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Classical and Quantum Mechanical Models of Many-Particle Systems

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Introduction

This Oberwolfach meeting was mainly devoted to the mathematical study of kinetic theory and its relationship with quantum mechanics. The workshop had 47 participants, and among them 12 "young participants", i.e. Ph.D. students or recent post-docs. One of them could even benefit from the new NSF project *US Junior Oberwolfach Fellows*.

Almost all of the participants have attended the complete workshop talks. On top of that, many informal scientific discussions as well as intense work on concrete mathematical problems have taken place among the participants.

The meeting was structured around three long "survey-style" talks of two hours each. In addition, there were talks of 30 minutes and a few short talks illustrating the posters.

The following three specific problems have been addressed:

- First, the use of entropy / entropy dissipation methods and their applications to the large time behaviour of kinetic equations (and parabolic equations). Some of the talks (and in particular the survey by C. Villani) were devoted to the most recent progress here: the so-called "hypocoercivity" concept.
- Secondly, the passage from classical or quantum N-particle-models toward kinetic equations. In particular, the survey of M. Pulvirenti was dedicated to the so-called weak coupling limit for classical and quantum systems: this is an asymptotics which recently attracted lots of attention, particularly, since it leads to Landau's equation and the Boltzmann equation with a quantum correction.
- Thirdly, the space-adiabatic perturbation theory for quantum dynamics, which is an efficient tool to separate slow and fast degrees of freedom (e.g. the motion of nuclei from the fast electron oscillations in the Born-Oppenheimer approximation). This survey of H. Spohn was closely followed by S. Teufel's talk on quantum dynamics in perturbed periodic structures.

Finally, many talks were concerned with other new achievements in kinetic theory. Among those, one can quote the announcement of important new results in the following subfields of kinetic theory: relativistic equations, shocks, solutions close to equilibrium, Bose- and Fermi-corrections to the Boltzmann equations etc.

Abstracts

The Einstein-Vlasov System - Cosmic Censorship

Håkan Andreasson

A central problem in general relativity is the cosmic censorship conjecture, i.e. the question about uniqueness in the large. This concerns the global properties of spacetime and a necessary prerequisite for attacking this problem is to obtain global existence results. In general this seems too difficult and symmetry assumptions on spacetime are imposed to reduce the complexity of the equations. It is also essential to carefully choose a matter model so that singularities do not form as a result of the matter model itself. A kinetic matter model has shown to be satisfying in this respect and the resulting system is the Einstein-Vlasov system. The global existence results for this system are reviewed in both the asymptotically flat case and in the cosmological case. In the latter case global existence results have been established for large initial data (for some symmetry classes), whereas in the asymptotically flat case only a small data result is known under the assumption of spherical symmetry. In order to investigate cosmic censorship for spherical symmetric gravitational collapse large data has to be considered and the difficulties (compared to the Vlasov-Poisson system) of this problem are discussed. A related model - the Nordström-Vlasov model - is also discussed. For this model global existence has recently been proved in the spherically symmetric case.

Self-similar solutions and self-similar asymptotics for the Boltzmann equation with elastic and inelastic interactions.

A. Bobylev

(joint work with Carlo Cercignani)

We present a review of recent results obtained jointly with Carlo Cercignani. The review is based on series of our publications in "Journal of Statistical Physics" in 2002-2003. We consider the spatially homogeneous non-linear Boltzman equation (BE) for elastic and inelastic Maxwell models. Then, it is easy to show at the formal level that the equation admits a class of self-similar solutions of the form $f(v,t) = A(t)F(v\exp(-at))$, $a = const$. Two main questions are: (a) does such non-negative solutions really exist? and (b) do they describe a large time asymptotics for some classes of initial data (self-similar asymptotics)? The answer to both questions is "yes". Moreover, we constructed two such solutions for the classical (elastic) BE in explicit form. For the same equation, we proved the existence of such solutions for any $a > 0$ and that they are asymptotic states for some (different for different a) classes of initial data having infinite second moment (energy). We note that the solutions are obviously eternal, they exist for both positive and negative values of time t, this is the first example of eternal solutions of BE. A by-product result was a clarification of the Krook-Wu conjecture (1977), we proved sufficient conditions under which the conjecture is true and large time asymptotics is described by the BKW mode.

In case of inelastic Boltzmann equation, we proved recent Ernst-Brito conjecture (2002): any solution having at $t = 0$ the finite moment of an order $p > 2$ has the self-similar large time asymptotics (this result was obtained jointly also with G. Toscani). It was also shown that the limiting self-similar solution has a power-like high energy tail for almost all values of the restitution coefficient.

Long-time behaviour through entropy methods

María J. Cáceres

(joint work with J. A. Carrillo and G. Toscani)

By using entropy methods we study the long-time behaviour of two equations; a linear inhomogeneous Boltzmann equation and a nonlinear fourth order parabolic equation.

The first problem concerns a linear kinetic equation: an inhomogeneous linear Boltzmann equation, to be more precise we work with the linear relaxation approximation. Using the entropy method proposed by Desvillettes and Villani for the linear Fokker-Planck equation we prove almost exponential convergence to the steady state (for more details [1]).

In the second problem we deal with a nonlinear fourth order parabolic equation and in this case we prove exponential convergence to the stationary solution. To prove exponential convergence by entropy methods we have to control the entropy production. It is done using Poincaré inequalities (see [2]).

References

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[2] Cáceres, M. J, Carrillo, J. A, Toscani, G.,*Long-time behaviour for a nonlinear fourth order parabolic equation* to appear in Trans. Amer. Math. Soc.

Asymptotic behaviour of nonlinear diffusion via mass-transportation methods

José A. Carrillo

(joint work with Robert J. McCann, Cédric Villani)

An algebraic decay rate is derived which bounds the time required for velocities to equilibrate in a spatially homogeneous flow-through model representing the continuum limit of a gas of particles interacting through slightly inelastic collisions. This rate is obtained by reformulating the dynamical problem as the gradient flow of a convex energy on an infinite-dimensional manifold. An abstract theory is developed for gradient flows in length spaces, which shows how degenerate convexity (or even non-convexity) — if uniformly controlled — will quantify contractivity (limit expansivity) of the flow in Wasserstein distance sense.

