Numerical and theoretical advances in quantum mechanics

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Recueil des résumés

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Clotilde Fermanian-Kammerer: Semiclassical gaussian states and dynamical approximation of quantum systems

Auteur correspondant clotilde.fermanian@u-pec.fr

In this talk we discuss methods for approximating of the solution of a semi-classical Schrödinger equation. Originated in a theoretical chemistry context, these methods have in common to strongly on the use of semiclassical Gaussian states.

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Mario Pulvirenti: ”Some considerations on the derivation of the Quantum Boltzmann equation”

In this talk I consider the problem of the derivation of the nonlinear Boltzmann equation from a quantum particle system in the weak-coupling limit, the very few rigorous results, the difficult open problems and possible perspectives.

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Peter Müller: ”Entanglement entropy for quasifree Fermi gases: area law versus logarithmic enhancement”

An overview is presented of Szeg\H{o}-type asymptotics for spectral projections of multi-dimensional continuum Schr\”odinger operators. Whenever possible we treat general test functions, including those which describe entanglement entropies of corresponding quasifree Fermi gases. Unfortunately, there exists no general theory which allows to deduce the leading asymptotic behaviour of entanglement entropies and whether they exhibit an area law or a logarithmically enhanced one. Therefore we focus on examples which shed some light on the underlying mechanism. We investigate stability, the role of spectral types versus dynamical (de-) localization and the relevance of the spatial structure of (generalised) eigenfunctions at the Fermi energy.

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David Krejcirik: Is the optimal rectangle a square?

We give a light talk on an optimality of a square in geometry and physics. First, we recollect classical geometric results that the square has the largest area (respectively, the smallest perimeter) among all rectangles of a given perimeter (respectively, area). Second, we recall that the square drum has the lowest fundamental tone among all rectangular drums of a given area or perimeter and reinterpret the result in a quantum-mechanical language of nanostructures. As the main body of the talk, we present our recent attempts to prove the same property in relativistic quantum mechanics, where the mathematical model is a matrix-differential (Dirac) operator with complex (infinite-mass) boundary conditions. It is frustrating that such an illusively simple and expected result remains unproved and out of the reach of current mathematical tools.

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Claudia Negulescu: ”Decoherence rhapsody in the photosynthesis process”

It is said that classical theories are sometimes inappropriate to describe very efficient biological processes in nature, which seem to be better understood via quantum mechanical models. We are however still very far from understanding how quantum features can survive in open quantum systems. In this talk I shall present two simple mathematical models for the illustration of the excitation energy transfer in photosynthesis complexes, and study numerically the environmental induced decoherence effect and its influence on the emergence of classicality in nature. The models are based on the Schrödinger equation, describing the propagation of an absorbed excitation through a spin-chain towards a reaction center, and this in permanent interaction with a vibrational environment.

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Anton Arnold: ”A hybrid WKB-based method for Schrödinger scattering problems in the semi-classical limit”

We consider 1D scattering problems related to quantum transport in diodes. We discuss the efficient numerical integration of ODEs like epsilon^2*u”+a(x)*u=0 for 0<epsilon«1 on coarse grids, but still yielding accurate solutions; including oscillatory (for given a(x)>0) and evanescent regimes (for a(x)<0), partly including turning points. In the oscillatory case we use a marching method that is based on an analytic WKB-preprocessing of the equation. Then we shall discuss two approaches to couple the oscillatory regime to smooth regimes across turning points and close to them: In the former (evanescent) case we use a FEM with WKB-ansatz functions; in the latter case an automated switching to a Runge-Kutta method with adaptive step size controller.

Co-authors: Claudia Negulescu; Kirian Döpfner, Jannis Körner; Christian Klein, Bernhard Ujvari

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Paola Pietra: ”An interface formulation for the Poisson equation in the presence of a semiconducting single-layer material”

We consider a semiconducting device with an active zone made of a single-layer material. The associated Poisson equation for the electrostatic potential (to be solved in order to perform self-consistent computations) is characterized by a surface particle density and an out-of-plane dielectric permit-

tivity in the region surrounding the single-layer. To avoid mesh refinements in such a region, we propose an interface problem based on the natural domain decomposition suggested by the physical device. Two different interface continuity conditions are discussed. Then, we present the corresponding variational formulations adapting the so called three-fields formulation for domain decomposition and the proper finite element method for their approximation. Finally, numerical experiments are shown to illustrate some specific features of this interface approach.
Co-author: Clement Jourdana, Univ. Grenoble Alpes, CNRS, Grenoble INP, LJK, Grenoble, France

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Christian Lubich: "Time integration of tree tensor networks"

First I report on recent numerical experiments with time-dependent tree tensor network algorithms for the approximation of quantum spin systems. I will then describe the basics in the design of time integration methods that are robust to the usual presence of small singular values, that have good structure-preserving properties (norm, energy conservation or dissipation), and that allow for rank (= bond dimension) adaptivity and also have some parallelism. This discussion of basic concepts will be done for the smallest possible type of tensor network differential equations, namely low-rank matrix differential equations. Once this simplest case is understood, there is a systematic path to the extension of the integrators and their favourable properties to general tree tensor networks.

