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Workshop on  
“Analytical and Computational Problems for Mixtures and Plasma  
Dynamics”

June 17-21 (except for 20), 2019

organized by  
Milana Pavić-Čolić, Liu Liu, Irene M. Gamba

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Abstracts

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Sona Akopian (Brown University)

**On  $L^p$  solutions of a special class of homogeneous Boltzmann equations in the Coulomb case**

**Abstract:** We study the well posed-ness in  $L^p$  of a family of spatially homogeneous Boltzmann equations with a Coulomb potential (and an angular cutoff), where the collision kernel is represented by a singular mass centered at very small scattering angles and relative velocities. This kernel was introduced by Bobylev and Potapenko in a 2013 paper where its corresponding collision operator was used to approximate the Landau collision integral. With this kernel, unlike in the classical Boltzmann equation so far, a global existence theory can be established in  $L^p$ , which, thanks to the grazing collisions limit (which does indeed hold for this particular class of collision kernels), gives hope for the search of global  $L^p$  solutions of the Landau equation in the Coulomb case.

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Alexander Bobylev (Keldysh Institute of Applied Mathematics, Russian Academy of Science, Moscow)

**On BGK-models for gas mixtures**

**Abstract:** In this talk we discuss a general problem of constructing consistent kinetic models of BGK type for gas mixtures is discussed. A particular model of this type for an arbitrary number of species with arbitrary collision law was recently proposed in [1]. The model features the same structure of the corresponding Boltzmann equations and fulfils all consistency requirements concerning conservation laws, equilibrium solutions, and H-theorem. The model is compared with other existing BGK models for mixtures. Possible applications to the plasma case are also briefly discussed. Hydrodynamics of the model is discussed in more detail in [2].

[1] Bobylev A.V., Bisi M., Groppi M., Spiga G., Potapenko I., A consistent BGK kinetic model for gas mixtures, *Kinet. Relat. Models*, 11 (2018), No.6, 1377-1393.

[2] Bisi M., Bobylev A.V., Groppi M. and Spiga G., Hydrodynamic equations from a BGK model for inert gas mixtures, 31st International Symposium on Rarefied Gas Dynamics, Glasgow, United Kingdom, July 2018, AIP Conf. Proc. (accepted for publication).

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**Laurent Boudin** (Sorbonne Université)

**Stability of the spectral gap for the Boltzmann multi-species operator linearized around non-equilibrium Maxwell distributions**

**Abstract:** In this talk, we consider the Boltzmann operator for mixtures with cutoff Maxwellian, hard potentials, or hard spheres collision kernels. In a perturbative regime around the global Maxwellian equilibrium, the linearized Boltzmann multi-species operator  $\mathbf{L}$  is known to possess an explicit spectral gap  $\lambda_{\mathbf{L}}$ , in the global equilibrium weighted  $L^2$  space. We study a new operator  $\mathbf{L}^\varepsilon$  obtained by linearizing the Boltzmann operator for mixtures around local Maxwellian distributions, where all the species evolve with different small macroscopic velocities of order  $\varepsilon$ ,  $\varepsilon > 0$ . This is a non-equilibrium state for the mixture. We establish a quasi-stability property for the Dirichlet form of  $\mathbf{L}^\varepsilon$  in the global equilibrium weighted  $L^2$  space. More precisely, we consider the explicit upper bound that has been proved for the entropy production functional associated to  $\mathbf{L}^\varepsilon$  and we show that the same estimate holds for the entropy production functional associated to  $\mathbf{L}^\varepsilon$ , up to a correction of order  $\varepsilon$ .

