

QMA Fall School

Topological Quantum Matter 2023

September 27 - 29, 2023

Penta Hotel in Leipzig



ct.qmat

**Complexity and Topology
in Quantum Matter**

Wednesday, September 27	
13:00 - 14:00	Arrival
14:00 - 14:10	Welcome note from organisers
14:10 - 14:30	Introduction to QMA/ct.qmat by Matthias Vojta <i>“Complexity and Topology – The Next 10 Years”</i>
14:30 - 16:00	Frédéric Mila <i>“Introduction to Frustrated Magnetism”</i>
16:00 - 16:30	Coffee Break
16:30 - 18:00	Felix Lüpke <i>“Van-der-Waals-Materials and Heterostructures studied by Scanning Tunneling Microscopy”</i>
18:30 - 20:00	Dinner
20:00 –	Poster Session
Thursday, September 28	
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08:30 - 10:00	Natalia Chepiga <i>“Chiral Transitions in Arrays of Rydberg Atoms”</i>
10:00 - 10:30	Coffee Break
10:30 - 12:00	Thierry Giamarchi <i>“An Introduction to Quantum Transport in Cold Atomic Gases”</i>
12:00 - 13:30	Lunch
13:30 - 15:00	Alexander B. Khanikaev <i>“Adiabatic Topological Photonics”</i>
15:00 - 15:20	Coffee Break
15:20 - 16:50	Weiwei Xie <i>“Exploring Novel Quantum Materials under High Pressure and High Temperature”</i>
17:00 - 19:00	City Tour
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10:00 - 10:30	Coffee Break
10:30 - 12:00	Philip J. W. Moll <i>“The Unusual Electron Transport in Metallic Kagome Nets ”</i>
12:00 - 14:00	Lunch
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14:30	Departure

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P5	Yu Wang, JMU Würzburg, Germany Observation of Zero Energy States of 1D Gadolinium Chains on Nb(110) Superconducting Surface
P6	Abdul-Vakhab Tcakaev, JMU Würzburg, Germany Intermixing-Driven Surface and Bulk Ferromagnetism in the Quantum Anomalous Hall Candidate $\text{MnBi}_6\text{Te}_{10}$
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Frédéric Mila

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Frédéric Mila graduated from École Polytechnique in Paris in 1983. At Orsay University, he pursued an advanced degree in solid-state physics and subsequently completed his education with a Ph.D. focusing on surface phonon theory in 1987. Over the course of six years, he held prestigious postdoctoral positions at ETH-Zürich, Rutgers University in the USA, and Neuchâtel University in Switzerland. In 1993, he secured a permanent position at CNRS (National Center for Scientific Research) and, in 2000, was appointed as a Professor of Theoretical Physics at Lausanne University. Since October 2003, he has held the position of a full Professor at the EPFL (École Polytechnique Fédérale of Lausanne), where he currently leads the Chair of Condensed Matter Theory.

Frédéric Mila is not only an expert in frustrated magnetism, but has as well co-authored the book “Introduction to Frustrated Magnetism”, published in 2011. He is known for his research including quantum-antiferromagnetism, spin liquids and the Shastry-Sutherland model.

“Introduction to Frustrated Magnetism”

14:30 - 16:00 Wednesday, September 27

In this lecture, I will give a self-contained introduction to frustrated magnetism, starting from the fundamental concept of classical degeneracy, and working out the main consequences of this degeneracy for classical and quantum magnets: algebraic correlations in spin-ice like models, thermal and quantum order-by-disorder, gapped spin liquids and resonating valence-bond phases, gapless algebraic spin liquids, and magnetization plateaus.