This talk is based on joint work with many colleagues and former and present students, among which I wish to single out Othmar Koch for the first mathematical work on dynamical low-rank approximation (DLRA) in 2007, Ivan Oseledets for jointly finding the first robust DLRA integrator (the projector-splitting integrator) in 2014, Gianluca Ceruti for jointly finding the Basis Update & Galerkin (BUG) integrators in 2021, and him and Hanna Walach and Dominik Sulz for the recent systematic extension from low-rank matrices to general tree tensor networks.

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Louise Gassot: "Zero-dispersion limit for the Benjamin-Ono equation on the torus"

We discuss the zero-dispersion limit for the Benjamin-Ono equation on the torus given a bell-shaped initial data. We prove that the solutions admit a weak limit as the dispersion parameter tends to zero, which is explicit and constructed from the Burgers' equation. The approach relies on the complete integrability for the Benjamin-Ono equation from Gérard, Kappeler and Topalov, and also on the spectral study of the Lax operator associated to the initial data in the zero-dispersion limit.

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Perelman

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Raffaele Carlone: ”A ionization model”

In the first part of the talk, it will be discussed the dynamics of a polaron (a quantum particle coupled to bosonic fields) in the quasi-classical regime: in such a regime, the effective dynamics for the quantum particles are approximated by the one generated by a time-dependent point interaction, i.e., a singular time-dependent perturbation of the Laplacian supported in a point.

In the second part, it will be analyzed the effective equation and, in particular: global well-posedness of the associated Cauchy problem under general assumptions on the potential and the initial datum and, for a monochromatic periodic potential; the asymptotic behavior of the survival probability of a bound state of the time-independent problem.

Joint work with M. Correggi, L. Tentarelli, M. Falconi, M. Olivieri, R. Figari, W. Borrelli

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Alessandro Teta: ”Many-particle systems with contact interactions in dimension three”

Hamiltonians with contact (or zero-range) interactions are useful models to analyze the behaviour of quantum systems at low energy in different contexts. In this talk we discuss the mathematical aspects of the construction of such Hamiltonians in dimension three as self-adjoint and lower bounded operators in the appropriate Hilbert space. We first consider the case of a system made of three identical bosons. In order to avoid the fall to the center phenomenon emerging in the standard Ter-Martirosyan Skornyakov (TMS) Hamiltonian, known as Thomas effect, we develop in detail a suggestion given in a seminal paper of Minlos and Faddeev in 1962 and we construct a regularized version of the TMS Hamiltonian. The regularization is given by an effective three-body force, acting only at short distance, that reduces to zero the strength of the interactions when the positions of the three particles coincide. The construction is then extended to the case of an arbitrary number of interacting bosons. The talk is based on a series of works in collaboration with G. Basti, C. Cacciapuoti, D. Ferretti, R. Figari, D. Finco and H. Saberbaghi.

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Serena Cenatiempo: ”A second order upper bound for the ground state energy of dilute Bose gases”

Back in 2009 H.-T. Yau and J. Yin established a second order upper bound for the ground state energy of dilute Bose gases in the thermodynamic limit, finally in agreement with a elebrated prediction due to Bogoliubov and, in more explicit terms, by Lee, Huang and Yang. In this talk we describe recent ideas allowing us to establish the same result for a larger class of potentials (namely repulsive and compactly supported potentials $V \in L^3(R^3)$), and via a simpler proof. Joint work with G. Basti and B. Schlein.

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Benjamin Schlein: ”Upper bounds on the ground state energy of dilute hard spheres”

We review some recent estimates on the energy of bosons interacting through hard-sphere potentials. We first discuss Bose gases in the Gross-Pitaevskii regime, in which N hard spheres with radius of order 1/N move on the unit torus; in this setting, we show an upper bound for the ground state energy, valid up to errors that vanish as N tends to infinity. We conclude presenting a simple new bound for hard spheres in the thermodynamic limit, resolving the ground state energy up to an error comparable with the so-called Lee-Huang-Yang corrections.

