# MP 7: Poster (joint session MP/QI)

Time: Tuesday 11:00–13:00 Location: Poster B

MP 7.1 Tue 11:00 Poster B

**Machine Learning Quantum Mechanical Ground States based on Stochastic Mechanics** — •Kai-Hendrik Henk and Wolfgang Paul — Martin-Luther-University, Halle(Saale), Germany

The Rayleigh-Ritz variation principle is a proven way to find ground states and energies for bound quantum systems in the Schrödinger picture. Advances in machine learning and neural networks make it possible to extend it from an analytical search from a subspace of the complete Hilbert space to the a numerical search in the almost complete Hilbert space. In this paper, we extend the Rayleigh-Ritz principle to Nelson's stochastic mechanics formulation of non-relativistic quantum mechanics, and propose a new algorithm to find the osmotic velocities $u(x)$, which contain the information of a quantum systems in this picture. As a proof of concept, we calculated $u(x)$ for one dimensional systems, the harmonic oscillator, the double well and the Pöschl-Teller potential. To obtain exited states, we calculate ground states of super symmetrical partner Hamiltonians for each of these potentials. We will show that this method is more efficient than the stochastic optimal control algorithm, that was the usual method to obtain osmotic velocities without going back to the Schrödinger equation.

MP 7.2 Tue 11:00 Poster B

**Quantum Dynamics on a Two-dimensional Comb: A Numerical Investigation** — •Ognen Kapetanoski and Irina Petreska — Ss. Cyril and Methodius University in Skopje, Faculty of Natural Sciences and Mathematics, Institute of Physics, Skopje, Macedonia

This study explores the quantum dynamics in anisotropic and heterogeneous media, using the comb model - a unique branched structure characterized by a backbone and lateral fingers. The focus is on the two-dimensional comb, which constitutes a simplified yet comprehensive model for theoretical investigation of the quantum motion under geometric constraints. The comb-like constraints are achieved by incorporating the Dirac delta function into the kinetic energy operator of the Schrödinger equation. Employing the finite difference approximation and the fourth-order Runge-Kutta method, the time-dependent Schrödinger equation is numerically solved. This enables the calculation of the wave functions and analysis of the probability density function. From the obtained results, localization of the wave packet due to the comb-like geometric constraints is evident. We also recall the previously derived analytical solutions on an infinite domain, expressed in terms of the Fox H-function. The comparative analysis between the analytical and numerical solution highlights the complexity of quantum transport phenomena, underscoring the challenges and potential of theoretical and computational approaches in quantum mechanics.

[1] T. Sandev, I. Petreska, E.K. Lenzi, *J. Math. Phys.* **59**, 012104 (2018).

MP 7.3 Tue 11:00 Poster B

**How to model an EUV-polariton?** — •Fridtjof Kerker[1,2], Christina Bömer[1,3], and Dietrich Krebs[1,2,3] — [1]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany — [2]Department of Physics - Universität Hamburg, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

In recent studies of x-ray parametric down-conversion (XPDC), unexpected imprints of a polaritonic excitation in the extreme ultraviolet (EUV) regime have been revealed. While polaritons, i.e., hybridized states of light and matter, exist in numerous contexts, they are largely unexplored at short wavelengths, such as the EUV spectral range. Under these conditions, new theoretical approaches are necessary to understand the phenomenon.

In this poster presentation, we introduce a first model of the EUV-polariton, which allows us to simulate its generation inside a diamond sample during XPDC. We derive the full scattering signal according to our model and find good agreement with the experimental XPDC data. We further employ our model to analyze the coupling strength of the observed EUV-polariton and discover it to reach up to the strong-coupling regime - notably without requiring an external enhancement-cavity. Our results provide first theoretical insights into this new kind of polariton and constitute a basis for future investigations into strong EUV-light-matter coupling.

MP 7.4 Tue 11:00 Poster B

**Driving chiral matter by chiral light** — •Alexandra Schrader, Benjamin Schwager, Christian Bohley, and Jamal Berakdar — Martin-Luther-Universität Halle-Wittenberg

Many chiral materials display a magneto-electric response which, in lowest order, can be expressed by a complex cross-coupling of the electric (magnetic) dipole moments to the magnetic (electric) fields. A number of physical properties depend on the material's chirality state and hence it is important to find ways to drive and separate objects according to their chirality. E.g., chiral molecules, which are crucial in drug manufacturing, can be chirality-specific separated by optical forces which act differently on different types of enantiomer. This theory contribution discusses how engineering the chiral characteristics of light through structuring both the spatial polarization and orbital phase allow to optimize the chiral forces and torques to steer chiral matter.

