New Challenges in Mathematical Modelling and Numerical Simulation of Superfluids

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Mauro Antezza: Solitons in a superfluid Fermi gas.

We will discuss recent results on the theoretical and experimental investigations on solitons in a superfluid Fermi gas along the BCS-BEC crossover. On the theory side, by solving the Bogoliubov de Gennes equations and looking for real and odd solutions for the order parameter, it has been shown that a dark soliton at unitarity posses a large density contrast and fermionic bound states. The superfluid gap is found to be significantly quenched by the presence of the soliton due to the occurrence of Andreev fermionic bound states localized near the nodal plane of the order parameter. By solving the time dependent Bogoliubov de Gennes equations, also the decay and collisions of dark solitons has been investigated. Recently, a cascade of Solitonic Excitations in a Superfluid Fermi gas has been experimentally observed.

Xavier Antoine: GPELab, an open source Matlab toolbox for the numerical simulation of Gross-Pitaevskii equations.

This talk presents GPELab (http://gpelab.math.cnrs.fr/ - Gross-Pitaevskii Equation Laboratory), an advanced easy-to-use and flexible Matlab toolbox for numerically simulating many complex physics situations related to Bose-Einstein Condensation (BEC). The model equation that GPELab solves is the Gross-Pitaevskii Equation (GPE). Robust and accurate numerical schemes are implemented for computing stationary solutions and the dynamics of BECs through the GPE. We will explain the pseudospectral schemes that are included in GPELab and will show some numerical examples including: 1d, 2d and 3d situations, general potentials, large classes of local and nonlocal nonlinearities, multi-components problems, fast rotating gazes. Joint work with Romain Duboscq.

Weizhu Bao: Quantized vortex stability and dynamics in superfluidity and superconductivity.

Quantized vortices have been experimentally observed in type-II superconductors, superfluids, nonlinear optics, etc. In this talk, I will review different mathematical equations for modeling quantized vortices in superfluidity and superconductivity, including the nonlinear Schrodinger/Gross-Pitaevskii equation, Ginzburg-Landau equation, nonlinear wave equation, etc. Asymptotic approximations on single quantized vortex state and the reduced dynamic laws for quantized vortex interaction are reviewed and solved analytically in several cases. Efficient and accurate numerical methods will be presented for computing quantized vortex lattices and ther dynamics. Direct numerical simulation results from different PDE models are reported for quantized vortex dynamics and they are compared with those from the reduced dynamics laws. Some open problems and emerging applications will be discussed. This is a joint work with Qiang Du, Dieter Jaksch, Alexander Klein, Qinglin Tang and Yanzhi Zhang.

Carlo Barenghi: Classical and non-classical flows of superfluids.

Superfluids are remarkable because they lack mechanisms of viscous dissipations, and because vorticity is concentrated in thin vortex lines - a property which arises from the existence and uniqueness of a macroscopic wave function. In this talk I shall review recent experiments and numerical simulations which reveal analogies and differences between the flow of ordinary fluids and the flow of superfluids. In particular, I shall describe conditions under which, in a homogeneous isotropic turbulent superfluid away from boundaries, the distribution of kinetic energy over the length scales is similar to the classical Kolmogorov distribution, and new insight into the properties of superfluid flow near boundaries.

Natalia Berloff: Polariton graph simulators.

We propose a platform for finding the global minimum of XY Hamiltonian with polariton graphs. We derive an approximate analytic solution to the spinless complex Ginzburg-Landau equation that describes the density and kinetics of a polariton condensate under incoherent pumping. The analytic expression of the wavefunction is used as the building block for constructing the XY Hamiltonian of two-dimensional polariton graphs. We illustrate examples of the quantum simulator for various classical magnetic phases on some simple lattice geometries: linear, triangular, square.

Christophe Besse: High-order numerical schemes for computing the dynamics of nonlinear Schrödinger equation.

