Conference

SEMI-CLASSICAL AND GEOMETRIC ASYMPTOTICS IN MATHEMATICAL PHYSICS

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Book of Abstracts

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SEMI-CLASSICAL ASYMPTOTICS FOR OPERATORS WITH NON TRIVIAL SUB-PRINCIPAL SYMBOL AND APPLICATION TO GRAPHENE EQUATION

We study the stationary 2-D Dirac equation for graphene with an axially symmetric potential, constant magnetic field and variable mass (impurity). The mass has no axial symmetry, and it plays the role of a perturbation. We are interested in (formal) semi-classical asymptotics of its solutions or, equivalently, quasi-modes of Dirac operator. The principal symbol of the operator defines a completely integrable system with a family of invariant Liouville tori. The subprincipal symbol (and, hence, the transport equation) turns out to be non-trivial. To solve it one has to impose two conditions on a torus: 1) it has to be Diophantine, and 2) it has to satisfy Bohr-Sommerfeld quantization rule. However, these two condtions may contradict to each other. Applying ideas by Lazutkin, Dobrokhotov, Rouleux and others, we show how to evade this condtradiction, and present an efficient algorithm for constructing quasi-modes. This is a joint work with S. Yu. Dobrokhotov and S. B. Kuksin.

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ARNOLD'S SCATTERING IN GRAPHENE

Arnold's interior scattering is typical local wave propagation at singular points of the eikonal equation on the geometrical optics level. We compute the semi-classical asymptotic of a model interiorly scattered wave described by the Dirac equation with a linear potential.

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WAVE PACKET SCATTERING OF DIRAC AND SCHRÖDINGER PARTICLES ON POTENTIAL BARRIERS IN GRAPHENE NANOSTRUCTURES

In monolayer graphene, the energy spectrum is gapless in two inequivalent points of the first Brillouin zone, which are usually called K and K'. In the vicinity of these points, low energy electrons exhibit a linear energy dispersion, so that, within a continuum model, they can be described as massless Dirac particles [1]. We investigate numerically the wave packet (WP) propagation in graphene in the presence of distributed circular potential steps in form of arrays. The calculations are performed within the continuum model, and the time propagation is made by a simple computational technique, based on the split-operator method. Numerical results show that the transmission probability decreases as the step barriers height increases, but only until a critical value is reached. Our results show also that, despite of Klein tunneling effect, the presence of these potential steps significantly changes the WP transmission, reflected coefficients and WP delay time in array region, especially for higher concentration of scatters and their distribution perpendicular direction of WP propagation (of 1 to 3 array cases and narrow channel in 3arrays). Some simple models of electronic device elements based of our studies are proposed. This is a joint work with Ph. Lambin and Kh. Rakhimov (Université de Namur, Belgium).

The work was carried out with financial support from RFBR (project No 17-51-150006).

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ABSENCE OF EIGENVALUES FOR THE FREE SCHRODINGER OPERATOR ON THE HALF-SPACE WITH NON SELF-ADJOINT BOUNDARY CONDITIONS

We study the free Schrödinger operator on the half-space with (possibly) non self-adjoint Robin boundary conditions. We prove, by developing multipliers technique in the sense of Morawetz, the absence of eigenvalues for this operator under explicit conditions on the boundary potential. The presence of point spectrum is also disproved in the self-adjoint setting under remarkable physically natural conditions.

The talk is based on a joint work with L. Fanelli (Rome) and D. Krejcirik (Prague).

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NEW INTEGRAL REPRESENTATIONS FOR MASLOV CANONICAL OPERATOR AND APPLICATIONS

Maslov canonical operator [1] (a closed object is the Fourier Integral Operator) allows one to construct the asymptotic solutions of evolution and stationary problems for a wide class of linear differential and pseudodifferential equations. The definition of Maslov canonical operator is connected with Lagrangian manifolds in the phase space and in particular, the canonical operator gives the description of the asymptotic solutions in the neighborhood of caustic and focal point (Lagrangian singularities). Near these objects Maslov's formulas have integral form and are based on partial Fourier transforms. The practical realization of such formulas is quite complicated and includes two steps: 1) expression the coordinates on the appropriate Lagrangian manifold via certain momenta in the phase space (which is not trivial as usual) and 2) the integration in these variables. We suggest [2] a construction based only on the integration in the coordinates on the Lagrangian manifold. Along with a theorem of Hörmander concerning fast-oscillating integrals, this allows to simplify crucially the process of calculation of asymptotic solutions in the neighborhood of caustic and focal point. This also shows the relationship of the canonical operator with many special function and allows to extend the range of applications of the canonical operator. As example we consider the problems about Airy-Bessel beams in optics [3] and the behavior of the edge front wave in the linear water wave theory [4] . This work was done together with V.E.Nazaikinskii and A.I.Shafarevich and was supported by Russian Scientific Fund (Project No 16-11-10282)

