THU 10: Foundational / Mathematical Aspects – Methods and Approximations

Time: Thursday 14:15–16:15 Location: ZHG103

THU 10.1 Thu 14:15 ZHG103

Shadow tomography for relativistic scattering experiments — Chau Nguyen, •Matthias Kleinmann, Otfried Gühne, Carmen Diez Pardos, and Gilberto Tetlalmatzi-Xolocotzi — University of Siegen, Germany

Scattering experiments produce relativistic particles that carry besides momentum information also spin, where the spin information of a decaying particle is accessible via the momenta of the decay particles. However, associating a consistent spin state to the particle proves to be difficult: In particular in the relativistic setting the spin state strongly depends on the reference frame, and with it, for example, change its purity and entanglement properties. This is further aggravated by the fact that each decaying particle has different momentum. We show that techniques from shadow tomography are best suited to handle this situation and that this can be used to infer a meaningful notion of entanglement, test the validity of the underlying physical model, and to extract information that can be otherwise difficult to access, like the ratio between different production channels.

THU 10.2 Thu 14:30 ZHG103

Absolute and relational many-body Green's function theories — •Ville Härkönen — Tampere University, Tampere, Finland

Quantum mechanics, now a century old, has relied heavily on the Coulomb problem and the Born-Oppenheimer (BO) approximation [1] for describing atoms, molecules, and solids. While the BO approximation is widely used, its limitations are evident in materials like superconducting hydrides.

Wave function methods are impractical for solids due to poor scaling, leading to alternatives like BO-based density functional theory and many-body Green's function theory. A beyond-BO Green's function approach was proposed in the 1960s [2], but it contains foundational issues [3].

We have developed an exact many-body Green's function theory to address these problems [4], revealing that quantum theory may need to be relational rather than absolute [5].

In this talk, we summarize recent developments in beyond-BO Green's function theory [4,5,6] and explore the implications of relational versus absolute frameworks in quantum mechanics [7].

[1] M. Born and R. Oppenheimer, Ann. Phys. (Leipzig) 389, 457 (1927).
[2] G. Baym, Ann. Phys. 14, 1 (1961).
[3] B. Sutcliffe, Adv. Chem. Phys. 114, 1 (2000).
[4] V. J. Härkönen, R. van Leeuwen, and E. K. U. Gross, Phys. Rev. B 101, 235153 (2020).
[5] V. J. Härkönen, arXiv:2503.01417 .
[6] V. J. Härkönen, Phys. Rev. B 106, 205137 (2022).
[7] J. B. Barbour, Br. J. Philos. Sci. 33, 251 (1982); L. Smolin, arXiv:1805.12.

THU 10.3 Thu 14:45 ZHG103

Geometry of quantum correlations — •Konrad Szymanski — Research Center for Quantum Information, Slovenská Akadémia Vied, Bratislava, Slovakia

Quantum mechanics gives rise to nonclassical correlations between observables, with rich mathematical theory behind and experimental importance: these correlations between observables affect metrological performance, entanglement detection, and phase transitions at zero temperature.

In this talk, numerical and analytical methods for the study of quantum correlations will be presented, focusing on the sets of admissible joint expectation values of observables and their covariance matrices. This framework will be illustrated through its application to entanglement characterization in photonic quantum states.

THU 10.4 Thu 15:00 ZHG103

Quantum into the mesoscopic: progress in matter-wave interference of massive sodium nanoclusters. — •Bruno E. Ramírez-Galindo[1,2], Sebastian Pedalino[1,2], Richard Ferstl[1,2], Klaus Hornberger[3], Stefan Gerlich[1], and Markus Arndt[1] — [1]University of Vienna, Faculty of Physics, Vienna, Austria — [2]University of Vienna, Vienna Doctoral School in Physics, Vienna, Austria — [3]University of Duisburg-Essen, Faculty of Physics, Duisburg, Germany

The wave-particle duality has been a cornerstone in quantum theory since Louis de Broglie's foundational insight in the early 20th century. Yet, some fundamental questions remain unresolved: Is there a limit in mass, size, or complexity beyond which quantum behavior gives way to classical physics? And, is it possible to realize quantum superpositions of mesoscopic matter states that are classically considered mutually exclusive - analogous to Schrödinger's cat being both dead and alive? In this work, we discuss experimental advances addressing these questions through matter-wave interference of sodium nanoclusters with physical sizes approaching the mesoscopic scale. We report on the use of a near-field Talbot-Lau interferometer equipped with three UV photo-depletion gratings, where recent measurements suggest its potential for testing the linearity of quantum mechanics and for enabling quantum-assisted precision measurements in nanocluster science.