Quantum Hydrodynamics and Diffusion models derived from the entropy principle

Pierre Degond

(joint work with F. Mehats (Toulouse, France) and C. Ringhofer (Tempe, USA))

In this work, we give an overview of recently derived quantum hydrodynamic and diffusion models. A quantum local equilibrium is defined as a minimizer of the quantum entropy subject to local moment constraints (such as given local mass, momentum and energy densities). These equilibria relate the thermodynamic parameters (such as the temperature or chemical potential) to the densities in a non-local way. Quantum hydrodynamic models are obtained through moment expansions of the quantum kinetic equations closed by quantum equilibria. We also derive collision operators for quantum kinetic models which decrease the quantum entropy and relax towards quantum equilibria. Then, through diffusion limits of the quantum kinetic equation, we establish various classes of models which are quantum extensions of the classical energy-transport and drift-diffusion models.

New applications of entropy methods

Jean Dolbeault

Entropy methods have been widely used over the last years. Still it seems that such ideas can be applied to many nonstandard settings. As an example, we may use these methods to obtain L^1 intermediate asymptotics for scalar conservation laws.

In a joint work with M. Escobedo, rates of convergence of nonnegative solutions of a simple scalar conservation law to their asymptotic states in a weighted L^1 norm have been obtained using entropy techniques. After an appropriate rescaling and for a well chosen weight, an exponential rate of convergence is obtained. Written in the original coordinates, this provides intermediate asymptotics estimates in L^1, with an algebraic rate. We also prove a uniform convergence result on the support of the solutions, provided the initial data is compactly supported and has an appropriate behaviour on a neighbourhood of the lower end of its support.

Mean Field Limit of Quantum Many-Body Models

Laszlo Erdös

We consider the evolution of N interacting quantum particles in the high density regime

$$i\partial_t \Psi_t = \Big(-\sum_{j=1}^{N} \Delta_j + \frac{1}{N}\sum_{j<k} U(x_j - x_k)\Big)\Psi \ .$$

We show how this N-body complex dynamics can be approximated by simpler one-body equations.

If the particles are bosons and the initial state is factorized, then the one particle marginal of Ψ_t converges to the solution of the Hartree equation that is a nonlinear Schrödinger equation with self consistent potential. We prove this fact for potentials that have at most Coulomb singularity [joint with H.T.Yau].

If the particles are fermions, then the typical velocity scales like $N^{1/3}$ by the Pauli exclusion principle. Therefore the correct scaling is semiclassical, with $\varepsilon = N^{-1/3}$,

$$i\varepsilon\partial_t \Psi_t = \Big(-\varepsilon^2\sum_{j=1}^{N} \Delta_j + \frac{1}{N}\sum_{j<k} U(x_j - x_k)\Big)\Psi.$$

For typical initial states, the exchange term is of order $O(\varepsilon^3)$ and thus factorized. We then prove that in the $N \to \infty$ limit the one particle marginal satisfies the semiclassical Hartree equation with accuracy $O(\varepsilon^3)$ [joint with A. Elgart, B. Schlein, H.T.Yau]. The exchange term is irrelevant up to this precision, therefore Hartree-Fock theory can be replaced by Hartree theory with high accuracy.

Classical Singular Solutions of Kinetic Equations for Bosons

Miguel Escobedo

In my conference, I present the construction of a classical singular solution to a Boltzmann equation for Bose particles derived by L. W. Nordheim and later by E. A. Uehling & G. E. Uhlenbeck. The construction is based on a fixed point argument and a linearization of the equation around a singular explicit solution. This is related with a conjecture linking the Bose Einstein condensation and the existence of a singular self similar solution of the Nordheim-Uehling-Ulenbeck equation.

Weak Coupling Limits for Classical and Quantum Systems

Raffaele Esposito and Mario Pulvirenti

We consider a system of N identical particle in the so-called weak-coupling (W-C) limit. It consists in scaling space and time hyperbolically (i.e. $x \to \varepsilon x, t \to \varepsilon t$, ε being a small parameter) and, simultaneously, rescaling the two-body interaction $\phi \to \sqrt{\varepsilon}\phi$ and letting the $N \to \infty$ as ε^{-d}, where $d = 3$ is the space dimension. Because of the smallness of the interaction, the behaviour of the system is not hydrodynamical, but rather kinetic. The goal is to derive kinetic equations for the one-particle distribution function in the limit $\varepsilon \to 0$.

We analyze both classical and quantum systems.

For classical systems we expect, in the limit, propagation of chaos and the following kinetic equation, (usually called Fokker-Planck-Landau equation):

$$(\partial_t + v \cdot \nabla_x)f = Q(f, f)$$

where the collision operator Q has the form:

$$Q(f, f)(v) = \int dv_1 \nabla_v G(|v - v_1|)(\nabla_v - \nabla_{v_1})ff_1$$

and G is the matrix:

$$G(|w|) = B\frac{w^2\mathbf{1} - w \bigotimes w}{|w|^3}$$

with the constant $B = \int_0^\infty \rho^3|\hat{\phi}(\rho)|^2 d\rho$ summarizing the properties of the potential. We present a formal argument partly inspired to [Balescu]. A rigorous proof seems indeed difficult even for short times.

