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# QMATH 12 Humboldt-Universität zu Berlin

Some conference series last for a few issues only, some have a longer life. It is hard to believe that the QMath one exists for more than quarter a century, starting from a two-day meeting convened in September 1987 in the Laboratory of Theoretical Physics, JINR, in Dubna. World changed a lot since then, countries have different names and borders, but the main topic of these conferences, mathematical methods and results in quantum physics, has not ceased to attract attention.

The series visited many places, after the first meetings in Dubna it was held in Liblice, Blossin, Ascona, Prague, Taxco, Giens, Moeciu, and Hradec Králové. Now it comes to Germany for

the second time, and to the very heart of Berlin. We are grateful to the Humboldt University for the hospitality and to the German mathematical-physics community for the efforts which made this meeting possible.

Within the general scope, which is the state of the art and new results in the «quantum part» of mathematical physics, each of the QMath conferences offered a different emphasis. For the Berlin issue the main topics will be spectral theory of Schrödinger operators, spectra of random operators, quantum field theory and relativistic quantum mechanics, interacting many body systems, and numerical methods in mathematical physics. There will be twelve plenary lectures, invited talks in topical sessions and a number of contributed ones – plenty to choose from.

On behalf of the conference scientific board I want to express hope that you will enjoy the programme and discussions with the other participants bringing inspiration for your future work. The QMath series has already a tradition of an important meeting in the intervals between international congresses of mathematical physics, and as any good tradition this one is certainly worth to be continued.

Pavel Exner (on behalf of the Organising Committee)





# Programme Overview

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	Friday, September 13, 2013
9.00	Plenary Talk Gueorgui Raykov
10.00	Coffee Break
10.30	Plenary Talk Amandine Aftalion
11.30	Plenary Talk Israel Michael Sigal
12.30	① Lunch Break
	Section A/C/D/E
1.30	
2.00	
2.30	
3.00	
03.30	Closing

# PROGRAMME COMMITTEE

Volker Bach (Braunschweig) Michael Demuth (Clausthal) Pavel Exner (Prague) Wolfgang König (Berlin) Alexander Mielke (Berlin) Hagen Neidhardt (Berlin) Reinhold Schneider (Berlin)

# LOCAL ORGANISING COMMITTEE

Wolfgang König (Berlin, Chair) Hagen Neidhardt (Berlin)

# HOST

Weierstrass Institute for Applied Analysis and Stochastics (WIAS) Research Group "Interacting Random Systems" Mohrenstr. 39 D-10117 Berlin

# CONFERENCE OFFICE

event lab. GmbH Dufourstraße 15 D-04107 Leipzig

Phone: +49-(0)341-240596-75 Fax: +49-(0)341-240596-51 E-Mail: jkaftan@eventlab.org





# CONFERENCE VENUE Universitätsgebäude am Hegelplatz Dorotheenstr. 24 10117 Berlin

**CONFERENCE DATES** 

Opening hours registration desk: Tuesday, September 10, 2013 08:00 am – 06:15 pm Wednesday, September 11, 2013 08:30 am – 06:15 pm Thursday, September 12, 2013 08:30 am – 06:15 pm Friday, September 13, 2013 08:30 am – 03:45 pm

# COFFEE AND LUNCH BREAKS

During the coffee breaks coffee, tea and small snacks (dessert fruit, cake) will be served.

For lunch you may purchase snacks in the cafeteria on the ground floor and the little restaurants around the university.

# TECHNICAL FACILITIES – SPEAKER'S PREVIEW

Facilities will be available to present Powerpoint (Office 2007) and PDF presentations in all rooms. The files (CD-R or USB-Stick) should be handed to the technical support in your lecture room lately in the break before your talk.

# CONFERENCE LANGUAGE

The official conference language is English.



# PUBLIC TRANSPORT

The venue can easily be reached by public transport from Berlin main station. Suburban train: No. 5, 7, 75 stop Friedrichstraße

# **REGISTRATION FEES**

The registration fee includes unlimited access to the scientific meetings, coffee breaks, proceedings as well as the name tag and delegate bags including abstracts.

# SOCIAL PROGAMME

Conference Dinner at the Restaurant "Cum Laude" Wednesday, September 11, 2013 Costs per Person: 40,00 EUR (includes a welcome drink and food from a buffet) Tickets are still available.

# SECTIONS, CHAIR PERSONS & SECTION SPEAKERS

# A: Spectral theory of Schrödinger operators

(organised by Michael Demuth, Pavel Exner and Hagen Neidhardt) *Werner Kirsch* Department of Mathematics and Informatics, Fernuniversität Hagen, Germany *Hynek Kovarik* Dipartimento di Matematica, Università degli studi di Brescia, Italy *Konstantin Pankrashkin* Laboratoire de mathématiques, Université Paris-Sud, France

# **B: Spectra of random operators**

(organised by Wolfgang König und Simone Warzel) *Marek Biskup* University of California, Los Angeles, USA *Hermann Schulz-Baldes* Department of Mathematics, Universität Erlangen, Germany *Emra Hamza* Egypt

# C: Quantum field theory and relativistic quantum mechanics

(organised by Marcel Griesemer) Jan Derezinski Faculty of Physics, University of Warsaw, Poland Jérémy Faupin Institut de Mathématiques de Bordeaux, France Christian Hainzl Department of Mathematics, Universität Tübingen, Germany



D: Interacting many body systems (organised by Volker Bach) *Christian Schilling* ETH Zürich, Institut für Theoretische Physik, Switzerland *Walter Pedra* Johannes Gutenberg-Universität Mainz, Germany *Benjamin Schlein* Institute for Applied Mathematics, University of Bonn, Germany

# **E: Numerical methods in Mathematical Physics**

(organised by Reinhold Schneider) *Virginie Ehrlacher* CERMICS – École des Ponts ParisTech, France *Jianfeng Lu* Mathematics Department, Duke University, USA *Gabriel Stoltz* CERMICS – École des Ponts ParisTech, France

# Proceedings

Proceedings will be published as a volume by **World Scientific**, a leading international publisher in science, technology and medicine. Participants are welcome to submit abstracts for this booklet until March 1, 2014. Please send your text as latex file to the Scientific Committee:

- Professor Wolgang König: koenig@wias-berlin.de
- Professor Pavel Exner: exner@ujf.cas.cz
- Dr. Hagen Neidhardt: neidhard@wias-berlin.de You will find detailed information online.

	Tuesday, September 10, 2013				
	📀 Hörsaal 1.101	<b>⊙</b> Room 1.102	<b>⊘</b> Room 1.103	<b>⊙</b> Room 1.205	
8.45	Opening Ceremony				
9.00	Plenary Talk E. Brian Davies				
10.00	Coffee Break				
10.30	Plenary Talk Fritz Gesztesy				
11.30	Plenary Talk Ari Laptev				
12.30	() Lunch Break				

	Section A		Section B	Section D
1.30	Invited Speaker Konstantin Pankrashkin		Fumihiko Nakano	Hans-Christoph Kaiser
2.00			Francisco Hoecker- Escuti	Shuji Watanabe
2.30	Olaf Post	Post Henrik Ueberschär	Invited Speaker Marek Biskup	Joachim Kerner
3.00	Stepan Manko	Tobias Weich		Ioannis Anapoliatnos

# 3.25 Coffee Break

	Section A		Section B	Section D
4.00	Evans Harrell	Franz Hanauska		Invited Speaker
4.30	Françoise Truc	Radek Novak	Christian Seifert	Christian Schilling
5.00	Evgeni Korotyaev	Jaroslav Dittrich	Invited Speaker Hermann Schulz- Baldes	Franz Achleitner
5.30	Hiroaki Niikuni	Igor Popov		Alexander Mielke



Tuesday

Session: Opening 8.45 - 9.00 am

Pavel Exner (Initiator of the Qmath) Alexander Mielke (Vice Director of WIAS)

Session: Plenary Talk 9.00 - 10.00 am

Chair: Michael Demuth

9.00 am Two non-self-adjoint spectral problems *E. Brian Davies (London / UK)* 

Session: Plenary Talk 10.30 am - 12.30 pm

Chair: Michael Demuth

10.30 am Applications of Weyl-Titchmarsh Operators *Fritz Gesztesy (Columbia / USA)* 

11.30 am Negative discrete spectrum of Schrödinger operators *Ari Laptev (London / UK)* 

12.30 – 1.30 pm Lunch Break

Session: Spectral theory of Schrödinger operators 1.30 - 3.25 pm

1.30 pm

Laplacian, wave equation and related operators on equilateral metric graphs Konstantin Pankrashkin (Orsay Cedex / France)

2.30 pm Shrinking fat graphs and convergence of operators and spectra *Olaf Post (Durham / UK)* 

3.00 pm

Approximations of general quantum-graph vertex couplings Stepan Manko (Decin / Czech Republic)

# Session: Spectral theory of Schrödinger operators 4.00 – 6.00 pm

4.00 pm

Eigenvalue distributions and the structure of graphs *Evans Harrell (Atlanta / USA)* 

# 4.30 pm Scattering theory for graphs isomorphic to a homogeneous tree at infinity *Françoise Truc (Saint-Martin-d'Hères / France)*

5.00 pm

Schrödinger operators on periodic discrete graphs *Evgeny Korotyaev (St. Petersburg / Russia)* 

5.30 pm

On the spectrum of periodic Schrödinger operators on a quantum graph with the  $\delta$ - $\delta$ - $\delta$  vertex conditions *Hiroaki Niikuni (Kyoto / Japan)* 

# 🤨 Hörsaal 1.102

Session: Spectral theory of Schrödinger operators 2.30 – 3.25 pm

2.30 pm

Quantum Limits for Point Scatterers on Flat Tori Henrik Ueberschär (Gif-sur-Yvette / France)

#### 3.00 pm

Experimental study of fractal Weyl law and the spectral gap in open quantum n-disk systems *Tobias Weich (Marburg / Germany)* 

#### Session: Spectral theory of Schrödinger operators 4.00 – 6.00 pm

#### 4.00 pm

On the discrete spectrum of linear operators in Banach spaces with nuclear perturbations *Franz Hanauska (Clausthal-Zellerfeld / Germany)* 

4.30 pm

Bound states in PT-symmetric layers Radek Novak (Prague / Czech Republic)

5.00 pm

Scattering through a straight quantum waveguide with combined boundary conditions Jaroslav Dittrich (Řež / Czech Republic)

5.30 pm Stokes graph *Igor Popov (St. Petersburg / Russia)* 



#### Session: Spectra of random operators 1.30 - 3.25 pm

1.30 pm

Level statistics for one-dimensional Schrödinger operator Fumihiko Nakano (Tokyo / Japan)

2.00 pm

Frequency concentration of the eigenfunctions of the Anderson model in the bulk of the spectrum at weak disorder.

Francisco Hoecker-Escuti (Chemnitz / Germany)

2.30 pm

Extreme order statistics for eigenvalues of random Schrödinger Hamiltonians Marek Biskup (Los Angeles / USA)

#### Session: Spectra of random operators 4.30 - 6.00 pm

4.30 pm

Cantor type spectra of Lebesgue measure zero for continuum one-dimensional quasicrystals *Christian Seifert (Hamburg / Germany)* 

5.00 pm

The role of invariants and disorder in two-dimensional topological insulators *Hermann Schulz-Baldes (Erlangen / Germany)* 

# 📀 Hörsaal 1.205

Session: Interacting many body systems 1.30 – 3.25 pm

1.30 pm

A Transient Drift-Diffusion Kohn-Sham Theory Hans-Christoph Kaiser (Berlin / Germany)

2.00 pm

Temperature dependence of the solution to the BCS gap equation for superconductivity and fixed point theorems

Shuji Watanabe (Maebashi / Japan)

2.30 pm

Interacting many-particle systems and Bose-Einstein condensation on general compact quantum graphs Joachim Kerner (Egham / UK)

3.00 pm

The ground state energy of the multi-polaron in the strong coupling limit *loannis Anapoliatnos (Stuttgart / Germany)* 

#### Session: Interacting many body systems 4.00 - 6.00 pm

4.00 pm

Quantum Marginal Problem and its Physical Relevance *Christian Schilling (Zurich / Switzerland)* 

5.00 pm

Traveling wave solutions in scalar conservation laws with anomalous diffusion *Franz Achleitner (Vienna / Austria)* 

5.30 pm

Entropy-driven dissipative coupling of quantum mechanics to simple heat baths *Alexander Mielke (Berlin / Germany)* 



	Wednesday, September 11, 2013				
	🤨 Hörsaal 1.101	<b>⊙</b> Room 1.102	<b>◎</b> Room 1.103	<b>◎</b> Room 1.205	
9.00	Plenary Talk Laszlo Erdös				
10.00	Coffee Break				
10.30	Plenary Talk Daniel Ueltschi				
11.30	Plenary Talk Peter Stollmann				
12.30	① Lunch Break				
	Section A		Section C	Section D	
1.30	Ricardo Weder	Jochen Schmid		Invited Speaker	
2.00	Hendrik Vogt	Jiri Lipovsky	Wojciech Dybalski	Walter Pedra	
2.30	Arne Jensen	Batu Güneysu	Invited Speaker	Horia Cornean	
3.00	Delio Mugnolo	Anton Boitsev	Jérémy Faupin	Anton Arnold	
3.25	Coffee Break				
	Section A		Section B		
4.00	Invited Speaker				
4.30	Werner Kirsch		Martin Gebert		
5.00	Andrii Khrabustovskyi	Daniel Schmidt	Invited Speaker Eman Hamza		
5.30	Takuya Mine	Alessandro Teta			
7.00	Get-together in the Res	taurant "Cum Laude"			

#### Session: Plenary Talk 9.00 - 10.00 am

# Chair: Alexander Mielke

## 9.00 am

Universality for random matrices and log-gases *Laszlo Erdös (Klosterneuburg / Austria)* 

## Session: Plenary Talk 10.30 am - 12.30 pm

## Chair: Alexander Mielke

10.30 am Probabilistic representations for quantum lattice systems Daniel Ueltschi (Coventry / UK)

# 11.30 am

Lifshitz tails via linear coupling of disorder *Peter Stollmann (Chemnitz / Germany)* 

# 12.30 – 1.30 pm Lunch Break

# Session: Spectral theory of Schrödinger operators 1.30 – 3.25 pm

#### 1.30 pm

High- and low- energy analysis and Levinson's theorem for the selfadjoint matrix Schroedinger operator on the half line

Ricardo Weder (Mexico City / Mexico)

# 2.00 pm

A weak Gordon type condition for absence of eigenvalues of one-dimensional Schrödinger operators Hendrik Vogt (Hamburg / Germany)

# 2.30 pm

Resolvent expansion for the discrete one dimensional Schrödinger operator *Arne Jensen (Aalborg / Denmark)* 

#### 3.00 pm

No boundary conditions for a diffusion equation on an interval *Delio Mugnolo (Ulm / Germany)* 



## Session: Spectral theory of Schrödinger operators 4.00 – 6.00 pm

4.00 pm

Spectral Theory for Block Matrices with Random Entries *Werner Kirsch (Hagen / Germany)* 

5.00 pm Periodic elliptic operators with predefined spectral gaps Andrii Khrabustovskyi (Karlsruhe / Germany)

5.30 pm

Two-solenoidal Aharonov-Bohm effect with quantized magnetic fluxes *Takuya Mine (Kyoto / Japan)* 

# 🥺 Hörsaal 1.102

Session: Spectral theory of Schrödinger operators 1.30 – 3.25 pm

1.30 pm

Adiabatic theorems with and without spectral gap condition for non-semisimple spectral values *Jochen Schmid (Stuttgart / Germany)* 

2.00 pm

Eigenvalue asymptotics for the damped wave equation on metric graphs *Jiri Lipovsky (Hradec Kralove / Czech Republic)* 

2.30 pm Generalized Schrödinger semigroups on infinite graphs Batu Güneysu (Berlin / Germany)

3.00 pm Boundary triplets approach for sum of tensor products of operators *Anton Boitsev (Saint-Petersburg / Russia)* 

## Session: Spectral theory of Schrödinger operators 5.00 – 6.00 pm

5.00 pm Eigenvalue Statistics of Random Block Operators Daniel Schmidt (Blacksburg / USA)

5.30 pm

Stability problem for a system of fermions with zero-range interactions *Alessandro Teta (Roma / Italy)* 

Session: Quantum field theory and relativistic quantum mechanics 2.00 – 3.25 pm

2.00 pm

Generalized asymptotic completeness in local relativistic QFT *Wojciech Dybalski (Zurich / Switzerland)* 

2.30 pm

On Rayleigh scattering in non-relativistic quantum electrodynamics Jérémy Faupin (Talence Cedex / France)

Session: Spectra of random operators 4.30 - 6.00 pm

4.30 pm Localization for Random Block Operators *Martin Gebert (Munich / Germany)* 

