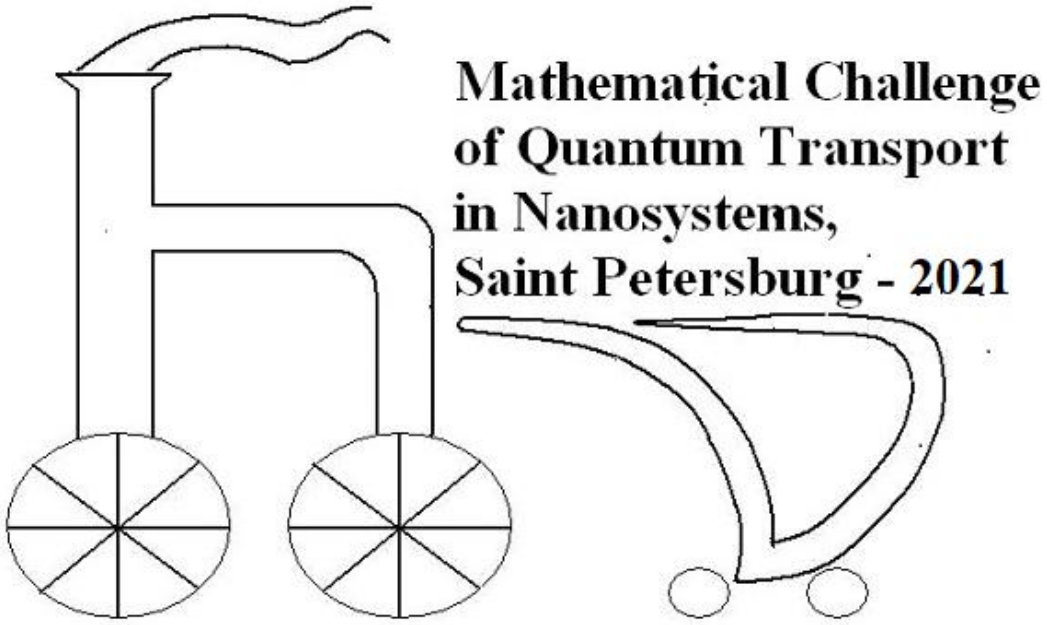
National Research University ITMO

MATHEMATICAL CHALLENGE OF QUANTUM TRANSPORT IN NANOSYSTEMS - PIERRE DUCLOS WORKSHOP International Conference

Saint Petersburg, September 20 – 22, 2021

Book of Abstracts



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Organized by the Saint Petersburg National Research University ITMO.

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Conference site: http://mathdep.ifmo.ru/mcqtn2021/

THE MAIN TOPICS OF THE CONFERENCE:

- Spectral theory
- Scattering
- Quantum transport
- Quantum communications and computations
- Topological structures

INVITED SPEAKERS

- **Pavel Exner (Rez, Czech Republic)**
- **Horia Cornean (Aalborg, Denmark)**
- **Pavel Kurasov (Stockholm, Sweden)**
- **Alexander Kiselev (Durham, USA)**
- **Valentin Zagrebnov (Marseille, France)**
- **Philippe Briet (Toulon, France)**
- **Claudio Cacciapuoti (Como, Italy)**
- **Giuseppe Cardone (Benevento, Italy)**
- **Alexander Motovilov (Dubna, Russia)**
- **Delio Mugnolo (Hagen, Germany)**
- **Ashok Chatterjee (Hyderabad, India)**
- **Davron Matrasulov (Tashkent, Uzbekistan)**
- **Mark Malamud (Moscow, Russia)**
- **Vladimir Lotoreichik (Prague, Czech Republic)**
- **Denis Borisov (Ufa, Russia)**
- **Victor Mikhaylov (St. Petersburg, Russia)**
- **Mikhail Belonenko (Volgograd, Russia)**
- **Sergey Levin (St. Petersburg, Russia)**
- **Vadim Malyshev (Moscow, Russia)**
- **A.Khrabustovskyi (Hradec Kralove, Czech Republic)**
- **Alexei Kiselev (St. Petersburg, Russia)**

Conference Program

Monday, 20.09.2021 (Moscow time)

09-55-10-00	Opening	
10-00 – 10-40	P.Exner	Quantum graphs with vertices of a preferred orientation
10-45 –11-25	D.Mugnolo	Torsional rigidity and spectral gap of quantum graphs
11-30 –12-10	H.Cornean	A new paradigm for bulk-edge correspondence
12-15 –12-55	P.Kurasov	On isospectral metric graphs
13-00 –13-40	A.Khrabustovskyi	Singular Schrödinger operators with prescribed spectral properties
15-00 –15-40	D.Borisov	Operators on quantum graphs with small edges
15-45 –16-25	V. Mikhaylov	On the method of the recovery of spectral data from dynamic one and related problems in inverse problems theory and signal processing
16-30 – 17-10	D.Matrasulov	Non-Hermittian quantum graphs: Quasiparticle transport, absorbing and scattering at the nodes