The aim of this talk is to present high-order numerical schemes for simulating the dynamics of systems of nonlinear Schrödinger/Gross-Pitaevskii equations. The usual high order numerical schemes based on time splitting technique can not be adapted for the computation of solutions to such equations in some situations. We introduce Runge-Kutta type schemes to obtain high order numerical schemes which can be used both for scalar and system of equations. We will consider exponential integrators such as exponential Runge–Kutta methods and Lawson methods, and high-order IMplicit-EXplicit (IMEX). We will show the properties of theses numerical schemes and develop a complete numerical study to investigate the properties of the schemes.

Marc Brachet: Helicity, topology and Kelvin waves in reconnecting quantum knots.

Helicity is a topological invariant that measures the linkage and knottedness of lines, tubes and ribbons. As such, it has found myriads of applications in astrophysics and solar physics, in fluid dynamics, in atmospheric sciences, and in biology. In quantum flows, where topology-changing reconnection events are a staple, helicity appears as a key quantity to study. However, the usual definition of helicity is not well posed in quantum vortices, and its computation based on counting links and crossings of vortex lines can be downright impossible to apply in complex and turbulent scenarios. We present a new definition of helicity which overcomes these problems. With it, we show that only certain reconnection events conserve helicity. In other cases helicity can change abruptly during reconnection. Furthermore, we show that these events can also excite Kelvin waves, which slowly deplete helicity as they interact nonlinearly, thus linking the theory of vortex knots with observations of quantum turbulence. Joint work with P.C. di Leoni and P.D. Mininni

Yongyong Cai: Ground states and dynamics of spin-orbit-coupled Bose-Einstein condensates.

We study analytically and asymptotically as well as numerically ground states and dynamics of two-component spin-orbit-coupled Bose-Einstein condensates (BECs) modeled by the coupled Gross-Pitaevskii equations (CGPEs).In fact, due to the appearance of the spin-orbit (SO) coupling in the two-component BEC with a Raman coupling, the ground state structures and dynamical properties become very rich and complicated. For the ground states, we establish the existence and non-existence results under different parameter regimes, and obtain their limiting behaviors and/or structures with different combinations of the SO and Raman coupling strengths. For the dynamics, we show that the motion of the center-of-mass is either non-periodic or with different frequency to the trapping frequency when the external trapping potential is taken as harmonic and/or the initial data is chosen as a stationary state (e.g. ground state) with a shift, which is completely different from the case of a two-component BEC without the SO coupling.

Rémi Carles: Time splitting methods and the semi-classical limit.

We consider the time discretization based on Lie-Trotter splitting, for the nonlinear Schrodinger equation, in the semi-classical limit, with initial data under the form of WKB states. Both the exact and the numerical solutions keep a WKB structure, on a time interval independent of the Planck constant. We prove error estimates, which show that the quadratic observables can be computed with a time step independent of the Planck constant. We give a flavor of the functional framework, based on time-dependent analytic spaces.

Frédéric Chevy: Counterflowing superfluids.

Since the discovery of superfluid 3He in 1972, the realization of a doubly-superfluid Bose-Fermi mixture has been one the major goals in the field of quantum liquids. However, due to strong repulsive interactions between helium atoms, the fraction of 3He inside 4He cannot exceed 6%. This high dilution of the fermionic species reduces dramatically its critical temperature from 2.5 mK for pure 4He to a predicted value of 40 ŒºK in the mixture. Despite decades of efforts, this range of temperature is still inaccessible to experimental investigation and has prevented the observation of a dual superfluid phase in liquid helium. In cold atoms however, Feshbach resonances make it possible to control the strength of interatomic interactions and realize stable Bose-Fermi mixtures. In my talk I will discuss the physical properties of weakly-coupled superfluid mixtures of 6Li and 7Li [1]. Superfluidity was revealed by the existence of a critical velocity below which the relative motion of the two species is undamped and the energy transfer between the two gases is coherent. We could interpret this critical velocity using a generalized Landau mechanism in which excitations are shed in both superfluids [2,3].

[1] I. Ferrier-Barbut et al., Science 345, 1035 (2014)
[2] Y. Castin et al., Comptes Rendus Physique 16, 241 (2015)

[3] M. Delehaye et al. Phys. Rev. Lett. 115, 265303 (2015)

Ionut Danaila: An overview of the BECASIM project: open source numerical simulators for the Gross-Pitaevskii equation.