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Felix Lüpke

Peter- Grünberg Institute, Forschungszentrum, Jülich, Germany

Dr. Felix Lüpke received his Ph.D. in 2017 at Peter Grünberg Institute (PGI-3) in Jülich, Germany. Subsequently, he joined as a postdoctoral fellow at Carnegie Mellon University, Pittsburgh, Pennsylvania in 2018. He was a postdoctoral research fellow of the Alexander von Humboldt Foundation at Oak Ridge National Laboratory from 2019-2020. At present, he holds the Junior Group Leader position at Forschungszentrum Jülich. This year he received DFG funding from the German Research Foundation for his outstanding research and now he wants to establish his own research group and become a professor. Dr. Felix Lüpke was awarded the Excellence Prize from the Jülich Research Center in 2019 for his doctoral work, where he modified the technology of a multi-tip scanning microscope and enabled it to decipher electronic properties of charge transport in quantum materials on the nanoscale. He is an expert in scanning probe techniques in the field of van der Waals materials. His research focuses on topological materials which, in combination with superconductors, allow to creation of Majorana states - potential candidates for future quantum computing. He further employs four-probe scanning tunneling microscopy to perform nanoscale transport measurements.

“Van-der-Waals Materials and Heterostructures Studied by Scanning Tunneling Microscopy”

16:30 - 18:00 Wednesday, September 27

Two-dimensional van der Waals (vdW) materials, such as graphene, have attracted great interest due to their unique properties and high tunability. Their layered nature further allows the assembly of vdW heterostructures, which opens new routes for the engineering of exotic optical and electronic quantum states. To study the properties of vdW samples, scanning tunneling microscopy (STM) has become an important tool, because it gives direct access to their structural and electronic properties. In my talk, I will summarize the development of STM on vdW samples and will present recent results of our work including topological insulators and superconductors [1-7].

[1] F. Lüpke et al., Nature Physics 16, 526 (2020)

- [2] W. Ko et al., PRB 102, 115402 (2020)
- [3] F. Lüpke et al., Nano Letters 14, 5674 (2022)
- [4] F. Lüpke et al., PRB 105, 035423 (2022)
- [5] K. Jin, et al., arXiv.2306.10305 (2023)
- [6] J. Martinez-Castro et al., arXiv.2304.08142 (2023)
- [7] F. Lüpke et al., arXiv:2208.13374v2 (2023)

Acknowledgements

We acknowledge support by the German Research Foundation's (DFG) Emmy Noether Programme and Priority programme 2244 ('2D Materials – Physics of van der Waals [hetero]structures', project nos. 443416235 and 422707584); the Alexander von Humboldt Foundation; Germany's Excellence Strategy - Cluster of Excellence Matter and Light for Quantum Computing (ML4Q); European Union's Horizon 2020 Research and Innovation Programme under Grant Agreement no 824109 (European Microkelvin Platform); the Helmholtz Nano Facility; APVV-20-0425, VEGA 2/0058/20, Slovak Academy of Sciences project IMPULZ IM-2021-42, COST action CA21144 (SUPERQUMAP) and EU ERDF (European regional development fund) Grant No. VA SR ITMS2014+ 313011W856.

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Natalia Chepiga

Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands

In 2017, she earned her PhD with distinction in Condensed Matter Physics from École Polytechnique Fédérale de Lausanne in Switzerland. Subsequently, between 2017 and 2020, she embarked on two postdoctoral positions, one at the University of Amsterdam in the Netherlands and the other at the University of California, USA. Since 2021, she has held the role of Assistant Professor at the Kavli Institute of Nanoscience, Delft University of Technology in the Netherlands.

“Chiral Transitions in Arrays of Rydberg Atoms”

08:30 - 10:00 Thursday, September 28

Investigation of the nature of commensurate-incommensurate transition out of period- p phase has a long history that goes back to the study of absorbed monolayers on surfaces. The problem has been revived by recent experiments on Rydberg atoms in a 1D trap with the phase diagram dominated by lobes of integer periodicities $p=2,3,4,5\dots$. Recent development of constrained DMRG algorithm that takes a full advantage of Rydberg blockade brings the study of chiral melting to a completely new level of accuracy. In my talk I will present the numerical evidences that transitions out of period-3 and period-4 phases change their nature along the critical lines: conformal points in the three-state Potts and Ashkin-Teller universality classes are surrounded by direct chiral transitions followed in turn by an opening of floating phases. Furthermore, I will show how the appearance and the extent of the chiral transition can be manipulated in multi-component Rydberg arrays. [1-5]

