MATHEMATICAL CHALLENGE OF QUANTUM TRANSPORT IN NANOSYSTEMS - PIERRE DUCLOS WORKSHOP

International Conference
Saint Petersburg, September 26 – 27, 2017

Book of Abstracts

ITMO UNIVERSITY

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- Horia Cornean (Aalborg, Denmark)
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- Raffaele Carlone (Napoli, Italy)
- Rodolfo Figari (Napoli, Italy)
- Andrey Badanin (St. Petersburg, Russia)
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Location
Saint Petersburg National Research University of Informational Technologies, Mechanics, and Optics, Lomonosova, 9, Saint Petersburg, 191002, Russia.

THE MAIN TOPICS OF THE CONFERENCE:
Spectral theory
Scattering
Quantum transport
Quantum communications and computations
Conference Program
Pierre Duclos Workshop

September 26, 2017
Room 1221
9:30 – 9:55 Registration (Pierre Duclos Workshop and Young Researches Symposium)
9:55 – 10:00 Opening

Chairman: Igor Popov

10:00 – 10:50 Johannes Brasche (Clausthal, Germany)
Approximation of eigenvalues of Schrödinger operators

10:50 – 11:40 Sylwia Kondej (Zielona Góra, Poland)
Quantum layers: resonance models

11:40 – 12:10 Coffee

Chairman: Sylwia Kondej

12:10 – 13:00 Raffaele Carlone (Napoli, Italy)
Nonlinear point interactions in d=2

13:00 – 13:50 Victor Mikhaylov (St. Petersburg, Russia)
Boundary Control method and De Branges spaces for canonical systems

13:50 – 15:00 Lunch

Chairman: Raffaele Carlone

15:00 – 15:50 S. Fassari, L.M. Nieto, M. Gadella and F. Rinaldi (Valladolid, Spain; Rome, Italy)
Level crossings of eigenvalues of the singularly perturbed harmonic oscillator in different dimensions

15:50 – 16:40 Stepan Botman (Kaliningrad, Russia)
Kinetic model of electron transport in cylindrical waveguide with rough surface

16:00 – 16:30 Coffee

Young Researchers Symposium-1 (YRS-1)

Chairman: Sergey Leble

16:30 – 16:40 Yaroslav Schmelev, Samsonov Eduard (St. Petersburg, Russia)
Investigation of the search algorithm perturbations in optical quantum computation

16:40 – 16:50 Ksenia Gubaidullina (Saint Petersburg, Russia)
Research of the stability of Grover's algorithm using a quantum computing platform

16:50 – 17:00 Natalya Gerasimenko (St. Petersburg, Russia)
Research of output parameters Y-led from asymmetry of its manufacture

17:00 – 17:10 Vladislav Gerasimenko (St. Petersburg, Russia)
Quantum optical circuits with thermal control

17:10 – 17:20 Vyacheslav Sheremetyev, Alexander Trifanov (St. Petersburg, Russia)
Testing Bell inequalities in frequency domain
17^{20} – 17^{30} **Natalya Shurygina**, Ksenia Gubaidullina (*St. Petersburg, Russia*)
Efficiency of the Grover’s algorithm searching for multiple solutions

17^{30} – 17^{40} **Irina Blinova**, Igor. Popov, Konstantin Pravdin (*St. Petersburg, Russia*)
Resonance states for Dirac operator on quantum graph

17^{40} – 17^{50} **Anton Boitsev**, Hagen Neidhardt, Igor Popov (*St. Petersburg, Russia; Berlin, Germany*)
Boundary triplets for point-like perturbation of Rashba Hamiltonian

18^{00}  **Conference Diner**

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**September 27, 2017**
Room 1221

**Chairman:** Johannes Brasche

10^{00} – 10^{50} **Rodolfo Figari** (*Napoli, Italy*)
Solvable models of Quantum Beating

10^{50} – 11^{40} **Wojciech Florek** (*Poznan, Poland*)
Lieb-Mattis theorem - revisited

11^{40} – 12^{10} **Coffee**

**Chairman:** Rodolfo Figari

12^{10} – 13^{00} **Sergey Simonov** (*St. Petersburg, Russia*)
Kac theorem for star-shaped graphs