5.00 pm

Spectral Transition for Random Quantum Walks on Trees *Eman Hamza (Cairo / Egypt)* 

# 📀 Hörsaal 1.205

Session: Interacting many body systems 1.30 – 3.25 pm

#### 1.30 pm

Conductivity Measure for Lattice Fermions from Joule's law Walter de Sigueira Pedra (São Paulo / Brazil)

#### 2.30 pm

Non-equilibrium steady-states for interacting open systems Horia Cornean (Aalborg / Denmark)

3.00 pm

Quantum Fokker-Planck models: kinetic vs. operator theory approaches Anton Arnold (Vienna / Austria)



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	Thursday, September 12, 2013				
	📀 Hörsaal 1.101		<b>⊙</b> Room 1.103		
9.00	Plenary Talk Eric Cances				
10.00	Coffee Break				
10.30	Plenary Talk Ivan Veselic				
11.30	Plenary Talk Jiři Černý				
12.20	Durah Draak				

# 12.30 🛞 Lunch Break

	Section A		Section C	Section E
1.30	Vladimir Lotoreichik	Anton Popov		Invited Speaker
2.00	Michal Jex	Alina Anikevich	Nuri Unal	Jianfeng Lu
2.30	Mark Malamud	Diana Barseghyan	<b>Invited Speaker</b> Jan Derezinski	Markus Bachmayr
3.00	Aleksey Kostenko	Ivan Melikhov		Andreas Arnold

# 3.25 Coffee Break

	Section A	Section C	Section E
4.00	Matěj Tušek	Oliver Matte	Invited Speaker
4.30	Yuri Kordyukov	Yana Butko	Gabriel Stoltz
5.00	Invited Speaker		Xiafeng Huang
5.30	Hynek Kovarik		Paul Racec

#### Session: Plenary Talk 9.00 – 10.00 am

Chair: Reinhold Schneider

# 9.00 am

Electronic structure calculation Eric Cances (Marne-la-Vallée / France)

# Session: Plenary Talk 10.30 am - 12.30 pm

# Chair: Reinhold Schneider

10.30 am

Equidistribution properties of eigenfunctions and solutions of PDE *Ivan Veselic (Chemnitz / Germany)* 

11.30 am

Aging in dynamics of disordered systems Jiři Černý (Vienna / Austria)

# 12.30 – 1.30 pm Lunch Break

# Session: Spectral theory of Schrödinger operators 1.30 – 3.25 pm

#### 1.30 pm

Self-adjoint Laplacians on partitions with delta- and delta'-couplings Vladimir Lotoreichik (Graz / Austria)

#### 2.00 pm

Discrete spectrum of Schrödinger operator with a strong  $\delta'$ -interaction supported by a planar loop *Michal Jex (Prague / Czech Republic)* 

#### 2.30 pm

1D Schödinger and Dirac operators with local point interactions Mark Malamud (Donetsk / Ukraine)

#### 3.00 pm

Spectral theory of 1-D Schrödinger operators with  $\delta'$ -interactions Aleksey Kostenko (Vienna / Austria)

# Session: Spectral theory of Schrödinger operators 4.00 – 6.00 pm

# 4.00 pm

Effective Hamiltonian for a thin curved quantum layer in a magnetic field *Matěj Tušek (Prague / Czech Republic)* 



#### 4.30 pm

Semiclassical spectral asymptotics for two-dimensional magnetic Schrödinger operators Yuri Kordyukov (Ufa / Russia)

5.00 pm

Spectral properties of two-dimensional Schrödinger operators *Hynek Kovarik (Brecia / Italy)* 

# 🥺 Hörsaal 1.102

Session: Spectral theory of Schrödinger operators 1.30 – 3.25 pm

1.30 pm

Discrete spectrum for quantum graph of Y-branching strips type Anton Popov (St. Petersburg / Russia)

2.00 pm

Estimates for numbers of negative eigenvalues of Laplacian for Y-type chain of weakly coupled ball resonators

Alina Anikevich (St. Petersburg / Russia)

2.30 pm

Spectral analysis of Schrödinger operators with unusual semiclassical behavior *Diana Barseghyan (Erlangen / Germany)* 

3.00 pm

Hartree-Fock approximation for particles storage problem *Ivan Melikhov (St. Petersburg / Russia)* 

# 📀 Hörsaal 1.103

Session: Quantum field theory and relativistic quantum mechanics 2.00 - 3.25 pm

2.00 pm

Quantum fluctations of photon in a time varying media: Coherent state approach Nuri Unal (Antalya / Turkey)

2.30 pm Massive and massless vector quantum fields Jan Derezinski (Warszawa / Poland)

#### Session: Quantum field theory and relativistic quantum mechanics 4.00 – 5.00 pm

4.00 pm Stochastic calculus and non-relativistic QED *Oliver Matte (Aarhus / Denmark)* 

#### Session: Numerical methods in Mathematical Physics 1.30 – 3.25 pm

1.30 pm

Time reversible Born Oppenheimer molecular dynamics Jianfeng Lu (Durham / USA)

2.30 pm

Error estimates for Gaussian approximations in quantum chemistry *Markus Bachmayr (Aachen / Germany)* 

3.00 pm

Approximation of high-dimensional inital value problems in the hierarchical Tucker format Andreas Arnold (Karlsruhe / Germany)

#### Session: Numerical methods in Mathematical Physics 4.00 – 6.00 pm

4.00 pm

The microscopic origin of the macroscopic dielectric permittivity of crystals *Gabriel Stoltz (Marne la Vallée / France)* 

5.00 pm

Critical Missing Equation of Quantum Physics for Understanding Atomic Structures *Xiaofei Huang (Sunnyvale / USA)* 

5.30 pm

Wigner-Eisenbud problem within finite volume method: Application to electronic transport in cylindrical nanowire heterostructures

Paul Racec (Berlin / Germany)





	Friday, September 13, 2013				
	📀 Hörsaal 1.101				
9.00	Plenary Talk Gueorgui Raykov				
10.00	Coffee Break				
10.30	Plenary Talk Amandine Aftalion				
11.30	Plenary Talk Israel Michael Sigal				
12.30	① Lunch Break				

#### 12.30 (1) Lunch Break

	Section A	Section D	Section C	Section E
1.30	Erik Skibsted	Invited Speaker Benjamin Schlein	Ivan Naumkin	Invited Speaker
2.00	Rainer Hempel		Wataru Ichinose	Virginie Ehrlacher
2.30	Carlos Villegas-Blas	Niels Benedikter	Invited Speaker Christian Hainzl	Christian Mendl
3.00	Petr Siegl			
03.30	Closing	-		

Friday

#### Session: Plenary Talk 9.00 - 10.00 am

#### Chair: Volker Bach

#### 9.00 am

A Trace Formula for Long-Range Perturbations of the Landau Hamiltonian *Gueorgui Raykov (Santiago de Chile / Chile)* 

#### Session: Plenary Talk 10.30 am - 12.30 pm

#### Chair: Volker Bach

10.30 am

Vortices, skyrmions and phase separation for a two component Bose Einstein condensates *Amandine Aftalion (Versailles / France)* 

#### 11.30 am

Magnetic Vortices, Nielsen-Olesen-Nambu strings and theta functions *Israel Michael Sigal (Toronto / Canada)* 

## 12.30 – 1.30 pm Lunch Break

#### Session: Spectral theory of Schrödinger operators 1.30 – 3.30 pm

#### 1.30 pm

Decay of eigenfunctions of elliptic PDE's *Erik Skibsted (Aarhus / Denmark)* 

#### 2.00 pm

L1-Estimates for eigenfunctions of the Dirichlet Laplacian on Euclidean domains *Rainer Hempel (Braunschweig / Germany)* 

#### 2.30 pm

On semiclassical limiting eigenvalue and resonance distribution theorems for unbounded perturbations of the hydrogen atom Hamiltonian

Carlos Villegas-Blas (Cuernavaca / Mexico)

#### 3.00 pm

Spectra of graphene nanoribbons with armchair and zigzag boundary conditions *Petr Siegl (Bern / Switzerland)* 

Closing 3.30 - 3.45 pm

Fritz Gesztesy



#### Session: Interacting many body systems 1.30 – 3.00 pm

1.30 pm

Quantitative Derivation of the Gross-Pitaevskii Equation *Benjamin Schlein (Bonn / Germany)* 

2.30 pm

Quantitative Derivation of the Gross-Pitaevskii Equation *Niels Benedikter (Bonn / Germany)* 

📀 Hörsaal 1.103

## Session: Quantum field theory and relativistic quantum mechanics 1.30- 3.30 pm

1.30 pm

High-energy and smoothness asymptotic expansion of the scattering mplitude for the Dirac equation and applications

Ivan Naumkin (Ciudad de México / Mexico)

2.00 pm

On the Feynman path integral for the Dirac equation in the general dimensional spacetime *Wataru Ichinose (Matsumoto / Japan)* 

2.30 pm

Estimates for numbers of negative eigenvalues of Laplacian for Y-type chain of weakly coupled ball resonators

Christian Hainzl (Tübingen / Germany)

# 📀 Hörsaal 1.205

Session: Numerical methods in Mathematical Physics 1.30 - 3.30 pm

1.30 pm

Greedy algorithms for electronic structure calculations of molecular systems *Virgine Ehrlacher (Marne la Vallée / France)* 

2.30 pm

The "strictly correlated electron" limit of the Hohenberg-Kohn functional *Christian Mendl (Munich / Germany)* 

# ABSTRACTS



King's College London, Mathematics, London

#### TWO NON-SELF-ADJOINT SPECTRAL PROBLEMS

We describe the asymptotic spectral behaviour of two large non- self-adjoint matrices. The first concerns a non-self-adjoint Anderson model, whose spectral behaviour is contrasted with some very recent work done jointly with Michael Levitin. This concerns a matrix ana- logue of an indefi nite self-adjoint linear pencil that concerns a Dirac operator with an inde finite potential. In some sense it is the simplest matrix example of its type, but its analysis is still far more complex than one might expect.

#### Fritz Gesztesy

University of Missouri, Department of Mathematics , Columbia

# APPLICATIONS OF WEYL-TITCHMARSH OPERATORS

We intend to present various applications of Weyl–Titchmarsh operators (i.e., energy-dependent Dirichlet-to-Neumann and Robin-to-Robin maps) to problems in spectral theory in connection with self-adjoint extensions of symmetric operators, Krein-type resolvent formulas, and the Krein-von Neumann extension. In particular, we will describe concrete applications to Schrödinger-type operators.

#### Ari Laptev

Imperial College London, Department of Mathematics, London

# NEGATIVE DISCRETE SPECTRUM OF SCHRÖDINGER OPERATORS

We shall discuss properties of the discrete spectrum of Schrödinger operators. Special attention will be paid to the two-dimensional case where necessary and sufficient conditions for the finiteness of the number of negative eigenvalues are still not known. Plenary Talk: Tuesday September 10 09.00 – 10.00 am

Plenary Talk Tuesday September 10 10.30 – 11.30 am

Plenary Talk Tuesday September 10 11.30 am – 12.30 pm Plenary Talk Wednesday September 11 9.00 – 10.00 am Laszlo Erdös

Institute of Science and Technology, Austria, Mathematics, Klosterneuburg

#### UNIVERSALITY FOR RANDOM MATRICES AND LOG-GASES

Eugene Wigner's revolutionary vision predicted that the energy levels of large complex quantum systems exhibit a universal behavior: the statistics of energy gaps depend only on the basic symmetry type of the model. These universal statistics show strong correlations in the form of level repulsion and they seem to represent a new paradigm of point processes that are characteristically different from the Poisson statistics of independent points. A prominent model for strongly correlated systems is the log-gas at inverse temperature  $\beta$ . For specific values of  $\beta = 1, 2, 4$  the model arises from the eigenvalue distribution of random invariant matrix ensembles. For other values of  $\beta$  there is no simple random matrix ensemble behind the log-gas but the local statistics is still universal. In this talk I present our earlier result on bulk universality and the recent result on edge universality.

This is a joint work with Paul Bourgade and Horng-Tzer Yau.

Plenary Talks

Plenary Talk Wednesday September 11 10.30 – 11.30 am Daniel Ueltschi

Warwick, Mathematics, Coventry

# PROBABILISTIC REPRESENTATIONS FOR QUANTUM LATTICE SYSTEMS

Quantum lattice models are relevant for the study of the electronic properties of condensed matter systems. They include spin systems (Heisenberg, XY,...), interacting fermions (Falicov-Kimball, Hubbard, t-J,...), or bosons (Bose-Hubbard,...). Their mathematical study is notoriously difficult. I will review various probabilistic representations that are obtained using Feynman-Kac methods. In particular, I will discuss certain random loop models that were originally proposed by Tóth (for the Heisenberg ferromagnet) and Aizenman-Nachtergaele (for the Heisenberg antiferromagnet). In these models, the quantum spin correlations are given by loop correlations.

Recently, extensions of these representations have been used in order to prove the existence of phase transitions in certain SU(2)-invariant spin 1 systems. Rather surprisingly, one can formulate a precise conjecture for the joint distribution of the lengths of the large loops, namely, they satisfy a Poisson-Dirichlet distribution. Among the consequences of these heuristics are some characterisations of the pure states.



Peter Stollmann

TU Chemnitz, Fakultät für Mathematik, Chemnitz

## LIFSHITZ TAILS VIA LINEAR COUPLING OF DISORDER

We explain a simple method for proving upper bounds on the Integrated Density Of States and present some old and new applications.

# Eric Cances

CERMICS - Ecole des Ponts ParisTech, Marne la Vallée Cedex 2 ELECTRONIC STRUCTURE CALCULATION

Electronic structure calculation is one of the main field of applications of quantum mechanics. It has become an essential tool in condensed matter physics, chemistry, molecular biology, materials science, and nanosciences.

In this talk, I will review the main numerical methods to solve the electronic Schroedinger equation and the Kohn-Sham formulation of the Density Functional Theory (DFT). The electronic Schroedinger equation is a highdimensional linear elliptic eigenvalue problem, whose solutions can be numerically approximated either by stochastic methods, or by sparse tensor product techniques. Kohn-Sham models are constrained optimization problems, whose Euler-Lagrange equations have the form of nonlinear elliptic eigenvalue problems. Recent progress has been made in the analysis of these mathematical models and of the associated numerical methods, which paves the road to highfidelity numerical simulations (with a posteriori error bounds) of the electronic structure of large molecular systems.

Ivan Veselic

TU Chemnitz, Mathematics, Chemnitz

# EQUIDISTRIBUTION PROPERTIES OF EIGENFUNCTIONS AND SOLUTIONS OF PDE

The property of a function being the solution of a partial differential equation or even the eigenfunction of a partial differential operator imposes a certain rigidity: the function cannot fluctuate arbitrarily over space. This is closely connected to unique continuation properties and the uncertainty principle. We discuss such problems with an underlying multiscale structure.

Plenary Talk Wednesday September 11 11.30 am – 12.30 pm

Plenary Talk Thursday September 12 9.00 – 10.00 am

Plenary Talk Thursday September 12 10.30 – 11.30 am Jiří Černý

Plenary Talk Thursday September 12 11.30 am – 12.30 pm

**Plenary Talk** 

9.00 - 10.00 am

Friday September 13 University of Vienna, Faculty of Mathematics, Vienna

#### AGING IN DYNAMICS OF DISORDERED SYSTEMS

I give a review of results on aging in dynamics of disordered systems that appeared during the past decade. Starting from the dynamics of true spin glasses, which originally motivated this research, I will discuss, among others, the trap models, various mean-field spin glasses, and, seemingly unrelated, random walk among random conductances. I will explain why aging in all these models can be explained using a universal mechanism bases on convergence of certain processes characterising the dynamics to Lévy processes, and then using the associated arc-sine law.

Gueorgui Raykov

Pontificia Universidad Católica de Chile, Matemáticas, Santiago de Chile

# A TRACE FORMULA FOR LONG-RANGE PERTURBATIONS OF THE LANDAU HAMILTONIAN

We consider the operator  $H = H_0 + V$  where  $H_0$  is the Landau Hamiltonian, i.e. the 2D Schrödinger operator with constant magnetic field B > 0, and  $V \in C(\mathbb{R}^2; \mathbb{R})$  is an electric potential which satisfies

$$\sup_{x\in\mathbb{R}^2}\langle x\rangle^\rho |V(x)|<\infty$$

with  $\rho \in (0,1)$ . First, we show that there exists a constant C > 0 such that the spectrum of H is contained in the set  $\bigcup_{q=0}^{\infty} \left(\lambda_q - C\lambda_q^{-\rho/2}, \lambda_q + C\lambda_q^{-\rho/2}\right)$ , where  $\lambda_q := B(2q+1), q \in \mathbb{Z}_+$ , are the Landau levels, i.e. the infinitely degenerate eigenvalues of  $H_0$ . The main part of the talk will be devoted to description of the asymptotic behaviour as  $q \to \infty$  of the trace  $\operatorname{Tr} \varphi(\lambda_q^{\rho/2}(H - \lambda_q))$  with  $\varphi \in C_0^{\infty}(\mathbb{R} \setminus \{0\})$ , under appropriate additional assumptions on V.

