MP 11: Many-body Theory II

Time: Thursday 9:30–11:50 Location: HL 102

MP 11.1 Thu 9:30 HL 102

Double or nothing: a Kolmogorov extension theorem for (bi)probabilities in quantum mechanics — •Davide Lonigro — Department of Mathematics, Università degli Studi di Bari Aldo Moro, Bari, Italy — Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

The family of multitime probability distributions obtained by repeatedly probing a quantum system generally violates Kolmogorov's consistency property, thus preventing us from interpreting such distributions as the result of the sampling of a single trajectory. We argue that, nonetheless, a pair of trajectories is sufficient. To this purpose, we prove a generalization of Kolmogorov extension theorem that applies to families of complex-valued bi-probability distributions (that is, defined on pairs of elements of the original sample spaces), and we employ this result in the quantum mechanical scenario. In this sense, rather than give up on trajectories, quantum mechanics requires to "double down" on them.

Joint work with D. Chruściński, Ł. Cywiński, F. Sakuldee, and P. Szańkowski.

MP 11.2 Thu 9:50 HL 102

Special techniques in the auxiliary equation method for solving nonlinear differential equations — •Alina-Maria Păuna — Department of Physics, University of Craiova, 13 A.I. Cuza Street, 200585 Craiova, Romania

This report refers to a special approach that can be used in the method of auxiliary equations to solve complex nonlinear differential equations. More precisely, we will consider the coupling between a nonlinear differential equation whose solutions are sought and an auxiliary equation with already known solutions. The coupling between the two equations allows to find the most general form of the considered nonlinear equation that remains compatible, in terms of its solutions, with the given auxiliary equation.

The approach will be illustrated for the particular case when the nonlinear equation to be solved is a second-order reaction-diffusion equation with polynomial coefficients. Such equations describe important nonlinear phenomena that occur in hydrodynamics, optics, or plasma physics. The general approach we are proposing will be illustrated on several nonlinear equations, by generating their solutions when the elliptic Jacobi equation is considered as an auxiliary equation

MP 11.3 Thu 10:10 HL 102

On the applicability of Kolmogorov's theory of probability for the description of quantum phenomena — •Maik Reddiger — Anhalt University of Applied Sciences, Germany

It is a common view that with his axiomatization of quantum mechanics von Neumann laid the foundations of a "non-commutative probability theory". As such, it is regarded a generalization of the "classical probability theory" due to Kolmogorov. Outside of quantum physics, however, Kolmogorov's axioms enjoy universal applicability. This raises the question of whether quantum physics indeed requires such a generalization of our conception of probability or if von Neumann's axiomatization of quantum mechanics was contingent on the absence of a mathematical theory of probability at the time.

Taking the latter view, I motivate an approach to the foundations of non-relativistic quantum theory that is based on Kolmogorov's axioms. It relies on the Born rule for particle position probability and employs Madelung's reformulation of the Schrödinger equation for the introduction of physically natural random variables. While an acceptable mathematical theory of Madelung's equations remains to be developed, one may nonetheless formulate a mathematically rigorous "hybrid theory", which is empirically almost equivalent to the quantum-mechanical Schrödinger theory. A major advantage of this approach is its conceptual coherence, in particular with regards to the question of measurement.

The talk is based on Reddiger, *Found. Phys.* **47**, 1317 (2017) and Reddiger & Poirier, *J. Phys. A: Math. Theor.* **56**, 193001 (2023).

20 min. break

MP 11.4 Thu 10:50 HL 102

TBMaLT, a flexible toolkit for combining tight-binding and machine learning — •Wenbo Sun[1], Guozheng Fan[1], Adam McSloy[2], Thomas Frauenheim[3], and Bálint Aradi[1] — [1]University of Bremen, Bremen 28359, Germany — [2]University of Bristol, Bristol BS8 1TS, United Kingdom — [3]Constructor University, Bremen 28759, Germany

Tight-binding approaches, especially the Density Functional Tight-Binding (DFTB) and the Extended Tight-Binding (xTB), allow for efficient quantum mechanical simulations of large systems and long time scales. They are derived from ab initio Density Functional Theory using pragmatic approximations and some empirical terms, ensuring a fine balance between speed and accuracy. Their accuracy can be improved by tuning the empirical parameters using machine learning techniques, especially when information about the local environment of the atoms is incorporated. As the significant quantum mechanical contributions are still provided by the tight-binding models, and only short-ranged corrections are fitted, the learning procedure is typically shorter and more transferable. As a further advantage, derived quantum mechanical quantities can be calculated based on the tight-binding model without the need for additional learning.

We have developed the open-source framework TBMaLT, which allows the easy implementation of such combined approaches. The toolkit currently contains layers for the DFTB method and an interface to the GFN1-xTB Hamiltonian, but due to its modular structure, additional atom-based schemes can be implemented easily.

MP 11.5 Thu 11:10 HL 102

A Multipolar Theory for the Color Palette of Periodic Metasurfaces — •Aso Rahimzadegan[1], Kevin Vynck[2,3], and Silvia Vignolini[1,4] — [1]Sustainale and Bio-Inspired Materials, Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [2]Univ. Claude Bernard Lyon,CNRS, Institut Lumière Matière, Villeurbanne, France — [3]Univ. Bordeaux, Institut d'Optique Graduate School, CNRS, Laboratoire Photonique Numerique et Nanosciences (LP2N), Talence, France — [4]Department of Chemistry, University of Cambridge, Cambridge, United Kingdom

Optical metasurfaces consist of 2D arrangements of nanoparticles can control the amplitude, phase, and polarization of an incidence field. Here, based on a developed comprehensive theory to describe the optical response of periodic metasurfaces, we explore the possible color coverage of metasurfaces made from isotropic coreshell particles. The color palette of metasurfaces in transmission and reflection is systematically explored and fundamental limits are investigated. The research bridges the gap between simulation and design by introducing a novel framework that translates desired color and iridescence outcomes into metasurface parameters.

MP 11.6 Thu 11:30 HL 102

Birth quota of non-generic degeneracy points — •Gergo Pinter[1,2], Gyorgy Frank[1,2], Daniel Varjas[3], and Andras Palyi[1,2] — [1]Department of Theoretical Physics, Budapest University of Technology and Economics, Hungary — [2]MTA-BME Exotic Quantum Phases Group, Budapest University of Technology and Economics, Hungary — [3]Department of Physics, Stockholm University, AlbaNova University Center, 106 91 Stockholm, Sweden

Let's think of a Hamiltonian system with a parameter space of dimension three - for example, it can be either the electronic band structure of a crystal or the Hamiltonian of two electrons in a double quantum dot depending on an external magnetic field. The generic degeneracy points of such systems are the Weyl points. For small perturbations the Weyl points are robust, while a non-generic twofold degeneracy point splits into Weyl points. What is the possible number of the Weyl points born from a non-generic degeneracy point? We show a strict upper bound for this number. https://arxiv.org/abs/2202.05825