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ON MINIMAL SOLUTIONS OF DIFFERENCE EQUATIONS WITH PERIODIC COEFFICIENTS

This talk is a review of results on entire and meromorphic solutions to difference equations in the complex plane. The space of solutions being infinite dimensional, it is natural to look for the solutions that grow most slowly with the distance from the real axis. We explain why such solutions simultaneously satisfy to two different difference equations, describe a series of cases when these two equations differ only by the values of the constant parameters and discuss quasi-classical asymptotics of the minimal solutions.

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EXCITED RESONANCE WIDTH FOR HELMHOLTZ RESONATORS WITH STRAIGHT NECK

We present joint works with Thomas Duyckaerts and André Martinez. We consider resonances associated with eigenvalues of the cavity of a general Helmholtz resonator with straight neck. Under the assumption that the neck stays away from the nodal set of the corresponding eigenstate in the case of excited eigenvalues, we obtain the optimal exponential lower bound on the width of the resonance.

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LONG RANGE VAN DER WAALS-LONDON INTERACTION
IN PSEUDO-RELATIVISTIC MOLECULES

We investigate a system of two neutral atoms with nuclei at fixed positions and electrons with pseudo-relativistic kinetic energy, interacting via Coulomb potential. The interaction energy between the atoms is defined as the ground state energy E_D, minus the ground state energy μ of these two atomes at infinite distance. We prove that the interaction energy $E_D - \mu$ is dominated by two negative terms, one term of order D^{-6} and a term of order D^{-8} with an error of order $\mathcal{O}(D^{-10})$. In addition we show that no odd negative powers appear in the interaction energy for a diatomic molecule.

To prove this main result, we derive estimates of the difference $E_D - \mu$ from above and below. For the estimate from below, we apply a partition of unity of the configuration space and minimize the energy functionals in the corresponding regions. For the estimate from above we construct a trial function with bounded support. These bounds coincide up to $\mathcal{O}(D^{-10})$.

The multipole expansion of the inter-atomic Coulomb potential gives us insight into the nature of the interaction energy. In particular, we can derive a natural choice for the trial function.

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SPECTRAL ASYMPTOTICS OF ROBIN LAPLACIANS ON POLYGONAL DOMAINS

Let $\Omega \subset \mathbf{R}^2$ be a curvilinear polygon and Q_Ω^γ be the Laplacian in $L^2(\Omega)$, $Q_\Omega^\gamma \psi = -\Delta\psi$, with the Robin boundary condition $\partial_\nu \psi = \gamma\psi$, where ∂_ν is the outer normal derivative and $\gamma > 0$. We are interested in the behavior of the eigenvalues of Q_Ω^γ as γ becomes large. We prove that there exists $N_\Omega \in \mathbf{N}$ such that the asymptotics of the N_Ω first eigenvalues of Q_Ω^γ is determined at the leading order by those of model operators associated with the vertices: the Robin Laplacians acting on the tangent sectors associated with $\partial\Omega$. In the particular case of a polygon with straight edges the N_Ω first eigenpairs are exponentially close to those of the model operators. Finally, we prove a Weyl asymptotics for the eigenvalue counting function of Q_Ω^γ for a threshold depending on γ, and show that the leading term is the same as for smooth domains.

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RESONANCES FOR LARGE RANDOM SAMPLES

The talk will be devoted to the description of the resonances generated by a large sample of random material. In one dimension, one obtains a very precise description for the resonances that directly related to the description fo the eigenvalues and localization centers for the full random model. In higher dimension, below a region of localization in the spectrum for the full random model, one computes the asymptotic density of resonances in some exponentially small strip below the real axis. This talk is partially based joint work with M. Vogel.