Partially supported by the Chilean Science Foundation *Fondecyt* under Grant 1130591.



#### Amandine Aftalion

CNRS-Universite de Versailles St-Quentin, Laboratoire de Mathematiques, Versailles

# VORTICES, SKYRMIONS AND PHASE SEPARATION FOR A TWO COMPONENT BOSE EINSTEIN CONDENSATES

The aim of this talk is to describe the main features arising in the description of a two component Bose Einstein condensate, under rotation and in the presence of Rashba spin orbit coupling. I will present a numerical classification of the ground states (regions of coexistence of the components, phase separation and symmetry breaking) and the types of topological defects, with and without spin orbit coupling. Analytical justifications of some phenomena will be made thanks to a nonlinear sigma model describing the condensate in terms of the total density, total phase and pseudo spin representation. In particular, we will estimate the total density in the Thomas fermi regime, and we will justify, that for certain values of the parameters, the experiment stabilizes a square lattice of vortices, whereas in previous experiments all lattices were triangular. This relies on the analytical derivation of a vortex energy that characterizes the type of vortex lattice. In the case of strong segregation, we will also present a Gamma convergence result to a perimeter minimization problem leading to symmetry breaking. Finally, we will show some insight into the spin orbit coupling problem and the relationship with ferromagnetic questions.

Israel Michael Sigal

University of Toronto, Mathematics, Toronto

# MAGNETIC VORTICES, NIELSEN-OLESEN-NAMBU STRINGS AND THETA FUNCTIONS

The Ginzburg-Landau theory was first developed to explain and predict properties of superconductors, but had a profound influence on physics well beyond its original area. It had the first demonstration of the Higgs mechanism and it became a fundamental part of the standard model in the elementary particle physics. The theory is based on a pair of coupled nonlinear equations for a complex function (called order parameter or Higgs field) and a vector field (magnetic potential or gauge field). They are the simplest representatives of a large family of equations appearing in physics and mathematics. (The latest variant of these equations is the Seiberg-Witten equations.) Geometrically, these are equations for the section of a principal bundle and the connection on this bundle. Besides of importance in physics, they contain beautiful mathematics (some of the mathematics was discovered independently by A. Turing Plenary Talk Friday September 13 10.30 – 11.30 am

Plenary Talk Friday September 13 11.30 am – 12.30 pm in his explanation of patterns of animal coats). In this talk I will review recent results involving key solutions of these equations – the magnetic vortices and vortex lattices, their existence, stability and dynamics, and how they relate to the modified theta functions appearing in number theory.

Invited Talk Tuesday September 10 1.30 – 2.25 pm

Invited Talk Wednesday September 11 4.00 – 4.55 pm Konstantin Pankrashkin University Paris-Sud, Laboratory of Mathematics, Orsay LAPLACIAN, WAVE EQUATION AND RELATED OPERATORS ON EQUILATERAL METRIC GRAPHS

In this talk we present some recent results concerning the spectral analysis of various operators associated with infinite equilateral metric graphs. In particular, we establish new relations between the continuous Laplacian, the normalized discrete Laplacian, the averaging operator and the solutions of the associated wave equation.

The talk is based on a joint work with Daniel Lenz.

#### Werner Kirsch

Fern Universität Hagen, Fakultät für Mathematik und Informatik, Hagen

#### SPECTRAL THEORY FOR BLOCK MATRICES WITH RANDOM ENTRIES

We discuss spectral properties of some block matrices whose entries are random Schrödinger operators. These operators model certain systems connected to superconductor physics. We will concentrate on matrices of the form

$$\begin{pmatrix} H & B \\ B & -H \end{pmatrix}$$

where either H or B or both may have random entries (e.g. on the diagonal).

We concentrate on properties of the density of states for those operators as well as on the question of Anderson localization.

#### References:

Kirsch, Werner; Metzger, Bernd; Müller, Peter: Random block operators J. Stat. Phys. 143 (2011), no. 6, 1035–1054.

Gebert, Martin; Müller, Peter: Localization for random block operators Oper. Theory Adv. Appl. 232, 229–246 (2013)



#### Hynek Kovarik

Università degli studi di Brescia, Dipartimento di Matematica, Brescia SPECTRAL PROPERTIES OF TWO-DIMENSIONAL SCHRÖDINGER OPERATORS

In this talk we will discuss the effect of a magnetic field on certain spectral properties of two-dimensional Schrödingier operators. Main attention will be paid to the estimates on the number of bound states and to the large time behavior of the associated heat semigroup and of the unitary group. In particular, it will be shown how certain magnetic fields accelerate the time decay of the heat semigroup and unitary group with respect to those generated by non-magnetic Schrödinger operators.

#### Alina Anikevich

St. Petersburg National Research University of Information Technologies, Mechanics and Optics, Natural Sciences, Saint Petersburg

# ESTIMATES FOR NUMBERS OF NEGATIVE EIGENVALUES OF LAPLACIAN FOR Y-TYPE CHAIN OF WEAKLY COUPLED BALL RESONATORS

Spectral problem for the Y-type chain of weakly coupled ball resonators is under discussion. More precisely, one deals with investigating negative eigenvalues for such chain. Y-bent system can be described as the central ball linking three semi-infinite chains that consist of balls of the same radius. Specifically, it is supposed that for each branch there is an axis passing through all coupling points between balls and all these three axis lie in the same plane. It is also supposed that the canters of balls, that are the closest ones to the central ball, are the vertices of an equilateral triangle. Two types of coupling in contact points between the balls are under investigation: the  $\delta$ -coupling and the  $\delta'$ -coupling. The transfer-matrix approach and the theory of operator extensions are employed. Upper estimates for number of negative eigenvalues for described above system for two mentioned earlier types of coupling are obtained. Invited Talk Thursday September 12 5.00 – 6.00 pm

> Thursday September 12 2.00 – 2.25 pm

Thursday September 12 3.00 - 3.25 pm Diana Barseghyan

Friedrich-Alexander-Universität Erlangen-Nürnberg, Mathematics, Erlangen SPECTRAL ANALYSIS OF SCHRÖDINGER OPERATORS WITH UNUSUAL SEMICLASSICAL BEHAVIOR

In first part of talk we analyze two-dimensional Schrödinger operators with the potential  $|xy|^p - \lambda (x^2 + y^2)^{p/(p+2)}$ , where  $p \ge 1$  and  $\lambda \ge 0$ . We show that there is a critical value of  $\lambda$  such that the spectrum for  $\lambda < \lambda_{crit}$  is below bounded and purely discrete, while for  $\lambda > \lambda_{crit}$  it is unbounded from below. In the subcritical case we prove upper and lower bounds for the eigenvalue sums.

The goal of second part of talk is to derive estimates of eigenvalue moments for Dirichlet Laplacians and Schrödinger operators in regions having infinite cusps which are geometrically nontrivial being either curved or twisted; we show how those geometric properties enter the eigenvalue bounds. The obtained inequalities reflect the essentially one-dimensional character of the cusps and we give an example showing that in an intermediate energy region they can be much stronger than the usual semiclassical bounds.

In rest part of talk we investigate Dirichlet Laplacian in a straight twisted tube of a non-circular cross section, in particular, its discrete spectrum coming from a local slowdown of the twist. We prove a Lieb-Thirring-type estimate for the spectral moments and present two examples illustrating how the bound depends on the tube cross section.

Irina Blinova, Anton Popov

St. Petersburg National Research University of Information Technologies, Mechanics and Optics, Higher Mathematics, St. Petersburg DISCRETE SPECTRUM FOR QUANTUM GRAPH OF Y-BRANCHING STRIPS TYPE

We consider a quantum graph with a hexagonal lattice consisting of three symmetrically coupled semi-infinite strips. We deal with the Schrödinger operator on the each edge of the graph  $\Gamma$ 

$$H = -\frac{d^2}{dx^2} \tag{1}$$

and  $\delta$ -type conditions as boundary conditions which are defined as follows

$$\begin{cases} f(x) \in C(\Gamma) ,\\ \sum_{e \in E_v} \frac{df}{dx_e}(v) = \alpha f(v). \end{cases}$$
(2)



September 12



Here  $\alpha$  is some fixed number,  $E_v := \{e \in E | v \in e\}$  is the set of edges adjacent to the vertex v. The sum is taken over all edges e incident to the vertex v and the derivatives are taken along e in the directions away from the vertex v (outgoing direction).

We prove the existence of the point spectrum of the corresponding operator, that is, the existence of bound states of electrons. We also specify the restrictions on the model parameters. For spectral analysis on metric graphs we use approach, based on the theory of self-adjoint extensions of symmetric operators in the Hilbert spaces. The method of transfer-matrices is used.

#### Anton Boitsev

NRU ITMO, Higher Mathematics, Saint-Petersburg

# BOUNDARY TRIPLETS APPROACH FOR SUM OF TENSOR PRODUCTS OF OPERATORS

Extension theory model for the Hamiltonian having a form of a sum of tensor products is considered. One of the operators is assumed to be self-adjoint. Boundary triplet is constructed in case the self-adjoint operator is bounded. A counterexample shows that in case of unbounded operator the surjectivity of the boundary operators may be lost. For the unbounded situation some extra-constructions are made and the boundary triplet is obtained. A particular example useful in physics is considered. Self-adjoint extensions are constructed in the framework of suggested approach.

# Jaroslav Dittrich

Nuclear Physics Institute ASCR, Theoretical Physics, Rez

# SCATTERING THROUGH A STRAIGHT QUANTUM WAVEGUIDE WITH COMBINED BOUNDARY CONDITIONS

Scattering through a straight two-dimensional quantum waveguide  $(-\infty, +\infty) \times (0, d)$  with the Dirichlet boundary condition on x < 0, y = 0 and x > 0, y = d, and the Neumann boundary condition on x < 0, y = d and x > 0, y = 0 is considered using stationary scattering theory. The energies between the two lowest transverse modes are considered only. The matching conditions at x = 0 are discussed, the existence of their solution is proved. The use of stationary scattering theory is justified showing its relation to the wave packets motion.

Wednesday September 11 3.00 – 3.25 pm

**Tuesday** September 10 5.00 – 5.25 pm Batu Güneysu

Humboldt University, Mathematics, Berlin

Wednesday September 11 2.30 – 2.55 pm

Tuesday

Tuesday September 10 4.00 – 4.25 pm

September 10 4.00 – 4.25 pm

#### GENERALIZED SCHRÖDINGER SEMIGROUPS ON INFINITE GRAPHS

In this talk, I will explain a new and unified concept of covariant Schrödinger type operators that act on sections in (possibly infinite dimensional) vector bundles over discrete graphs, which relies on a discrete notion of unitary covariant derivatives. With this notion at hand, it is possible to introduce a natural concept of stochastic parallel transport along the paths of the underlying Markoff process, which in turn allows a very general covariant Feynman-Kac type probabilistic representation of the corresponding vector bundle valued Schrödinger semigroups, even if the graph is "locally infinite". I will also explain some spectral theoretic applications of this Feynman-Kac formula.

This is joint work with Ognjen Milatovic and Francoise Truc.

#### Franz Hanauska

TU Clausthal, Mathematik, Clausthal-Zellerfeld

# ON THE DISCRETE SPECTRUM OF LINEAR OPERATORS IN BANACH SPACES WITH NUCLEAR PERTURBATIONS

Let  $Z_0$  be a bounded operator in a Banach space X with purely essential spectrum and K a nuclear compact operator in X. With methods of complex analysis we study the discrete spectrum of  $Z_0 + K$  and derive a Lieb-Thirring type inequality. We can obtain estimates for the number of eigenvalues in certain regions of the complex plane and an estimate for the asymptotics of the eigenvalues approaching to the essential spectrum of  $Z_0$ . Instead of nuclear operators we are also able to treat the more general case of operators with p-summable approximationnumbers.

#### Evans Harrell

Georgia Institute of Technology, Mathematics, Atlanta, GA EIGENVALUE DISTRIBUTIONS AND THE STRUCTURE OF GRAPHS

We consider the spectra of three self-adjoint matrices associated with a combinatorial graph, viz., the adjacency matrix A, the graph Laplacian  $H = -\Delta$ , and the normalized graph Laplacian L. Using a) variational techniques, and b) identities for traces of operators and Chebyshev's inequality, we present some bounds on gaps, sums, Riesz means, and the statistical distribution of eigenvalues of these operators, and relate them to the structure of the graph.



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### Rainer Hempel

TU Braunschweig, Mathematics, Braunschweig

# L1-ESTIMATES FOR EIGENFUNCTIONS OF THE DIRICHLET LAPLACIAN ON EUCLIDEAN DOMAINS

For  $d \in \mathbb{N}$  and  $\Omega \neq \emptyset$  an open set in  $\mathbb{R}^d$ , we study the eigenfunctions  $\Phi$  of the Dirichlet Laplacian  $-\Delta_\Omega$ , acting in the Hilbert space  $L_2(\Omega)$ . Here  $\Omega$  may be bounded, of finite volume or of infinite volume, but our results only pertain to eigenfunctions  $\Phi$  that are associated with a discrete eigenvalue  $\lambda$  of  $H_\Omega$ . We first establish that all such  $\Phi$  belong to  $L_1(\Omega)$ . We then turn to eigenvalues  $\lambda$ below the infimum of the essential spectrum where we obtain bounds on the  $L_1$ norm of  $\Phi$  which are independent of the volume of  $\Omega$ ; these bounds involve the  $L_2$ -norm of  $\Phi$  and spectral data. Our bounds complement well-known estimates for the  $L_\infty$ -norm of  $\Phi$ . As an application, we study the *heat content* of  $\Omega$  where we assume that  $H_\Omega$  has compact resolvent. We show that the heat content of  $\Omega$  is finite for t > 0 iff the *heat trace* of  $\Omega$  is finite, and we produce a two-sided estimate for these quantities.

This is joint work with M. van den Berg (Bristol) and J. Voigt (Dresden).

#### Arne Jensen

Aalborg University, Department of Mathematical Sciences, Aalborg

# RESOLVENT EXPANSION FOR THE DISCRETE ONE DIMENSIONAL SCHRÖDINGER OPERATOR

Given a discrete Schrödinger operator

(Hu)[n] = -(u[n+1] + u[n-1] - 2u[n]) + (Vu)[n]

with a fairly general (nonlocal) interaction V we obtain asymptotic expansions around the two thresholds 0 and 4 of the resolvent of H.

Joint work with K. Ito, Tsukuba University, Japan.

Friday September 13 1.30 – 1.55 pm

Wednesday September 11

2.30 - 2.55 pm

Michal Jex

Thursday September 12 2.00 – 2.25 pm Czech Technical University in Prague, Department of Physics, FNSPE, Prague DISCRETE SPECTRUM OF SCHRÖDINGER OPERATOR WITH A STRONG Î'-INTERACTION SUPPORTED BYA PLANAR LOOP

We study the discrete spectrum of a generalized Schrödinger operator in  $L^2(\mathbb{R}^2)$  describing an attractive strongly singular interaction of  $\delta'$  type supported by a  $C^4$ -smooth closed curve  $\Gamma$  of length L without self-intersections. We characterize this singular interaction by the coupling parameter  $\beta>0$ . We are interested in the properties of the spectrum in the strong coupling limit, i.e. when the coupling parameter approaches zero  $\beta \to 0_+$ . For such situation it is shown that the number of eigenvalues can be written as  $\frac{2L}{\pi\beta} + \mathcal{O}(|\ln\beta|)$ . Furthermore we are able to write the j-th eigenvalue in the same limit as  $-\frac{4}{\beta^2} + \mu_j + \mathcal{O}(\beta |\ln\beta|)$ . In the previous expression  $\mu_j$  is the j-th eigenvalue of the Schrödinger operator on  $L^2(0,L)$  with periodic boundary conditions and the potential  $-\frac{1}{4}\gamma^2$  where  $\gamma$  denotes the signed curvature of  $\Gamma$ .