We then pass to analyze what happens for the quantum case. We also expect that propagation of chaos hold for the Wigner function of the system, but, due to different nature of the Quantum Scattering, now the one-particle Wigner function is expected to satisfy a "classical" Boltzmann equation:

$$(\partial_t + v \cdot \nabla_x)f = Q(f, f) \tag{1}$$

with Q given by:

$$Q(f, f)(v) = \int dv_1 \int d\omega B(\omega; v, v_1)(f'f'_1 - ff_1)$$

Here B denotes the quantum cross-section in the Born approximation. We give plausibility arguments for that. Moreover, we study the Wigner Hierarchy for the Wigner transforms of the reduced density matrices and express them as a sum on suitable graphs. We show that a suitable subseries, based on graphs involving instantaneous collision-recollision events, provides the dominant terms and its sum converges to the solution of (1). For details on this, see [BCEP].

When the statistics is taken into account the structure of the equation is modified in the following way:

$$Q(f, f)(v) = \int dv_1 \int d\omega B_\pm(\omega; v, v_1)[f'f'_1(1 \pm f)(1 \pm f_1) - ff_1(1 \pm f')(1 \pm f'_1)]$$

where $\pm$ is chosen according to the Bose-Einstein or Fermi-Dirac statistics respectively.

The new terms arise from the fact that the initial family of Wigner functions must satisfy suitable symmetry conditions in order to be compatible with the statistics. The Quantum Statistics does not affect the propagation of chaos, which holds on the kinetic scale, but modifies the structure of the collision term, since collisions take place on the microscopic scale.

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[BCEP] D. Benedetto, F. Castella, R. Esposito and M. Pulvirenti:Some Considerations on the derivation of the nonlinear Quantum Boltzmann Equation, *Journal of Statistical Physics*, to appear

Convergence to Equilibrium for Reaction-Diffusion Systems

Klemens Fellner
(joint work with Laurent Desvillettes)

We consider reaction-diffusion systems on bounded domains modelling chemical substances with individual diffusivities, which react in a reversible way according the principle of mass-action kinetics. The considered examples feature unique steady states, which can be characterised as minimising states of a non-increasing entropy functional. The production rate of the entropy functional - the so called entropy dissipation - combines the effects of the diffusion- as well as of the reaction process.

We compute an explicit bound on the rates for the exponential convergence of solutions towards the steady state. Therefore, we explicitly estimate the entropy dissipation below in terms of the relative entropy with respect to the steady state, such that exponential convergence in entropy follows immediately. The established estimates are not sharp but "good". Moreover, we proof Cziszar-Kullback type inequalities to conclude convergence in L^1.

Semi-classical Analysis of Energy Transfers for Generic Codimension 3 Crossings

Clotilde Fermanian Kammerer

It is known since the works of Landau and Zener in the 1920' that energy levels crossing yields **energy transfer at leading order**. This transfer has been precisely calculated by Hagedorn and Joye for Schrödinger equation with matrix-valued potential when the initial data is a Gaussian wave packet (Hagedorn 94, Hagedorn-Joye 98). We describe two results (Fermanian- P. Gérard 02-03, Fermanian 03) in which the transfer is calculated in terms of Wigner measures for any uniformly bounded initial data. We consider a general system of two equations of pseudo-differential type presenting a crossing of codimension 3. Its symbol is a hermitian matrix admitting two eigenvalues which cross on a codimension 3 set called crossing set. We are concerned with the evolution of **Wigner measures** associated with a family of solutions to this system. There exist two types of genericity assumptions (Colin de Verdière 03, Fermanian-Gérard 03) which yield two different geometric contexts. Under these assumptions, we calculate the energy transfer which happens above the crossing set. The point is that this transfer does not occur at microlocal scale: a second level of observation at the scale $\sqrt{h}$ is required. We decompose Wigner measures by means of **two-scale Wigner measures** and obtain formula of Landau-Zener type for the traces of these measures on the crossing set. Besides, the nature of the two-scale Wigner measure used and the shape of the decomposition depend on which of the two types of genericity assumptions we make.

A Derivation of the Time-Dependent Hartree-Fock Equations from the N-body Schrödinger equation

François Golse

(joint work with C. Bardos, A. Gottlieb and N. Mauser: see [1, 2])

We consider the N-body Schrödinger equation with binary interactions embodied by some radial bounded potential, and coupling constant of the order of $1/N$.

Given an initial data for the N-body Schrödinger equation that is (close to) a Slater determinant built on an arbitrary N-uple of wave functions that is orthonormal in L^2, we prove that, for any positive time, the single-body, reduced density matrix converges in trace-norm to the solution of the TDHF (time-dependent Hartree-Fock) equations.

The method of proof is based on a priori estimates on the BBGKY hierarchy; a major difficulty being that solutions to the TDHF equations are not exact solutions of the limiting, infinite BBGKY hierarchy as $N \to +\infty$. However, these solutions satisfy a hierarchy of equations that we show are close in trace-norm to the infinite BBGKY hierarchy.

References

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Long time asymptotics to a third- and a fourth-order non-linear equations

Maria Pia Gualdani

In the last years the so called " entropy dissipation method" has been succesfully applied to prove asymptotic decay (sometimes optimal) to non-linear second order problems. But this method can be also used for higher order equations, like in our case, where we use it in order to show exponential decay of solutions to the steady-state for a non-linear third- and fourth-order problem.

A nonlinear energy method in the Boltzmann theory

Yan Guo

Upon linearizing around a given Maxwellian $\mu(v) = e^{-|v|^2}$, we can rewrite the Boltzmann equation as:

$$\partial_t g + v \cdot \nabla_x g + Lg = \Gamma(g, g), \tag{2}$$

for perturbations g such that $f = \mu + \mu^{1/2} g$, and $L \geq 0$ being the well-known linear collision operator. In the presence of $x-$dependence, as an operator, L is *not* positive definite so that Lg seems to offer little help for proving asymptotic stability or global existence. Recently, I have demonstrated that

$$\sum_{|\nu| \leq 4} (L\partial^\nu g, \partial^\nu g) > 0 \tag{3}$$

in appropriate sense, for *all small solutions* g to the full nonlinear equation (2) which preserve the mass, momentum and energy of μ. Here ν denotes the both temporal as well as spatial derivatives. It is well-known that $\langle Lg, g\rangle$ is positive definite with respect to the microscopic part $\{\mathbf{I}-\mathbf{P}\}g$, where

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

being the standard projection (the macroscopic part) to the null space of L. The proof for the coersivity relies on new nonlinear estimates for the macroscopic coefficients $a(t,x)$, $\mathbf{b}(t,x)$ and $c(t,x)$, in terms of the microscopic part $\{\mathbf{I}-\mathbf{P}\}g$, via the full nonlinear Boltzmann equation (2). Such an positivity estimate leads to asymptotic stability of Maxwellians in high Sobolev norms. Based on more delicate nonlinear estimates, I was able to construct global in time classical solutions near Maxwellians for the Landau equation, and for various versions of Vlasov-Maxwell-Boltzmann system even in the presence of a self-consistent magnetic field.