- [1] N. Chepiga and F. Mila, Phys. Rev. Lett. 122, 017205 (2019)
- [2] N. Chepiga and F. Mila, SciPost Phys. 6, 33 (2019).
- [3] N. Chepiga and F. Mila, Nature Communications 12, 1 (2021)
- [4] I. A. Maceira, N. Chepiga, and F. Mila, Phys. Rev. Res. 4, 043102 (2022).
- [5] N. Chepiga, arxiv:2308.12838 (2023)

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Thierry Giamarchi

Theory of Quantum Matter, Université de Genève, Switzerland

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Thierry Giamarchi earned his physics degree from Ecole Normale Supérieure in Paris and obtained his PhD in 1987 from Paris XI University, focusing on "Localization and Interactions in one-dimensional quantum fluids". After a postdoc at Bell Laboratories, he became a professor at the University of Geneva in 2002. In recognition of his remarkable contributions, he was awarded the Aragam prize from the French Academy of Sciences in 2000. Furthermore, he is widely known for his book "Quantum Physics in One Dimension", published in 2003, which became a foundational work in the literature of one-dimensional systems.

His research delves into strongly interacting one-dimensional quantum systems, exploring phases like the Luttinger Liquid, Bose glass, and Bragg glass. He also collaborates with experimental groups in low-dimensional systems, including cold atomic gases.

"An Introduction to Quantum Transport in Cold Atomic Gases"

10:30 - 12:00 Thursday, September 28

Measuring the conductivity or other transport quantity is a routine measure in material science and solid state physics. It is however in principle a very complicated quantity to compute, since it is a case where the system is out of equilibrium. This is particularly the case when interactions between particles or disorder play a major role in the physics of the system. Recently cold atomic gases have provided a remarkable playground to study such quantum transport and stimulate further theoretical studies. I will review in this presentation the basic ideas in this field and discuss some of the recent results that have been obtained in connections with experiments in cold atomic gases, as well as discuss some of the challenges of the field.

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Alexander B. Khanikaev

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Dr. Alexander Khanikaev is currently a professor City University of New York in the department of electrical engineering and the Physics department. Previously, He was a Assistant Professor of Physics at Queens College. He obtained Ph.D degree in physics from M. V. Lomonosov Moscow State University, Russia. He did post-doctoral research work at Toyohashi University of Technology, Japan and University of Texas, Austin. Since 2020 he is a Fellow of Optical Society of America and He has been awarded NSF Special Creativity Award from the Division of Materials Research in 2021. He has a very unique area of interest that is to investigate topological properties of photonic and polaritonic systems. He mainly uses nano-patterned 2D materials, like graphene, hBN, transition metal dichalcogenides, etc. In addition, he has explored extensively nonreciprocal and nonlinear photonic nanostructures and plasmonic metamaterials by using infrared spectroscopy with special interest on bio-molecules.

“Adiabatic Topological Photonics”

14:00 - 15:30 Thursday, September 28

Topological phases of matter represent a new realm of physics that has been attracting significant attention across diverse fields, from inherently quantum systems (e.g., condensed matter and lattices of trapped ions) to purely classical photonic and acoustic metamaterials. In the context of photonics, topological phases offer resilience to defects and disorder and bring novel opportunities to control light with pseudo-spin degrees of freedom. However, topological photonic systems can suffer from limitations associated with their bosonic nature, including partial breakdown of topological properties due to their symmetry-protected origin and radiative leakage. In this article, we introduce the concept of adiabatic topological photonic interfaces, which helps to overcome these issues. We demonstrate theoretically and confirm experimentally that

adiabatic topological metasurfaces with slowly varying synthetic gauge fields significantly improve the guiding features of spin-Hall and valley-Hall topological photonic structures, which are commonly used in the design of symmetry-protected topological devices. Adiabatic variation in the domain wall profiles leads to the delocalization of topological boundary modes, which makes them less sensitive to details of the lattice, perceiving the structure as an effectively homogeneous Dirac metasurface. As a result, the topological modes showcase enhanced bandgap crossing behavior, longer radiative lifetimes and propagation distances, while retaining their topological resilience.