13^{00} – 13^{50} **Sergey Leble** (*Kaliningrad, Russia*)
Cyclic-periodic ZRP structures and generalized Bloch functions

13^{50} – 15^{00} **Lunch**

**Chairman:** Wojciech Florek

15^{00} – 15^{50} **Andrey Badanin** (*St. Petersburg, Russia*)
Resonances of the Euler-Bernoulli operators on the half-line

15^{50} – 16^{00} **Tatyana Pankratova** (*St. Petersburg, Russia*)
N wells in a circle. Splitting of lower eigenvalues

16^{00} – 16^{30} **Coffee**

**Young Researchers Symposium-2 (YRS-2)**

**Chairman:** Andrey Badanin

16^{30} – 16^{40} **Maria Shumova** (*Saint Petersburg, Russia*)
Mathematical modeling of the process of sedimentation magnetic nanoparticles on the vessels wall

16^{40} – 16^{50} **Daria Golovina** (*St. Petersburg, Russia*)
Reproduction of the evolution of the liquid front profile in inhomogeneous nanoporous media

16^{50} – 17^{00} **Svetlana Ezhenkova** (*St. Petersburg, Russia*)
Sedimentation of nanoparticles in a liquid regarding their Brownian diffusion

17^{00} – 17^{10} **Maria. Faleeva** (*St. Petersburg, Russia*)
Distance of quantum gate matrix from the subspace of tensor products matrices as a characteristic of the gate
17^{10} – 17^{20} **Dmitry Nikiforov**, Igor Popov (*St. Petersburg, Russia*)

Time dependent graph: classical and quantum wave dynamics

17^{20} – 17^{30} **Maria Smolkina** (*St. Petersburg, Russia*)

GS energy in a chain of two Holstein-Hubbard rings in the presence of Rashba spin-orbit interaction

17^{30} – 17^{35} **Closing**
Abstracts

Resonances of the Euler-Bernoulli operators on the half-line
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We consider resonances for the Euler-Bernoulli differential operators on the half-line. The coefficients of this operator are positive and constants outside a finite interval. The Euler-Bernoulli operator is a specific case of the forth order differential operator. It describes the relationship between the thin beam's deflection and the applied load. In particular, these operators can be applied to study the wave propagation in carbon nanotubes.

We determine asymptotics of a counting function of resonances in complex discs at large radius, describe the forbidden domain for resonances, and obtain trace formulas in terms of resonances. We show that this operator does not have any eigenvalues and resonances if and only if its coefficients are constants on the whole half-line.

This is a joint work with E. Korotyaev.

Resonance states for Dirac operator on quantum graph
I.V. Blinova, I.Y. Popov, K.V. Pravdin
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The Dirac operators on quantum graphs of various geometries are considered. Scattering problems for the graphs with two semi-infinite edges are solved. Resonances and resonance states are considered. Methods: Lax-Phillips approach in the scattering theory and functional model. Results: Completeness theorems for the resonance states.

Boundary triplets for point-like perturbation of Rashba Hamiltonian
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We consider spin-orbit coupled quantum system with the Hamiltonian having a tensor structure. The main operator is the Rashba spin-orbit coupled operator in three dimensional space. We construct a boundary triplet for such an operator.
Kinetic model of electron transport in cylindrical waveguide with rough surface

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In this work the problem of electron transport in cylindrical nanowires is considered. In the proposed model nanowire is treated as waveguide with some scattering indicatrix introduced to describe specular and nonspecular scattering cases. Employing the kinetic approach, Kolmogorov equation is used to calculate subsequently nonequilibrium distribution function and resistivity of the system.

Approximation of eigenvalues of Schrödinger operators

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We shall describe methods how to approximate the eigenvalues of Schrödinger operators with the aid of point interaction Hamiltonians. As it is well known convergence of closed quadratic forms implies convergence in the norm resolvent sense of the associated self-adjoint operators; we shall give a sharp estimate on the rate of convergence. This general result can be used to estimate the error term in the approximation of eigenvalues.