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'The Vlasov-Poisson-Boltzmann system near Maxwellians.' Comm. Pure Appl. Math. LV, 1104-1135 (2002).

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'Classical solutions to the Boltzmann equation for molecules with an angular cuoff.' Arch. Rational. Mech. Anal., 169, 305-353 (2003).

'Stability of relativistic Maxwellians in a collisional plasma' (with R. Strain) submitted 2003.

Regularity for the Vlasov-Poisson system in a convex domain

Hyung Ju Hwang

Abstract. We consider the initial-boundary value problem in a convex domain for the Vlasov-Poisson system. Boundary effects play an important role in such physical problems that are modelled by the Vlasov-Poisson system. We establish the global existence of classical solutions with regular initial boundary data under the absorbing boundary condition. We also prove that regular symmetric initial data lead to unique classical solutions for all time in the specular reflection case.

Kinetic Models of Fokker-Planck Type for Multilane Traffic Flow

Reinhard Illner

We discuss kinetic descriptions of traffic dynamics and present a class of new models of Fokker-Planck type . These models incorporate (nonlocal and time-delayed) braking and acceleration terms consistent with realistic time scales. Correlation assumptions are made such that braking and acceleration terms depend only on macroscopic densities and the relative speeds with respect to the average speed; the braking term includes lane change probabilities, and reasonable assumptions on the dependencies of these probabilities on the traffic situation lead to multivalued fundamental diagrams, consistent with traffic observations. This part of the work is based on joint work with Axel Klar and Thorsten Materne from Darmstadt.

The velocity diffusion coefficients included in the original model vanish at the average speed; this is because drivers "going with the flow" have neither motivation or need to brake or accelerate. The original model is therefore degenerately parabolic in velocity space. An interesting consequence is that the model permits discontinuous equilibria, and solutions of the spatially homogeneous model will usually converge to such an equilibrium. Inclusion of such discontinuities in the calculation of the fundamental diagram adds further values to the diagram. If a residual positive diffusivity is added to the diffusion coefficient (probably a realistic modification), the discontinuous equilibria disappear, but strong gradients at average speed may persist for a long time (metastability).

Traffic observations (made on the A5 in Germany) suggest that in certain density regimes the traffic densities in adjacent lanes will synchronize. This is shown analytically for caricatures of the new traffic models by Fourier expansion techniques (joint work with Vladislav Panferov). Numerical studies done by Michael Herty concerning synchronization for the full model, emergence of discontinuous equilibria and the formation of stop-and-go waves due to nonlocalities and reaction times behind bottlenecks will also be reported.

Propagation through Conical Crossings: an Asymptotic Semigroup

Caroline Lasser
(joint work with Stefan Teufel)

Time-dependent Born-Oppenheimer approximation allows us to think of nucleonic motion in molecules as governed by the occupied electronic energy bands. We study the special case of two such bands of cone-like shape intersecting on a codimension two manifold of nucleonic configuration space, as it is the case in photodissociation processes. In this situation, non-adiabatic transitions between the electronic subspaces occur to leading order in the semi-classical approximation.

We approximate the corresponding time-dependent Schrödinger equation's solution by evolving the initial data's Wigner function with an asymptotic semigroup. This semigroup is the forwards semigroup of a Markov process defined through classical transport on the bands and jumps in between them with transition probabilities given by a Landau-Zener type formula.

This explicit description translates into an algorithm, which can be regarded as a rigorous counterpart of chemical physics' trajectory surface hopping methods.

Ground state energies for quantum systems composed of infinitely many particles

Claude Le Bris

We review a series of works, in collaboration with Xavier Blanc (Laboratoire Jacques-Louis Lions, Paris), Isabelle Catto (University Paris 9), and Pierre-Louis Lions (Collège de France, Paris) on the ground state energies for systems composed of an infinite number of particles. The framework is that of quantum chemistry, where the state of matter is modelled though variational problems that couple a classical description of the nuclei with a quantum description of the electrons. Starting from a model for the molecule (finite number N of nuclei-say of unit charge- and an equal finite number N of electrons), a prototypical example being the Thomas-Fermi-von Weizsäcker model, we pass to the limit when N goes to infinity. When the nuclei are enforced to sit on the sites of a periodic lattice, asymptotically filling the entire lattice $\mathbf{Z}^3$, then the problem is solved by the so-called bulk limit problem for periodic crystals (series of work by I. Catto, LB and P.-L. Lions). But one can ask the question : is the minimal energy configuration periodic or not, a problem which is indeed known in the physics literature as the crystal problem. For such quantum problems, only one-dimensional results can be proven so far (X. Blanc and LB, Nonlinear Analysis, 2001). Alternatively, one may ask whether it is possible to pass to the N goes to infinity limit when the nuclei are not arranged periodically. A construction is developped in (Blanc/LB/Lions, CPDE 2002) that allows one to properly define the energy of this infinite system, under very weak and natural conditions on the geometric arrangement of the nuclei.