The purpose of the French BECASIM project (Bose-Einstein Condensates: Advanced SIMulation Deterministic and Stochastic Computational Models, HPC Implementation, Simulation of Experiments) is to develop robust and reliable numerical simulators, based upon new mathematically sound methods and modern high performance computing strategies. Several numerical systems for solving various forms of the Gross-Pitaevskii equation have been developed in the framework of the project: GPELab (a Matlab based spectral code), GPFEM (a FreeFem++ based finite-element code) and GPS (a spectral/compact finite- difference MPI-OpenMP Fortran code). After a short presentation of the main characteristics of these open source codes, we illustrate their capabilities by showing simulations of configurations corresponding to physical experiments of Bose-Einstein condensates.

Anne De Bouard: Inhomogeneities and temperature effects in Bose-Einstein condensates.

We will review in this talk some mathematical results concerning stochastic models used by physicist to describe BEC in the presence of fluctuations (that may arise from inhomogeneities in the confinement parameters), or BEC at finite temperature. The results describe the effect of those fluctuations on the structures âĂî e.g. vortices âĂî which are present in the deterministic model, or the convergence to equilibrium in the models at finite temperature. We will also describe the numerical methods which have been developed for those models in the framework of the ANR project Becasim. These are joint works with Reika Fukuizumi, Arnaud Debussche, and Romain Poncet.

Qiang Du: Nonlocal models and their numerical discretization.

Nonlocal models have appeared in many applications including superfluids. Recent development of nonlocal vector calculus and nonlocal calculus of variations provides a systematic mathematical framework for the analysis of nonlocal continuum models given in the form of partial-integral equations. In this lecture, we consider a few related examples of nonlocal models such as nonlocal Ginzburg-Landau and nonlocal Schrödinger equations, as well as nonlocal models with heterogeneous localization. A particular focus is on connections with their local limit given by traditional local PDEs and their monolithic numerical discretization.

Arnaldo Gammal: Three-dimensional vortex structures in a rotating dipolar Bose-Einstein condensate.

We study three-dimensional vortex lattice structures **in** purely dipolar Bose-Einstein condensate (BEC). By using the mean-field **approximation,** we obtain a stability diagram for the vortex states in purely dipolar BECs as a function of harmonic trap aspect ratio (λ) and dipole-dipole interaction strength (D) under rotation. Rotating the condensate

within the unstable region leads to collapse while in the stable region furnishes stable vortex lattices of dipolar BECs. We analyse stable vortex lattice structures by solving the three-dimensional time-dependent Gross-Pitaevskii equation in imaginary time. Further, the stability of vortex states is examined by evolution in real-time. We also investigate the distribution of vortices in a fully anisotropic trap by increasing eccentricity of the external trapping potential. We observe the breaking up of the condensate in two parts with **an equal number of** vortices on each when the trap is sufficiently weak, and the rotation frequency is high.
Joint work with Ramavarmaraja Kishor Kumar, Thangarasu Sriraman, Henrique Fabrelli, Paulsamy Muruganandam.

Jean-Claude Garreau: Symmetries and dynamics in a quantum-chaotic system.

Symmetries are quintessential in the understanding of physical systems. This is particularly true in chaotic, quantum-chaotic or quantum-disordered systems. Using a cold-atom realization of the kicked rotor, we can exploit the influence of the time-reversal or parity symmetry on its dynamics. This is particularly interesting as such a system, is a paradigma for all these problems: Classical hamiltonian chaos, through the well-known Äústandard map; quantum chaos in which it displays characteristic phenomena as dynamical localization and quantum resonances, and disorder, where it is a âÄúquantum simulator for the Anderson model in any dimension. I will present the latest experimental results obtained by our group.

Dieter Jaksch: Plasmonics in layered superconductors.