Nonlinear point interactions in d=2

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We consider a two-dimensional nonlinear Schrödinger equation with concentrated nonlinearity. In both the focusing and defocusing case we prove local well-posedness, i.e., existence and uniqueness of the solution for short times, as well as energy and mass conservation. In addition, we prove that this implies global existence in the defocusing case, irrespective of the power of the nonlinearity, while in the focusing case blowing-up solutions may arise.
Sedimentation of nanoparticles in a liquid regarding their Brownian diffusion
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Sedimentation of nanoparticles in a liquid is investigated by using the methods of mathematical modelling. Based on the model of nanoparticles' sedimentation under the action of gravitational forces, an analytical model of nanoparticles' sedimentation regarding their Brownian diffusion is constructed. The dependence of the particle size distribution on the coordinate for particles of different sizes is studied.

Distance of quantum gate matrix from the subspace of tensor products matrices as a characteristic of the gate
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A way of estimation of independence of quantum bit transformation by a quantum gate is suggested. It is based on a modification of Eckart-Young-Mirsky theorem. The corresponding parameter is obtained as the distance of the matrix from the subspace of matrices which are tensor products of one-qubit matrices. The procedure of the parameter computing is described. A few examples are considered.

Solvable models of Quantum Beating
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In a solvable model of a one dimensional double well potential, I will examine the suppression of quantum beating. The potential is realized as two focusing nonlinear point interactions. The investigation of the beating dynamics is reduced to the study of a system of coupled nonlinear Volterra integral equations. For various values of geometric and dynamical parameters it will be shown that already for a nonlinearity exponent well below the critical value there is complete suppression of the typical beating behavior characterizing the linear quantum case.
Level crossings of eigenvalues of the singularly perturbed harmonic oscillator in different dimensions

S. Fassari, L.M. Nieto, M. Gadella and F. Rinaldi
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In this brief presentation we wish to point out the striking difference between level crossings of eigenvalues of the harmonic oscillator perturbed by a renormalisable point interaction in one (delta'-interaction) or three dimensions (three-dimensional delta) and those occurring in the corresponding two-dimensional model.

Joint work with L.M. Nieto, M. Gadella and F. Rinaldi. Based also on previous work with S. Albeverio.

Lieb-Mattis theorem - revisited
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The Lieb-Mattis theorem (LMT, also known as the Lieb-Schultz-Mattis theorem) stated in 1962 is in fact based to the Perron (1907) and the Frobenius (1912) theorems. It has been formulated for magnetic (quantum spin) systems, but it has been used in many other fields. For many years it has been applied mainly to lattice (infinite) systems, in which case only its ”stronger” version is applicable. This fact has led to, among others, unfounded simplification that bipartiteness (in the sense of the LMT) is opposite to frustration. However, in the case small spin systems (e.g. magnetic molecules including single molecule magnets) or systems with special topology, a ”weak” version of the LMT can be used. It means that it is possible to have geometrically frustrated spin systems which are bipartite. Therefore, such systems have to show (and they really show) the so-called Lieb-Mattis Level Order (LMLO). Moreover, in the case of many analogous (usually larger) systems the LMLO is present despite the lack of bipartiteness. It is argued that this fact could be explained basing on some generalizations of the Perron-Frobenius theory.

Research of output parameters Y-led from asymmetry of its manufacture
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The Y-beam splitter is the simplest integral-optical element, which can be used, for example, in quantum random number generators. Ideally, the probability of
receiving a signal at each of the outputs is 50%, and the losses are inconsiderable. It should be noted, however, that the properties of a real Y-beam splitter differ from the properties of an ideal Y-beam splitter. The aim of this work is to study the ratio of the intensities at the input and output of the beam splitter as a function of the angle of variation of the output branches from the input branch.

To perform the calculations, we used the Finite Difference Time Domain Photonics Simulation Software from OptiWave Systems (OptiFDTD). It is a graphical user interface that allows you to define the waveguide geometry, parameters of medium and sources, and also allow to changes these parameters through scripts in the Visual Basic language.

To evaluate the limits in which it is necessary to consider possible combinations of the angles of the variation of the output branches of the beam splitter from the input one, the symmetrical case of the Y-scheme was considered.