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WAVE PACKET DYNAMICS AND ELECTRONIC PROPERTIES
OF NOVEL PERFORATED BILAYERED GRAPHENE

Here we present the comprehensive study of electronic and transport properties of novel structures based on bilayered graphene and graphene nanoribbons. By means of wave packet dynamical calculations together with DFT methods dependence of the electronic and transport properties on the geometry configuration of the pores in bilayered graphene nanoribbons were performed, such as pore size and distance between the pores. Also transport characteristics of bilayered graphene nanoribbons with pores were studied in details. In such structure pores plays the major role in the connection between the layers of the ribbons. Propagation of the electron wave packet from the top to bottom layers of considered nanostructures were analyzed in details. Dependence of spectral function on the electrode applying configurations was obtained. The work was carried out with financial support from the Ministry of Education and Science of the Russian Federation in the framework of Increase Competitiveness Program of NUST MISiS (No 2-2017-001). D.G.K. and L.A.C. also acknowledge to financial support of RFBR No 17-51-150006.

This is a joined work with G.Mark (Pirogov Russian National Research Medical University, Moscow), P. Vancso (Institute of Technical Physics and Materials Science, Budapest), and L. A. Chernozatonskii (Emanuel Institute of Biochemical Physics, Moscow).

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SEMI-CLASSICAL ASYMPTOTICS AND THE DENSITY OF STATES
IN GRAPHENE UNDER STM TIP

Our study [1] is related to the question: how much the tip of a scanning tunneling microscope (STM) affects the measured values. We study the influence of the potential induced by the microscope tip on the electronic states in a two-dimensional crystal. We consider the two-dimensional stationary Schrödinger and Dirac equations with a radial symmetric potential that simulates the STM tip. We construct semiclassical asymptotic forms for generalized eigenfunctions and study the local density of states that corresponds to the microscope measurements. We show that in the case of the Dirac equation, the tip distorts the measured density of states for all energies. This is a joint work with J. Brüning, S. Yu. Dobrokhotov and M. I. Katsnelson.

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ASYMPTOTICS IN PROBLEMS WITH LOCALIZED FUNCTIONS ON THE RIGHT-HAND SIDE AND IN THE BOUNDARY DATA

We consider problems of the following two types for a Helmholtz type equation: (i) the right-hand side is a function localized near some point of the domain: (ii) the equation is equipped with inhomogeneous boundary conditions, the boundary data being given by a function localized near some point of the boundary. The characteristic size of these sources is assumed to be of the order of the wave length. The high-frequency asymptotics of the solutions of these problems is constructed in terms of Maslov's canonical operator on pairs of Lagrangian manifolds under the assumption that there are no grazing rays involved.

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GRAPH SPECTRAL CHARACTERIZATION OF THE XY MODEL ON COMPLEX NETWORKS

There is recent evidence that the XY spin model on complex networks can display three different macroscopic states in response to the topology of the network underpinning the interactions of the spins. In this seminar, I shall introduce a different way to characterise the macroscopic states of the XY spin model based on the spectral decomposition of time series using topological information about the underlying networks. In this work [1], we use three different classes of networks to generate time series of the spins for the three possible macroscopic states. We then apply the temporal Graph Signal Transform technique to decompose the time series of the spins on the eigenbasis of the Laplacian. From this decomposition, we produce spatial power spectra, which summarise the activation of structural modes by the non-linear dynamics, and thus coherent patterns of activity of the spins. Remarkably, these signatures of the macroscopic states are independent of the underlying networks and can thus be used as universal signatures for the macroscopic states.

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QUANTUM THEORY IN REAL OR QUATERNIONIC HILBERT SPACE :
HOW THE COMPLEX HILBERT SPACE STRUCTURE EMERGES
FROM POINCARÉ SYMMETRY

In principle, the lattice of elementary propositions of a generic quantum system admits a representation in real, complex or quaternionic Hilbert spaces as established by Soler's theorem (1995) closing a long standing problem that can be traced back to von Neumann's mathematical formulation of Quantum Mechanics. However up to now there are no examples of quantum systems described in Hilbert spaces whose scalar field is different from the set of complex numbers. We show that elementary relativistic systems cannot be described by irreducible strongly-continuous unitary representations of SL(2;**C**) on real or quaternionic Hilbert spaces as a consequence of some peculiarity of the generators related with the theory of polar decomposition of operators. Indeed such a "naive" attempt leads necessarily to an equivalent formulation on a complex Hilbert space. Although this conclusion seems to give a definitive answer to the real/quaternionic-Quantum-Mechanics issue, it lacks consistency since it does not derive from more general physical hypotheses as the complex one does. Trying a more solid approach, in both situations we end up with three possibilities: an equivalent description in terms of a Wigner unitary representation in a real, complex or quaternionic Hilbert space. At this point the "naive" result turns out to be a definitely important technical lemma, for it forbids the two extreme possibilities. In conclusion, the real/quaternionic theory is actually complex. This improved approach is based upon the concept of von Neumann algebra of observables. Unfortunately, while there exists a thorough literature about these algebras on real and complex Hilbert spaces, an analysis on the notion of von Neumann algebra over a quaternionic Hilbert space is completely absent to our knowledge. There are several issues in trying to define such a mathematical object, first of all the inability to construct linear combination of operators with quaternionic coefficients. Restricting ourselves to unital real *-algebras of operators we are able to prove the von Neumann Double Commutant Theorem also on quaternionic Hilbert spaces. This is a joint work with Valter Moretti.