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Liviu Ignat: ”Asymptotic behavior of solutions for some diffusion problems on metric graphs”

In this talk we present some recent result about the long time behavior of the solutions for some diffusion processes on a metric graph. We study evolution problems on a metric connected finite graph in which some of the edges have infinity length. We show that the asymptotic behaviour of the solutions of the heat equation (or even some nonlocal diffusion problems) is given by the solution of the heat equation, but on a star shaped graph in which there is only one node and as many infinite edges as in the original graph. In this way we obtain that the compact component that consists in all the vertices and all the edges of finite length can be reduced to a single point when looking at the asymptotic behaviour of the solutions. We prove that when time is large the solution behaves like a gaussian profile on the infinite edges. When the nonlinear convective part is present we obtain similar results but only on a star shaped tree.

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Paolo Antonelli : ”Stability of Cnoidal Waves for the Damped Nonlinear Schrödinger Equation”

We consider the cubic nonlinear Schrödinger (NLS) equation with a linear damping on the one dimensional torus and we investigate the stability of some solitary wave profiles within the dissipative dynamics. The undamped cubic NLS equation is well known to admit a family of periodic waves given by Jacobi elliptic functions of cnoidal type. We show that the family of cnoidal waves is orbitally stable. More precisely, by considering a sufficiently small perturbation of a given cnoidal

wave at initial time, the evolution will always remain close (up to symmetries of the equation) to the cnoidal wave whose mass is modulated according to the dissipative dynamics.
Since cnoidal waves are not exact solutions to the damped NLS, the perturbation is forced away from the family of solitary wave profiles. To achieve our result and control this secular growth, we construct an approximated solitary wave profile that embodies the first order effects of the damping. The perturbation around the approximated profile is controlled by means of a Lyapunov functional, for which we derive suitable decay estimates.

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Raffaele Carlone: "A ionization model"

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In the second part, it will be analyzed the effective equation and, in particular: global well-posedness of the associated Cauchy problem under general assumptions on the potential and the initial datum and, for a monochromatic periodic potential; the asymptotic behavior of the survival probability of a bound state of the time-independent problem.

Joint work with M. Correggi, L. Tentarelli, M. Falconi, M. Olivieri, R. Figari, W. Borrelli

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Cristian Cazacu: "Uncertainty principles: sharp constants, extremal functions and stability results"

First of all, in this talk we focus on two well-known uncertainty principles applied to special classes of vector fields and we show that the sharp constants improve with respect to case of scalar fields whereas minimizers are described explicitly. These results are also extended to more general functional inequalities of Caffarelli-Kohn-Nirenberg type. Secondly, we provide optimal constants for the stability inequalities for the Heisenberg uncertainty principle and a class of Caffarelli-Kohn-Nirenberg inequalities. For the the Heisenberg uncertainty principle we introduce a new deficit function different from what is considered in the literature and then obtain the best constants. In addition, we recover the stability inequalities with optimal constants with respect to the deficit functions considered in the literature. These results are based on joint works written in collaboration with Joshua Flynn, Nguyen Lam and Guozhen Lu. C.C. was partially supported by the grant no. PN-III-P1-1.1-TE-2021-1539, CNCS - UEFISCDI, Romania.

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Lucrezia Cossetti: "A limiting absorption principle for time-harmonic isotropic Maxwell and Dirac equation"

In this talk we investigate the L^p − L^q mapping properties of the resolvent associated with the time-harmonic isotropic Maxwell and perturbed Dirac operator. As spectral parameters close to the spectrum are also covered by our analysis, we establish a L^p − L^q type limiting absorption principle for these operators. Our analysis relies on new results for Helmholtz systems with zero order non-Hermitian perturbations. The talk is based on a joint work with R. Mandel and on an ongoing project with R. Schippa.

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Loïc Le Treust: "The Dirac bag model in strong magnetic field"

We study Dirac operators on two-dimensional domains coupled to a magnetic field perpendicular to the plane. We focus on the infinite-mass boundary condition (also called MIT bag condition). In the case of bounded domains, we establish the asymptotic behavior of the low-lying (positive and negative) energies in the limit of strong magnetic field.

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Pierangelo Marcati: "Existence and Stability of almost finite energy weak solutions to the Quantum Euler Maxwell system"