MP 7.5 Tue 11:00 Poster B

**Particle dynamics on quantum membranes** — •Lars Meschede, Benjamin Schwager, and Jamal Berakdar — Martin-Luther-Universität Halle-Wittenberg

We are working on an approach for an effective description of particles confined to a thin tubular neighborhood of a curved, dynamical, lower-dimensional submanifold (e.g. membranes). In addition to the well-known geometric potential due to confinement to a static submanifold, the dynamical degrees of freedom give rise to new effective, dynamical scalar and vector potentials. The coupling of the particles to the underlying space itself allows the transfer of energy and momentum to the manifold. In the case of membranes, the coupled dynamics of the particles and the membrane can be described by a (quantum) field theory of two interacting fields, which also yields an equation governing the membrane dynamics in the presence of particles confined to it. This setup can be seen as an elastic field analog of an electromagnetic cavity. If one considers the non-relativistic case, the Lagrangian and the necessity of the existence of a new effective vector potential follow from the invariance requirement under Galilean transformations. An additional coupling of the particles to the external electromagnetic field allows radiative excitations of vibrational modes of the membrane. This approach could be of interest for the description of the long-wavelength coupled electron-membrane dynamics on flexible 2D structures.

MP 7.6 Tue 11:00 Poster B

**Electron-phonon and Coulomb intercation in twisted bilayer graphene aligned on WSe$_2$** — •Sonia Haddad[1,2] and Jihang Zhu[3] — [1]Laboratoire de Physique de la Matière Condensée, Faculté des Sciences de Tunis, Université Tunis El Manar, Campus Universitaire 1060 Tunis, Tunisia — [2]Institute for Theoretical Solid State Physics, IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [3]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, Dresden 01187, Germany

The origin of the superconducting state, emerging at the so-called magic-angle (MA), in twisted bilayer graphene (TBG) is still an open question. However, there is a general consensus on the key role of the flat electronic bands occuring at the MA. Recently, a stable superconducting state has been observed in TBG aligned on WSe$_2$ at small twist angles compared to MA, which calls into question the relevance of the flat bands. Here we address the role of SOC induced in TBG by its proximity to WSe$_2$. Based on the continuum model, we study the effect of the SOC on the electron-phonon interaction and on the screened Coulomb potential. Our results show that the latter is the key factor for the stability of the superconducting phase, which is expected to be due to a Kohn-Luttinger mechanism.

MP 7.7 Tue 11:00 Poster B

**Microscopic mechanism of photo-induced tip-surface currents driven by near-infrared pulses** — •Carlos Bustamante[1], Franco Bonafé[1], Simon Maier[2], Rupert Huber[2], and Angel Rubio[1] — [1]Max Planck Institute for the Structure an Dynamics of Matter, Hamburg, Germany. — [2]Department of Physics, University of Regensburg, Regensburg, Germany.

The control of photo-induced currents from a tip using terahertz laser pulses, when combined with electronic microscopy, has allowed the study of ultrafast dynamics at the atomic scale. Although the charge transfer process has been described by simplified models, further improvement of this technique to achieve shorter time scales and better resolution at the atomic scale requires an ab initio framework. In this work, we have studied the electron dynamics of a tip-surface arrangement described atomistically, when interacting with near-infrared single-cycle laser pulses using TDDFT. Our results provide further insight into the nature of the photo-current induced by the laser pulse, its dependence on the electric field amplitude of the laser and the role of multiphoton absorption.

MP 7.8 Tue 11:00 Poster B

**Slow Modes in Dissipatively Stabilized Superconductors** — •Tom Zander and Sebastian Diehl — Universität zu Köln, D-50937 Cologne, Germany

Topological states of fermionic matter can be induced by purely dissipative dynamics. Other interesting states can exhibit superfluidity or superconductivity. The states which are cooled into, irregardless of the initial state, are called 'dark states'.

We construct an interacting field theory using the Keldysh formalism to investigate a system of 1d fermions cooling into a superconducting dark state. Using the Hubbard-Stratonovich transformation, as well as other tools of quantum field theory, we derive, in the long wavelength limit, the effective slow mode action for the Goldstone and hydrodynamic modes.