Some layered superconductors support weakly damped plasma waves, involving oscillatory tunneling of the superfluid between capacitively coupled planes. Such Josephson plasma waves are highly nonlinear, and exhibit striking phenomena like cooperative emission of coherent terahertz radiation, superconductor-metal oscillations and soliton formation. In recent experiments it was shown that terahertz Josephson plasma waves in cuprate superconductors can be parametrically amplified through the cubic tunneling nonlinearity [1]. This parametric amplification is sensitive to the relative phase between pump and seed waves and may be optimized to achieve squeezing of the order parameter phase fluctuations or single terahertz-photon devices. In this talk I will present a simple model describing this physics in terms of coupled superfluid order parameters with optical driving applied to their boundaries. I will compare experimental and theoretical results and discuss challenges in obtaining numerically accurate solutions in the parameter regime of relevance to the experiments.

[1] Srivats Rajasekaran, Eliza Casandruc, Yannis Laplace, Daniele Nicoletti, Genda D. Gu, Stephen R. Clark, Dieter Jaksch, Andrea Cavalleri, https://arxiv.org/abs/1511.08378

Robert Jerrard: Nearly parallel vortex filaments in the 3d Gunzburg-Landau equations.

Starting from the Gross-Pitaevskii free energy, we derive a free-energy functional energy that characterizes the fine-scale structure of a finite collection of nearby, nearly-parallel vortex filaments in equilibrium. (This is joint work with Andres Contreras.) Time permitting, we will also report on some related dynamical questions.

Michikazu Kobayashi: Quantum nature and statistical law in quantum turbulence.

Quantum turbulence in quantum fluid features a spatially and dynamically complicated structure of quantized vortices with quantized circulation. Quantized vortices are (i) vortices with finite circulation, and (ii) stable topological line defects. In a fully developed turbulence, the first character of vortices becomes dominant in large scales, giving Kolmogorov's -5/3 power law spectrum as a classical analoque of quantum turbulence. Here, I talk about two topics of quantum turbulence where the second character of vortices becomes dominant. The first topic is the laminar-turbulent transition of quantum fluid. In the case of quantum fluid, we can easily separate laminar and turbulent states as a system with or without vortices. Defining the "order parameter" of turbulence as the vortex density, we find that the laminar-turbulent transition can be regarded as the non-equilibrium phase transition belonging to the temporally-directed percolation universality class. The key concept is that vortices has a finite energy barrier to be nucleated and cannot be re-nucleated after annihilated near the transition point. The second topic is topological protection of the helicity conservation. In general, the helicity is not conserving quantity in quantum fluid because it discretely changes when vortices reconnect. However, vortices have topological charges besides circulations, and we can topologically control the reconnection process by changing topological charges of vortices. Actually, reconnection process is topologically prohibited by non-Abelian topological charges of vortices. We find that helicity is conserved and cascade in quantum turbulence with vortices having non-Abelian topological charges, obtaining a new power law spectrum of turbulence.

Mathieu Lewin: Superfluidity and Bogoliubov theory: rigorous derivation for mean-field many-body systems.

One of the most famous problem is to understand the occurence of superfluidity in cold Bose gases, starting from many-body quantum mechanics. A physical explanation was provided by Landau and Bogoliubov in terms of the excitation spectrum, but a mathematical proof of this effect is still lacking. I will review recent advances in this direction for the simpler mean-field model, where the interaction has an intensity of order $1/N$, with N the number of particles in the system. Joint works with Phan Thanh Nam, Nicolas Rougerie, Benjamin Schlein, Sylvia Serfaty and Jan Philip Solovej.

Philippe Parnaudeau: A hybrid code for solving the Gross-Pitaevskii equation.

We present a new robust, efficient and scalable numerical code: GPS (Gross-Pitaevskii Solver). GPS computes the stationary solutions and the dynamics of the Gross-Pitaevskii Equation (GPE), used as model for Bose- Einstein Condensates (BEC), quantum turbulence, or ultracold quantum gases (in optical lattices for example). In order to obtain most accurate solutions, two spectral-like discretizations of mathematical operators are implemented in GPS.We have parallelized the code via a two-level communication scheme using MPI across nodes and OpenMP within nodes. GPS has shown good scalability up to 100 000 cores. Capabilities of GPS are highlighted by reproducing some experimental configurations (giant vortex).

Bartosz Protas: On Some Variational Optimization Problems in Classical Fluids and Superfluids.