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**Esther S. Daus** (Technical University of Vienna)

**Multi-species cross-diffusion population models: existence of solutions and derivation from underlying particle models**

**Abstract:** In the first part of this talk, we focus on the proof of the existence of global-in-time weak solutions to reaction-cross-diffusion systems for an arbitrary number of competing population species. In the case of linear transition rates, the model extends the two-species population model of Shigesada, Kawasaki, and Teramoto. The existence proof is based on a refined entropy method and a new approximation scheme. Global existence follows under a detailed balance or weak cross-diffusion condition, where the detailed balance condition is related to the symmetry of the mobility matrix, which mirrors Onsager's principle in thermodynamics. The second part of the talk links at the formal level the entropy structure of the cross-diffusion system satisfying the detailed balance condition with the entropy structure of a reversible microscopic many-particle Markov process on a discretised space. Moreover, we present a very recent proof of a rigorous mean-field limit from a stochastic particle model to a cross diffusion model. These results are based on a joint work with Xiuqing Chen and Ansgar Juengel, a joint work with Helge Dietert and Laurent Desvillettes, and a joint work with Li Chen and Ansgar Juengel.

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**Erica Belen De La Canal** (University of Texas at Austin)

**$L^p$  estimates for the solution of the system of Boltzmann equations for monatomic gas mixtures**

**Abstract:** The Boltzmann equation is a classical model for a gas at low or moderate densities. In the single species case, the transport equation for  $f$  in the space homogeneous case reads

$$\partial_t f = Q(f, f).$$

When we consider a mixture of  $I$  monatomic gases, each species will be described by its own distribution function, each one satisfying a Boltzmann like equation. So we will have a system of Boltzmann equations.

It has been proved recently, by I. Gamba and M. Pavić-Colić, the existence and uniqueness of the vector value solution to the system of Boltzmann equations, by obtaining generation and propagation of polynomial moments. Following the ideas developed for moments, I will present the gain of integrability and propagation of  $L^p$  norms for the vector value solution. This is work in progress with I. Gamba and M. Pavić-Čolić.

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**Helge Dietert** (Université Paris Diderot)

### **On Cucker-Smale dynamical systems with degenerate communication**

**Abstract:** The Cucker-Smale model is a kinetic model for the alignment of a system of agents. I will report on joint work with Roman Shvydkoy, where we study the case of a degenerate communication kernel. Like the study of hypocoercivity, I will present results how the combination of a degenerate communication kernel and the transport give global alignment.

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**Marina Ferreira** (University of Helsinki)

### **Multicomponent coagulation equation for aerosol dynamics**

**Abstract:** In the atmosphere, aerosol particles collide and merge forming bigger particles. To investigate this phenomenon we consider a coagulation equation for the particle size distribution with source at the small particles. We prove existence and non-existence of stationary non-equilibrium solutions for two different classes of kernels. To account for different types of particles, we then consider a multicomponent coagulation equation. We study the shape of solutions for large times and show that the mass concentrates along straight lines in the size space.

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**Irene M. Gamba** (University of Texas at Austin)

### **Multi-component gas system models: The billiard mixing for mixtures**

**Abstract:** The lecture will focus on the mathematics of kinetic systems for mixtures of gases with different masses. This corresponds to a Boltzmann system for the evolution of vector valued probability distribution densities for non-local bi-linear collisional forms modeling ‘mixing’ of their states. The collision or interaction law, as much as the modeling of the transition probability rates, which modeled by a quantification of differential cross section for pairwise interactions, are crucial components in the dynamics. We will present some recent rigorous properties developed for the multi-component gas system described by coupled Boltzmann equations corresponding to the dynamics of elastic mixing of particles characterized by their identical shapes (spheres) but different masses, both in monoatomic and polyatomic cases.

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**François Golse** (École Polytechnique)

### **Partial Regularity in Time for the Landau Equation (with Coulomb Interaction)**

**Abstract:** We prove that the set of singular times for weak solutions of the space homogeneous Landau equation with Coulomb potential constructed as in [C. Villani, Arch. Rational Mech. Anal. 143 (1998), 273-307] has Hausdorff dimension at most  $1/2$ . (joint work with M.P. Gualdani, Cyril Imbert and Alexis Vasseur)

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**B erence Grec** (Universit  Paris Descartes)