MP 7.9 Tue 11:00 Poster B

**Energy conserving adaptive QM/MM method using an extended Hamiltonian approach** — •Marvin Nyenhuis and Nikos Doltsinis — Institute for Solid State Theory, University of Münster, Wilhelm-Klemm-Straße 10, 48149 Münster

We present an extended Hamiltonian formalism that introduces a fictitious switching particle with mass $\mu_k$ which propagates a system between two different potential energy surfaces ($V_{k-1} \to V_k$) during a hybrid ab initio (QM) and classical force field (MM) molecular dynamics simulation by mixing both potentials via a switching function $g(\lambda_k) \in [0,1]$.

$$\mathcal{H} = \sum_{I=1}^{N} \frac{\mathbf{P}_I^2}{2M_I} + \sum_{j=1}^{k} \frac{\Delta V_j}{|\Delta V_j|} \frac{1}{2} \mu_j \dot{\lambda}_j^2 + \underbrace{g(\lambda_k) V_{k-1}(\mathbf{R}) + \{1 - g(\lambda_k)\} V_k(\mathbf{R})}_{V_{\mathrm{mix}}}$$

The Hamiltonian consists of the kinetic energy of all nuclei $I \in \{1, \ldots, N\}$ with mass $M_I$, kinetic energy of all completed $\lambda_j$, $j \in \{1, \ldots, (k-1)\}$ and running switching procedures ($\lambda_k$) as well as the mixed potential energy $V_{\mathrm{mix}}$ depending on all nuclear positions $\mathbf{R}$. Each $\lambda_k$ is propagated from 0→1 and describes the progress of switching.

MP 7.10 Tue 11:00 Poster B

**Numerical simulations of stochastic optimal control model for navigation of finite size microswimmers** — •Malte Thumann — Institut für Numerische und Angewandte Mathematik, Universität Göttingen

Using stochastic optimal control theory, we study the optimal navigation of finite size microswimmers in the presence of a fluid flow and thermal fluctuations in two-dimensional space. The resulting Hamilton-Jacobi-Bellmann (HJB) equation is a nonlinear convection-diffusion type partial differential equation (PDE) that describes the optimal torque an active swimmer must satisfy to navigate towards a desired target. This equation is numerically solvable in a three-dimensional phase space (position and orientation) for a given set of initial conditions. We discretise the HJB equation in a finite element framework known as the discontinuous Galerkin method, which operates over a trial space of functions that are only piecewise continuous. This allows for a more stable and flexible discretisation scheme, in particular to cope with the challenging task of implementing singular boundary conditions arising from the stochastic optimal control approach. Using the optimal torque solution, we perform stochastic simulations to determine the optimal mean microswimmer path. Our work emphasises that finite element methods are a suitable discretisation technique to handle PDEs arising in theoretical biophysics in a non-trivial setting with complex geometries, singularities, or higher order local approximations.

MP 7.11 Tue 11:00 Poster B

**Perturbative Series Expansions for Two-Particle Bound-State Energies in the Thermodynamic Limit: A Green's Function Approach** — •Maximilian Bayer, Patrick Adelhardt, and Kai Phillip Schmidt — Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Staudtstr. 7, 91058 Erlangen, Germany

The investigation of (quasi-)particle bound states has been a focal point in quantum mechanics research, tracing its roots back to the solutions of the Hydrogen atom. In the realm of solid-state systems, the emergence of two-quasi-particle bound-states, such as excitons, Cooper pairs or magnon-magnon bound-states in spin systems, gives rise to unique material properties. Our interest lies in developing general techniques for systematically computing the energies associated with such bound-states on lattice systems in a perturbative manner.

We introduce an approach based on zero-temperature Green's functions (Resolvents), capable of generating series expansions for these energies in the thermodynamic limit, eliminating the need for exact diagonalization and Rayleigh-Schrödinger perturbation theory on finite systems. This technique is universal in the dimensionality of the system and accommodates fermionic, bosonic, and hard-core bosonic particles, only requiring finite-range interactions.

By reducing the eigenvalue equation into the determinant of a finite matrix we obtain a finite expression even for infinite systems. This expression allows for the extraction of bound-state energies either exactly for fixed perturbation parameters or in the form of a power series, if such a series exists.