Analysis of the results showed that the nature of the main source of losses varies depending on the angle of variation of the output branches of the Y-beam-splitter from the input. At small angles, losses are associated with a long overlap region, where the cross section increases constantly, which leads to a violation of the in-phase condition and a partial output of the signal beyond the waveguide boundary. As the angles increase, the overlap zone is reduced, which also reduces this type of loss. However, in this case, the area where the output branches are separated starts to behave like a slit on which a part of the light diffracts, with the larger the angle, the higher the loss. In such a situation, one can find an angle for which the losses are minimal (about 27-29°).

In modeling the asymmetric case, the most interesting result was the difference in the "behavior" of the intensity ratios at angles close to symmetric, depending on the underlying cause of the losses.

Quantum optical circuits with thermal control

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Quantum calculations, which are more and more relevant today, can be implemented in many ways. One of the possibilities is to represent the qubit in the form of a two-photon state in a system of two interacting waveguides. In this paper we consider the possibility of constructing a temperature-controlled logical circuit in such a system.

The possibility of influencing the output parameters of the circuit from two X-beam splitters connected by two waveguides, one of which can be heated, was shown several years ago [1,2], but the idea did not develop in quantum calculations. To begin with, it is necessary to determine the state designation: for a pure state \( |0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \)
we denote the situation when the photon is in the conventionally upper waveguide, and $|0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ - in the lower one. We shall denote the mixed state $|\psi\rangle = \begin{pmatrix} \alpha + \beta \\ \alpha - \beta \end{pmatrix}$.

To construct an arbitrary logical function, it suffices to use some combination of operators $\hat{X}, \hat{Y}, \hat{Z}$ defined in the matrix form as follows:

$$
\hat{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{Y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{Z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
$$

(1)

In addition, we need the Hadamard operator:

$$
\hat{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}
$$

(2)

An arbitrary controllable operator $\hat{O}_\gamma$, denoted by the lower index $\gamma$, in contrast to the uncontrolled operator, works by definition for $\gamma=1$, and doesn't work for $\gamma=0$. For simplicity, only real operators will be considered below.

It is easy to show that the determined from (1) $\hat{Z}$ when it exposed to $|\psi\rangle$ gives $\begin{pmatrix} \alpha \\ -\beta \end{pmatrix}$, what can be interpreted as introducing a phase difference in $\pi$ into the lower branch of the circuit. The temperature-controlled operator $\hat{Z}_\gamma$ in this case will simply be a miniature heater mounted on the lower waveguide (see Figure 1).

*Fig. 1. Schematic diagram of the operator $\hat{Z}_\gamma$

Operator $\hat{H}$ we need to get operator $\hat{X}$ from $\hat{Z}$, since from (2), (1) and simple calculations it follows that $\hat{H}\hat{Z}\hat{H}=\hat{X}$. In this case, the definition of the Hadamard operator is satisfied by the X-beam splitter, to which the lower branch is attached $\hat{Z}$ (see Figure 2).

Fig. 2. Schematic diagram of the operator $\hat{H}$
Reproduction of the evolution of the liquid front profile in inhomogeneous nanoporous media

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Nowadays inhomogeneous nanoporous materials are widely used in biophysics and biomedicine in many aspects: immunoisolation, tissue engineering, as biosensors, etc. In all these fields it is often required to reproduce in synthesized non-organic nanoporous medium the specific pattern of evolution of the liquid front profile observed in organic nanoporous medium.

The purpose of our work is to select the inhomogeneous nanoporous medium for realization of the sought-out pattern of the liquid front propagation. The combination of the continuity equation for the incompressible flow and the approximation of Darcy's law gives us the numerical model of the liquid front propagation in inhomogeneous nanoporous media with varying porosity and pore size. Then the porosity and/or pore radius distribution can be set as a polynomial with unknown coefficients.

Minimization of the difference between modelled evolution of the liquid front profile and sought-for one by selecting the coefficients of the polynomials gives us the desired result — the parameters of the inhomogeneous nanoporous medium, in which the liquid will propagate as needed.