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Gas Dynamics Beyond Navier-Stokes

David Levermore

Compressible fluid dynamical systems are traditionally derived from a kinetic theory by either a Hilbert or Chapman-Enskog expansion in small Knudsen number. These derivations fail to produce formally well-posed systems beyond the compressible Navier-Stokes system, which arises as a first order correction to the Euler system. Here we offer an alternative derivation that produces a family of compressible fluid dynamical systems. The first two systems are again the Euler and Navier-Stokes systems, but one can go further. Every system in the family dissipates entropy and is formally well-posed over domains without boundary. The validity of these systems formally extends into transition regimes. These systems extend the compressible Navier-Stokes system and also extend a class of systems developed by Maxwell, Kogan, Sone, and others that are not derivable from the Navier-Stokes system.

Boltzmann equation and fluid dynamics

Tai-Ping Liu

Consider the Boltzmann equation for hard spheres. We describe several results on the behaviour of the Boltzmann solutions. With Shih-Hsien Yu we show through the time-asymptotic stability analysis that the Boltzmann shocks previously constructed are physical, that is, they are positive. To make uses of the techniques for viscous conservation laws for the stability analysis, the Boltzmann equation as well as the H-Theorem are decomposed into macro-micro parts. Yu then uses this and the introduction of the generalized Hilbert expansion to constructed Boltzmann solutions which converge to a given piecewise smooth Euler solutions with shocks. Yu and the author analyze the Green function for the linearized Boltzmann equation. We use the spectral analysis to construct the fluid waves, which exhibit the weak Huygen's principle. The particle-like waves in the Green function are constructed through a Picard-type iterations.

Isotropic Distributional Solutions to the Boltzmann Equation for Bose-Einstein Particles

Xuguang Lu

We consider the spatially homogeneous Boltzmann equation for Bose-Einstein particles. Physical background and derivation of such quantum models can be found in Chapter 17 of the book *The Mathematical Theory of Non-Uniform Gases* (Third Edition,1970) by T. Chapman and T.G. Cowling. We show that, because of taking quantum effect into account, the Boltzmann collision integral operator has a stronger nonlinear structure that makes us only able to deal with the hard sphere model and the equation has to be taken a weak form, and solutions (called distributional solutions) in the weak form have to be set (at least in the present level) in the class of isotropic positive Borel measures. Existence and moment production estimate of global isotropic distributional solutions that conserve the mass and energy are proven by taking weak limit of L^1-approximate solutions. As an application of the weak form of the equation, we show that a Bose-Einstein distribution plus a Dirac δ-function is an equilibrium state if and only if it satisfies a kinetic low temperature and an exact ratio of the Bose-Einstein condensation.

On the 3-D Wigner-Poisson-Fokker-Planck system

CHIARA MANZINI
(joint work with Anton Arnold, Elidon Dhamo)

WPFP problem is a well-known model of an *open* quantum system: the evolution of the (Wigner) quasi-distribution function on the phase space describes the *irreversible* dynamics of the system. We have presented a well-posedness result of the three-dimensional, whole space case. Due to the definition of the self-consistent potential in the (nonlinear) pseudo-differential operator, the state space for our analysis is an L^2-space, with a symmetric weight in the velocity and in the position variables, and the unknown function has to be differentiable (in the velocity variable) in the same space. The quantum FP operator is uniformly elliptic under the same algebraic condition among its coefficients, which guarantees that the system is quantum-mechanically correct, moreover, the linear (unbounded) operator in the WFP equation generates a C_0 semigroup in the weighted space and the derivatives of its solution decay in time in the weighted space, in a small time interval. A fixed point argument in the space of the solution of the linear equation gives the local-in-time result; the derivation of a priori estimates is a work in progress.

Kinetic models of interface motion

ROSSANA MARRA

We consider a kinetic model for a system of two species of particles based on two coupled Vlasov-Boltzmann equations with self-consistent forces given in terms of a non-negative, compactly supported and monotone potential. We prove by minimizing the entropy functional under the constraints on the total energy and total masses that the equilibria are Maxwellian with the same temperature, zero mean velocity and densities minimizing the macroscopic free energy functional $\mathcal{F}$. We prove that at low temperature the only minimizers of $\mathcal{F}$ on a torus for fixed total masses are spatially homogeneous profiles of densities, while at high T the minimizers are non constant functions ρ_i in L^1, with $\nabla\rho_i \in L^1$ and symmetric monotone, by using compactness argument and rearrangement inequalities. The behaviour of the system in the so-called late stages of relaxation to equilibrium is studied by scaling space as ϵ^{-1} and time as ϵ^{-2} and choosing the range of the potential ϵ^{-1} in the Vlasov-Boltzmann eq.s (sharp interface limit). At time zero there is an interface Γ_0 separating regions of different phases and the velocity field is zero, so to study the incompressible regime. By formal Hilbert expansions we prove that the rescaled velocity field is in the limit $\epsilon \to 0$ solution of the incompressible Navier-Stokes equation everywhere but on the interface. It is continuous while the pressure is discontinuous on Γ_t and satisfy the Laplace's law $(p^+ - p^-) = -\sigma K(r,t)$ with σ the surface tension and K the mean curvature of the interface Γ_t, which moves in its normal direction ν with velocity given by $v_{\Gamma_t}(x) = u(x,t) \cdot \nu(x,t)$.

http://people.roma2.infn.it/∼marra

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A Boltzmann equation for elastic, inelastic and coalescing collisions

Stephane Mischler

In this talk we consider a spatially homogeneous Boltzmann model for particles undergoing elastic, inelastic and coalescing collisions. More precisely, defining the phase space of mass-momentum variable $y := (m, p) \in Y := (0, \infty) \times \mathbf{R}^3$ the underlying microscopical collisional mechanisms are the following: when two *pre-collisional* particles $\{y, y_*\}$ collide, they result in one or two *post-collisional* particle(s) $\{y_{**}\}$ or $\{y', y'_*\}$, such that

$$\underline{\text{elastic or inelastic collision}}: \qquad \{y\}+\{y_*\} \longrightarrow \{y'\}+\{y'_*\} \quad \text{with} \quad \begin{cases} m' = m, \quad m'_* = m_* \\ p' + p'_* = p + p_* \\ \mathcal{E}' + \mathcal{E}'_* \leq \mathcal{E} + \mathcal{E}_*, \end{cases}$$

where $\mathcal{E} = |p|^2/m$ is the kinetic energy, or

$$\underline{\text{coalescence}}: \qquad \{y\} + \{y_*\} \longrightarrow \{y_{**}\} \quad \text{with} \quad \begin{cases} m_{**} - b = m + m_* \\ -A p_* = p + p_*. \end{cases}$$

