the above process.

This way we generate M random time dependent signals which produce the random capacity $\mu(x,t)$ according to (3). For each realization of this process we solve one realization of the conservation law (1), modeling so the random breakdown of elements in the chain.

Note that the conservation law (1) exhibits, despite of its simple form, a rather interesting feature. Since the flux function F is uniformly bounded from above by $\mu(x,t)$, it will necessarily become discontinuous if the flux coming from the left exceeds this value. This can be the case if $\mu(x,t)$ is discontinuous in the stage variable x, which will certainly happen if $\mu(x,t)$ is generated randomly by the algorithm above. Since mass has to be conserved, the discontinuity in the fluxes has to be compensated by $\delta-$ functions in the density ρ.

The aim of this work is to derive an evolution equation for the expectation $\langle \rho(x,t) \rangle$ of the density ρ given by the stochastic process above. This provides us with a rather inexpensive way to estimate the behavior of long supply chains, with random breakdowns of individual processors, by solving directly one rather simple conservation law for the expectation. The main result of the present paper is, that the expectation $\langle \rho(x,t) \rangle$ satisfies an initial boundary value problem for a conservation law of the form

$$(a)\ \partial_t \langle \rho(x,t) \rangle + \partial_x F_E(\bar{\tau}, C, V, \langle \rho \rangle) = 0, \quad F_E(\bar{\tau}, C, V, \langle \rho \rangle) = \bar{\tau} C [1 - \exp(-\frac{V \langle \rho \rangle}{C})] \ ,$$

$$(b)\ F_E|_{x=0} = \lambda(t), \quad \langle \rho(x,0) \rangle = 0$$

where the piecewise constant functions $\bar{\tau}$ and C are given by

$$\bar{\tau}(x) = \sum_{m=0}^{M-1} \chi_{[\gamma_m, \gamma_{m+1})}(x) \frac{\tau_m^{up}}{\tau_m^{up} + \tau_m^{down}}, \quad C(x) = \sum_{m=0}^{M-1} \chi_{[\gamma_m, \gamma_{m+1})}(x) c_m \ .$$

The result is derived in a limiting regime for large time scales and many parts and processors. So, it holds when the behavior of the chain, given by the stochastic version of (1), is considered on a time scale where a large number of parts arrive and the on / off switches of the processors happen very frequently. Similar models

have been used on a heuristical basis, in the context of clearing functions, in [9, 11]. Our result basically states two facts.

- For a large number of parts the function $\min\{\mu, V\rho\}$ is, under the expectation, replaced by the function $\mu[1-\exp(-\frac{V\rho}{\mu})]$ which has the same limiting behavior for large and small densities (the limits $\rho \to 0$ and $\rho \to \infty$).
- The effect of the random on / off switches can be incorporated into the model by replacing μ by the on- capacity c and multiplying the whole flux function by the average time $\frac{\tau^{up}}{\tau^{up}+\tau^{down}}$ the processor is on.

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