MP 7.12 Tue 11:00 Poster B

**Comparison the determination techniques of the effective refractive index of all-dielectric metasurface as a graphene layer substrate using finite-element electromagnetic simulations** — •Zoya Eremenko and Aliaksei Charnukha — Leibniz Institute for Solid State and Materials Research

We proposed the use of the resonant all-dielectric metasurface as a graphene layer substrate. The task is to define the effective refractive index of such a metasurface to have the possibility to control the surface plasmon polariton propagation length. We studied some techniques to define the effective refractive index of the metasurface. The first one is determining the band structure of a two-dimensional photonic crystal with a square lattice of the defined metasurface structure and obtained the eigen frequencies at definite relation between metasurface unit cell parameters. The second one is retrieval of the effective parameter technique from S-parameters defined from simulations results. Thus, such techniques give the opportunity to use any structure configuration of the resonant all-dielectric metasurfaces.

MP 7.13 Tue 11:00 Poster B

**Thermalization of black holes and the SYK model** — •Zhuo-Yu Xian[1], Yuxuan Liu[2], Shao-Kai Jian[3], Yi Ling[4], and Jiasheng Liu[5] — [1]Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany — [2]Institute of Quantum Physics, School of Physics, Central South University, Changsha 418003, China — [3]Department of Physics and Engineering Physics, Tulane University, New Orleans, Louisiana, 70118, USA — [4]Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, China School of Physics, University of Chinese Academy of Sciences, Beijing 100049, China — [5]Ludwig-Maximilians-Universität München, Geschwister-Scholl-Platz, 1 D-80539 München

We investigate the evolution of entanglement and Heisenberg operators within open and strongly coupled systems interacting with its environment, in the frameworks of both the doubly holographic model and the Sachdev-Ye-Kitaev (SYK) model. In both cases, the entanglement within the system initially increases as a result of internal interactions; however, it eventually dissipates into the environment. We also study the operator size growth in the Lindbladian SYK model and analytically obtain the suppression of the growth due to the dissipation. The dynamic behaviors of the entanglement and the opeartor size observed in these two models are attributable to the competition between the internal interaction of the system and the external interaction with the environment.

MP 7.14 Tue 11:00 Poster B

**Conceptual-Mathematical Approach for the Derivation of Effective Field Theories from QCD- & Gauge Theories (Large 48x48 matrices in QCD from Hubbard-Stratonovich transformations)** — •Bernhard Mieck — Keine Institution

An effective field theory of BCS quark pairs is derived from an ordinary QCD-type path integral with SUc(Nc=3) non-Abelian gauge fields. We consider the BCS quark pairs as constituents of nuclei and as the remaining degrees of freedom in a coset decomposition SO(N,N) /U(N) x U(N) of a corresponding total self-energy matrix taking values as generator within the so(N,N) Lie algebra. The underlying dimension (N = Nf x 4 x Nc) is determined by the product of isospin- 'Nf = 2' (flavour- 'Nf = 3') degrees of freedom, by the 4x4 Dirac gamma matrices with factor '4' and the colour degrees of freedom 'Nc = 3'; therefore, the smallest, total self-energy generator has Lie algebra so(N,N) with N = 24. We distinguish between a total unitary sub-symmetry U(N) for purely density related parts of the quarks, which are taken into account as background fields and as invariant vacuum states in a SSB, and between the BCS terms of quarks as coset elements so(N,N) / u(N). These HST's are sufficient to achieve a path integral entirely determined by self-energy matrices for the coset decomposition. Concerning homotopies, we attain the nontrivial Hopf mapping Π_{3}(S^2)=Z from consideration of Fujikawa-anomalies and would like to point again the possibility for further nontrivial homotopies, as e.g. Π_{7}(S^4) = Z or Π_{2^n -1}( S^( 2^(n-1) ) ) = Z.

MP 7.15 Tue 11:00 Poster B

**Wave function of the universe in the presence of trans-Planckian censorship** — •Vikramaditya Mondal — School of Physical Sciences, Indian Association for the Cultivation of Science, Kolkata 700032, India

The wave function for a closed de Sitter universe has been computed, demanding consistency with the recently proposed Trans-Planckian Censorship Conjecture (TCC). We extend the Einstein-Hilbert action to contain a complex-valued term that provides an exponentially decaying weight for the geometries violating TCC in the Lorentzian path integral sum while working in the minisuperspace approach to quantum cosmology. This postulated modification suppresses the probability of the evolution of the universe into configurations that violate TCC. We show that due to the presence of this suppression factor, the Hubble rate of the universe at the end of the inflation gets subdued and assumes a value less than what is expected classically. Moreover, the consequences of this quantum gravity-motivated correction in the primordial power spectrum are discussed as well.