Andrii Khrabustovskyi

Karlsruhe Institute of Technology, Department of Mathematics, Karlsruhe PERIODIC ELLIPTIC OPERATORS WITH PREDEFINED SPECTRAL GAPS

We denote by  $\mathcal{L}_{\mathrm{per}}$  the set operators in  $\mathbb{R}^n$  of the form

$$\mathcal{A} = -\frac{1}{b} \operatorname{div}(a\nabla)$$

where a(x), b(x) are  $\mathbb{Z}^n$ -periodic measurable real functions satisfying

$$\exists \alpha, \beta > 0 : \ \alpha \le a(x) \le \beta, \ \alpha \le b(x) \le \beta$$

In the talk we discuss the following result obtained in [1]: for an arbitrary L > 0 and for arbitrary pairwise disjoint intervals  $(\alpha_j, \beta_j) \subset [0, L], j = 1, \ldots, m$   $(m \in \mathbb{N})$  we construct the family of operators  $\{\mathcal{A}^{\varepsilon} \in \mathcal{L}_{per}\}_{\varepsilon}$  such that the spectrum of  $\mathcal{A}^{\varepsilon}$  has exactly m gaps in [0, L] when  $\varepsilon$  is small enough, and these gaps tend to the intervals  $(\alpha_j, \beta_j)$  as  $\varepsilon \to 0$ .



Section A



Russian Academy of Sciences, Institute of Mathematics, Ufa

# SEMICLASSICAL SPECTRAL ASYMPTOTICS FOR TWO-DIMENSIONAL MAGNETIC SCHRÖDINGER OPERATORS

Let (M,g) be a two-dimensional compact oriented Riemannian manifold (possibly with boundary), and let  $\mathbf{A}$  be a real-valued differential 1-form on M. We consider the Schrödinger operator with magnetic potential  $\mathbf{A}$  (the magnetic Laplacian), which is the second order differential operator on M defined by  $H^h = (ih d + \mathbf{A})^*(ih d + \mathbf{A})$  (here h > 0 is a semiclassical parameter). If M has non-empty boundary, we assume that the operator  $H^h$  satisfies the Dirichlet boundary condition.

Let  $\mathbf{B} = d\mathbf{A}$  be the magnetic field, which is a closed 2-form on M. One can write  $\mathbf{B} = b dx_g$ , where  $b \in C^{\infty}(M)$  and  $dx_g$  is the Riemannian volume form. We assume that  $b_0 = \min_{x \in M} |b(x)| > 0$ , the set  $\{x \in M : |b(x)| = b_0\}$  is a single point  $x_0$ , which belongs to the interior of M, and the magnetic field b is non-degenerate at  $x_0$  (the case of discrete wells).

First, we state complete asymptotic expansions for the low-lying eigenvalues  $\lambda_0(H^h) \leq \lambda_1(H^h) \leq \lambda_2(H^h) \leq \ldots$  of the operator  $H^h$  as  $h \to 0$  (in semiclassical limit). Then we discuss the asymptotic behavior of the eigenvalues of  $H^h$  contained in the interval  $(-\infty, h(b_0 + \epsilon)]$  for some  $\epsilon > 0$ .

This is joint work with Bernard Helffer.

#### Evgeny Korotyaev

St. Petersburg State University, Math. Phys., St. Petersburg

### SCHRÖDINGER OPERATORS ON PERIODIC DISCRETE GRAPHS

We consider Schroedinger operators with periodic potentials on periodic discrete graphs. We show that the spectrum of the Schroedinger operator consists of an non-empty absolutely continuous part (which is a union of finite number of spectral bands, i.e., open intervals) plus finite number of flat bands, i.e., eigenvalues of infinite multiplicity. The following results are obtained:

 Estimates of the Lebesgue measure of the spectrum in terms of geometric parameters of the graph. Moreover, for some classes of graphs these estimates become identities.

 Detailed analysis of all bands for specific periodic graphs, including the face-centered cubic lattice and the graphene.

3) The existence and positions of the flat bands for specific graphs; in particular, for any integer N there exists a graph, such that the corresponding LaplaThursday September 12 4.30 – 4.55 pm

Tuesday September 10 5.00 – 5.25 pm cian has two spectral bands and N flat bands between the bands,

4) Stability estimates of bands and gaps in terms of potentials.

The proof is based on the constructed Floquet theory.

This is a joint result with Nataliya Saburova.

Aleksey Kostenko

Thursday September 12 3.00 – 3.25 pm

University of Vienna, Faculty of Mathematics, Vienna

# SPECTRAL THEORY OF 1-D SCHRÖDINGER OPERATORS WITH δ''-INTERACTIONS

We study 1-D Schrödinger operators with  $\delta'$ -interactions. Firstly, we consider Hamiltonians with  $\delta'$ -interactions concentrated on discrete sets. Using the extension theory approach [1], we establish a connection between the spectral properties (self-adjointness, lower semiboundedness etc.) of Hamiltonians with  $\delta'$ -interactions and the corresponding spectral properties of a certain class of Krein–Stieltjes strings. Further, using the form approach [2], we study lower semibounded Hamiltonians. Finally, it turns out that one can define  $\delta'$ -interactions with the help of quasi-differential expressions [3]. The latter allows us to introduce a  $\delta'$ -interaction on a set of Lebesgue measure zero (e.g., Cantor type set) and then to analyze the spectral properties of these Hamiltonians.

1. A. Kostenko and M. Malamud, 1–D Schrödinger operators with local point interactions on a discrete set, J. Differential Equations 249, 253–304 (2010).

2. A. Kostenko and M. Malamud, *Spectral analysis of semibounded Schrödinger operators with*  $\delta'$ *-interactions*, Ann. Henri Poincaré (2013), to appear. (ArXiv:1212.1691)

3. J. Eckhardt, A. Kostenko, M. Malamud and G. Teschl, *Schrödinger oper*ators with  $\delta'$ -interactions on a Cantor type set, submitted.



# Jiri Lipovsky

University of Hradec Kralove, Department of Physics, Hradec Kralove EIGENVALUE ASYMPTOTICS FOR THE DAMPED WAVE EQUATION ON METRIC GRAPHS

Linear damped wave equation on finite metric graphs is considered and its asymptotical spectral properties are researched. In the case of linear damped wave equation on an abscissa there is one high frequency abscissa, one sequence of eigenvalues with real part approaching to a constant value. In the case of a graph the location of high frequency abscissas can be determined only by the averages of the damping function on each edge. For a graph with equilateral edges we find lower and upper bounds on the number of high frequency abscissas depending on the number of its edges and its structure.

This is a joint work with prof. Pedro Freitas.

Vladimir Lotoreichik

Graz University of Technology, Institute of Computational Mathematics, Graz

# SELF-ADJOINT LAPLACIANS ON PARTITIONS WITH DELTA- AND DELTA'-COUPLINGS

In the talk I will discuss self-adjoint Laplace operators acting on partitions of Euclidean spaces into finite number of bounded and unbounded Lipschitz domains. The problem becomes non-trivial when we pose boundary conditions which connect neighboring domains in the partition. Spectral properties of the corresponding self-adjoint Laplacians turn out to be related to combinatorial properties of the partition such as the number of colors sufficient to color all the domains in a way that any two neighboring domains are associated with distinct colors.

This talk is based on the joint work with Jussi Behrndt and Pavel Exner.

Wednesday September 11 2.00 – 2.25 pm

Thursday September 12

1.30 – 1.55 pm

Thursday September 12 2.30 – 2.55 pm Mark Malamud

Institute of Applied Mathematics and Mechanics, Donetsk

# 1D SCHRÖDINGER AND DIRAC OPERATORS WITH LOCAL POINT INTERACTIONS

Let  $X = \{x_n\}_{n=1}^{\infty} \subset \mathbb{R}_+$  be a discrete set and  $d_* := \inf_{n \in \mathbb{N}} |x_{n+1} - x_n|$ . Consider the Schrödinger operator  $H_{X,\alpha,q}$  associated with the differential expression

$$H_{X,\alpha,q} = -\frac{d^2}{dx^2} + q(x) + \sum_{k=1}^{\infty} \alpha_k \delta(x - x_k), \quad \alpha_k \in \mathbb{R},$$
(3)

and its counterpart  $D_{X,\alpha,Q}$  associated with the Dirac differential expression

$$D^{c} + Q := -i c \frac{d}{dx} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \frac{c^{2}}{2} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \begin{pmatrix} q_{11} & q_{12} \\ q_{12} & q_{22} \end{pmatrix}.$$
 (4)

Here c > 0 denotes the velocity of light. Our approach to the spectral properties of operators  $H_{X,\alpha,q}$  and  $D_{X,\alpha,Q}$  with point interactions is based on a new connection of these operators with Jacobi matrices of certain classes. We show that the spectral properties of  $H_{X,\alpha} = H_{X,\alpha,0}$  like self-adjointness, discreteness, lower semiboundedness, and discreteness (finiteness) of the negative spectrum correlate with the corresponding spectral properties of Jacobi matrices of certain classes. Based on this connection, we will discuss necessary and sufficient conditions for the operators  $H_{X,\alpha}$  to be self-adjoint, lower-semibounded, to have finite negative spectrum, as well as to be discrete (in the case  $d_* = 0$ ). Self-adjointness and discreteness of  $D_{X,\alpha,Q}$  on finite and infinite intervals will also be discussed. The property of both operators  $H_{X,\alpha,q}$  and  $D_{X,\alpha,Q}$  to have either absolutely continuous or purely singular spectrum will be discussed too. The talk is based on the results of the papers [1]-[4].

#### Stepan Manko

Czech Technical University in Prague, Department of Physics, Faculty of Nuclear Science and Physical Engineering, Decin

# APPROXIMATIONS OF GENERAL QUANTUM-GRAPH VERTEX COUPLINGS

We discuss one of the central questions in quantum graph models concerning the way in which the wave functions are coupled at the graph vertices. If n edges meet at a vertex, in the absence of external fields the requirement of probability current conservation leads to the condition coupling the vectors of boundary values of the wave functions and their derivatives with the coefficients being determined by an  $n \times n$  unitary matrix. This tells us, in particular, that such a coupling may depend on  $n^2$  real parameters. P. Exner, along with



Tuesday

September 10

3.00 - 3.25 pm

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his coauthors, described how to realize the general  $n^2$ -parametric vertex coupling in terms of zero-distance limit of Dirac's delta functions. This effectively gives the practical prescription to realize the full connection conditions by using the continuous wave functions with the discontinuous gradients. We will give a solution to the problem within the framework of the real-world quantum mechanics, i.e., we are going to show how to realize the general  $n^2$ -parametric vertex coupling by using the wave functions that are continuous together with their derivatives.

The talk is based on a joint project with P. Exner.

#### Ivan Melikhov

National Research University of Information Technologies, Mechanics and Optics, Math, Saint Petersburg

# HARTREE-FOCK APPROXIMATION FOR PARTICLES STORAGE PROBLEM

The research deals with problem of particles storage in nanolayers. It can be useful in developing of the nanostructured hydrogen accumulator. The possibility to store particles, or in physical terms existence of the bound state, means the existence of the discrete spectrum of the corresponding Hamiltonian. In this work a few interacting particles with predefined spins are placed into a deformed waveguide. Delta potential of the interacting is assumed. Three types of the deformation are studied: i) a local boundary perturbation ii) two layers coupled through a window iii) a curved layer. To simplify the multi-particle Schrodinger equation the Hartree-Fock approximation is used. The eigenvalue problem is solved numerically with the help of the finite element method. Computations for different numbers and spins of particles are done. The output of the program is the minimal deformation which keeps boundary state of the system. Those results help to choose the most efficient type of deformation and system configuration. Thursday September 12 4.00 – 4.25 pm

#### Takuya Mine

Kyoto Institute of Technology, Graduate School of Science and Technology, Kyoto

# TWO-SOLENOIDAL AHARONOV-BOHM EFFECT WITH QUANTIZED MAGNETIC FLUXES

We consider the motion of a quantum particle confined in a plane under the influence of two infinitesimally thin magnetic solenoids perpendicular to the plane. Provided that two fluxes equal the quantum of magnetic flux, we give the generalized eigenfunctions of the corresponding Hamiltonian using various Mathieu functions. As a consequence, we give an explicit formula for the scattering amplitude using some special value of Mathieu functions.

### Delio Mugnolo

University of Ulm, Analysis, Ulm

# NO BOUNDARY CONDITIONS FOR A DIFFUSION EQUATION ON AN INTERVAL

I consider a one-dimensional diffusion equation subject to integral constraints on the total mass and the barycenter, instead of more common boundary conditions. It turns out that the natural operator theoretical setting is that of some space of distributions on the torus. Prior to applying energy methods, a new integration-by-parts-type formula has to be deduced. This eventually allows to prove well-posedness and Weyl-type spectral asymptotics.

This is joint work with Serge Nicaise (Valenciennes, France).

Wednesday September 11 3.00 – 3.25 pm

Wednesday

September 11 5.30 – 6.00 pm



Hiroaki Niikuni

Doshisha University, Faculty of Science and Engineering, Kyoto

# ON THE SPECTRUM OF PERIODIC SCHRÖDINGER OPERATORS ON A QUANTUM GRAPH WITH THE $\hat{i} \cdot \hat{i}' \cdot \hat{i}'$ VERTEX CONDITIONS

In this talk, we discuss the spectrum of periodic Schrödinger operators on a quantum graph with the  $\delta$ - $\delta$ - $\delta$  vertex conditions. Put  $\mathbb{J} = \{0, 1, 2\}$  and  $\mathcal{Z}_1 = \mathbb{Z} \times \mathbb{J}$ . For  $(n, j) \in \mathcal{Z}_1$ , we put  $\kappa_n = \frac{\sqrt{3}}{4}(-1)^n(1, 0, 0)$ ,  $\mathbf{e}_0 = (0, 0, 1)$ ,

$$\begin{split} \mathbf{e}_{n,0} &= (0,0,1), \quad \mathbf{e}_{n,1} = \kappa_{n+1} - \kappa_n + \frac{\mathbf{e}_0}{2}, \quad \mathbf{e}_{n,2} = \kappa_{n+2} - \kappa_{n+1} - \frac{\mathbf{e}_0}{2}, \\ \mathbf{r}_{n,0} &= \kappa_n + \frac{3n}{2} \mathbf{e}_0, \quad \mathbf{r}_{n,1} = \mathbf{r}_{n,0} + \mathbf{e}_0, \quad \mathbf{r}_{n,2} = \mathbf{r}_{n+1,0}. \end{split}$$

Using these notations, we define the sefments  $\Gamma_{n,j} = \{\mathbf{x} = \mathbf{r}_{n,j} + t\mathbf{e}_{n,j} | 0 \le t \le 1\}$  for  $(n, j) \in \mathcal{Z}_1$ . Each segment  $\Gamma_{n,j}$  is oriented by the vector  $\mathbf{e}_{n,j}$  from the initial point  $\mathbf{r}_{n,j}$  to the terminal point  $\mathbf{r}_{n,j} + \mathbf{e}_{n,j}$ . We consider the graph

$$\Gamma^1 = \bigcup_{\alpha \in \mathcal{Z}_1} \Gamma_\alpha.$$

(We see the figure of the graph in the talk.) For  $(\beta_A, \beta_B) \in \mathbb{R}^2 \setminus \{(0,0)\}$ and  $q \in L^2(0,1)$ , we define the Schrödinger operators in the Hilbert space  $L^2(\Gamma^1) = \bigoplus_{\alpha \in \mathcal{Z}_1} L^2(\Gamma_\alpha)$  as follows:

$$(Hf_{\alpha})(x) = -f_{\alpha}''(x) + q(x)f_{\alpha}(x), \quad x \in (0,1), \quad \alpha = (n,j) \in \mathcal{Z}_1,$$

$$\mathrm{Dom}(H) = \begin{cases} \bigoplus_{\alpha \in \mathcal{Z}_1} (-f''_\alpha + qf_\alpha) \in L^2(\Gamma^1), \\ -f'_{n,0}(1) + f'_{n,1}(0) - f'_{n,2}(1) = \beta_A f_{n,1}(0), \\ f_{n,1}(0) = f_{n,0}(1) = f_{n,2}(1), \\ f'_{n+1,0}(0) - f'_{n,1}(1) + f'_{n,2}(0) = \beta_B f_{n,1}(1), \\ f_{n,1}(1) = f_{n+1,0}(0) = f_{n,2}(0) \quad \text{for} \quad n \in \mathbb{Z} \end{cases}$$

The boundary condition in Dom(H) is called the  $\delta$ - $\delta$ - $\delta$  vertex condition.