**A numerical scheme for a kinetic model for mixtures in the diffusive limit using the moment method**

**Abstract:** In this talk [1], we consider a multi-species kinetic model in a one-dimensional setting with a diffusive scaling. More precisely, assuming that both Knudsen and Mach numbers of order  $\varepsilon > 0$ , we can write, for each species  $1 \leq i \leq p$ , the Boltzmann equation for mixtures [3] on the distribution function  $f_i^\varepsilon = f_i^\varepsilon(t, x, v)$

$$\varepsilon \partial_t f_i^\varepsilon + v \partial_x f_i^\varepsilon = \frac{1}{\varepsilon} \sum_{k=1}^p Q_{ik}(f_i^\varepsilon, f_k^\varepsilon), \quad \text{in } R_+ \times \Omega \times R, \quad (1)$$

where  $Q_{ik}$  is the multi-species Boltzmann collision operator, and  $\Omega$  is an open interval on  $R$ . For each species, macroscopic quantities, such as its concentration and its flux, can be obtained as the first moments of its distribution function

$$c_i^\varepsilon(t, x) = \int_R f_i^\varepsilon(t, x, v) dv, \quad c_i^\varepsilon(t, x) u_i^\varepsilon(t, x) = \int_R v f_i^\varepsilon(t, x, v) dv.$$

Formally, it has been proved [2] that the moments of the solutions to the Boltzmann equation for mixtures converge to  $(c_i, c_i u_i)$  solutions of the Maxwell-Stefan equations when  $\varepsilon$  tends to zero, in the equimolar diffusion setting. This formal convergence is obtained by the moment method [5], relying on an ansatz on the distribution functions that they are at local Maxwellian states with different macroscopic velocities  $\varepsilon u_i^\varepsilon$  of order  $\varepsilon$ .

In the context of kinetic equations for mixtures, previous approaches [4] are not adapted to the diffusive scaling we are dealing with. We therefore propose a new numerical scheme, mimicking the analytical analysis (moment method), approximating the solutions of the kinetic model both in a rarefied regime and in the diffusion limit. We prove some *a priori* estimates (mass conservation and nonnegativity), as well as existence of a solution to the numerical scheme. We also present numerical simulations illustrating the asymptotic-preserving behavior of the scheme, and its capacity to describe uphill diffusion phenomena for mixtures.

[1] A. Bondesan, L. Boudin, and B. Grec. A numerical scheme for a kinetic model for mixtures in the diffusive limit using the moment method. *Numerical Methods for Partial Differential Equations*, 35(3):1184–1205.

[2] L. Boudin, B. Grec, and V. Pavan. The Maxwell-Stefan diffusion limit for a kinetic model of mixtures with general cross sections. *Nonlinear Anal.*, 159:40–61, 2017.

[3] L. Desvillettes, R. Monaco, and F. Salvarani. A kinetic model allowing to obtain the energy law of polytropic gases in the presence of chemical reactions. *Eur. J. Mech. B Fluids*, 24(2):219–236, 2005.

[4] S. Jin and Q. Li. A BGK-penalization-based asymptotic-preserving scheme for the multispecies Boltzmann equation. *Numer. Methods Partial Differential Equations*, 29(3):1056–1080, 2013.

[5] C. D. Levermore. Moment closure hierarchies for kinetic theories. *J. Statist. Phys.*, 83(5-6):1021–1065, 1996.

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**Jeffrey Haack** (Los Alamos National Laboratory)

## Consistent BGK model for high energy density plasma mixtures

**Abstract:** We derive a conservative multispecies BGK model that follows the spirit of the original, single species BGK model by ensuring pairwise conservation of momentum and kinetic energy and that the model satisfies Boltzmann's H-Theorem. The derivation emphasizes the connection to the Boltzmann operator, which allows for direct inclusion of information from a molecular dynamics validated effective Boltzmann model. We also develop a complete hydrodynamic closure via the Chapman-Enskog expansion, including a general procedure to generate symmetric diffusion coefficients based on this model. We further extend the model to include the effect of degeneracy on the electron plasma species. We employ this model to investigate kinetic effects on interfacial mixing of the shell-fuel interface in inertial confinement fusion, as well as experiments performed on the Z pulsed power facility.