We prove the existence of global in time, finite energy, weak solutions to a quantum magneto hydrodynamic system [7] (QMHD) with large data, modeling a charged quantum fluid interacting with a self generated electromagnetic field. The analysis of QMHD relies upon the use of Madelung transformations. The rigorous derivation requires nontrivial smoothing estimates, which are obtained by assuming slightly higher regularity for the electromagnetic potential. These assumptions are motivated by the nonlinear dependence of the hydrodynamic system in terms of the underlying wave function dynamics, which is supercritical with respect to the bare energy bounds. [2,3,4]
Due to quantum effects on the dispersive properties of QMHD, our approach requires neither smallness nor high regularity, unlike a large amount of existing literature for Euler Maxwell's classical system [9,8]. In fact, the difficulty posed by the presence of the nonlinear electromagnetic force field (Lorentz) severely restricts the possibility to get existence and stability results in the general framework of finite energy solutions. In the classical case the dispersion is not able to deal with the transport of a nontrivial vorticity, therefore almost GWP holds in a life span, reciprocal of the amplitude of the vorticity. GWP can be proved in the irrotational case, where in any case smallness and high regularity assumptions are needed.
For a quantum MHD system the irrotationality and the presence of a highly nonlinear quantum stress tensor induce much stronger dispersive properties, as a byproduct of a close relationship with the classical Maxwell Schrödinger system. Therefore the core argument is shifted to the analysis of the nonlinearities related to the formulation of the hydrodynamic variables through the Madelung transformations. The analysis carried out shows that it is necessary to go through nontrivial smoothing estimates and these require us to assume regularity conditions, just above the energy norms, for the initial data of the Maxwellian electromagnetic potential. In the same regime of regularity, with the help of suitable local smoothing estimates, we also prove stability of both the hydrodynamic variables and the Lorentz force associated with the electromagnetic field. These results can be found in [6]

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Luigi Barletti: ”Functional calculus in phase-space and application to electron hydrodynamics in graphene”

We present a systematic method to compute the formal semiclassical expansion of functional calculus in the framework of the phase-space representation of quantum mechanics. This is particularly useful to compute subleading corrections to the classical Maxwell-Boltzmann, Fermi-Dirac or other local equilibrium distributions. We also show how these results can be applied to derive quantum corrections to electron hydrodynamics in graphene.

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Vittorio Romano: ”Analytical and simulation aspects of charge transport in graphene”

The last years have witnessed a great interest for 2D-materials due to their promising applications. One of the most investigated is graphene which is considered as a potential new material to be exploited in nano-electronic and optoelectronic devices.
Charge transport in graphene can be described with several degrees of physical complexity [1]. At quantum level an accurate model is represented by the Wigner equation but in several cases its semiclassical limit, the Boltzmann equation, constitutes a fully acceptable model. However, the numerical difficulties encountered in the direct solution of both the Wigner and the semiclassical Boltzmann equation has prompted the development of hydrodynamical, energy transport and drift diffusion models, in view of the design of a future generation of electron devices where graphene replaces standard semiconductors like silicon and gallium arsenide. Moreover, thermal effects in low dimensional structures play a relevant role and, therefore, phonon transport must be also included.

Interesting new mathematical issues related to the peculiar features of graphene arise. The main aspects will be discussed and recent results [2-13] illustrated in the perspective of future developments, in particular the design and optimization of graphene field effect transistors.

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Hajer Bahouri: ”On the global well-posedness for the derivative nonlinear Schrödinger equation on the real line”

In this joint work with Galina Perelman, we have been interested in the question of global well-

posedness for the derivative nonlinear cubic Schrödinger equation on the real line. This equation known as (DNLS) appeared in the 80's in the study of the one-dimensional compressible magneto-hydrodynamic equation in the presence of the Hall effec and the propagation of circular polarized nonlinear Alfvèn waves in magnetized
plasmasa. The local existence issue for this equation is well understood in the scale of Sobolev spaces for about twenty years. However, the problem of global existence is more challenging: the central difficulty of the DNLS equation as compared to other integrable equations like the cubic nonlinear Schrödinger equation (NLS) is its defect of coercivity and new ideas were needed to show that the solutions are global. In this work, by combining profile decomposition techniques with the integrable structure of the equation, we were able to establish a global existence result for (DNLS) in
H^s, $s \geq 1/2$.

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Cristian Cazacu: "Uncertainty principles: sharp constants, extremal functions and stability results"

First of all, in this talk we focus on two well-known uncertainty principles applied to special classes of vector fields and we show that the sharp constants improve with respect to case of scalar fields whereas minimizers are described explicitly. These results are also extended to more general functional inequalities of Caffarelli-Kohn-Nirenberg type. Secondly, we provide optimal constants for the stability inequalities for the Heisenberg uncertainty principle and a class of Caffarelli-Kohn-Nirenberg inequalities. For the the Heisenberg uncertainty principle we introduce a new deficit function different from what is considered in the literature and then obtain the best constants. In addition, we recover the stability inequalities with optimal constants with respect to the deficit functions considered in the literature. These results are based on joint works written in collaboration with Joshua Flynn, Nguyen Lam and Guozhen Lu. C.C. was partially supported by the grant no. PN-III-P1-1.1-TE-2021-1539, CNCS - UEFISCDI, Romania.