The operator H is self-adjoint. The spectrum of H is closely related to the corresponding Hill operator  $L := -d^2/dx^2 + q$  in  $L^2(\mathbb{R})$ , where  $q \in L^2(0,1)$  is extended to the periodic function on  $\mathbb{R}$  with the period 1. Let  $\theta(x, \lambda)$  and  $\varphi(x, \lambda)$  be the solutions to  $(Ly)(x, \lambda) = \lambda y(x, \lambda)$  subject to the initial conditions

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$$\theta(0,\lambda) = 1, \quad \theta'(0,\lambda) = 0 \quad \text{and} \quad \varphi(0,\lambda) = 0, \quad \varphi'(0,\lambda) = 1,$$

respectively. We put

$$\begin{split} F(\lambda) &= 2\Delta^2(\lambda) + \frac{\theta(1,\lambda)\varphi'(1,\lambda)}{4} - \frac{5}{4} \\ &+ \frac{1}{4}\{(2\beta_A + \beta_B)\theta(1,\lambda) + (\beta_A + 2\beta_B)\varphi'(1,\lambda) + \beta_A\beta_B\varphi(1,\lambda)\}\varphi(1,\lambda), \end{split}$$

where  $\Delta(\lambda)$  is the Lyapunov function for L, namely,  $\Delta(\lambda) := (\theta(1, \lambda) + \varphi'(1, \lambda))/2$ . Furthermore, let  $\sigma_D(L)$  be the Dirichlet spectrum of L, and  $\sigma_\infty(H)$  the set of eigenvalues of H with the multiplicity  $\infty$ . Then, we have  $\sigma(H) = \sigma_\infty(H) \cup \sigma_{ac}(H)$ , where

$$\sigma_{\infty}(H) = \sigma_D$$
 and  $\sigma_{ac}(H) = \{\lambda \in \mathbb{R} | F(\lambda) \in [-1, 1]\}.$ 

We next describe the band structure of  $\sigma_{ac}(H)$ . Suppose that q is even and  $\beta_A\beta_B \leq 0$ . Let  $\lambda_{0,0}^+, \lambda_{0,2}^-, \lambda_{0,4}^+, \lambda_{0,4}^-, \lambda_{0,4}^+, \ldots$ , and  $\lambda_{0,1}^-, \lambda_{0,1}^+, \lambda_{0,3}^-, \lambda_{0,3}^+, \ldots$ , be the non-decreasing sequences of the periodic and anti-periodic eigenvalues of H, respectively. Then, we have

$$\lambda_{0,0}^+ < \lambda_{0,1}^- < \lambda_{0,1}^+ < \lambda_{0,2}^- \le \lambda_{0,2}^+ < \lambda_{0,3}^- < \lambda_{0,3}^+ < \lambda_{0,4}^- \le \lambda_{0,4}^+ < \dots$$

Furthermore, the absolutely continuous spectrum of H has the band structure:

$$\sigma_{ac}(H) = \bigcup_{j=1}^{\infty} [\lambda_{0,j-1}^+, \lambda_{0,j}^-].$$

In the talk, we give the asymptotics of the band edges.

#### Radek Novak

Nuclear Physics Institute, The Academy of Sciences of the Czech Republic, Department of Theoretical Physics, Rez

## BOUND STATES IN PT-SYMMETRIC LAYERS

We consider the Laplacian in a tubular neighbourhood of a hyperplane subject to non-Hermitean  $\mathcal{PT}$ -symmetric Robin-type boundary conditions. They bring the non-self-adjointness into the problem as the probability current does not vanish on either component of the boundary and the layer therefore behaves as an open system. We analyse the influence of the perturbation in the boundary conditions on the threshold of the essential spectrum using the Birman-Schwinger principle. Our aim is to derive a sufficient condition for ex-



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istence, uniqueness and reality of discrete eigenvalues. We show that discrete spectrum exists when the perturbation acts in the mean against the unperturbed boundary conditions and we are able to obtain the first term in its asymptotic expansion in the weak coupling regime.

### Igor Popov

St. Petersburg National Research University of Information Technologies, Mechanics and Optics, Higher Mathematics, St. Petersburg

# STOKES GRAPH

The system of one-dimensional Stokes and continuity equations with varying viscosity  $\eta$  and density  $\rho$  can be reduced to the Schrödinger equation with a specific potential:

$$v'' - \frac{\eta'}{\eta} \frac{\rho'}{\rho} v = 0.$$

Here v = v(x) is the flow velocity. It opens an interesting perspective. Particularly, consider the Scrödinger operator  $L = -\frac{d^2}{dx^2} + \frac{\eta'}{\eta}\frac{\rho'}{\rho}$  on a segment [a, b] with the boundary condition v'(a) = v'(b) = 0. If  $-\frac{\eta'}{\eta}\frac{\rho'}{\rho} > \varepsilon > 0$ , then our equation can present an equation for the eigenfunction of the operator, and the eigenfunction, correspondingly, gives us the velocity distribution.

Another intriguing perspective is related with graphs. Let us consider a metric graph with the Scrödinger operator L on each edge. Taking into account the above treatment we will call it the Stokes graph. It is necessary to determine boundary conditions at vertices. Consider a vertex (let it be zero point) with noutput edges. From physical conditions one has  $\rho_1(0) = \rho_2(0) = ...\rho_n(0) =$  $\rho(0)$  and  $v'_1(+0) = v'_2(+0) = ...v'_n(+0) = v'(0)$ . The last condition is related with the pressure continuity. Here  $v'_j(+0)$  is the derivative in the outgoing direction at the vertex 0. The continuity equation gives us for this vertex:

$$\sum_{j=1}^{n} v_j = -\left(\frac{\rho(0)}{\sum_{j=1}^{n} \rho'_j(+0)}\right) v'(0).$$

It is analogous to well-known  $\delta'$ -coupling condition for quantum graph. The coupling constant is related with the density derivative.

The problem of the Stokes graph is related with the spectral and the scattering problems for the corresponding quantum graph. Cases of various graph geometries are considered. It gives us interesting properties of the corresponding Stokes flows. Tuesday September 10 5.30 – 6.00 pm Tuesday September 10 2.30 – 2.55 pm

### Olaf Post

Durham University, Mathematics, Durham

SHRINKING FAT GRAPHS AND CONVERGENCE OF OPERATORS AND SPECTRA

In this talk, we give an overview of the convergence of Laplace-like operators on domains or manifolds that shrink to a metric graph. We discuss the operators appearing in the limit on the metric graph, as well as the consequences such as convergence of the spectrum.

#### Jochen Schmid

Stuttgart, Mathematik, Stuttgart

# ADIABATIC THEOREMS WITH AND WITHOUT SPECTRAL GAP CONDITION FOR NON-SEMISIMPLE SPECTRAL VALUES

We present adiabatic theorems with and without spectral gap condition for operators  $A(t) : D(A(t)) \subset X \to X$  in a Banach space X with not necessarily (weakly) semisimple spectral values  $\lambda(t)$ . We thereby generalize recent results of Avron, Fraas, Graf, Grech - and, in particular, the classic adiabatic theorems for self-adjoint operators - in various directions: most importantly, we no longer require the considered spectral values  $\lambda(t)$  to be semisimple (in the case with spectral gap) or weakly semisimple (in the case without spectral gap), but - in the latter case, for instance – rather allow  $A(t)|_{P(t)D(A(t))} - \lambda(t)$  to be merely nilpotent and  $A(t)|_{(1-P(t))D(A(t))} - \lambda(t)$  to be merely injective with dense range in (1 - P(t))X for some (then unique) projections P(t) commuting with A(t). Additionally, we impose fairly mild regularity conditions on  $t \mapsto A(t), \lambda(t), P(t)$ and, in particular, allow the domains of the operators A(t) to be time-dependent which, for instance, yields a simple alternative approach to the adiabatic theorems of Bornemann for operators defined by symmetric sesquilinear forms a(t). As a simple application to the adiabatic switching of perturbative potentials, we derive a Gell-Mann and Low theorem for not necessarily isolated eigenvalues, thereby extending a recent result of Brouder, Panati, Stoltz.





Virginia Tech, Mathematics, Blacksburg, VA

#### EIGENVALUE STATISTICS OF RANDOM BLOCK OPERATORS

We derive a criterion that allows us to establish an n-level Wegner estimate; that is, an upper bound on the probability that a local Hamiltonian has at least neigenvalues in a given energy interval. We demonstrate its usefulness by verifying the input conditions of our criterion for a certain class of random Schrödinger operators with two internal degrees of freedom. This gives the usual (1-level) Wegner estimate for these operators, as well as a weakened Minami estimate.

This work was supported in part by NSF grant DMS-1210982.

# Petr Siegl

University of Bern, Mathematical Institute, Bern

# SPECTRA OF GRAPHENE NANORIBBONS WITH ARMCHAIR AND ZIGZAG BOUNDARY CONDITIONS

We study the spectral properties of the two-dimensional Dirac operator on bounded domains together with the appropriate boundary conditions which provide a (continuous) model for graphene nanoribbons. These are of two types, namely the so-called armchair and zigzag boundary conditions, depending on the line along which the material was cut. In the former case, we show that the spectrum behaves in what might be called a "classical" way, while in the latter we prove the existence of a sequence of finite multiplicity eigenvalues converging to zero and which correspond to edge states.

### Erik Skibsted

Aarhus Universitet, Institut for Matematiske Fag, Aarhus

# DECAY OF EIGENFUNCTIONS OF ELLIPTIC PDE'S

Consider a real elliptic polynomial Q on  $\mathbb{R}^d$  and the operator  $H = Q(-i\nabla) + V$ on  $L^2 = L^2(\mathbb{R}^d)$  for a suitable class of real decaying potentials V = V(x). For any eigenfunction  $\phi \in L^2$ ,  $(H - E)\phi = 0$ , the *critical decay rate* is defined as

$$\sigma_{\rm cri} = \sup\{\sigma \ge 0 \mid e^{\sigma|x|} \phi \in L^2\}$$

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If  $0 < \sigma_{\rm cri} < \infty$  we prove the existence of a pair  $(\omega, \xi) \in S^{d-1} \times \mathbb{R}^d$ satisfying the following system of equations with  $\sigma = \sigma_{\rm cri}$ :

$$Q(\xi + i\sigma\omega) = E,$$
  

$$\nabla_{\xi}Q(\xi + i\sigma\omega) = \mu\omega; \ \mu = \omega \cdot \nabla_{\xi}Q(\xi + i\sigma\omega).$$

If the system has a solution for a given  $\sigma > 0$  we call  $\sigma$  *exceptional*.

If *E* is not a critical value of the polynomial *Q* then indeed  $0 < \sigma_{\rm cri}$ , and the eigenfunction  $\phi$  can not be super-exponentially decaying, that is indeed  $\sigma_{\rm cri} < \infty$  (our proof of the latter result requires a somewhat strong decay condition on *V*).

These results generalize well-known results for one-body Schrödinger operators. Although being very different the exceptional numbers share common features with the possible decay rates for *N*-body Schrödinger operators, determined by thresholds. In particular the set of exceptional numbers is in a typical situation countable, in fact finite, and there are no spurious elements, more precisely any exceptional number occurs as the critical decay rate for an eigenfunction with energy *E* for some potential. For example for the bilaplacian  $\Delta^2$ ,  $\sigma = E^{1/4}$  is the only exceptional number for E > 0 while  $\sigma = (-E/4)^{1/4}$  is the only exceptional number for E < 0, and in both cases this number is the critical decay rate for an eigenfunction with energy *E* for some potential (in fact possibly for a compact support potential).

Françoise Truc

Grenoble 1, Institut Fourier, St Martin d'Hères

# SCATTERING THEORY FOR GRAPHS ISOMORPHIC TO A HOMOGENEOUS TREE AT INFINITY

We describe the spectral theory of the adjacency operator of a graph which is isomorphic to a homogeneous tree at infinity. Using some combinatorics, we reduce the problem to a scattering problem for a finite rank perturbation of the adjacency operator on a homogeneous tree. We develop this scattering theory using the classical recipes for Schrödinger operators in Euclidian spaces.



# Matěj Tušek

Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Department of Mathematics, Prague EFFECTIVE HAMILTONIAN FOR A THIN CURVED QUANTUM LAYER IN A MAGNETIC FIELD

The Dirichlet Laplacian between two parallel hypersurfaces in Euclidean spaces of any dimension in the presence of a magnetic field is considered in the limit when the distance between the hypersurfaces tends to zero. In three dimensions, this operator corresponds to the Hamiltonian of the so-called quantum layer in a magnetic field. We prove that, after some obvious renormalization, the Laplacian converges in the norm-resolvent sense to a Schrödinger operator on the limiting hypersurface whose electromagnetic potential is expressed in terms of principal curvatures and the projection of the ambient vector potential to the hypersurface. As an application, we obtain an effective approximation of bound-state energies and eigenfunctions of the original system.

# Henrik Ueberschär

CEA Saclay, Gif-sur-Yvette

# QUANTUM LIMITS FOR POINT SCATTERERS ON FLAT TORI

The Laplacian with a delta potential, also known as a point scatterer, on a at torus is a popular model in Quantum Mechanics to study the transition between integrability and chaos in quantum systems. In a 1990 paper Petr Seba investigated numerically the spectrum and wave functions of a point scatterer in a rectangular billiard and found evidence of level repulsion and the random wave conjecture-features which are usually associated with quantum systems whose classical dynamics is chaotic.

In this talk I will discuss which semiclassical measures can arise for a point scatterer on a at 2d torus. It turns out the answer depends on the choice of lattice. In the case of the square lattice I will discuss a proof of Quantum Ergodicity. For irrational lattices I will construct semiclassical measures which are localised in momentum.

This is joint work with Pär Kurlberg (KTH Stockholm) and Zeev Rudnick (Tel Aviv).

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Thursday September 12 4.00 – 4.25 pm Friday September 13 2.30 – 2.55 pm Carlos Villegas-Blas Universidad Nacional Autonoma de Mexico, Instituto de Matematicas, Cuernavaca, Cuernavaca

# ON SEMICLASSICAL LIMITING EIGENVALUE AND RESONANCE DISTRIBUTION THEOREMS FOR UNBOUNDED PERTURBATIONS OF THE HYDROGEN ATOM HAMILTONIAN.

Let us consider the hydrogen atom Hamiltonian

$$H_{\hbar} = -\frac{\hbar^2}{2}\Delta_{R^3} - \frac{1}{|\mathbf{x}|}$$

The discrete spectra of  $H_{\hbar}$  consists of eigenvalues  $E_k(\hbar) = \frac{-1}{2\hbar^2k^2}$ , k = 1, 2, ...,with growing multiplicity  $d_k = k^2$ . Considering  $\hbar = \frac{1}{N}, N = 1, 2, ...$  and noticing that E = -1/2 is an eigenvalue of all the operators  $H_{1/N}$ , A. Uribe and C. Villegas-Blas have shown a limiting eigenvalue distribution theorem consisting in studying the distribution of eigenvalues within clusters of eigenvalues around E = -1/2 in the semiclassical limit  $N \to \infty$  after introducing a bounded perturbation  $\epsilon(\hbar)Q_{\hbar}$ , with  $\epsilon(\hbar) = O(\hbar^{1+\delta}), \delta > 0$ , and  $Q_{\hbar}$  a bounded pseudo-differential operator of order zero. The limiting distribution involves averages of the principal symbol of  $Q_{\hbar}$  along the classical orbits of the Kepler problem on the surface energy E = -1/2. This talk is about extensions of this theorem for unbounded perturbations like the Stark and Zeeman effects. In the Stark case, we actually have a limiting resonance distribution theorem.

This is joint work with Peter Hislop.

### Hendrik Vogt

TU Hamburg-Harburg, Institut für Mathematik, Hamburg

# A WEAK GORDON TYPE CONDITION FOR ABSENCE OF EIGENVALUES OF ONE-DIMENSIONAL SCHRÖDINGER OPERATORS

We show absence of eigenvalues for one-dimensional Schrödinger operators  $-\Delta + \mu$  under the condition that the measure  $\mu$  can be approximated by periodic measures in a suitable sense. Roughly speaking, we require that there are arbitrarily large periods p>0 such that the three "pieces"  $\mathbf{1}_{[-p,0]}\mu$ ,  $\mathbf{1}_{[0,p]}\mu$  and  $\mathbf{1}_{[p,2p]}\mu$  look very similar. This type of study is motivated by models of quasicrystals, where the corresponding potential is locally close to being periodic.

The important new aspect is that the distance of the three pieces is measured in a Wasserstein type metric and not in the total variation metric as in previous results. For linear combinations of Dirac measures this means that

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not only the coefficients but also the positions of the Dirac deltas are allowed to vary. Thus, in models of quasicrystals, the positions of atoms may be slightly perturbed from a quasiperiodic lattice.

#### Ricardo Weder

Universidad Nacional Autonoma de Mexico, Instituto de Investigaciones en Matematicas Aplicadas y en Sistemas, Mexico City

# HIGH- AND LOW- ENERGY ANALYSIS AND LEVINSON'S THEOREM FOR THE SELFADJOINT MATRIX SCHROEDINGER OPERATOR ON THE HALF LINE

The matrix Schrödinger equation with a selfadjoint matrix potential is considered on the half line with the general selfadjoint boundary condition at the origin. When the matrix potential is integrable, the high-energy asymptotics are established for the related Jost matrix, the inverse of the Jost matrix, and the scattering matrix. Under the additional assumption that the matrix potential has a first moment, it is shown that the scattering matrix is continuous at zero energy, and a explicit formula is provided for its value at zero energy. The small-energy asymptotics are established also for the related Jost matrix, its inverse, and various other quantities relevant to the corresponding direct and inverse scattering problems. Furthermore, Levinson's theorem is derived, relating the number of bound states to the change in the argument of the determinant of the scattering matrix.