THU 10.5 Thu 15:15 ZHG103

Tunneling Modeled via First-Passage Times — •Philipp Tesch, Kai-Hendrik Henk, and Wolfgang Paul — MLU Halle-Wittenberg

Since quantum mechanics lacks a self-adjoint time operator, time is not an observable in the standard formalism. As a result, time measurements such as tunneling durations are not directly accessible within the conventional framework. In 1966, Edward Nelson introduced a stochastic mechanics approach to describe quantum systems [1]. In this framework, quantum systems are treated as open systems undergoing conservative, time-reversible diffusion processes. This is modeled by Brownian motion guided by velocity fields. This framework is applied for quantum tunneling in symmetric double-well potentials. Instead of tunneling, particles overcome the finite potential barrier due to energy fluctuations. Ground states are obtained numerically via the stationary Schrödinger equation, from which probability densities and osmotic velocities are calculated. Solving the stochastic differential equations to simulate sample paths of particles allows us to compute first-passage times across the potential barrier under two different threshold criteria. An inverse relation between mean first-passage times τ and the energy splitting ΔE in double-well potentials emerges. Furthermore, this framework allows for a detailed study of the probability distribution of tunneling times (modelled as first passage times), which can be addressed by attosecond spectroscopy [2].

[1] E. Nelson, *Phys. Rev.* 150 (1966) [2] A. S. Landsmann et al., *Optica* 1 (2014)

THU 10.6 Thu 15:30 ZHG103

Approximations in light-matter interaction — •Leonhard Richter, Daniel Burgarth, and Davide Lonigro — Department Physik FAU Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

I will present recent advances in quantifying the quality of approximations such as the rotating-wave approximation. Specifically, I present bounds on the norm difference between the unitary evolutions generated by the full Hamiltonian and the approximation applied to the same initial state. As full-quantum models of light-matter interaction are unbounded in energy, the derived error bounds depend on the particular initial state of the system and convergence is only given in the strong and not in the uniform sense. The central method enabling such derivation in these settings is based on repeated integration-by-parts of the difference of two unitary evolutions.

THU 10.7 Thu 15:45 ZHG103

The perils of finite dimensional approximations — •Felix Fischer — FAU Erlangen, Staudtstr. 7 91058 Erlangen

When numerically simulating the unitary time evolution of an infinite-dimensional quantum system, one is usually led to treat the Hamiltonian H as an "infinite-dimensional matrix" by expressing it in some orthonormal basis of the Hilbert space, and then truncate it to some finite dimensions. However, the solutions of the Schrödinger equations generated by the truncated Hamiltonians need not converge, in general, to the solution of the Schrödinger equation corresponding to the actual Hamiltonian. In some cases, the approximate solutions do not converge to any valid state at all, whilst in others they converge to the dynamics generated by a "wrong" Hamiltonian different from the initial one. In this talk, I present multiple necessary and sufficient

conditions for the convergence of finite dimensional approximations to the correct dynamics. Multiple examples from quantum chemistry and quantum optics illustrate the convergence issues which can appear in practice. Using our abstract results, I discuss why these issues arise and showcase how to ensure convergence to the correct dynamics we aim to simulate.

THU 10.8 Thu 16:00 ZHG103

Improved Gerchberg-Saxton Approach to the One-Dimensional Pauli Phase Retrieval Problem — Felipe de Andrade Ferreira da Silva, Karen Fernanda Pagnoni, and •Alexys Bruno-Alfonso — Department of Mathematics, School of Sciences, UNESP - São Paulo State University, Bauru, 17033-360, Brazil

The iterative Gerchberg-Saxton algorithm retrieves the phases of a Fourier pair from the corresponding intensities. It can deal with the one-dimensional phase-retrieval Pauli problem: the calculation of the state representations $\psi(x)$ and $\phi(k)$ from the probability densities $\rho(x)=|\psi(x)|^2$ and $\mu(k) = |\phi(k)|^2$. We improve the algorithm in several ways. First, we find compatibility tests between two given densities $\rho(x)$ and $\mu(k)$. Second, we enhance the algorithm stability by adding two stages after each Fourier transformation: (i) we replace the exact absolute value of the transform by its weighted harmonic mean with the approximate one, (ii) we multiply the transform by a factor that reproduces the expected values and variances of x and k as given by $\rho(x)$ and $\mu(k)$.