Under general assumptions on the collision rates, we state existence and uniqueness of a solution $0 \leq f \in C([0, \infty); X)$ for any initial datum $0 \leq f_{in} \in X$, where $X := \{g : Y \rightarrow \mathbf{R},\ g\,(m^{-1} + m + \mathcal{E})^2 \in L^1(Y)\}$. This shows in particular that the cooling effect (due to inelastic collisions) does not occur in finite time.

In the long time asymptotic, we prove that the solution converges to a mass-dependent Maxwellian function (when only elastic collisions are considered), to a velocity Dirac mass (when elastic and inelastic collisions are considered) and to 0 (when elastic, inelastic and coalescing collisions are taken into account). We thus show in the latter case that the effect of coalescence is dominating in large time. Our proofs gather deterministic and stochastic arguments.

On Fluctuation Spectra of Plasma and Fluid Shear Flow

P. J. Morrison

Phase space density fluctuations of a plasma are obtained by a novel method that parallels conventional partition function calculations of statistical physics. The Hamiltonian that describes linear fluctuations about general stable equilibria is diagonalized by a linear transformation of the form:

$$q_k(v, t) = \epsilon_R(k, v)\, Q'_k(v, t) + \epsilon_I(k, v)\, H[Q'_k]\,, \tag{4}$$

where $\epsilon_I := -\pi\omega_p^2 f_0'/k^2$, with f_0 being the equilibrium distribution function, $H[\cdot]$ the Hilbert transform, and $\epsilon_R = 1 + H[\epsilon_I]$, which allows exact calculation of the partition functional integral. For electric field fluctuations we obtain

$$\langle E_k(u) E^*_{k'}(u') \rangle = \frac{16}{\beta} \frac{\epsilon_I}{u|\epsilon|^2}\, \delta_{k,k'} \delta(u - u')\,, \tag{5}$$

where $\beta = 1/K_B T$, the frequency $\omega = ku$, and k is the wavenumber. The corresponding phase space fluctuations are governed by

$$\langle f_k(v) f^*_{k'}(v')\rangle = \delta_{k,k'} \frac{k^2}{\pi^2 e^2 \beta} \times$$
$$\left\{ \frac{\epsilon_I(v)}{v}\delta(v-v') - \frac{1}{\pi}\frac{\epsilon_R(0)}{|\epsilon(0)|^2}\frac{\epsilon_I(v')\epsilon_I(v)}{vv'} \right\}. \tag{6}$$

Our calculations clear up ambiguous statements in the plasma literature about equipartition. Similar results are obtained for fluid fluctuations about shear flow in a channel.

Explicit spectral gap estimates for the linearized Boltzmann and Landau operators with hard potentials

Clément Mouhot

(joint work with Céline Baranger, ÉNS Cachan, France)

We prove explicit spectral gap estimates for the linearized Boltzmann operator with hard potentials (and hard spheres). We prove that it can be reduced to the Maxwellian case, for which explicit estimates are already known by diagonalization. The idea of the proof is to work on the Dirichlet form and to introduce suitable intermediate collisions and triangular inequality in order to skip the regions where the collision kernel vanishes, i.e essentially for small relative velocities. The idea is the following: performing a collision with small relative velocity is the same than performing two collisions with great relative velocity, provided that the pre- and post-collisional velocities are the same. Moreover when a collision with small relative velocity occurs, at the same time, two collisions with great relative velocity occur, which give the same pre- and post-collisional velocities, and which produce *at least the same amount of entropy.* Thus we replace the former by the latters. The method is constructive, does not rely on Weyl's Theorem and does not require Grad's splitting. Estimates are thus valid for cutoff as well as non cutoff collision operators. In a second part, we use the fact that the Landau operator can be expressed as the limit of the Boltzmann operator as collisions become grazing in order to deduce explicit spectral gap estimates for the linearized Landau operator with hard potentials.

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Algebraic properties of the Fokker-Planck equations and applications.

Francis Nier

We presented three kinds of algebraic structures associated with the operator

$$K = v.\partial_x - \frac{1}{m}\partial V(x).\partial_v - \frac{\gamma_0}{m\beta}\left(-\partial_v + \frac{m\beta}{2}v\right).\left(\partial_v + \frac{m\beta}{2}v\right),$$

involved in the Fokker-Planck (or Kramers) equation, and the Witten Laplacian on 0-forms ($m = \beta = \gamma_0 = 1$ here)

$$\Delta^{(0)}_\Phi = -\Delta_{x,v} + |\nabla_{x,v}\Phi(x,v)|^2 - \Delta_{x,v}\Phi$$

with

$$\Phi(x,v)=\frac{1}{2}\left(\frac{v^2}{2}+V(x)\right).$$

These algebraic properties are : 1) The operator K can be written X_0+b^*b where X_0 is the classical hamiltonian field associated with $p(x,v)=\frac{m}{2}v^2+V(x)$ and b, b^* are the annihilation-creation operators associated with the harmonic oscillator in the velocity variable. It looks like a type-II Hörmander hypoelliptic operator; 2) The Witten Laplacian can be written as a sum of squares $\Delta^{(0)}_{V/2}=\sum_{j=1}^{d}L_j^*L_j$ with $L_j=X_j-iY_j$, $X_j=\partial_{x_j}$ and $Y_j=i\partial_{x_j}V(x)$; 3) The Witten Laplacian $\Delta^{(0)}_{V/2}$ also writes $d^{(0),*}_{V/2}d^{(0)}_{V/2}$ where $d^{(0)}_{V/2}=e^{-V/2}d_xe^{V/2}$ is the distorted differential. These properties combined with adapted hypoelliptic techniques lead to: 1) In the qualitative analysis, almost necessary and sufficient conditions for the exponential in time return to the thermodynamical equilibrium $Ce^{-\Phi(x,v)}\in L^2(\mathbb{R}^{2d}_{x,v},\ dx)$; 2) From the quantitative point of view to accurate lower an upper bounds for the exponential rate of return to the equilibrium in terms in the physical parameters, mass, temperature and friction coefficient.