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Lingbing He (Tsinghua University)

## On semi-classical limit of spatially homogeneous quantum Boltzmann equation

**Abstract:** The quantum Boltzmann equations for Fermi-Dirac and Bose-Einstein statistics proposed by Uehling and Uhlenbeck (after Nordheim) should be derived from the evolution of real Fermions and Bosons in the so called weak-coupling limit. Since Fokker-Planck-Landau equation is the effective equation associated with a dense and weakly interacting gas of classical particles, it is not surprising that the semi-classical limits of the solutions to quantum Boltzmann equations are expected to be solutions to the Fokker-Planck-Landau equation. In this talk, we will show that these limits can be justified mathematically. It is based on a joint work with Xuguang Lu and Marrio Pulvirenti.

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Gernot Heiel (University of Vienna)

## The dynamical systems approach to spatially homogenous Einstein-Vlasov cosmology

**Abstract:** In conventional cosmology the universe is assumed to be spatially homogenous and spatially isotropic, and its matter content is modeled as perfect fluid with linear equation of state. In theoretical and mathematical cosmology, deviations from this approach have been investigated with respect to both, the strong symmetry assumptions on the spatial geometry, and the modeling of the matter as ideal fluid. In my talk I will consider spatially homogenous Einstein-Vlasov cosmology, i.e. spacetimes which are spatially homogenous, but not necessarily spatially isotropic, and whose matter content is modeled as collision free kinetic gas (freely falling particles/galaxies). One approach to analyse such models, initiated by Rendall (1996), is to impose certain symmetry assumptions on the Vlasov distribution function, by which the Einstein-Vlasov system reduces to an autonomous dynamical system on  $R^n$ . Investigations then focus on a dynamical systems analysis of these equations, in particular yielding the exact past and future asymptotic solutions – i.e. the behaviour of these cosmologies close to big-bang or big-crunch singularities, or towards a forever expanding future. After some background and a short review of the corresponding body of literature, I will summarise our current results which completed this body: Our investigation of one class of these models – *Kantowski-Sachs cosmology with Vlasov matter*; Fajman & Heiel 2019 Class. Quantum Grav..

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Maxime Herda (Inria Lille - Nord Europe)

## Asymptotic behaviors of the Vlasov-Poisson-Fokker-Planck equation

**Abstract:** In this talk, we will be interested in the Vlasov-Poisson-Fokker-Planck equation describing the evolution of charged particle under electrostatic interactions and collisions. We will show how to

close hypocoercive and hypoelliptic estimates uniformly in some parameters of the equation (Debye length and mean free path between collisions). These estimates will allow us to build solutions, quantify regularization effects as well as large-time behavior of solutions. Thanks to the uniformity in the parameters, we will obtain explicit dependence of the rates of decay in asymptotic regimes of the parameters. Finally, these uniform estimates will allow us to justify strong convergence to some macroscopic limits such as the drift-diffusion equation in the diffusive scaling. This work is a collaboration with L. Miguel Rodrigues (Univ. Rennes).

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**Hélène Hivert** (École Centrale de Lyon)

**An asymptotic preserving scheme for a kinetic equation describing propagation phenomena**

**Abstract:** The run-and-tumble motion of bacteria such as *E. coli* can be represented by a kinetic equation considered with an hyperbolic scaling. The propagation of fronts is highlighted by geometric optics approximation, that makes the problem non-linear. The stiff front limit is then governed by a Hamilton-Jacobi equation, in which the Hamiltonian is implicitly defined. In this setting, stiff terms appear in the kinetic equation when getting close to the asymptotic. As a consequence, an appropriate strategy has to be used for the numerical resolution of the problem. I will present the construction of an asymptotic-preserving scheme, designed to deal with these difficulties. It is based on a formal asymptotic analysis of the kinetic equation, and a careful treatment of the nonlinearity of the problem.

