

DOCTORAL STUDIES COURSE UNIT DESCRIPTION

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| Name of subject | Scientific Field | Faculty | Center/Institute/ Department |
| Selected Topics in Theoretical Physics (10 ECTS credits) | Physics N 002 | Faculty of Physics | Institute of Chemical Physics |
| Student's workload | Hours | Student's workload | Hours |
| Lectures | | Consultations | 50 |
| Individual study | 200 | Seminars | |

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| Course annotation | | | |
| <p>Classical stochastic processes Markov chains. Chapman–Kolmogorov equation. Branching processes. Fokker–Planck equation. Continuous-time random walk. Diffusion processes. Anomalous diffusion.</p> <p>Irreversibility in classical physics System–bath interaction. Liouville equation. Master equation. Hydrodynamic equations. Fluctuation–dissipation theorem. BBGKY hierarchy equations.</p> <p>Relativistic quantum mechanics and introduction into quantum field theory Klein–Gordon equation. Dirac equation. Formulation of quantum mechanics using Lagrange formalism. Time-evolution operator. Path integrals. Second quantization of the identical particles. Field operators. Quantization of the electromagnetic field. Casimir effect</p> <p>Theory of open quantum systems Density operator. Deduced density operator. Interaction picture. Irreversibility in quantum mechanics. Dissipation and decoherence. Projection super-operators. Förster and Redfield transfer rates.</p> | | | |
| List of literature | | | |
| <ol style="list-style-type: none"> 1. J. Chmeliov, V. Butkus, L. Valkūnas. Kvantinė fizika, Vilniaus universiteto leidykla, 2020. 2. S. Weinberg. The Quantum Theory of Fields. Cambridge University Press, 1995. 3. M. O. Caceres. Non-equilibrium Statistical Physics with Application to Disordered Systems, Springer, 2017. 4. V. May, O. Kühn, Charge and Energy Transfer Dynamics in Molecular Systems, Wiley, 2011. 5. M. Yang and G. R. Fleming, Chem. Phys. 275, 355 (2002). | | | |
| Consulting teachers | Scientific degree | Pedagogical name | Main scientific works published in a scientific field in last 5 year period |
| Jevgenij Chmeliov | PhD | Assoc. Prof. | <ol style="list-style-type: none"> 1. V. Mascoli, A. Gelzinis, J. Chmeliov, L. Valkūnas, R. Croce, “Light-Harvesting Complexes Access Analogue Emissive States in Different Environments”, Chemical Science, 2020, 11, 5697. 2. H. van Amerongen, J. Chmeliov, “Instantaneous Switching between Different Modes of Non-Photochemical Quenching in Plants. Consequences for |

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| | | | <p>Increasing Biomass Production”, <i>Biochimica et Biophysica Acta – Bioenergetics</i>, 2020, 1861, 148119.</p> <p>3. M. Tutkus, F. Saccon, J. Chmeliov, O. Venckus, I. Ciplys, A. V. Ruban, L. Valkunas, “Single-molecule microscopy studies of LHCII enriched in Vio or Zea”, <i>Biochimica et Biophysica Acta – Bioenergetics</i>, 2019, 1860, 499–507.</p> <p>4. S. Farooq, J. Chmeliov, E. Wientjes, R. Koehorst, A. Bader, L. Valkunas, G. Trinkunas, H. van Amerongen, “Dynamic feedback of the photosystem II reaction center on photoprotection in plants”, <i>Nature Plants</i>, 2018, 4, 225–231.</p> <p>5. M. Tutkus, J. Chmeliov, D. Rutkauskas, A. V. Ruban, L. Valkunas, “Influence of the Carotenoid Composition on the Conformational Dynamics of Photosynthetic Light-Harvesting Complexes”, <i>The Journal of Physical Chemistry Letters</i>, 2017, 8, 5898–5906.</p> |
| Andrius Gelžinis | PhD | Assoc. Prof. | <p>1. A. Gelzinis, D. Abramavicius, J. P. Ogilvie, L. Valkunas, Spectroscopic properties of photosystem II reaction center revisited, <i>J. Chem. Phys.</i> 147, 115102, 2017.</p> <p>2. A. Gelzinis, E. Rybakovas, L. Valkunas, Applicability of transfer tensor method for open quantum system dynamics, <i>J. Chem. Phys.</i> 147, 234108, 2017.</p> <p>3. E. Rybakovas, A. Gelzinis, L. Valkunas, Simulations of absorption and fluorescence lineshapes using the reaction coordinate method, <i>Chem. Phys.</i> 515, 242–251, 2018.</p> <p>4. A. Gelzinis, L. Valkunas, Analytical derivation of equilibrium state for open quantum system, <i>J. Chem. Phys.</i> 152, 051103, 2020. A. Gelzinis, E. Rybakovas, L. Valkunas, Applicability of transfer tensor method for open quantum system dynamics, <i>J. Chem. Phys.</i> 147, 234108, 2017.</p> <p>5. Y. Braver, L. Valkunas, A. Gelzinis, Benchmarking the forward–backward trajectory solution of the quantum-classical Liouville equation, <i>J. Chem. Phys.</i> 152, 214116, 2020.</p> |

Certified during Doctoral Committee session 02/02/2022, protocol No. (7.17 E) 15600-KT-32

Committee Chairman prof. S. Juršėnas