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The Nordström-Vlasov system

Gerhard Rein

(joint work with Håkan Andréasson)

When describing a large, self-gravitating collisionless ensemble of mass points in a relativistic set up the physically correct model is the Einstein-Vlasov system. The available results indicate that the Vlasov description of the matter content in a relativistic spacetime is preferable to other matter models when studying questions such as the cosmic censorship hypotheses or more generally, global properties of the spacetime. However, the Einstein-Vlasov system is difficult to analyze from a PDE point of view. Hence mathematically simpler relativistic toy models which share at least some features of the true model are desirable. One such model is the Nordström-Vlasov system:

$$\partial_t f+\frac{p}{\sqrt{1+|p|^2}}\cdot\nabla_x f-\left[\left(\partial_t\phi+\frac{p}{\sqrt{1+|p|^2}}\cdot\nabla_x\phi\right)p+\frac{1}{\sqrt{1+|p|^2}}\nabla_x\phi\right]\cdot\nabla_p f=0,$$

$$\partial_t^2\phi-\triangle_x\phi=-e^{4\phi}\int f\,\frac{dp}{\sqrt{1+|p|^2}}.$$

The spacetime is a Lorentzian manifold with metric $g_{\mu\nu}=e^{2\phi}\mathrm{diag}(-1,1,1,1)$. The particles move along geodesics of this metric, and their distribution on phase space is given by $f(t,x,e^{\phi}p)$, $x,p\in\mathbb{R}^3$. The system is covariant, allows for relativistic effects like gravitational radiation, has the correct Newtonian limit, namely the Vlasov-Poisson system, but due to the scalar nature of the field ϕ it is much less difficult to analyze than the Einstein-Vlasov system.

Unique classical solutions to the corresponding Cauchy problem exist and can be extended as long as the growth of the particle momenta can be controlled. Furthermore, the system has global weak solutions for general initial data and global classical solutions for initial data which are spherically symmetric and where all particles have angular momenta bounded away from 0. Analogues of the latter two results are not known for the Einstein-Vlasov system.

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Macroscopic and quantum mechanical models for semiconductors

Joachim Rehberg

The reported work is devoted to the coupling of macroscopic and quantum mechanical models for semiconductors. On one hand, Van Roosbroeck's system turned out to be a powerful tool for the description of many features of semiconductors. However, there are effects (tunnelling, e.g.) which only can be described by quantum mechanics. Thus we aim at so called hybrid models, in which some part is described by a macroscopic model and another part by a quantum mechanical model. The combination of the two models rests on the two following principles:

Principle I There is an electrostatic potential φ, living on the whole domain, and which is governed by Poisson's equation

$$-\nabla\big(\varepsilon\nabla\varphi\big) = D - n + p - N + P \qquad \text{(+ boundary conditions)},$$

(D denoting the impurities, n, p the quantum mechanical densities of electrons and holes, and N, P the macroscopic densities of electrons and holes).

Principle II The normal components of the corresponding (species) current densities coincide at the (fictive) boundary between the two regions.

Applications of the Desvillettes-Villani Approach to the Convergence to Equilibrium for Nonhomogeneous Kinetic Models

Christian Schmeiser

For spatially nonhomogeneous kinetic equations, the entropy dissipation inequality is not sufficient for proving quantitative results on the convergence to global equilibrium, since the entropy dissipation vanishes whenever the distribution is in local equilibrium. In this talk, the application of an entropy-entropy dissipation procedure (as developed by L. Desvillettes and C. Villani) overcoming this problem to several kinetic models is reviewed. The models include linear non-micro-reversible interaction of particles with a background medium, nonlinear interaction of fermions with a background medium, a linearized version of a cometary flow model, as well as some discrete velocity models. The method leads to systems of ordinary differential inequalities of different sizes, depending on the details of the mechanisms driving the distribution away from nonglobal local equilibria.

Kinetic schemes for the Saint-Venant equations with source terms

CHIARA SIMEONI

Hyperbolic conservation laws with source terms arise in many applications, especially as a model for geophysical flows, and their numerical approximation leads to specific difficulties.

Numerical schemes based on "fictitious" kinetic models are introduced for the Saint-Venant equations for shallow water, in order to take source terms like the bottom topography and friction into account in the Upwind Interface Source method [2]. In the framework of the finite volume method, we use a formal description of the microscopic behaviour of the physical systems to define numerical fluxes at the interfaces of an unstructured mesh [1].

Applications to the simulation of experimental data and the numerical modelling of avalanches are discussed, motivated by the interest in recovering the results of experimental studies on the free-surface flows over a complex topography [3] and to describe the stopping mechanism of a granular mass in presence of friction terms like the Coulomb threshold [4].