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Weiwei Xie

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Weiwei Xie completed her Bachelors degree in chemistry in 2010 at Nankai University, Tianjin, China. Following this she joined Gordon Miller's group at Iowa State University to study intermetallics. There she was lucky enough to study under both Gordon Miller and John Corbett, who are both giants in their fields. This sparked her growing interest in solid-state chemistry, with employing varying synthetic methods becoming a focus during this time. Following the completion of her PhD in 2014, she then went on to do her postdoc with another great in the field of solid-state chemistry, Robert Cava. She spent two years there, during which she broadened the scope of materials of interest to superconductors. All of this led to her joining Louisiana State University as an Assistant Professor in 2016, before moving on to Rutgers University as an Assistant Professor in 2020 and most recently, becoming an Associate Professor at Michigan State University in 2022. Over the course of the last eight years, she has earned numerous awards, including the Beckman Young Investigator award in 2018, the Rainmaker Emerging Scholar for Research and Creative Activity in 2020 and the NSF Career Award in 2020. Throughout all of this she has maintained a keen interest in elucidating crystal structures of solid-state materials and linking these to their respective physical properties, finding novel superconducting and topologically non-trivial materials and trying to understand the effect that high pressures can have on the structure and properties of the materials.

“Exploring Novel Quantum Materials under High Pressure and High Temperature”

16:00 - 17:30 Thursday, September 28

Pressure, an intensive variable, is a virtually unexplored pathway to new quantum materials. The application of high pressure can yield dramatic new examples of quantum materials. In this presentation, I will discuss how high pressure can be used to tune unexpected physical properties in magnetic topological materials and low dimensional materials. High pressure neutron scattering techniques will be the focus of the discussion. The use of high pressure and high temperature synthesis can

stabilize the exotic quantum phenomena detected by high pressure neutron scattering. I will also introduce our new lab-based in-situ high pressure and high temperature single crystal X-ray diffraction technique, which can guide us to synthesize materials rationally under high pressure and high temperature. Furthermore, we are utilizing artificial intelligence (AI) to search for the metastable phase under high pressure, which enables us to explore a much larger phase space and discover new quantum materials. These advancements in high pressure techniques and the integration of AI have opened up new avenues for discovering and understanding quantum materials.

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Michael Sentef

Theoretical Solid State Physics, University of Bremen, Germany

Prof. Michael Sentef received his PhD degree in Physics on “Electronic correlations in insulator, metals and superconductors” at the University of Augsburg in 2010. Then he joined as a postdoctoral fellow in Stanford University and SLAC from 2011-2014. Then he moved back to Germany and joined as a postdoctoral fellow at the University of Bonn for one year. In 2015-2016, he became a Group leader at the Max Planck Institute for the Structure and Dynamics of Matter, Hamburg. From 2016 to 2022, he was the group leader of the Emmy Noether research group on “theoretical description of ultrafast spectroscopies in solids.” Then he became an associate professor of Physics at the University of Bristol, UK for one year. At present, he holds the position of professor of Theoretical solid-state physics at the University of Bremen.

His research is focused on light-matter control of quantum materials which includes ultrafast dynamics of condensed matter, theory of time-resolved pump-probe spectroscopies, novel light-induced nonequilibrium states of matter, floquet states in driven quantum many-body systems. His group investigate the materials interacting with light in ways that can probe and modify key materials properties.

“Light-Matter Control of Quantum Materials”

08:30 - 10:00 Friday, September 29

Advances in time-resolved pump-probe spectroscopies have enabled us to follow the microscopic dynamics of quantum materials on femtosecond time scales. This gives us a glimpse into the inner workings of how complex, emergent functionalities of quantum many-body systems develop on ultrafast time scales or react to external forces. The ultimate dream of the community is to use light as a tuning parameter to create new states of matter on demand with designed properties and new functionalities, perhaps not achievable by other means. In this talk I will discuss recent progress in controlling and engineering properties of quantum materials through light-matter interaction [1]. I will highlight work on Floquet engineering — the creation of effective Hamiltonians by time-periodic drives — on sub-cycle time scales [2,3] combining theory and pump-probe experiments at the limits of energy and time resolution. I will then showcase recent theories on inducing superconductivity with light by employing

enhanced light-matter interaction in the near-field involving polaritonic excitations [4,5].