Tuesday, 21.09.2021 (Moscow time)

10-00 – 10-40	M. Malamud	Scattering matrices for singular perturbations and elliptic BV problems
10-45 –11-25	V. Lotoreichik	Isoperimetric inequality for the two-dimensional magnetic Robin Laplacian
11-30 –12-10	Alexei Kiselev	Lindblad dynamics of mixed polarization states
12-15 –12-55	Ph. Briet	A model of Sheared Nanoribbons
14-00 –14-40	A.Motovilov	Quantum speed limits for the time evolution of a subspace
14-45–15-25	S.Levin	On coordinate asymptotics of the Schroedinger operator absolutely continuous spectrum eigenfunctions of the *n* three-dimensional charged quantum particles system
15-30 – 16-10	V.Malyshev	Coulomb law as information transmission by virtual particles
16-15- 16-55	M.Belonenko	Two-dimensional non-topological solutions of Maxwell's equations in the environment of strained carbon nanotubes with impurities
17-00-17-40	Alexander Kiselev	The Flow of Polynomial Roots Under Differentiation
18-00-18-10	A.Belolipetskaya	Non-Weyl asymptotic for Dirac operator on quantum graph with general coupling conditions
18-20-18-30	P.Gilev	Simulation of the quantum imaging with the Shor code
18-40 – 18-50	A.Vorobiev	Asymptotics of resonances for waveguides separated by semitransparent barrier with small window
18-50 – 19-00	T.Yurova	A model of acoustic scattering by a cell with nanoparticles inserted

Wednesday, 22.09.2020 (Moscow time)

10-00 –10-40	C. Cacciapuoti	Three-body Hamiltonians with zero range interactions
10-45 –11-25	G. Cardone	Planar Waveguide with “Twisted” Boundary Conditions and Small Width
11-30 –12-10	I.Lobanov	To be announced
12-15 –12-55	A.Chatterjee	To be announced
13-00 –13-40	V.Zagrebnov	To be announced

Abstracts

Non-Weyl asymptotic for Dirac operator on quantum graph with general coupling conditions

Anna Belolipetskaia

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In the past few decades, quantum graphs have been the subject of active research. In this work, we study the Weyl asymptotics of the resonance states of the Dirac operator on a quantum graph with general coupling conditions. If instead of the Dirac operator we consider the Schrödinger operator, then many results have been obtained on the topic of the Weyl asymptotics of resonance states on quantum graphs. For example, it was shown that in the problem for the Schrödinger operator with general coupling conditions, the so-called effective matrix affects the form of the asymptotics. An effective matrix was first described by P. Exner and J. Lipovsky. Later E.B.Davies, P.Exner and J.Lipovsky investigated the eigenvalues of the effective matrix and obtained a criterion for the non-weyl asymptotics of resonance states of the Schrödinger operator on quantum graphs with general coupling conditions. In this work, a similar study will be carried out for the Dirac operator. In particular, an effective matrix for the Dirac operator will be constructed, and the asymptotics of the resonance states of the Dirac operator on a quantum graph with general coupling conditions will be investigated through the study of the effective matrix.

Two-dimensional non-topological solutions of Maxwell's equations in the environment of strained carbon nanotubes with impurities

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For a system of impurity carbon nanotubes, the exact expression is obtained for nonlinearity depending on two gauge fields. One of fields is interpreted as a mechanical stress field. Second of fields is interpreted as electromagnetic field. Based on the obtained nonlinearity, the solutions of Maxwell's equations are analyzed. It is shown that there are two-dimensional non-topological stable solutions that can be interpreted as light bullets.

Operators on quantum graphs with small edges

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We consider a general second order self-adjoint elliptic operator on an arbitrary metric graph with finitely many edges. These small edges are obtained via rescaling by a small positive parameter. The coefficients in the differential expression are varying, and they, as well as the matrices in the boundary conditions, can also depend on the small parameter and we assume that this dependence is analytic. Under a natural non-resonance condition we prove that the resolvent of the considered operator is analytic in the small parameter and it can be expressed by a Taylor-like series. We establish the convergence of the spectrum of the perturbed operator to that of the limiting operator. The convergence of the spectral projectors is proved as well. We show that the eigenvalues of the perturbed operator converging to limiting discrete eigenvalues are analytic in the small parameter and the same is true for the associated perturbed eigenfunctions.