In this presentation we discuss some analytical and computational aspects of two families of variational optimization problems with common structure arising in classical and quantum fluids. The first question concerns the numerical minimization of the Gross-Pitaevskii energy functional subject to the normalization constraint on the wavefunction. While such problems can be efficiently solved with gradient-based approaches using suitable Sobolev gradients, the presence of the nonlinear constraint makes it difficult to use the conjugate-gradients method to accelerate the convergence. Recognizing that that the nonlinear constraint defines a smooth manifold in the solution space, we demonstrate how the method of conjugate gradients can be adapted to this problems using concepts of Riemannian optimization such as vector transport along the manifold. We will present computational results illustrating an improved performance of this optimization approach as compared to the standard steepest-descent method. The aforementioned variational structure is also shared by a class of optimization problems recently proposed to probe the sharpness of certain fundamental estimates in classical fluid mechanics. These estimates characterize extreme (potentially singular) behavior in viscous incompressible flows and in the second part of the presentation we will survey recent results concerning these problems. We will emphasize, in partcular, the insights obtained by tracing out different branches of extremal solutions.[joint work with I. Danaila and D. Ayala]

Nick Proukakis: Quantum Fluid Mixtures: Modelling Phase Separation & Dynamics of Atomic Bose-Einstein Condensates.

Mixtures of quantum fluids, accessible in controlled ultracold atomic experiments, constitute an exciting system to study phase mixing and non-equilibrium dynamics of interacting quantum gases. In this talk, we give a brief overview of our recently formulated self-consistent kinetic model to study such systems at finite-temperature [1], where both components are partially-condensed. Within this scheme, both condensates and thermal atoms are coupled together through both the mean-field interactions and all possible collisional processes, and this creates an interesting system, whose hydrodynamicity is controllable through variations of temperature, trap frequencies and trap geometries [2]. Our studies also raise interesting questions on the route to thermalisation [3] and the related approach to equilibrium following a quench [4]. By numerically analysing the miscibility-immiscibility phase diagram for a particular mixture, we introduce an improved criterion for the determination of the phase separation boundary and propose its experimental mapping by monitoring the damping rate of the dipole oscillations [5]. Our model is also suited to describing the recently achieved double superfuid Bose-Fermi mixture, for which initial results are also shown.

We acknowledge funding from the EPSRC.

[1] M Edmonds, K-L Lee, N P Proukakis, Phys Rev A 91,011602(R) (2015).
[2] M Edmonds, K-L Lee, N P Proukakis, Phys Rev A 92,063607 (2015).
[3] K-L Lee, N P Proukakis (in preparation)
[4] I-K Liu et al., Phys. Rev. A 93, 023628 (2016)
[5] K-L Lee et al., arXiv:1604.08063

Etienne Sandier: Young measures for homogenization of phase transition models.

I will present a framework which combines ideas of Dal Maso-Modica and Alberti-Müller and which we believe to be efficient for the study of non-convex homogenization problems, random or not. Joint work with S. Serfaty and L. Berlyand.

Didier Smets: Leapfrogging for the axisymmetric Gross-Pitaevskii equation.

The leapfrogging is the name given to a regime of interaction between vortex rings with the same axis of symmetry in incompressible fluids. We will explain where it comes from and indicate a rigorous derivation in the case of the axisymmetric Gross-Pitaevskii equation.

Henk Stoof: Order parameter fluctuations in the holographic superconductor.

We investigate the effect of order parameter fluctuations in the holographic superconductor. In particular, following an introduction to the concept of intrinsic dynamics, we compute the intrinsic spectral functions of the order parameter in both the normal and the superconducting phase. We also present a vector-like large-N version of the Ginzburg-Landau model that accurately describes our long- wavelength results in both phases. Our results indicate that the holographic superconductor describes a relativistic multi-component superfluid in the universal regime of the BEC-BCS crossover.

Qinglin Tang: Numerical methods on simulating dynamics of the nonlinear Schrödinger equation with rotation and/or nonlocal interactions.