[1] M. A. Sentef, “Licht treibt Materie an“, Physik-Journal, März 2023

[2] M. Schüler and M. A. Sentef, <https://doi.org/10.1016/j.elspec.2021.147121>

[3] S. Ito et al., Nature 616, 696-701 (2023), <https://www.nature.com/articles/s41586-023-05850-x>

[4] C. J. Eckhardt et al., arXiv:2303.02176

[5] S. Chattopadhyay et al., arXiv:2303.15355

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Philipp J. W. Moll

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Hamburg, Germany

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Philipp Moll received his Ph.D. in 2012 from ETH Zurich in Switzerland. After continuing his research there for the next two years, he moved to the University of California at Berkeley as a post-doctoral fellow in 2014. In 2016, he moved back to Germany, where he joined the Max Planck Institute for the Chemical Physics of Solids in Dresden as a leader of the research group "Physics of Microstructured Quantum Matter". Then, in 2018, he was appointed as an assistant professor at the Institute of Materials at EPFL, Switzerland, where he heads the Laboratory of Quantum Materials. Since 2021 he has been appointed Director at the Max Planck Institute for the Structure and Dynamics of Matter in Hamburg.

Prof. Moll is a recipient of the Nicholas Kurti Science Prize (2018), the ABB Award of the Swiss Physical Society (2014), and was selected as a World Economic Forum Young Scientist in 2020. He has also been awarded ERC Starting Grant in 2017, ERC Consolidator Grant in 2022, and a Professorial Fellowship from the Swiss National Science Foundation in 2018.

Prof. Moll studies quantum materials at the microscale. He is particularly interested in topological metals, unconventional superconductors and other strongly correlated electron systems. He is developing new techniques for the fabrication of high-quality crystalline microstructures for measurements of electrical transport, magnetization or thermal conductivity.

"The Unusual Electron Transport in Metallic Kagome Nets"

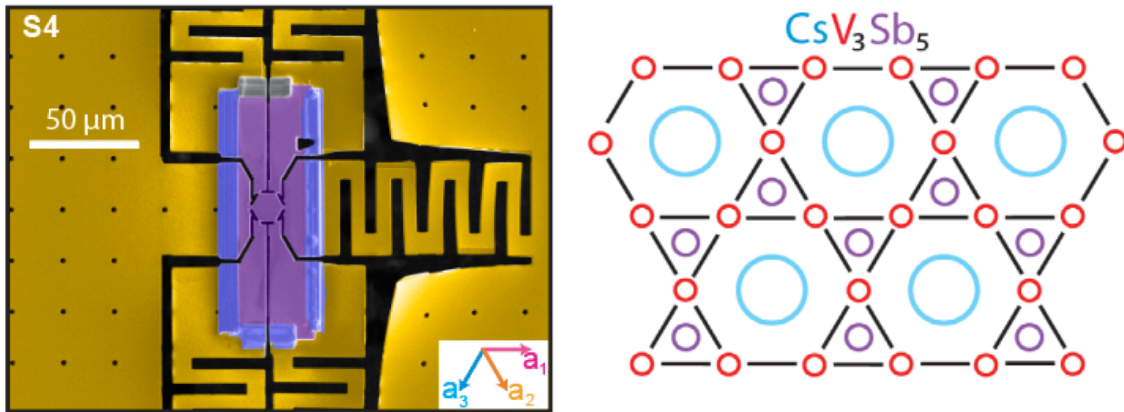
10:30 - 12:00 Friday, September 29

Materials that can host different states of electronic order form a recurring theme in physics and materials science, and they are of particular interest if they are coupled strongly. A famous example are ferroelectrics, in which electric polarization and magnetism not only coexist but are strongly linked. This both unveils a rich physics of correlated states, and also opens unexpected application avenues as the coupling promises to manipulate one state by a stimulus that primarily acts on another – say

switching magnetism using electric fields.