A model of Sheared Nanoribbons

Ph. Briet

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In this talk I will present a joint work with David Krejcirik and Hamza Abdou Soimadou (PHD student). It concerns the study of a new model of 2-dimensional waveguide, I will describe various results we obtain about the spectral analysis of the corresponding self-adjoint operator.

Three-body Hamiltonians with zero range interactions

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We consider the problem of defining quantum Hamiltonians for a system of N-particles with zero range interactions, also known as point interactions. Such Hamiltonians ara characterized by the fact that the only physical parameter defining the interaction is the two body scattering length. In dimension three the mathematical construction of these Hamiltonians for N larger than three is not trivial. A natural construction, based on the analogy with the two-particle case, leads to the so called Ter-Martirosyan Skornyakov (TMS) Hamiltonian and the fall to the center phenomenon known as Thomas effect. Following a suggestion given by Minlos and Faddeev in a seminal paper published in 1962, reprised by Albeverio, Høegh-Krohn and Wu in 1981, we construct a regularized version of the TMS Hamiltonian which is self-adjoint and bounded from below. Furthermore, we show that the Hamiltonian is the norm resolvent limit of Hamiltonians with rescaled non local interactions, also called separable potentials, with a suitably renormalized coupling constant.

The talk is based on a joint work with Giulia Basti, Domenico Finco, and Alessandro Teta.

Ref.: https://arxiv.org/abs/2107.07188

Planar Waveguide with “Twisted” Boundary Conditions and Small Width

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We consider a planar waveguide with "twisted" boundary conditions. By twisting we mean a special combination of Dirichlet and Neumann boundary conditions. Assuming that the width of the waveguide goes to zero, we identify the effective (limiting) operator as the width of the waveguide tends to zero, establish the uniform resolvent convergence in various possible operator norms, and give the estimates for the rates of convergence. We show that studying the resolvent convergence can be treated as a certain threshold effect and we present an elegant technique which justifies such point of view.

A new paradigm for bulk-edge correspondence

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We consider 2d random ergodic Schrödinger operators with long range magnetic fields on domains with and without boundary. By extending the gauge covariant magnetic perturbation theory to infinite domains with boundary, we prove that the celebrated bulk-edge correspondence is just a particular case of a much more general paradigm, which also includes the theory of diamagnetic currents and of Landau diamagnetism.
More precisely, we obtain a formula which states that the derivative of a large class of bulk partition functions with respect to the external constant magnetic field is equal to the expectation of a corresponding edge distribution function of the velocity component which is parallel to the edge. Neither spectral gaps, nor mobility gaps, nor topological arguments are required. The equality between the bulk and edge indices, as stated by the conventional bulk-boundary correspondence, is obtained as a corollary of our purely analytical arguments by imposing a gap condition and by taking a "zero temperature" limit. This is joint work with M. Moscolari and S. Teufel.

Quantum graphs with vertices of a preferred orientation

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We discuss quantum graphs with the vertex coupling violating the time-reversal invariance. As a case study we analyze a simple example in which the asymmetry is maximal at a fixed energy. This leads to an interesting topological property, namely that high-energy scattering depends crucially on the vertex parity; we will demonstrate implications of this fact for spectral and transport properties in several classes of graphs, both finite and infinite periodic ones. We will show other time-asymmetric graphs and identify a class of such couplings which exhibits a nontrivial PT-symmetry despite being self-adjoint. The results come from a common work with Marzieh Baradaran, Ji\v{r}\'{\i} Lipovsk\'{y}, and Milo\v{s} Tater

Simulation of the quantum imaging with the Shor code

Pavel Gilev

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This research shows behaviour of a scheme which based on quantum imaging. The main difference with the pure quantum imaging scheme is addition of the Shor code for main (transported) qubit. This act leads to more distributed load and error rate on qubits but significantly increases the number of qubits in the scheme.

Singular Schrödinger operators with prescribed spectral properties

Andrii Khrabustovskyi

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In this talk we illustrate how one can construct Schrödinger operators on a bounded interval with predefined essential and discrete spectra. The required structure of the spectrum is realized by a special choice of a sequence of point interactions of δ or δ' types.

This is a joint work with Jussi Behrndt (TU Graz).