### References:

[1] T. Aktosun, M. Klaus, R. Weder, Small-energy analysis for the selfadjoint matrix Schrödinger operator on the half Line, J. Math. Phys. **52** (2011) 102101, 24 pp, arXiv:1105.1794 [math-ph].

[2] T. Aktosun, R. Weder, High-energy analysis and Levinson's theorem for the selfadjoint matrix Schrödinger operator on the half line, J. Math. Phys <u>54</u> (2013) 012108, 27pp, arXiv:1206.2986 [math-ph].

The talk is based on a joint work with T. Aktosun and M. Klaus

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### Tobias Weich

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# Philipps Universität Marburg, Fachbereich Mathematik, Marburg EXPERIMENTAL STUDY OF FRACTAL WEYL LAW AND THE SPECTRAL GAP IN OPEN QUANTUM N-DISK SYSTEMS

The study of resonances in open quantum systems with fractal repeller is a fruitful topic in mathematical physics which attained much attention in recent years. One central question is the problem of counting resonances which led after some pioneering work of Sjöstrand [1] to the conjecture of the fractal Weyl law [2]. Another important point is the determination of a spectral gap, i.e. an upper bound on the imaginary part of the quantum resonances. Also here recent progress has been made in establishing rigorous bounds in terms of the topological pressure of the underlying classical system (see e.g. [3]).

Up to now the study of resonance distribution in open quantum systems with fractal repeller was restricted to mathematics and numerical studies, but there was no experimental verification, as it is very challenging to extract resonances from experimental data.

We present the first experimental studies addressing the question of the fractal Weyl law and spectral gap [4,5]. Using the equivalence between Schrödinger and Helmholtz equation we can study "quantum" n-disk systems by a microwave setup. The resonances are extracted from the measured microwave signal by the method of harmonic inversion and the number of resonances as a function of their wave number and their width distribution is compared to the mathematical predictions.

#### Grigoriy Zhislin

Nizhny Novgorod State Universitet, General and Applied Physics, N.Novgorod

# PERMUTATION SYMMETRY FOR N-PARTICLE HAMILTONIANS DISCRETE SPECTRUM STUDY WHEN N TENDS TO INFINITY

Let us consider the energy operator H(n) of the relative motion of quantum system Z, consisting of n identical particles of nucleon type with short-range potentials V of interparticle interaction. Let  $B_k = (b_1, b_2, \ldots, b_k)$  and  $I_k = (i_1, i_2, \ldots, i_k)$  be arbitrary systems of k integers, for which  $i_1 > 0$ ,  $i_s < i_t$ ,  $b_s \ge b_t$  when s < t;  $b_s > 0$  for s < k;  $b_k \ge 0$ ; if  $b_k = 0$ , then  $i_1 > 1$ . We denote by  $E(n;k) = E(n;I_k,B_k)$  the set of all types  $A = (n_1,n_2,\ldots,n_p)$  of symmetric groupe  $S_n$  irreducible representations, which are determined by decompositions  $n = n_1 + n_2 + \ldots + n_p$  of the number n into the sum of p positive integers  $n_s, n_s \ge n_t$  for s < t, where  $n_{i_s} \le b_s, s = 1, 2, \ldots, q, q = k$  if  $b_k > 0$ , q = k - 1 if  $b_k = 0$  and k > 1; p is arbitrary if  $b_k > 0$  and  $p < i_k$  if  $b_k = 0$ . Thus E(n;k) be the set of all irreducible representations types A of the groupe  $S_n$ .

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that correspond to Young schemes with p lines, for which the length of  $i_s$ -th line is not greater than  $b_s$ , s = 1, 2, ..., q, where q = k if  $b_k > 0$ , q = k - 1 if  $b_k = 0$ , k > 1; the number p of lines in the scheme is arbitrary if  $b_k > 0$  and  $p < i_k$  if  $b_k = 0$ .

Let for any A from E(n,k) P(A) be projector (in the space of the considered system relative motion states) on the subspace the states of permutational symmetry of the type A. We set H(n,k,A) = P(A)H(n) and denote by H(n,k) the sum of the operatops H(n,k,A) over all A from E(n,k). We proved the following

**Theorem.** Let the integral over  $\mathbb{R}^3$  of potential V(x, y, z) be negative. Then for any fixed k and any sets  $I_k$ ,  $B_k$  there is such infinite increasing sequence of positive integers  $N_t$ , t = 1, 2, ..., that for  $n = N_t$  the discrete spectrum of the operator H(n, k) is not empty.

It means that for each  $n = N_t$  there is at least one type  $A = A(N_t)$  from E(n,k), for which the discrete spectrum of the operator H(n,k,A) is not empty and consequently the considered system Z is stable in the space of symmetry A states.

Before this time similar result was known only for k = 1,  $B_k = B_1 = (b_1)$ ,  $I_k = I_1 = (i_1)$ , when  $i_1 = 1$ ,  $b_1 > 0$  or  $i_1 > 1$ ,  $b_1 = 0$ .

The work is supported by RFBR grant 11-01-00458-a.

### Marek Biskup

University of California, Department of Mathematics, Los Angeles

# EXTREME ORDER STATISTICS FOR EIGENVALUES OF RANDOM SCHRÖDINGER HAMILTONIANS

I will describe the conclusions of an ongoing work with Wolfgang König on eigenvalue extreme order statistics for random Schrödinger operators over the hypercubic lattice with i.i.d. on-site potentials whose law lies in a (well-defined) neighborhood of doubly-exponential tails. A key conclusion is that the extreme eigenvalues for the Hamiltonian in a box of side L lie, after proper shift and scaling, in the Gumbel universality class. As part of the analysis we also control the spatial decay of the corresponding eigenfunctions. An interesting feature of our method is that, thanks to the focus on extreme points of the spectrum, we are able to substitute most of the standard techniques for proving Anderson localization with percolation-based arguments.

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**Tuesday** September 10 4.00 – 4.25 pm Hermann Schulz-Baldes

Friedrich-Alexander-Universität Erlangen, Department Mathematik, Erlangen

THE ROLE OF INVARIANTS AND DISORDER IN TWO-DIMENSIONAL TOPOLOGICAL INSULATORS

According to a widely accepted definition, a topological insulator is a (often free) Fermion system which has surface modes that are not exposed to Anderson localization due to topological constraints given by non-trivial invariants. Prime examples are quantum Hall systems, but there are other classes in the Altland-Zirnbauer classification (specified by time, particle-hole and chiral symmetries) which lead to non-trivial topological insulators in this sense. The talk focuses on the two-dimensional cases and reviews rigorous results on basic toy models.

#### Eman Hamza

Cairo

# SPECTRAL TRANSITION FOR RANDOM QUANTUM WALKS ON TREES

We consider random quantum walks on a homogeneous tree of degree 3 describing the discrete time evolution of a quantum particle with internal degree of freedom in  $\mathbb{C}^3$  hopping on the neighboring sites of the tree in presence of static disorder. The one time step random unitary evolution operator of the particle depends on a unitary matrix  $C \in U(3)$  which monitors the strength of the disorder. We show the existence of open sets of matrices in U(3) for which the random evolution has either pure point spectrum almost surely or purely absolutely continuous spectrum. We also establish properties of the spectral diagram which provide a description of the spectral transition driven by  $C \in U(3)$ .

### Martin Gebert

Universität München, Mathematisches Institut, München

# LOCALIZATION FOR RANDOM BLOCK OPERATORS

We investigate the spectral properties of a certain type of random block operators arising in a mean field approximation of the BCS theory of dirty superconductors. We prove a Wegner estimate and Lifschitz tails at the inner band edges. Using these ingredients and a multi-scale analysis, we prove dynamical localization in a neighbourhood of the inner band edges.

This is joint work with Peter Müller.



Francisco Hoecker-Escuti

Technische Universität Chemnitz, Fakultät für Mathematik, Chemnitz

FREQUENCY CONCENTRATION OF THE EIGENFUNCTIONS OF THE ANDERSON MODEL IN THE BULK OF THE SPECTRUM AT WEAK DISORDER.

In an important paper in 2002, W. Schlag, C. Shubin and T. Wolff proved that, in a small coupling constant regime  $\lambda \ll 1$ , the mass of the eigenfunctions of the Anderson model  $H_{\omega} = \triangle + \lambda V_{\omega}$  having their energies in the bulk of the spectrum, concentrate essentially in rings of size  $\lambda^{2+\epsilon}$  in Fourier space. Their result is valid in dimensions 1 and 2 (in dimension 2 one restricts the operator to a box). The purpose of this talk is to show that the same phenomenon appears in any dimension.

# Fumihiko Nakano

Gakushuin University, Department of Mathematics, Tokyo

# LEVEL STATISTICS FOR ONE-DIMENSIONAL SCHROEDINGER OPERATOR

We study the level statistics of one-dimensional Schrödinger operator with random potential decaying like  $x^{-\alpha}$  at infinity. We consider the point process  $\xi_L$ consisting of the rescaled eigenvalues and show that : (i)(ac spectrum case) for  $\alpha > \frac{1}{2}$ ,  $\xi_L$  converges to a clock process, and the fluctuation of the eigenvalue spacing converges to Gaussian. (ii)(critical case) for  $\alpha = \frac{1}{2}$ ,  $\xi_L$  converges to the limit of the circular  $\beta$ -ensemble.

This is a joint work with S. Kotani.

# **Christian Seifert**

Hamburg University of Technology, Institute of Mathematics, Hamburg

# CANTOR TYPE SPECTRA OF LEBESGUE MEASURE ZERO FOR CONTINUUM ONE-DIMENSIONAL QUASICRYSTALS

We consider an ergodic family  $(H_{\omega})_{\omega\in\Omega}$  of continuum one-dimensional Schrödinger operators, where we allow for measures as potentials. We show that the random operator H has Cantor type spectra of Lebesuge measure zero under suitable finite local complexity conditions on the potentials. Such operator families appear in the study of quasicrystalline models.

The talk is based on joint work with Daniel Lenz (FSU Jena, Germany) and Peter Stollmann (Chemnitz University of Technology, Germany).

Tuesday September 10 2.00 – 2.25 pm

**Tuesday** September 10 1.30 – 1.55 pm

Tuesday September 10 4.00 – 4.25 pm Jeremy Faupin

Université de Bordeaux 1, Institut de Mathématiques de Bordeaux, Talence Cedex

# ON RAYLEIGH SCATTERING IN NON-RELATIVISTIC QUANTUM ELECTRODYNAMICS

In this talk we consider a particle system coupled to the quantized electromagnetic field in the standard model of non-relativistic QED. We prove Asymptotic Completeness for Rayleigh scattering on the states for which the photon number operator is uniformly bounded in time. This result is obtained, in particular, thanks to propagation estimates for photons justifying that asymptotically as time tends to infinity, photons propagate at the speed of light.

Joint work with I.M. Sigal

# Jan Derezinski

University of Warsaw, Faculty of Physics, Warszawa

# MASSIVE AND MASSLESS VECTOR QUANTUM FIELDS

Even though quantization of the (free) Proca and Maxwell equation is one of the classic subjects of relativistic quantum field theory, I have never been satisfied with its discussion in the usual textbooks. There are at least two issues, that are confusing: there are several methods to quantize, and the nature of the massless limit is quite delicate. In my talk I will discuss several approaches to the quantization of vector fields. I will also describe its massless limit, which is quite singular – the number of spin degress of freedom jumps from 3 to 2.

## Christian Hainzl

University of Tübingen, Mathematik, Tübingen

# GROUND STATE PROPERTIES OF GRAPHENE IN HARTREE-FOCK THEORY

We study the Hartree-Fock approximation of graphene in infinite volume, with instantaneous Coulomb interactions. First we construct its translation-invariant ground state and we recover the well-known fact that, due to the exchange term, the effective Fermi velocity is logarithmically divergent at zero momentum. In a second step we prove the existence of a ground state in the presence of local defects and we discuss some properties of the linear response to an external electric field.

This is joint work with M. Lewin and Ch. Sparber.



Thursday September 12 2.30 – 3.25 pm

Section C

Invited Talk

Invited Talk

Wednesday

September 11 2 30 - 3 25 pm

Invited Talk Friday September 13 2.30 – 3.25 pm

#### Yana Butko

Bauman Moscow State Technical University, Department of Fundamental Sciences, Moscow

# FEYNMAN FORMULAS AND FEYNMAN PATH INTEGRALS FOR DESCRIPTION OF QUANTUM DYNAMICS

A new approach to describe quantum evolution is presented. This approach is based on Feynman formulas. Feynman formula is a representation of a solution of an evolution equation by a limit of iterated n-fold integrals when n tends to infinity. One succeeds to obtain such representations for solutions of different classes of evolution equations on various geometrical structures. Sometimes one succeeds to get Feynman formulas containing only integrals of elementary functions. Such Feynman formulas allow to calculate solutions of evolution equations directly and, consequently, to model quantum dynamics numerically.

The limits of iterated integrals in Feynman formulas often coincide with functional integrals (i.e. integrals over infinite dimensional path spaces) with respect to probability measures (such integrals are called Feynman-Kac formulas) or with respect to Feynman type pseudomeasures (such integrals are called Feynman path integrals). First, the representations of solutions of evolution equations by Feynman-Kac formulas allow to investigate the considered dynamics by means of stochastic analysis, e.g., by the method of Monte-Carlo. And the approach of Feynman formulas provides a new way to establish Feynman-Kac formulas. Second, the limits of iterated finite dimensional integrals in some Feynman formulas can be used to define rigorously several Feynman path integrals over paths both in configuration and in phase space. And, on the other hand, the iterated integrals themselves reveal, in turn, the tool to calculate Feynman path integrals. Besides, different types of Feynman formulas for the same evolution equation allow to connect some Feynman path integrals with functional integrals with respect to probability measures. This gives another way to calculate Feynman path integrals and, moreover, develops deeper connections between quantum mechanics and stochastic analysis. Furthermore, the approach of Feynman formulae allows to distinguish different procedures of guantization in the language of Feynman path integrals.

Different types of Feynman formulae will be presented in the talk. It is planned to consider the cases of the Cauchy and Cauchy–Dirichlet problems for parabolic and Schroedinger type equations in a Euclidean space and in a Riemannian manifold; pseudo-differential equations related to stochastic jump processes (including diffusion of particles with variable mass and the processes generated by relativistic Hamiltonian and fractional Laplacian), multiplicative and additive perturbations of the dynamics. It is also planned Thursday September 12 5.00 – 5.25 pm to discuss Feynman formulae for evolution semigroups generated by different procedures of quantization of a polynomial Hamilton function. Further, it is supposed to present a construction of phase space Feynman path integrals, allowing to distinguish different procedures of quantization, and to discuss Feynman path integrals which correspond to the Feynman formulas mentioned in the talk. Some of the considered results are obtained in collaboration with O.G. Smolyanov, R.L. Schilling and M.G. Grothaus.

The work has been supported by the Grant of the President of Russian Federation, the Grant of the Ministry of education and science of Russian Federation, DFG, Erasmus Mundus, DAAD.

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Ya.A. Butko. Feynman formulas and functional integrals for diffusion with drift in a domain on a manifold, Math. Notes, N3 (2008), 301-316.

Ya.A. Butko. Function integrals corresponding to a solution of the Cauchy-Dirichlet problem for the heat equation in a domain of a Riemannian manifold, J. Math. Sci., N1 (2008), 2629-2638.

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Ya.A. Butko. Functional Integrals for the Schroedinger Equation on a Compact Riemannian manifold, Math. Notes N2 (2006), 194-200.





ETH Zurich, Institut f. Theoretische Physik, Zurich

# GENERALIZED ASYMPTOTIC COMPLETENESS IN LOCAL RELATIVISTIC QFT

We formulate a generalized concept of asymptotic completeness and show that it holds in any massive relativistic quantum field theory satisfying the Haag-Kastler axioms. It remains valid in the presence of pairs of oppositely charged particles in the vacuum sector, which invalidate the conventional property of asymptotic completeness. Our result can also be recast as a criterion characterizing the class of theories with complete particle interpretation in the conventional sense. This criterion is formulated in terms of certain asymptotic observables (Araki-Haag detectors) whose existence, as strong limits of their approximating sequences, is the main technical step of our analysis. It is accomplished with the help of a novel propagation estimate, which is also relevant to scattering theory of quantum mechanical dispersive systems.