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**Shi Jin** (Shanghai Jiao Tong University)

**Semiclassical computational methods for quantum dynamics with band-crossing and uncertainty**

**Abstract:** Band-crossing is a quantum dynamical behavior that contributes to important physics and chemistry phenomena such as quantum tunneling, Berry connection, chemical reaction etc. In this talk, we will discuss some recent works in developing semiclassical methods for band-crossing in surface hopping. For such systems we will also introduce an "asymptotic-preserving" method that is accurate uniformly for all wave numbers, including the problem with random uncertain band gaps.

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**Jang Jin Woo** (University of Pennsylvania)

**On the Landau equation with the specular reflection boundary condition**

**Abstract:** In this talk, I will introduce a recent work on the global well-posedness of the Landau equation (1936) in a general bounded domain, which has been a long-outstanding open problem. This work proves the global stability of the Landau equation in an  $L_{x,v}^\infty$  framework with the Coulombic potential in a general smooth bounded domain with the specular reflection boundary condition for initial perturbations of the Maxwellian equilibrium states. Our methods consist of the generalization of the well-posedness theory for the Fokker-Planck equation (HJV-2014, HJJ-2018) and the extension of the boundary value problem to a whole space problem, as well as the use of a recent extension of De Giorgi-Nash-Moser theory for the kinetic Fokker-Planck equations (GIMV-2016) and the Morrey estimates (Polidoro-Ragusa-1998) to further control the velocity derivatives, which ensures the uniqueness. This is a joint work with Y. Guo, H. J. Hwang, and Z. Ouyang.

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**Christian Klingenberg** (Würzburg University)

### **On a multi-species kinetic model of plasma, theory and numerics**

**Abstract:** A kinetic description for evolving gases is given by the Boltzmann equations. This equation is very complicated, so in practice a simplification of the collision operator, namely the so called BGK model, is considered. For an adequate description of a plasma, where treating the different ions is important, one is led to multi-species kinetic models. A new model of this type, arising in inertial confinement fusion, is introduced, where the collision frequency depends on the microscopic velocity. This model is an extension of the model in C. Klingenberg, M. Pirner, G. Puppo: “A consistent kinetic model for a two-component mixture with an application to plasma”, *Kinetic and Related Models* Vol. 10, No. 2 (2017). The fact that now the collision frequency depends on the microscopic velocity gives rise to the need to prove important theoretical properties for this new model, like conservation properties and the H-theorem. These theorems open the way to solving these equations numerically. We present an algorithm for doing this.

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**Liu Liu** (University of Texas at Austin)

### **Micro-macro decomposition based asymptotic-preserving numerical schemes for collisional nonlinear kinetic equation**

**Abstract:** We first extend the micro–macro decomposition method for multiscale kinetic equations from the BGK model to general collisional kinetic equations, including the Boltzmann and the Fokker–Planck Landau equations. Such a scheme allows the computation of multiscale collisional kinetic equations efficiently in all regimes, including the fluid regime in which the fluid dynamic behavior can be correctly computed even without resolving the small Knudsen number. A distinguished feature of these schemes is that although they contain implicit terms, they can be implemented explicitly. These schemes preserve the moments (mass, momentum and energy) exactly thanks to the use of the macroscopic system which is naturally in a conservative form. We further utilize this conservation property for more general kinetic systems, using the Vlasov–Ampère and Vlasov–Ampère– Boltzmann systems as examples. The main idea is to evolve both the kinetic equation for the probability density distribution and the moment system, the later naturally induces a scheme that conserves exactly the moments numerically if they are physically conserved.