The Flow of Polynomial Roots Under Differentiation

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The question about the behavior of gaps between zeros of polynomials under differentiation is classical and goes back to Marcel Riesz. In this paper, we analyze a nonlocal nonlinear partial differential equation formally derived by Stefan Steinerberger to model dynamics of roots of polynomials under differentiation. Interestingly, the same equation has also been recently obtained formally by Dimitri Shlyakhtenko and Terence Tao as the evolution equation for free fractional convolution of a measure [51] - an object in free probability that is also related to minor processes for random matrices. The partial differential equation bears striking resemblance to hydrodynamic models used to describe the collective behavior of agents (such as birds, fish or robots) in mathematical biology. We consider periodic setting and show global regularity and exponential in time convergence to uniform density for solutions corresponding to strictly positive smooth initial data. In the second part of the paper we connect rigorously solutions of the Steinerberger's PDE and evolution of roots under differentiation for a class of trigonometric polynomials. Namely, we prove that the distribution of the zeros of the derivatives of a polynomial and the corresponding solutions of the PDE remain close for all times. The global in time control follows from the analysis of the propagation of errors equation, which turns out to be a nonlinear fractional heat equation with the main term similar to the modulated discretized fractional Laplacian $(-\Delta)^{1/2}$.

Lindblad dynamics of mixed polarization states

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We study quantum dynamics of mixed polarization states using exact solutions of the Lindblad master equation for multi-mode bosonic systems. It is shown that the dynamical regimes of depolarization and dynamics of the normalized Stokes parameters are governed by intermode couplings that determine anisotropy of the Lindblad relaxation superoperator. Both the dynamical and environment induced couplings are found to affect the regimes of disentanglement and dynamics of the mutual information.

On isospectral metric graphs

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We present a new family of isospectral metric graphs. The isospectrality of these graphs is explained studying Steklov subspaces associated with their subgraphs.

On coordinate asymptotics of the Schroedinger operator absolutely continuous spectrum eigenfunctions of the *n* three-dimensional charged quantum particles system

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We suggest an ansatz which describes a leading term of coordinate asymptotics at infinity in configuration space of the *n* three-dimensional charged quantum particles Schroedinger operator absolutely continuous spectrum eigenfunctions. The description of the result coincides with the previously known constructions in the asymptotic configurations studied earlier (for example, for like-charged particles). The Schroedinger equation discrepancy for the suggested ansatz decreases faster than the potential uniformly in all angular variables at infinity in configuration space.

Isoperimetric inequality for the two-dimensional magnetic Robin Laplacian

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In this talk, we consider the two-dimensional magnetic Robin Laplacian with a negative boundary parameter on a bounded and sufficiently smooth domain. The respective magnetic field is chosen to be homogeneous. Among a certain class of domains, we prove that the disk maximizes the ground state energy under the fixed perimeter constraint provided that the magnetic field is of moderate strength. This class of domains includes, in particular, all domains that are contained upon translations in the disk of the same perimeter and all centrally symmetric domains. Our result generalizes the isoperimetric inequality for the Robin Laplacian without magnetic field due to Antunes, Freitas, and Krejcirik.

This talk is based on a joint work with Ayman Kachmar.

Scattering matrices for singular perturbations and elliptic BV problems

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Let A be a symmetric operator in a Hilbert space H with infinite deficiency indices $n_{\pm}(A)=\infty$. We investigate the scattering matrix of two extensions A_0 and A_1 assuming that they are resolvent comparable, i.e. their resolvent difference is of trace class. The scattering matrix is expressed by means of the limit values of the abstract Weyl function. The latter is defined in the framework of double B-generalized boundary triples demonstrating an interesting feature of our approach.

The abstract result is applied to different realizations of Schrodinger differential expressions in exterior domains in R^2. In particular, if A_D and A_N are the Dirichlet and Neumann realizations, then the scattering matrix of the scattering system $\{A_D, A_N\}$ is expressed by means of the limit values of the Dirichlet-to-Neumann map. The latter is the classical object naturally appeared in the theory of boundary value problems of the second order elliptic operators.

The talk is based on joint results with J. Behrndt and H. Neidhardt published in [1] and some new results.

[1] \ J. Behrndt, M.M.Malamud, H.Neidhardt, Scattering matrices and Dirichlet-to-Neumann maps, Journal of Functional Analysis, V. 273 (2017), p. 1970 -- 2025..

Coulomb law as information transmission by virtual particles

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In classical physics, fields move point particles via Newtonian mechanics with Lorentz forces, and particles create fields via Maxwell equations. Both pictures have quite rigorous mathematical theories. However, consistency of united system of these equations had never been proved. In quantum physics QFT seems to cover everything but rigorous QFT does not still exist. Moreover instead, often scattering pictures with virtual particles are used. In this talk classical picture with information transmission (by virtual particle) between two particles will be presented in detail. Unexpectedly, it gives rigorous deduction (without Maxwell equations) of 3-dimensional Coulomb force between two particles in question.