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[2] V.Moretti, M.Oppio. "Quantum theory in quaternionic Hilbert space: How Poincaré symmetry reduces the theory to the standard complex one", submitted to Rev. Math. Phys.]

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DIRICHLET SPECTRUM OF CONICAL LAYERS

In this talk I will discuss some spectral properties of Hamiltonians related to a quantum particle constrained to live in a neighborhood of a surface with hard-wall boundary conditions. Such systems are well studied and I will focus on the specific case of conical surfaces. These geometries proved to have an interesting behavior: when the cone is smooth (except in its vertex), the essential spectrum is a half-line and there is an infinite number of bound states accumulating to the threshold of the essential spectrum.

In a first time, I will review recent results quantifying this accumulation then, in a second time, I will detail how the smoothness of the cone impacts the number of eigenvalues.

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HEAT FLUCTUATIONS IN THE TWO-TIME MEASUREMENT FRAMEWORK AND ULTRAVIOLET REGULARITY

Since Kurchan's seminal work (2000), two-time measurement statistics (also known as full counting statistics) has been shown to have an important theoretical role in the context of Quantum Statistical Mechanics, as they allow for an extension of the celebrated fluctuation relation to the quantum setting.

After defining these statistics and recalling their connection to the quantum fluctuation relation, I will present some result about heat fluctuations. We show that heat fluctuation description differs considerably form it classical counterpart, in particular a crucial role is played by ultraviolet regularity conditions .

For bounded perturbations, we give sufficient ultraviolet regularity conditions on the perturbation for the moments of the heat variation to be uniformly bounded in time, and for Fourier transform of the heat variation distribution to be analytic and uniformly bounded in time in a complex neighborhood of 0.

On a set of canonical examples, with bounded and unbounded perturbations, we show that our ultraviolet conditions are essentially necessary. If the form factor of the perturbation does not meet our assumptions, the heat variation distribution exhibits heavy tails. The tails can be as heavy as preventing the existence of a fourth moment of the heat variation. This is a joint work with T.Benoist, and R. Raquépas.

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DIRAC OPERATORS WITH LORENTZ SCALAR SHELL INTERACTIONS

We discuss the spectral properties of 3D Dirac operators with interactions of a special type supported by a compact smooth surface. Some qualitative results on the (non-)existence of eigenvalues are obtained. In addition, we study the behavior of the eigenvalues in the large mass limit, in this case the asymptotics is governed by an effective Schroedinger-type operator on the surface with curvature-dependent potentials. Based on a joint work with Markus Holzmann (Graz) and Thomas Ourmières-Bonafos (Orsay), to be published in Reviews in Mathematical Physics.

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WHISPERING GALLERY WAVES IN SHALLOW-WATER GEO-ACOUSTIC WAVE-GUIDES

The horizontal refraction phenomena in a shallow-water waveguide with the bottom relief featuring curved isobaths is studied. This situation can be met in areas of a coastal slope that are characterized by curvilinear coastal line, e.g. lagoons and bays, as well as in lakes. Typical curvature radius of isobaths can be estimated for the bathymetric data, and usually amounts to few kilometers. It is shown that for amplitudes of normal modes, describing distribution of acoustic pressure in horizontal plane, under certain conditions whispering gallery waves can exist. The energy of these waves is concentrated in the neighborhood of horizontal rays propagating along the isobath. A relation between the waveguide parameters ensuring the whispering gallery formation is derived. A WKB theory of radial whispering gallery modes is developed, and azimuthal wavenumbers are computed from the WKB quantization condition. The possibility of excitation and observation of the whispering gallery waves in realistic shallow-water waveguides is discussed, and the respective simulation results are presented. This is a joint work with Boris Katsnelson, University of Haifa, Israël.