Wataru Ichinose

Shinshu University, Mathematical Sciences, Matsumoto

# ON THE FEYNMAN PATH INTEGRAL FOR THE DIRAC EQUATION IN THE GENERAL DIMENSIONAL SPACETIME

The Dirac equation in the general dimensional spacetime

$$\begin{split} i\hbar\frac{\partial u}{\partial t}(t) &= H(t)u(t) \\ &:= \left[c\sum_{j=1}^{d}\widehat{\alpha}^{(j)}\left(\frac{\hbar}{i}\frac{\partial}{\partial x_{j}} - eA_{j}(t,x)\right) + \widehat{\beta}mc^{2} + eV(t,x)\right]u(t) \end{split}$$

is considered, where constant matrices  $\widehat{\alpha}^{(j)}$  and  $\widehat{\beta}$  are assumed to be simply Hermitian.

In this talk the Feynman path integral for the Dirac equation above is determined mathematically in the form of the sum-over-histories satisfying the superposition principle, i.e. the "sum" of the probability amplitudes with a common weight over all possible paths that go in any direction at any speed forward and backward in time.

It is noted that our Feynman path integral is determined not in configuration space, but in phase space.

Wednesday September 11 2.00 – 2.25 pm

Friday

September 13 2.00 – 2.25 pm Oliver Matte

#### Thursday September 12 4.30 – 4.55 pm

# Aarhus Universitet, Instut for Matematik, Aarhus C STOCHASTIC CALCULUS AND NON-RELATIVISTIC QED

We consider Feyman-Kac type formulas for the standard model of nonrelativistic quantum electrodynamics. In particular, the spin degrees of freedom may be taken into account. We present a new derivation of the Feyman-Kac formulas by means of the stochastic calculus in Hilbert spaces and explain how the corresponding stochastic differential equations can be used to discuss regularity properties of a Fock space operator-valued semigroup kernel associated with the Hamiltonian.

The talk is based on joint work with Batu Güneysu and Jacob Møller.

#### Ivan Naumkin

Universidad Nacional Autonoma de Mexico UNAM, Instituto de Investigaciones en Matemáticas Aplicadas y Sistemas, Mexico DF

# HIGH-ENERGY AND SMOOTHNESS ASYMPTOTIC EXPANSION OF THE SCATTERING MPLITUDE FOR THE DIRAC EQUATION AND APPLICATIONS

In this talk we present explicit formulae for the on-diagonal singularities of the scattering amplitude for the Dirac equation with short-range electromagnetic potentials and for its high-energy expansion. Using these formulae we prove the uniqueness of the inverse scattering problem, both at fixed-energy and at high-energy. We also discuss a method for the unique reconstruction of the electric potential and the magnetic field.

This talk is based on join work with Ricardo Weder, Instituto de Investigaciones en Matematicas Aplicadas y en Sistemas, Universidad Nacional Autonoma de Mexico, Mexico.

Friday

September 13

1.30 - 1.55 pm



# Nuri Unal

Akdeniz, Physics, Antalya

# QUANTUM FLUCTATIONS OF PHOTON IN A TIME VARYING MEDIA: COHERENT STATE APPROACH

We discuss the quantization of electromagnetic fields in a media with time varying dielectric permittivity,  $epsilon(t) = epsilon_0expetat$ . For each mode of oscillations, the quantum fluctations of the vector potential are converted into the damping harmonic oscillator. Then, we derive the quasi-coherent states for a damping harmonic oscillator and discuss the quantum fluctations of the electric and magnetic fields. Additionally, we derive non stationary quantum states in the configuration space of a photon and discuss the mean value and uncertainities in the photon numbers.

Thursday September 12 4.00 – 4.25 pm Christian Schilling

Invited Talk Tuesday September 10 4.00 – 4.55 pm

# ETH Zürich, Institute for Theoretical Physics, Zürich

### QUANTUM MARGINAL PROBLEM AND ITS PHYSICAL RELEVANCE

The question whether given marginals for subsystems of a multipartite quantum system are compatible to a common total state is called Quantum Marginal Problem (QMP). We present the solution found by A.Klyachko some years ago and the main steps for its derivation. Applying those concepts to fermionic systems leads to constraints on (mathematically) possible occupation numbers, strengthening Pauli's exclusion principle. By studying a natural physical model we find evidence that few-fermion ground states approximately saturate those generalized Pauli constraints. This effect of *quasi-pinning* is physically relevant since it corresponds to very specific and simplified structures of the corresponding *N*-fermion state. Our findings suggest a generalization of the Hartree-Fock approximation.

#### Walter de Siqueira Pedra

Universidade de São Paulo, Departamento de Física-Matemática, Sao Paolo CONDUCTIVITY MEASURE FOR LATTICE FERMIONS FROM JOULE'S LAW.

The concept of conductivity measure has been introduced for the first time by Klein, Lenoble and Müller for non-interacting lattice fermions in presence of disorder. We show how such measures can be obtained from Bochner's theorem and Joule's law, which says that electric resistance in conducting media is related to (positive) heat production. Our approach can be applied to fermions with short range interactions and in presence of disorder. We prove, moreover, that the conductivity measure is the Fourier transform of a time-correlation function of current fluctuations, i.e. it satisfies Green-Kubo relations.

Invited Talk Wednesday September 11 1.30 – 2.25 pm



### Benjamin Schlein

University of Bonn, Institute for Applied Mathematics, Bonn

#### HARTREE-FOCK DYNAMICS FOR WEAKLY INTERACTING FERMIONS.

For fermionic systems, the mean field regime is naturally linked to a semiclassical limit. Asymptotically, the many body evolution can be described by the classical Vlasov equation. A better approximation to the Schroedinger dynamics is given by the Hartree-Fock (or the Hartree) equation. In this talk, we will show precise bounds on the difference between the Schroedinger and the Hartree-Fock dynamics, for initial data close to Slater determinants with the correct semiclassical structure.

This is a joint work with Niels Benedikter and Marcello Porta.

Franz Achleitner

Vienna University of Technology, Institute for Analysis and Scientific Computing, Vienna

# TRAVELING WAVE SOLUTIONS IN SCALAR CONSERVATION LAWS WITH ANOMALOUS DIFFUSION

We consider scalar conservation laws with anomalous diffusion,

$$\partial_t u + \partial_x f(u) = \partial_x \mathcal{D}^{\alpha} u, \quad (t, x) \in \mathbb{R}_+ \times \mathbb{R},$$
(5)

for a density  $u: \mathbb{R}_+ \times \mathbb{R} \to \mathbb{R}$ ,  $(t, x) \mapsto u(t, x)$ , a smooth flux function f(u) and a non-local operator

$$(\mathcal{D}^{\alpha}u)(x) = \frac{1}{\Gamma(1-\alpha)} \int_{-\infty}^{x} \frac{u'(y)}{(x-y)^{\alpha}} dy$$
(6)

with  $0 < \alpha < 1$ .

We prove the global solvability for the associated Cauchy problem in  $L^{\infty}$ , i.e. the existence of a unique mild solution for the Cauchy problem with essentially bounded initial datum, by following the analysis of Droniou, Gallouet and Vovelle [3] in case of an anomalous diffusion realized by a fractional Laplacian. The crucial property is the non-negativity of the semigroup generated by  $\partial_x \mathcal{D}^{\alpha}$ , which is a consequence of its interpretation as an infinitesimal generator of an  $(\alpha + 1)$ -stable Levy process [5], and allows to prove a maximum principle for solutions of the Cauchy problem.

To analyze the existence of traveling wave solutions connecting different far-field values, we work with the original representation of  $\mathcal{D}^{\alpha}$ , and obtain the traveling wave equation in form of a nonlinear Volterra integral equation. As-

Invited Talk Friday September 13 1.30 – 2.25 pm

Tuesday

September 10 5.00 – 5.25 pm suming (even a bit less than) convexity of the flux function and that the solutions of the associated linear Volterra integral equation form a one-dimensional subspace of  $H^2(\mathbb{R}_-)$ , we can show the existence and uniqueness of monotone solutions satisfying the entropy condition for classical shock waves of the underlying inviscid conservation law. This requires to extend the well known results for the existence of viscous shock profiles, which solve (local) ordinary differential equations.

Moreover, we prove the dynamic nonlinear stability of the traveling waves under small perturbations, similarly to the case of the standard diffusive regularization, by constructing a Lyapunov functional.

For more details, we refer to our article [1].

Finally, we will provide an example of a single layer shallow water flow, where the pressure is governed by a nonlinear conservation law with the aforementioned nonlocal diffusion term and additional dispersion term [4], and report on our recent progress in the analysis of smooth shock profiles [2].

#### References

- F. Achleitner, S. Hittmeir and Ch. Schmeiser, On nonlinear conservation laws with a nonlocal diffusion term, *Journal of Differential Equations*, 250(4) (2011), pp. 2177 – 2196.
- [2] F. Achleitner, C. Cuesta and S. Hittmeir, Existence and Stability of travelling wave solutions in Korteweg-de Vries-Burgers equation with nonlocal diffusion, work in progress.
- [3] J. Droniou, T. Gallouet and J. Vovelle, Global solution and smoothing effect for a non-local regularization of a hyperbolic equation, J. Evol. Equ., 3 (2003), pp. 499–521.
- [4] A. Kluwick, E. A. Cox, A. Exner and C. Grinschgl, On the internal structure of weakly nonlinear bores in laminar high Reynolds number flow, Acta Mech., 210 (2010), pp. 135–157.
- [5] Ken-iti Sato, Lévy processes and infinitely divisible distributions, Cambridge University Press, (1999).

#### Ioannis Anapolitanos

Universität Stuttgart, Mathematics, Stuttgart

# THE GROUND STATE ENERGY OF THE MULTI-POLARON IN THE STRONG COUPLING LIMIT

We consider the Fröhlich *N*-polaron Hamiltonian in the strong coupling limit and bound its ground state energy from below. In particular, our lower bound confirms that the ground state energy of the Fröhlich polaron and the ground state energy of the associated Pekar-Tomasevich variational problem are asymptotically equal in the strong coupling limit. We generalize the operator approach that was used to prove a similar result in the N = 1 case by Lieb and Thomas, and apply a Feynman-Kac formula to obtain the same result for an arbitrary particle number N > 1.



Tuesday September 10 3.00 – 3.25 pm

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### Anton Arnold

Vienna University of Technology, Inst. for Analysis & Sc. Computing, Wien QUANTUM FOKKER-PLANCK MODELS: KINETIC VS. OPERATOR THEORY APPROACHES

Dissipative open quantum systems like quantum-Fokker-Planck models play an important role for quantum Brownian motion, quantum optics, and the numerical simulation of nano-semiconductor devices. Their time evolution can be described either by quantum kinetic Wigner function models or in the density matrix formalism. In this talk we compare both approaches w.r.t. the existence of a unique (normalized) steady state and the large-time convergence to it.

Dissipative open quantum systems like quantum-Fokker-Planck models play an important role for quantum Brownian motion, quantum optics, and the numerical simulation of nano-semiconductor devices. Their time evolution is determined on one hand by the Hamiltonian of the considered system, and on the other hand by its one-way coupling to a heat bath. Their mathematical description can be based on quantum kinetic Wigner function models or on the density matrix formalism.

In this talk we compare the analytic features of both approaches. We shall focus on the existence of a unique (normalized) steady state and large-time convergence to it (in trace class norm). This involves tools from semigroup theory, spectral theory, operator theory, and quantum probability. In the operator formalism, the proofs cover quadratic confinement potentials along with subquadratic perturbations. In the kinetic approach we can (at present) only treat small, smooth perturbations of the quadratic potential. But here we obtain exponential convergence rates for the large-time behavior which is not yet available in the density matrix framework.

References: A. Arnold, I. Gamba, M.P. Gualdani, S. Mischler, C. Mouhot, C. Sparber: The Wigner-Fokker-Planck equation: stationary states and large time behavior, Math. Mod. Methods Appl. Sc. 22, No. 11 (2012) 1250034.

A. Arnold, F. Fagnola, L. Neumann: Quantum Fokker-Planck models: the Lindblad and Wigner approches, "Quantum Probability and related Topics - Proceedings of the 28th Conference" (Series: QP-PQ: Quantum Probability and White Noise Analysis - Vol. 23), J.C. Garcia R. Quezada, S.B. Sontz (Eds.), World Scientific 2008.

A. Arnold, C. Sparber: Quantum dynamical semigroups for diffusion models with Hartree interaction, Comm. Math. Phys. 251, no.1 (2004) 179-207.

Wednesday September 11 3.00 – 3.25 pm

### Niels Benedikter

Friday September 13 2.30 – 2.55 pm

# University of Bonn, Institute for Applied Mathematics, Bonn QUANTITATIVE DERIVATION OF THE GROSS-PITAEVSKII EQUATION

In typical experiments, Bose-Einstein condensates are initially prepared in a trapping potential. The trap is then released to observe the evolution of the condensate. The dynamics have been found to be described by the non-linear Gross-Pitaevskii equation. On a more fundamental level, condensates can be described as a quantum gas of N particles interacting through a potential with very short scattering length (of the order 1/N, i.e. describing rare but strong collisions). This poses the question whether the Gross-Pitaevskii equation can be derived from the Schrödinger equation in the limit of large N. Due to the presence of strong correlations, this question is mathematically much more intricate than for mean-field models, which at first sight appear to be formally similar.

Taking explicitly into account two-particle correlations by a Bogoliubov transformation, we find a natural class of initial data in Fock space for which the evolution is correctly described by the Gross-Pitaevskii equation (on the level of one-particle observables). More precisely, we prove that the one-particle reduced density matrix of the system evolved by the full Schrödinger equation can be approximated in trace norm by the density matrix evolved by the Gross-Pitaevskii equation, up to an error of order  $N^{-1/2}$  at any fixed time.

### Horia Cornean

Aalborg University, Department of Mathematical Sciences, Aalborg

# NON-EQUILIBRIUM STEADY-STATES FOR INTERACTING OPEN SYSTEMS

We give sufficient conditions for the existence of steady-state Green-Keldysh correlation functions for interacting mesoscopic systems coupled to reservoirs (semi-infinite leads). The partitioning and partition-free scenarios are treated on an equal footing. Moreover, our time-dependent scattering approach proves the independence of the steady-state quantities from the initial state of the sample, and that the stationary current vanishes when the bias is zero.

This is joint work with V. Moldoveanu (Bucharest) and C.-A. Pillet (Toulon).



Wednesday

September 11

2.30 - 2.55 pm



#### A TRANSIENT DRIFT-DIFFUSION KOHN-SHAM THEORY

We propose a drift-diffusion Kohn–Sham system providing a thermodynamically motivated model for charge transport in heterogeneous semiconductor materials with non-local operators for the charge carrier densities and currents.

The theory is in the general framework of Transient Density Functional Theory, yet, the evolution is not governed by the semigroup of the Schrödinger operator, but by the driving force to equilibrium.

One ends up with an abstract evolution equation of parabolic type such that the free energy of the complex quantum system decays along trajectories of the evolution system. Tuesday September 10 1.30 – 1.55 pm

Tuesday

September 10

2.30 – 2.55 pm

#### Joachim Kerner

Royal Holloway, University of London, Mathematics, Egham

# INTERACTING MANY-PARTICLE SYSTEMS AND BOSE-EINSTEIN CONDENSATION ON GENERAL COMPACT QUANTUM GRAPHS

In recent years, quantum graphs have become useful models in quantum chaos as well as other areas of physics. Most of the results, however, concern oneparticle quantum graphs only. In this talk, we will introduce models of interacting many-particle systems on general compact quantum graphs. The models will incorporate two types of interactions, singular interactions localised at the vertices and contact interactions which are also present along the edges. Subsequently, we use the developed models to discuss Bose-Einstein condensation in interacting many-particle systems on general quantum graphs. We show that a many-particle system, interacting with singular external potentials only, shows condensation if and only if the interaction is not fully repulsive. We then implement particle-particle interactions and show, as a final result, that repulsive hard-core interactions suppress Bose-Einstein condensation. Most importantly, this result holds independently of the singular interactions in the vertices. Alexander Mielke

Tuesday September 10 5.30 – 6.00 pm

# Weierstrass Institute for Applied Analysis and Stochastics, Berlin ENTROPY-DRIVEN DISSIPATIVE COUPLING OF QUANTUM MECHANICS TO SIMPLE HEAT BATHS

Pure quantum mechanics can be formulated as a Hamiltonian system in terms of the density matrix. The von Neumann entropy can be used to model dissipative effects, in particular for the coupling to dissipative macroscopic systems such as heat baths. Following O"ttinger (2010) we use the GENERIC framework (General Equations for Non-Equilibrium Reversible Irreversible Coupling) to construct thermodynamically consistent evolution equations as a sum of a Hamiltonian and a gradient-flow contribution.

The dissipation mechanism is modeled via the canonical correlation operator, which is the inverse of the Kubo-Mori metric for density matrices and which is strongly linked to the von Neumann entropy for quantum systems. Thus, one recovers the dissipative double-bracket operators of the Lindblad equations but encounters a correction term for the consistent coupling to the dissipative dynamics.