The model simulating the two-dimensional liquid front propagation in inhomogeneous nanoporous medium was written in C++. The problem of the function minimization (as function we set the standard deviation between modelled evolution of the liquid front profile and the sought-for one) was solved by variation of the Nelder-Mead method.
Research of the stability of Grover's algorithm using a quantum computing platform

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By the IBM quantum computing platform, algorithms can be explored on a real processor. Investigating the algorithm working on a real platform of the quantum processor, one can see its real stability to the effects of distortions of the quantum circuit and compare it with theoretical calculations. It is also possible to personally introduce distortions into the scheme by quantum operators, and to study their influence on the operation of the algorithm. This experiment allowed to compare the calculations of a real quantum computer and a simulation of 2-qubit Grover's algorithm. The comparison showed that with a perturbation amount of about 85%, the stability of the IBM quantum computer is consistent with the simulation results.

Quantum layers: resonance models

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We consider two and three dimensional models of quantum layers with a delta potential preserving symmetry and inducing embedded eigenvalues. We show that after the breaking symmetry the embedded eigenvalues turn to resonances determined by the second sheet poles of the resolvent.

We analyze various types of “perturbants” which lead to breaking symmetry. Finally, we discuss how the widths of resonances depend on breaking symmetry parameters.

Cyclic-periodic ZRP structures and generalized Bloch functions

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Systems of zero-range potentials (ZRP) with a space group symmetry are studied. The quantum states of electrons in such pseudopotentials are built as common eigenstates of the Hamiltonian and the symmetry group operators. In a case of continuous spectrum the eigenfunctions are interpreted as generalized Bloch functions. A scattering problem for opposite directed generalized Bloch waves is formulated. A solutions are build as a linear combination of the 3D spherical waves,
that satisfy boundary conditions, specific for ZRPs. Examples of benzene-like and nanotube-like structures are presented.

**Boundary Control method and De Branges spaces for canonical systems**

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We study the connections between the Boundary Control method and De Branges method for inverse problems for the canonical systems. We consider the case of smooth positive Hamiltonian and the special canonical systems: the one-dimensional Schrödinger and Dirac operators on the half-line and semi-infinite discrete Schrödinger Operator.

The talk is based on joint works with A.S. Mikhaylov (PDMI RAS, SPbSU).

**Time dependent graph: classical and quantum wave dynamics**

Dmitry Nikiforov, Igor Popov  
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Quantum graphs with the Schrödinger and wave equations on edges were considered. Edge lengths vary in time. Wave dynamics for the two cases are considered. Comparison of the results was made.

**N wells in a circle. Splitting of lower eigenvalues**

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I consider a two-dimensional stationary Schrödinger equation having a smooth potential $V$ with $N$ identical wells which differ only by space translation. Points $M_k$, $k=1, \ldots, N$, the bottoms of these wells, are situated on a circle $C$ of radius $r_0$ and divide this circle in $N$ equal parts. Each point $M_k$ we put in a Cartesian system of coordinates $x_k, y_k$ such that in $M_k x_k = y_k = 0$. We consider rectangles $D_k = \{(x_k, y_k) : \left| x_k \right| \leq \alpha, \left| y_k \right| \leq b\}, k = 1,\ldots,N$, such that $\bigcup D_k \ni C$, and $\bigcup D_k = \cdots = \bigcup D_N$.

In polar coordinates $(r, \varphi)$ we may assume that

$$V = \frac{\alpha^2}{2} (r - r_0)^2 + \frac{\omega^2}{2} \sin^2 \frac{N \varphi}{2}.$$
In this assumption we find splitting formula for lower eigenvalues of a corresponding Schrödinger operator \( \Delta E_n = \frac{\hbar}{\hbar^2(1 + O(\hbar^n))}, n = (n_1; n_2), n_1 = 0, 1, ..., n_2 = 0, 1, ..., \ b = \frac{4}{N^2} \pi \omega^2 \).

**Spectral analysis of the bottom of the spectrum of 2-dimensional periodic Hamiltonians in slowly varying magnetic fields**

Radu Purice

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Consider a periodic Schroedinger operator in two dimensions, perturbed by a weak magnetic field whose intensity slowly varies in space. We show in great generality that the bottom of the spectrum of the corresponding magnetic Schroedinger operator develops spectral islands separated by gaps, reminding of a Landau-level structure.