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On Quantum Fokker-Planck models

CHRISTOF SPARBER
(joint work with Anton Arnold)

In the modelling of *open quantum systems*, one is often forced to take into account *dissipative and diffusive effects*. The non-unitary time evolution of such systems is then usually described by *Markovian master equations* of the following form:

$$\begin{cases} \dfrac{d}{dt}\rho = \mathcal{L}(\rho), \quad t > 0, \\ \rho\big|_{t=0} = \rho_0 \in \mathcal{J}_1(\mathcal{H}). \end{cases}$$

Here, $\mathcal{J}_1(\mathcal{H})$ denotes the space of *density matrices*, *i.e.* the cone of positive self-adjoint trace-class operators ρ over some Hilbert space $\mathcal{H}$. It is well known that if $\mathcal{L}$ is a bounded linear operator, it has to be in the so called *Lindblad class* to satisfy the basic physical requirements of *complete positivity* and *mass conservation*. In the given talk we present recent results on the (global) well-posedness of a concrete family of unbounded generators $\mathcal{L}$, formally in the *Lindblad class*. Diffusive effects are modelled by Lindblad operators which are linear combinations of the position and momentum operators. Moreover particle-particle interactions are accounted for by a nonlinear mean-field approximation of *Hartee* type.

preprint available at: http://wwwmath.uni-muenster.de/u/arnold/publik.html

Space-adiabatic perturbation theory in quantum dynamics

Herbert Spohn

The space-adiabatic perturbation theory is a systematic tool to separate slow and fast degrees of freedom for quantum systems. Under the gap assumption, in the Hilbert space of all states there is an almost invariant subspace, where almost refers to the fact that leaking out of that subspace is $\mathcal{O}(\epsilon^\infty)$ with ϵ the adiabaticity parameter. On the almost invariant subspace the time evolution is well approximated by an effective Hamiltonian, which can be computed in an expansion in ϵ. In practice one only computes the first order correction, in exceptional cases also the second order. The first order has interesting novel physics and is known also as geometric, respectively Berry, phase.

The method is explained in complete detail in

S. Teufel, *Adiabatic Perturbation Theory in Quantum Dynamics*, Lecture Notes in Mathematics 1821, Springer, Berlin 2003.

There also a number of examples are worked out, in particular the Dirac equation, the Born-Oppenheimer approximation, and electrons in a periodic potential with slowly varying external electromagnetic potentials and possibly an additional strong uniform magnetic field.

In my presentation I used the Born-Oppenheimer approximation as a guiding example.

Quantum dynamics in perturbed periodic structures

Stefan Teufel

(joint work with G. Panati and H. Spohn)

We consider the Schrödinger equation

$$i\varepsilon\partial_t\psi(t) = \left[\tfrac{1}{2}\left(-i\varepsilon\nabla_x + A(\varepsilon x)\right)^2 + V_\Gamma(x) + \phi(\varepsilon x)\right]\psi$$

with periodic potential V_Γ and with non-periodic "external" electromagnetic potentials A and ϕ for small $\varepsilon > 0$. This scaling limit corresponds to slow variation of the external potentials on the scale of the lattice Γ.

It is shown how to translate this problem into a space-adiabatic problem and how to use space-adiabatic perturbation theory, as presented in the talk of H. Spohn, in order to derive the semiclassical limit. As a result we obtain for each isolated Bloch band E_n the so-called semiclassical model of solid-state physics, i.e. the following classical equations of motion for a particle with phase space coordinates (q,p),

$$\begin{aligned}\dot q &= \nabla_v\Big(E_n(v) - \varepsilon\, B(q)\cdot M_n(v)\Big) + \varepsilon\,\dot v \wedge \Omega_n(v)\\ \dot v &= -\nabla_q\Big(\phi(q) - \varepsilon\, B(q)\cdot M_n(v)\Big) + \dot q \wedge B(q)\,.\end{aligned}$$

Here $v = p - A(q)$ is the kinetic momentum and $B = \mathrm{curlA}$ is the magnetic field. The terms of order ε are the first order corrections to the semiclassical model as (partly) predicted by Niu et al. Ω_n is the curvature of the Berry connection of the nth Bloch bundle and M_n the Rammal-Wilkinson 2-form. The first order corrections provide a semiclassical explanation for the quantization of the Hall conductivity in quantum Hall systems.

This is joint work with G. Panati and H. Spohn and appeared in Commun. Math. Phys. **242**, 547–578 (2003).

Kinetic models of granular gases

Giuseppe Toscani

We investigate the asymptotic behaviour of certain models of dissipative systems obtained from a suitable modification of Kac caricature of a Maxwellian gas. It is shown that global equilibria different from concentration are possible if the energy is not finite. These equilibria are distributed like stable laws, and attract initial densities which belong to the normal domain of attraction. If the initial density is assumed of finite energy, with higher moments bounded, it is shown that the solution converges for large–time to a profile with power law tails. These tails are heavily dependent of the collision rule.

Convergence to equilibrium for kinetic equations

Cedric Villani

I presented a state of the art about the study of equilibration rates for some basic kinetic equations (Boltzmann, Landau, Fokker-Planck...). Essentially all known methods are based on the study of a Lyapunov functional ("entropy", "free energy" or "weighted L^2 norm"), thereafter called entropy. There are two very different cases.

Case 1 ("coercivity"): the entropy production vanishes only at equilibrium. This is usually true only for spatially homogeneous models. In many cases one can establish functional inequalities comparing the entropy production with the entropy itself, depending only on regularity a priori estimates and implying convergence to equilibrium like $O(t^{-\infty})$.

Case 2 ("hypocoercivity"): there are a lot of states for which the entropy production vanishes, but only one of them is the equilibrium, because of the action of some nondissipative term in the equation. Then much more details of the dynamics should be retained; I presented a general method to handle that, devised with Desvillettes, and sketched some developments.

Nonequilibrium steady states for the Kac and Boltzmann equation

Bernt Wennberg

(joint work with Yosief Wondmagegne (Chalmers, Göteborg))

We study the stationary Kac equation in the presence of

an external force field and a Gaussian thermostat, and investigate the behaviour of a solution to this equation for varying field strength. We prove that for a weak field, the stationary density is continuous, but for a strong field the density has a singularity. Monte Carlo simulations illustrating the same are also presented.

http://www.ceremade.dauphine.fr/˜bares/hyke/2003/06/068.pdf

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