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CAUSTICS IN GRPAHENE :
CONSTRUCTION OF A UNIFORM SEMI-CLASSICAL APPROXIMATION
AND COMPARISON WITH TIGHT-BINDING RESULTS

We study above-barrier scattering of Dirac electrons by a smooth electrostatic potential combined with a coordinate-dependent mass in graphene. We assume that the potential and mass are sufficiently smooth, so that we can define a small dimensionless semiclassical parameter h. This setup naturally leads to focusing and the formation of a so-called cusp caustic. We construct an asymptotic solution for the wavefunction near this caustic in the form of the Maslov canonical operator. This construction is greatly simplified by introducing so-called eikonal coordinates on the Lagrangian manifold and by using a recently proposed new representation [1]. The matrix character of the Dirac equation gives rise to a nontrivial semiclassical phase in the wavefunction, which makes this problem different from a scalar wave equation. Because of this semiclassical phase, the leading-order approximation is no longer sufficient to describe the wavefunction near the cusp, and one has to use the uniform approximation [2]. In this talk, I will place particular emphasis on the numerical implementation of this uniform approximation and compare it with tight-binding calculations of real graphene samples. We show that the semiclassical phase can have a significant effect on the position of the intensity maximum. The observed effects are opposite for graphene's two valleys and can be very well captured within the uniform approximation. Additional information about the system can be obtained by incorporating the semiclassical phase into the equations of motion. This is a joined work with D. Minenkov, M.I. Katsnelson, and S.Dobrokhotov.

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[2] J. N. L. Connor and D. Farrelly, J. Chem. Phys. 75, 2831 (1981)

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MONODROMY MATRICES FOR HARPER EQUATION

Let us consider the difference equations of the form

$$\Psi(z+h) = M(z)\Psi(z), \quad z \in \mathbf{C} \tag{1}$$

where $M : \mathbf{C} \to \mathrm{SL}(2, \mathbf{C})$ is a given matrix-valued 1-periodic function, and $h > 0$ is a small constant parameter.

One can show that the space of solutions to (1) is a two-dimensional module over the ring of h-periodic functions, i.e., given two linearly independent solutions of this equation, any other solution equals their linear combination with h-periodic coefficients.

Since M is 1-periodic, the space of solutions of (1) is invariant with respect to the shift $z \mapsto z+1$. Being restricted to the space of solutions of (1) the corresponding shift operator can be represented by 2×2 matrices that are h-periodic in z. These matrices are called monodromy matrices, see the review [Fe] and references to it. In the quasiclassical limit $h \to 0$, we describe monodromy matrices for an important class of equations arising when studying a well known model (Harper equation) from the solid state physics.

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HOMOGENEIZATION OF THE STATIONARY MAXWELL SYSTEM WITH PERIODIC COEFFICIENTS

We study homogenization of a stationary Maxwell system with periodic coefficients in $\mathbf{R}^3$ and in a bounded domain $\mathcal{O} \subset \mathbf{R}^3$. Assume that the dielectric permittivity and the magnetic permeability are given by $\eta(\frac{x}{\varepsilon})$ and $\mu(\frac{x}{\varepsilon})$, $\varepsilon > 0$. Here η and μ are positive definite and bounded 3×3-matrix-valued functions, periodic with respect to some lattice. The classical results show that, as $\varepsilon \to 0$, the solutions of the Maxwell system with such coefficients converge weakly in L^2 to the solution of the homogenized Maxwell system with the effective coefficients η^0 and μ^0. We improve the classical results and find approximations for the solutions in the L^2-norm. The approximations involve not only the solution of the homogenized Maxwell system, but also some correctors of zero order. For the problem in $\mathbf{R}^3$, the error of approximation is $\mathcal{O}(\varepsilon)$, while for the problem in a bounded domain the error is $\mathcal{O}(\sqrt{\varepsilon})$. This is explained by the boundary influence.

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INTERMEDIATE EIGENVALUE STATISTICS

A key question in the field of quantum chaos concerns the link between the statistics of the spacings of eigenvalues of a Schrödinger operator and the underlying classical dynamics. Berry and Tabor predicted in 1977 that a generic integrable system should satisfy Poissonian spacing statistics in the semiclassical limit (provided the mean spacing is normalized suitably). On the contrary, Bohigas, Giannoni and Schmit conjectured in 1984 that generic chaotic systems should have spacing statistics which coincide with the predictions of random matrix theory. I will review which progress has been made at the rigorous mathematical level and I will then address the case of certain "pseudo-integrable" billiards whose statistics is intermediate beween Poissonian and RMT.