In this talk, I will present some efficient numerical methods for simulating dynamics of the nonlinear Schrödinger equation (NLSE) with nonlocal potential and rotation term. The method consists two main merits: (i) a rotating Lagrangian coordinate transformation will be presented to eliminate the rotation term. (ii) efficient and accurate numerical methods will then be presented to evaluate nonlocal potential of different types. Finally, some interesting applications and phenomena will also be presented.

Mechthild Thalhammer: High-order Magnus integrators for non-autonomous linear evolution equations.

The class of commutator-free Magnus integrators is known to provide a favourable alternative to standard interpolatory Magnus integrators, in particular for large-scale applications arising in the time integration of non-autonomous linear evolution equations. A high-order commutator-free Magnus integrator is given by a composition of several exponentials that comprise certain linear combinations of the values of the defining operator at specified nodes. Due to the fact that previously proposed commutator-free Magnus integrators of order five or higher involve negative coefficients in the linear combinations, severe instabilities are observed for spatially semi-discretised partial differential equations of parabolic type or for master equations describing dissipative quantum systems, respectively. In order to remedy this issue, two different approaches for the design of efficient Magnus integrators of orders four, five, and six are pursued: (i) the study of commutator-free Magnus integrators involving complex coefficients with positive real part, and (ii) the study of unconventional Magnus integrators that comprise in addition a single exponential involving a commutator. Numerical experiments for test equations of Schrödinger and parabolic type confirm that the identified novel Magnus integrators are superior to Magnus integrators previously proposed in the literature.
This is joint work with Sergio Blanes and Fernando Casas.

Makoto Tsubota: Inhomogeneous quantum turbulence in a channel.

Most of previous numerical works on quantum turbulence in superfluid helium were performed for periodic boundary conditions. This was chiefly because there was no information on inhomogeneous flow in a channel. However, the recent visualization experiments found inhomogeneous flow profile in a channel (1). Being motivated by these experiments, we study numerically the dynamics of quantized vortices in a square channel. The first problem is thermal counterflow. When the normal fluid profile is prescribed to be inhomogeneous, we revealed the inhomogeneous profile and dynamics of vortices (2) and found the logarithmic velocity profile of the superfluid velocity (3). The logarithmic velocity profile is the most important statistical law in turbulent boundary layer in classical fluid mechanics, discovered by this work for the first time in quantum turbulence. The second problem is coflow in which superfluid and normal fluid flow along the same direction (4). We investigated the vortex dynamics in coflow to find a characteristic attractor in which vortices are absorbed (5).

(1) A. Marakov et al., Phys. Rev. B 91, 094503 (2015).
(2) S. Yui, M. Tsubota, Phys. Rev. B 91, 184504 (2015).
(3) S. Yui, K. Fujimoto, M, Tsubota, Phys. Rev. B 92, 224513 (2015).
(4) E. Varga, S. Babuin and L. Skrbek, Phys. Fluids 27, 065101 (2015).
(5) S. Ikawa, M. Tsubota, Phys. Rev. B 93 (in press).

Hanquan Wang: An efficient splitting Fourier pseudospectral method for Vlasov-Poisson-Fokker-Planck system.

In this paper, we propose an efficient splitting Fourier pseudospectral method for Vlasov-Poisson-Fokker-Planck system. The numerical integration for the system is performed using the splitting method in time and Fourier pseudospectral method in the phase space, wherein Fourier Galerkin method is applied in space direction and Fourier collocation method is used in velocity direction, respectively. The algorithm provides spectral accuracy in phase space and can be implemented efficiently with the fast Fourier transform and technique of diagonalization, respectively. Numerical results in both two-dimensional and four-dimensional phase space by the proposed numerical method are shown and proves the good agreement with the theory and previous studies.

Xiaofei Zhao: Numerical methods on discretizing the fractional Laplacian.

Recently, the fractional partial differential equations with the fractional Laplacian has attracted great attention from both physicists and mathematicians. The fractional Laplacian, representing an infinitesimal generator of a symmetric α-stable Levy process, is a nonlocal operator, which introduces considerable challenges for both the mathematical analysis and numerical simulations. In this talk, we will present various numerical methods for discretizing the fractional Laplacian and provide the error analysis and comparison between methods.