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**Alessia Nota** (University of Bonn)

### **Homoenergetic Solutions for the Boltzmann Equation**

**Abstract:** We consider a particular class of solutions of the Boltzmann equation, known as homoenergetic solutions, which are useful to describe the dynamics of Boltzmann gases under shear, expansion or compression in nonequilibrium situations. While their well posedness theory has many similarities with the theory of homogeneous solutions of the Boltzmann equation, their long time asymptotics differs completely, due to the fact that these solutions describe far-from-equilibrium phenomena. Indeed, the long-time asymptotics cannot always be described by Maxwellian distributions. For several collision kernels the asymptotics of homoenergetic solutions is given by particle distributions which do not satisfy the detailed balance condition. In this talk I will describe different possible long-time asymptotics of homoenergetic solutions of the Boltzmann equation, as well as some open problems in this direction. This is a joint work with R.D.James and J.J.L.Velázquez.

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**Marlies Pirner** (University of Vienna)

## **BGK models for gas mixtures: Modelling and theory**

**Abstract:** A kinetic description for evolving gases with a simplification of the collision operator is given by the BGK model. I shall present such a model for gas mixtures. It is a multi-species model, for we can show conservation properties, H-Theorem, Existence and Uniqueness of solutions and results on the large time behaviour. Moreover, the model can be extended to polyatomic multi-species gases, ES-BGK models and velocity dependent collision frequencies.

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**Chiara Saffirio** (Universität Zürich)

## **From the many-body quantum dynamics to the Vlasov equation**

**Abstract:** We review some results on the joint mean-field and semiclassical limit of the N-body Schrödinger dynamics leading to the Vlasov equation, which is a model in kinetic theory for charged or gravitating particles. The results we present include the case of singular interactions and provide explicit estimates on the convergence rate, using the Hartree-Fock theory for interacting fermions as a bridge between many-body and Vlasov dynamics.

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**Francesco Salvarani** (Università degli Studi di Pavia)

## **On the Maxwell-Stefan diffusion equations for multicomponent gaseous mixtures**

**Abstract:** The diffusive behavior of multicomponent gaseous mixtures has recently gained interest in the mathematical community. In this talk, I will study a system describing diffusive phenomena for a mixture in a non-isothermal setting, derived from the Boltzmann system for gaseous mixtures. I will prove local existence and uniqueness of the solution and discuss some related questions.

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**Anna Sczekutovwicz** (University of Texas at Austin)

## **Velocity Dependent Coulomb Logarithm In The Landau Limit Of The Boltzmann Equation**

**Abstract:** We propose to study numerical and analytically recent developments on a new spectral formulation of the Fokker-Planck-Landau (FPL) operator with velocity dependent Coulomb logarithm that fully revisits the derivation of the FPL limit operator as a grazing collision form starting from the classical Boltzmann operator form for binary elastic interactions where the transition probability rates depending on the scattering angle dominates the glancing limiting dynamics. The key problem is that using Rutherford cross section forms in the Boltzmann collision operator results in a logarithmic singularity. A revised derivation of the scattering cross section can be obtained noticing that the scattering angle depends on the impact parameter with is proportional to the total cross section. This observation yields an impact parameter depending on the angle and the relative speed resulting in a nonlinear relation between the total cross section and the relative particle speed, with a scattering angle with an angular cut-off condition depending on Debye length  $\lambda D$  given the range of charged particles being screened from one another. Then, the resulting cross section has a stronger physical meaning as the angular cut-off condition that depends on  $\lambda D$ , and thus differs significantly from the one used in the classical formal derivation where the cut-off is given by a small constant that is completely unrelated to the Debye length between the two-body interaction.

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**Raphael Winter** (University of Bonn)



## Convergence to the Landau equation from the truncated BBGKY hierarchy in the weak-coupling limit

**Abstract:** We show that in macroscopic times of order one, the solutions to the truncated BBGKY hierarchy (to second order) converge in the weak coupling limit to the solution of the nonlinear spatially homogeneous Landau equation. The truncated problem describes the formal leading order behavior of the underlying particle dynamics, and can be reformulated as a non-Markovian hyperbolic equation which converges to the Markovian evolution described by the parabolic Landau equation. The analysis in this paper is motivated by Bogolyubov's derivation of the kinetic equation by means of a multiple time scale analysis of the BBGKY hierarchy.

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