In particular, we consider a model where a quantum system is coupled to two simple heat baths. In the limit of large heat capacities but different temperatures of the heat baths, one can study the non-equilibrium steady state and its energy flux through the quantum mechanical system.

A. Mielke. Dissipative quantum mechanics using GENERIC, WIAS preprint 1710, 2012. To appear in "Proceedings of the Conference "Recent Trends in Dynamical Systems, Springer Verlag, 2013".

#### Shuji Watanabe

Gunma University, Division of Mathematical Sciences, Graduate School of Engineering, Maebashi

# TEMPERATURE DEPENDENCE OF THE SOLUTION TO THE BCS GAP EQUATION FOR SUPERCONDUCTIVITY AND FIXED POINT THEOREMS

In previous literature, the existence and uniqueness of the solution to the BCS gap equation for superconductivity were established for each fixed temperature. But the temperature dependence of the solution was not covered. For example, how the solution varies with the temperature was not pointed out, and it was not shown that the solution is continuous with respect to the temperature. Since studying the temperature dependence of the solution is very important, we address this problem. On the basis of the Schauder fixed-point theorem, we



Tuesday

September 10 2.00 – 2.25 pm first give another proof of the existence and uniqueness of the solution so as to show how the solution varies with the temperature. More precisely, we show that the solution belongs to a certain set, from which we see how the solution varies with the temperature. On the basis of the Banach fixed-point theorem, we then show that the solution is indeed continuous with respect to both the temperature and the wavevector when the temperature satisfies a certain condition.

Shuji Watanabe, *The solution to the BCS gap equation and the second-order phase transition in superconductivity*, Journal of Mathematical Analysis and Applications **383** (2011), 353-364.

Shuji Watanabe, Addendum to 'The solution to the BCS gap equation and the second-order phase transition in superconductivity', Journal of Mathematical Analysis and Applications **405** (2013), 742–745.

Shuji Watanabe, *An embedding theorem of Sobolev type for an operator with singularity*, Proceedings of the American Mathematical Society **125** (1997), 839–848.

#### Jianfeng Lu

Duke University, Mathematics Department, Durham TIME REVERSIBLE BORN OPPENHEIMER MOLECULAR DYNAMICS

Ab initio molecular dynamics in which the ionic forces are obtained from electronic structure calculations is widely used in many fields. Conventional Born-Oppenheimer dynamics suffers from time irreversibility, while Car-Parrinello molecular dynamics has issues when the system has a tiny gap or is gapless. A time reversible modified Born Oppenheimer molecular dynamics (TRBOMD) was proposed recently. In this talk, we will analyze this time reversible dynamics, in particular, we will identify conditions such that the dynamics well approximate the physical time evolution. Invited Talk Thursday September 12 1.30 – 2.25 pm Invited Talk Thursday September 12 4.00 – 4.55 pm

Invited Talk

1.30 - 2.25 pm

Friday September 13

### Gabriel Stoltz

# Ecole des Ponts, CERMICS, Marne la Vallée

# THE MICROSCOPIC ORIGIN OF THE MACROSCOPIC DIELECTRIC PERMITTIVITY OF CRYSTALS

The aim of this talk is to present a study of the response of crystals to external, static or time-dependent forcings. The mathematical treatment relies on the properties of localized defects and their time evolutions. In particular, it provides a mathematical analysis of the Adler-Wiser formula relating the (possibly frequency dependent) macroscopic relative permittivity tensor to the microscopic structure of the crystal at the atomic level. It also gives sound foundations to the random phase approximation, a fundamental ingredient of the GW approximation to compute accurate band gaps in photovoltaic materials.

### Virgine Ehrlacher

École des Ponts ParisTech, CERMICS, Marne la Vallée GREEDY ALGORITHMS FOR ELECTRONIC STRUCTURE CALCULATIONS OF MOLECULAR SYSTEMS

In this talk, a new greedy algorithm for the resolution of electronic structure calculations for molecular systems will be presented. The principle of this numerical method consists in computing an approximation of the ground state wavefunction of the molecule, solution of the many-body Schrödinger equation, as a sum of Slater determinants where each of these Slater determinants are computed iteratively as the best possible, in a sense which will be made clear in the talk. The advantage of this new family of methods relies in the fact that the resolution of the original high-dimensional problem is replaced with the resolution of several low-dimensional problems, which enables one to circumvent the curse of dimensionality inherent to the resolution of the electronic problem. The convergence results we proved for our algorithms will be detailed, along with some convergence rates in finite dimension.

This is joint work with Davide Bianco, Eric Cances, Majdi Hochlaf and Tony Lelièvre

QMATH 12 Umboldt-Universität zu Berlin

### Andreas Arnold

Karlsruhe Institute of Technology, Department of Mathematics, Karlsruhe APPROXIMATION OF HIGH-DIMENSIONAL INITAL VALUE PROBLEMS IN THE HIERARCHICAL TUCKER FORMAT

In this talk we will show how the hierarchical Tucker format can be used to approximate the solution of a high-dimensional initial value problem. Moreover we will present an *a posteriori* error bound for the dynamical approximation.

The multiconfiguration time-dependent Hartree method (MCTDH) proposed by Meyer, Manthe and Cederbaum approximates the solution of the Schrödinger equation on a low-dimensional ansatz manifold. Wang and Thoss extended the MCTDH theory to a multilayer formulation. The idea behind this formalism can be transferred to the approximation of high-dimensional initial value problems. For this purpose the set of tensors in the hierarchical Tucker format can be considered as a low-dimensional ansatz manifold. This format is closely related to the multilayer formulation, as each of these tensors can be decomposed recursively into sums of products of lower-dimensional tensors. In order to obtain a time-dependent approximation on the manifold, equations of motion for the parameters of the format were derived from the Dirac-Frenkel variational principle. The equations of motion lead to a new non-linear initial value problem of moderate size, which approximates the primary one. As time-dependent partial differential equations can be approximated by ordinary differential equations through a suitable space-discretization, this ansatz is also a promising approach for the numerical solution of high-dimensional time-dependent partial differential equations.

The presented results are closely related to a recent work of Lubich, Rohwedder, Schneider and Vandereycken.

#### Markus Bachmayr

RWTH Aachen, IGPM, Aachen ERROR ESTIMATES FOR GAUSSIAN APPROXIMATIONS IN QUANTUM CHEMISTRY

Gaussian-type orbitals are the most widely used basis functions in molecular simulations. However, the known mathematical results explaining their high approximation efficiency apply only to very restricted situations. We present new results towards a systematic error analysis of such approximations in the conThursday September 12 3.00 – 3.25 pm

Thursday September 12 2.30 – 2.55 pm text of Hartree-Fock and Kohn-Sham models. We consider on the one hand approximations based on Hermite Gaussians, where algebraic convergence rates can be characterized in terms of appropriate notions of regularity. On the other hand, we study approximations by even-tempered Gaussians, which are much more closely related to the Gaussian bases used in practice. Here we obtain almost exponential convergence in  $H^1$ -norm for approximations of functions with radial parts of the form  $r^n e^{-\gamma r}$ . Via linear combinations, in principle this also yields error estimates for the approximation of more general wavefunctions, but the constants arising in the estimates lead to quite restrictive conditions on the approximands. Furthermore, we also point out connections to approximations based on low-rank tensor representations and wavelet bases, where error estimates can be obtained by similar techniques.

### Xiaofei Huang

eGain Communications, Sunnyvale CRITICAL MISSING EQUATION OF QUANTUM PHYSICS FOR UNDERSTANDING ATOMIC STRUCTURES

Our current understanding of electron motions in an atom is just like the Kepler era at understanding planetary motions in our solar system. We know the mathematical formula for describing the electron orbit (the electron cloud to be more accurate). However, we do not know why it must satisfy the formula and how an electron moves from one orbit to another. This paper postulates that the answers to these two critical questions may lie in a global optimization equation that nature deploys so that atoms and molecules can find their ground states, i.e., the global minimal energy states. The electron orbits are the equilibrium points of the equation and the orbit jumping can be understood as the energy minimization process defined by the equation.

Specifically, it is desirable for nature to deploy an evolutionary strategy for atoms and molecules to evolve from arbitrary initial states to their lowest energy states, even when their energy landscapes are full of local minima. Such a point of view can serve as a theoretical basis for us to understand why atoms and molecules in nature are stable and have definite and unchangeable structures and properties. Otherwise, if those basic constituents of nature can easily get stuck at arbitrary states other than their ground states, then there is no way to ensure their stability and consistency. Consequently, the universe will fall into chaos and it is impossible to have everything including life because all living organisms are made of the large size molecules, called proteins.

The global optimization equation can be derived from the cooperative optimization algorithm recently proposed by the author for attacking hard optimiza-





tion problems. It can also be viewed as a generalization of classical gradient descent from hard decision making to soft one at assigning decision variables. It is called the soft-decision gradient descent here. A hard decision, for example, can be x=0 or x = 1. A soft decision can be x=0 with a probability-like preference p=0.3 and x=1 with p=0.7. The classical gradient descent assigns decision variables with hard decisions at any given time instance. It suffers terribly with the local minimum problem. Its soft-decision based generalization can greatly alleviate the local minimum problem of its classical counterpart by eliminating local minima via energy landscape smoothing.

In mathematics, the soft-decision gradient descent is complementary to the time-dependent Schrödinger equation, a key equation in quantum mechanics. The former describes the dynamics for an energy-dissipative many-body system while the later describes that for an energy-conservative one. The soft-decision gradient descent can be obtained simply by replacing the imaginary number i by the number -1 in the time-dependent Schrödinger equation. In particular, it has the following form:

$$-\hbar\frac{\partial}{\partial t}\Psi = H\Psi - \langle H\rangle\Psi,$$

where  $\hbar$  is the reduced Planck constant,  $\Psi$  is the wavefunction describing the state of a system, H is the Hamiltonian operator corresponding to the total energy of the system, and  $\langle H \rangle$  is the expected value of H. The second term on the right side of the equation,  $\langle H \rangle \Psi$ , is solely for the normalization of the wavefunction  $\Psi$ . There is no need for the time-dependent Schrödinger equation  $(i\hbar \, \partial \Psi/\partial t = H\Psi)$  due to its unitary transformation property.

Most importantly, we can see that this soft-decision gradient descent falls back to the stationary Schrödinger equation at any equilibrium point. That is, assume that the dynamics of a many-body system is governed by the softdecision gradient descent. Starting from any initial state, it always converges to an equilibrium state, called a stationary state in physics, satisfying the stationary Schrödinger equation. Most likely the algorithm converges to the lowest energy equilibrium state, called the ground state in physics, because other equilibrium states are not stable. Any small disturbing force, such as quantum vacuum fluctuation or background radiation, will shake the system out of a stationary state of a higher energy level and it will converge to the ground state eventually.

The soft-decision gradient descent could be the critical, undiscovered law for

quantum mechanics to answer why and how atoms and molecules in the universe have definite and unchangeable structures and properties. The bizarre behaviors of the quantum world, such as wave-particle duality, uncertainty principle, quantum state superposition, and the quantization of electron energy will make sense from the perspective of this global optimization algorithm. They are simply the characteristics of the algorithm. It should be interesting to verify the theory by conducting experiments such as observing the process of molecular conformations through the study of their spectrums.

The current quantum theory only answers the question on what are atomic structures and properties. It misses the answers to the question on "why" and the question on "how". As a consequence, nobody can truly understand the theory beyond simply applying formulas to calculate. Physicist Richard Feynman once said: "Anyone who claims to understand quantum theory is either lying or crazy". Albert Einstein also said: "God does not play dice with the universe". The logic of quantum mechanics remains incomplete as long as we do not have the answers to these two fundamental questions.

As a consequence, the current methods for computing the atomic/molecular structures, such as Hartree-Fock method and density functional theory, are cumbersome and suffer many restrictions and limitations. The soft-decision gradient descent presented here not only possibly offers an answer to the "how" question, but also is a simple numeric method for computing both the ground-state as well as any excited state of a many-body quantum system in a straightforward way. It offers many advantages over classical methods in computational physics and chemistry in terms of computational complexity, generality, easiness to understand, and the possibility to visualize.

In general, the soft-gradient descent is a new mathematical principle for optimization based on energy landscape smoothing. It has already demonstrated remarkable performances in the fields like decoding codes for HDTV, image processing, stereo vision, and game theory. Most importantly, it defines a generic evolutionary strategy for a society of multiple competing individuals to reach an equilibrium state which is both personally optimal and globally optimal. It

could be served as a general mathematical model of cooperation in the studies of joint decision optimization for democratic society, intra-neuron interactions in perception, self-organization and regulation in cell biology, and many more.



### **Christian Mendl**

# Technische Universität München, Mathematics, Munich THE "STRICTLY CORRELATED ELECTRON" LIMIT OF THE HOHENBERG-KOHN FUNCTIONAL

This talk is concerned with practical (numerical) solutions and physical applications of the "strictly correlated electron" (SCE) limit of the Hohenberg-Kohn functional first studied by Seidl, Perdew, Levy, Gori-Giorgi and Savin. In this limit, one tries to find the minimum internal repulsion energy for N electrons in a given one-particle density. Until now the treatment based on the calculation of so-called comotion functions is feasible only for spherically symmetric densities and strictly one-dimensional systems. An alternative approach is the Kantorovich dual formulation, allowing general geometries. For this purpose, a nested optimization method has been developed in C.B. Mendl and L. Lin, Phys. Rev. B 87, 125106 and will be presented in the first part of the talk.

The SCE limit relaxes the famous N-representability problem to a "density representability problem" since the functional depends only on the square of the wavefunction. This gives rise to a hierarchy of approximations based on a representing k-point density with k < N, see Friesecke, Mendl, Pass, Cotar, Klüppelberg, arXiv:1304.0679. These approximations have been incorporated into a self-consistent Kohn-Sham calculation for small atoms and are the focus of the second part of the talk.

A promising application of the SCE theory are quantum dots in the low density regime. We present preliminary numerical results, including a comparison with quantum Monte Carlo calculations from the literature. Friday September 13 2.30 – 3.30 pm Thursday September 12 5.30 – 6.00 pm

#### Paul Racec

Weierstrass Institute for Applied Analysis and Stochastics, Research group 'Partial Differential Equations', Berlin

# WIGNER-EISENBUD PROBLEM WITHIN FINITE VOLUME METHOD: APPLICATION TO ELECTRONIC TRANSPORT IN CYLINDRICAL NANOWIRE HETEROSTRUCTURES

A challenge for modeling electronic transport in nanowire-based devices is the open character of the quantum system, i.e. the active region of the nanowire is in contact with electrical leads. One can describe the charge transport between the leads by the means of scattering theory. The direct computation of scattering states in two- and three-dimensional geometries requires a considerable computational effort. The R-matrix formalism is a potent means to reduce the computational costs by using the eigensolutions of the Wigner–Eisenbud problem, that means an eigenproblem for the electronic Schrödinger operator in effective mass approximation on a bounded domain with mixed hard- and soft-wall boundary conditions.

Our numerical approach to solve the Wigner–Eisenbud problem is based upon a 2D Delaunay triangulation of the rotationally symmetric device domain and the node-centered finite volume method (FVM). We study how the anisotropy of the effective mass tensor acts on the uniform approximation of the first K eigenvalues and eigenvectors and their sequential arrangement. There exists an optimal uniform Delaunay discretization with matching anisotropy with respect to the effective masses of the host material. For a centrifugal potential one retrieves the theoretically established first-order convergence, while second-order convergence is recovered only on uniform grids with an anisotropy correction.

This is a joint work with Stanley Schade and Hans-Christoph Kaiser.



Alessandro Teta

"Sapienza" Universita' di Roma, Matematica, Roma

# STABILITY PROBLEM FOR A SYSTEM OF FERMIONS WITH ZERO-RANGE INTERACTIONS

We study the stability problem for a non-relativistic quantum system in dimension three composed by N>1 identical fermions, with unit mass, interacting with a different particle, with mass m, via a zero-range interaction of strength  $\alpha \in R$ . We construct the corresponding renormalized quadratic (or energy) form  $F_\alpha$  and we find a value of the mass  $m^*(N)$  such that for  $m>m^*(N)$  the form  $F_\alpha$  is closed and bounded from below. As a consequence,  $F_\alpha$  defines a unique self-adjoint and bounded from below Hamiltonian and therefore the system is stable. On the other hand, we also show that the form  $F_\alpha$  is unbounded from below for  $m < m^*(2)$ . In analogy with the well-known bosonic case, this suggests that the system is unstable for  $m < m^*(2)$  and the so-called Thomas effect occurs.

Reference: Correggi M., Dell'Antonio G., Finco D., Michelangeli A., Teta A., Stability for a system of N fermions plus a different particle with zero-range interactions. *Reviews in Mathematical Physics* **24**, no. 5, (2012) 1250017.

Wednesday September 11 5.30 – 6.00 pm

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