**Investigation of the search algorithm perturbations in optical quantum computation**

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We consider optical implementations of the Grover’s algorithm. Different realization of the circuits was presented. The Elements of the algorithm can be fabricated from integrated optical waveguides on a silica-on-silicon chip. The optical quantum computation allows us to create Grover’s algorithm on a chip with some distortions. In this case we investigate the search algorithm perturbations for different implementations.

**Kac theorem for star-shaped graphs**

Sergey Simonov

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We consider a Schrodinger operator on a star-shaped graph with self-adjoint matching conditions at the interior vertex. This operator is a finite-dimensional perturbation of the Dirichlet decoupling operator in the resolvent sense. The graph can have infinite edges, and Schrodinger operators on individual edges with Dirichlet boundary conditions are supposed to be self-adjoint. The main result is a
generalization of Kac theorem on multiplicity for one-dimensional perturbations. The classical theorem of I. S. Kac says that the singular spectrum of a Schrodinger operator on the whole real line is simple for any potential which is in the limit point case on both infinities. We will also discuss more general self-adjoint matching conditions. The talk is based on joint work with Harald Woracek.

**Testing Bell inequalities in frequency domain**

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Our work deals with Bell inequalities in three-qubit case under frequency bin coding. Started from two particle system and using algebraic approach to electro-optic phase modulation of quantum light [1] we obtained the results that were consistent with other authors [2-3]. Then violation of Bell inequalities in more general Mermin form [4] was demonstrated numerically as a solution of quantum optimization problem, which in fact confirm nonlocal properties of our three parted quantum system.

**References**


**Mathematical modeling of the process of sedimentation magnetic nanoparticles on the vessels wall**

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During the recent decades increasing attention attracts the use nanoparticles with magnetic properties in biomedicine. It is due to the possibility of its remote management under the influence of external magnetic field to concentrate them in a particular area of the human body and control of medical exposure using magnetic resonance imaging (MRI). This method of control is more safety than X-rays one [1]. Magnetic nanoparticles are used in many areas of medicine such as in targeted
delivery of drugs in the human body, in the diagnosing of diseases as contrast agents for MRI, in local controlled hyperthermia, in cytological studies [2].

The present work investigates the process of blood vessels embolization with the use of magnetic nanoparticles. The process of embolization occurs in two stages. The first stage is the introduction substance with magnetic nanoparticles into the vessel which dispose on the vessel wall under the influence of the magnetic field. The second stage is application of the optical heating. Under the heating the particles transfer heat to the blood and after that and blood vessels coagulation occur in the necessary area.

The experiment to study the magnetically-driven drug delivery in a blood vessel of human and embolization process with the use of magnetic nanoparticles was conducted [3]. This work performed mathematical modeling of this experiment. By the results mathematical model of embolization process was created. Obtained results qualitatively correspond with the experimental data. The conditions when embolization with optical heating is possible were obtained.

References:

Efficiency of the Grover’s algorithm searching for multiple solutions

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In this work, we investigated Grover's algorithm for searching a group of elements. This algorithm differs from the classical Grover only with an oracle, which marks not one element, but a group of them. Comparison of the modified algorithm with the classical one shows that probability of finding the selected elements is lower. The influence of various types of perturbations to the initial state on the efficiency of the algorithm is considered.

One of the most known Grover’s algorithm applications is doing quantum search. In the beginning, we have $2^n$-element amplitude vector, where $n$ — is the number of qubits. Then we apply Hadamard gate to provide equal superposition.
Mark one or multiple elements satisfying search condition. Calculate number of Grover iterations necessary in terms of our task and then perform them. As the result, we get transformed amplitudes vector, where element(s) searched for have largest values in comparison to other elements.

Thus, it is shown, how the following parameters affect the result: number of elements satisfying the condition, number of qubits we perform search on, degree of perturbations to the initial amplitudes state.

**GS energy in a chain of two Holstein-Hubbard rings in the presence of Rashba spin-orbit interaction**

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The model of two Holstein-Hubbard rings in the presence of Rashba spin-orbit interaction was obtained and the first steps to study the effect of Rashba spin-orbit interaction were also made. First, the phonons degrees of freedom were eliminated by the conventional Lang-Firsov transformation and then the spin-dependence was removed by performing the unitary transformation. The effective electronic Hamiltonian was diagonalized by using the Hartree-Fock approximation and the GS energy was obtained.