Also two rigorous many particle models will be presented:

1. model of electric current, that appears by self-organization in many electron system, interacting via Coulomb force,
2. one-dimensional many particle model of ball lightning.

Non-Hermittian quantum graphs: Quasiparticle transport, absorbing and scattering at the nodes

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Quantum graphs attracted much attention as effective and powerful tool for modeling of quantum transport in low-dimensional branched structures and networks. Particle motion in quantum graphs can be described in terms of Schrodinger or Dirac equations on metric graphs. These latter are the branched wires connected to each other according to some rule, which is called topology of a graph. An important feature of quantum graphs comes from the fact that one can achieve tuning of the quantum transport by choosing proper topology of a graph or controlling transmission through the nodes. In an approach, where such processes are described in terms of quantum mechanical wave functions on graphs, all these can be done by imposing proper boundary conditions at the vertices (nodes). Apparently, such boundary conditions should keep self-adjointness of the problem, i.e. quantum graph should be Hermitian. General form of vertex boundary conditions, providing self-adjointness of the problem was derived in early stage of the quantum graph theory. In this work we extend well developed theory of quantum graphs to the case of non-Hermittian, more precisely, PT-symmetric quantum graphs. This is done by introducing so-called (skew) PT-symmetric inner product at the nodes, leading to PT-symmetric vertex boundary conditions. Relation of such PT-symmetric vertex conditions with absorbing ones is revealed. Scattering, reflectionless transmission and absorption of quasiparticles in Hermitian and PT-symmetric quantum graphs is studied in detail.

On the method of the recovery of spectral data from dynamic one and related problems in inverse problems theory and signal processing

Victor Mikhailov, Alexander Mikhailov

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We consider several different problems: the spectral estimation problem in signal processing theory, classical moment problems in mathematical analysis and the inverse problem for the Schr\"odinger Equation with Non-self-adjoint Matrix Potential (we will mainly focus our attention on the last one). The common point is the method the aforementioned problems can be solved by: it is the application of the Boundary control method and recovery spectral data from the dynamical one.

Quantum speed limits for the time evolution of a subspace

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By a quantum speed limit one usually understands an estimate on how fast a quantum system can evolve between two distinguishable states. The most known quantum speed limit exist in the form of the celebrated Mandelstam-Tamm inequality that bounds the speed of the evolution of a state in terms of its energy dispersion. In contrast to the basic Mandelstam-Tamm inequality, we are concerned not with a single state but with a (possibly infinite-dimensional) subspace which is subject to the Schroedinger evolution. By using the concept of maximal angle between subspaces we derive optimal bounds on the speed of such a subspace evolution. These bounds may be viewed as further generalizations of the Mandelstam-Tamm inequality. In the latest study, we extend some of our initial results [1] to the case of unbounded Hamiltonians.

This is a joint work with Sergio Albeverio.

[1] S. Albeverio and A.K. Motovilov, Quantum speed limits for time evolution of a system subspace, arXiv:2011.02778 (2020) [8 pages].

Torsional rigidity and spectral gap of quantum graphs

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We develop the theory of torsional rigidity - a quantity routinely considered for Dirichlet Laplacians on bounded planar domains - for Laplacians on metric graphs. Using a variational characterization that goes back to Pólya, we develop surgical principles that, in turn, allow for isoperimetric-type inequalities comparing the torsional rigidity of general metric graphs with that of intervals of the same total length. We also derive sharp bounds on the spectral gap of a quantum graph in terms of its torsional rigidity: this is particularly attractive since computing the torsional rigidity reduces to inverting a finite matrix.

Asymptotics of resonances for waveguides separated by semitransparent barrier with small window

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Two-dimensional quantum waveguides with common semitransparent wall are considered. It is assumed that there is a small window in the separating wall. It leads to appearance of a resonance below the second threshold of the continuous spectrum. Semitransparent wall is considered as a potential supported by a hypersurface. We use method of asymptotic expansions of boundary problems solutions. It allows us to obtain the main terms of the asymptotic expansion explicitly.

A model of acoustic scattering by a cell with nanoparticles inserted

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A solvable model for scattering of ultrasound waves by a cell with inserted nanoparticles is suggested. The cell is considered as a domain with a boundary formed by a potential supported by a surface. Nanoparticles are presented by point-like potentials. The asymptotics of the Green function with the singularity at the surface is obtained. Resonances induced by point-like potentials are studied. An application of the result to explanation of selective cancer cell membrane destruction in ultrasonic field is discussed.