Recently, materials based on the structural motif of the Kagome web have attracted significant attention for their tendency to host such strongly coupled phases. In particular, the centro-symmetric layered Kagome metal $(\text{K,Cs})\text{V}_3\text{Sb}_5$ have entered the focus of experimental and theoretical research. They host a charge-density-wave type transition at elevated temperatures ~ 100 K, followed by a superconducting transition at 3K (exact values depend on composition). Yet there is another type of electronic order which thus far eludes exact microscopic identification. A series of experimental probes detects the onset of anomalous behavior around $T' \sim 30 - 40$ K, including thermal Hall, μSR , NMR, magnetic torque, Kerr rotation. The anomalous low-temperature state carries the characteristics of a chiral, nematic and time-reversal-symmetry breaking fluid (all of which are under most active debate currently).

Yet what crystallizes out of the current state of experimental data is a highly entangled system which is extraordinarily responsive to external perturbations. This materials main strength is equally its weakness, the unusual degree of coupling between states can hinder its systematic investigation. However, it is already clear that it provides a platform to explore strongly coupled correlated phases, and as a result it displays a thus-far unknown electromagnetic response, a diode in which the forward direction can be switched by the application of a magnetic field. I will review the current state of the field, and discuss ongoing projects in my department.



[1] C. Guo et al., Nature 611, 461-466 (2022)

[2] X. Huang et al., PRB 106, 064510 (2022)

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List of Poster Abstracts

Quantum Transport Properties of the Superconducting Weyl Semimetal

Ankit Kumar, IFW Dresden, Germany



P1

Novel quantum materials with band structures showing both topologically non-trivial nature and superconducting properties, in the last decade, a lot of interest due to the interplay between superconductivity and topologically protected electronic surface states and related exciting possibilities of application in the emergent quantum technologies.

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2D High Temperature Superconductor Integration in Contact Printed Circuit Boards

P2

Christian Niclaas Saggau, IFW Dresden, Germany

Inherent properties of superconducting $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ films, such as their high superconducting transition temperature T_c , the efficient Josephson coupling between neighboring CuO layers, and fast quasiparticle relaxation dynamics, make them a promising platform for advances in quantum computing and communication technologies. However, preserving two-dimensional superconductivity throughout the device fabrication is an outstanding experimental challenge due to the fast degradation of its superconducting properties when exposed to moisture, organic solvents, and heating sources. Here, to realize functional superconducting devices based on the sensitive two-dimensional material, we develop a novel fabrication technique relying on the cryogenic dry transfer of printable circuits embedded into a silicon nitride membrane. This approach separates the circuit fabrication stage requiring chemically reactive substances and ionizing physical processes from the creation of the thin superconducting structures. Apart from providing electrical contacts in a single transfer step, the membrane encapsulates the surface of the crystal shielding it from the environment. The fabricated atomically thin $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ devices show a high superconducting transition temperature T_c of 91 K equal to that of the bulk crystal and stable superconducting properties.

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Flat Bands of Surface States in Chiral Symmetric Superconductors

P3

Clara Johanna Lapp, TU Dresden, Germany

Noncentrosymmetric superconductors can support flat bands of zero-energy surface states in part of their surface Brillouin zone. This requires that they obey time-reversal symmetry and have a sufficiently strong triplet-to-singlet-pairing ratio to exhibit nodal lines. These bands are protected by a winding number that relies on chiral symmetry, which is realized as the product of time-reversal and particle-hole symmetry. We here reveal a way to stabilize a flat band in the entire surface Brillouin zone, while the bulk dispersion is fully gapped. The necessary ingredient is an additional spin-rotation symmetry that forces the direction of the spin-orbit-coupling vector not to depend on the momentum component normal to the surface, which allows us to block diagonalize the Bogoliubov-de Gennes Hamiltonian. We define a winding number which leads to flat zero-energy surface bands due to bulk-boundary correspondence. In addition, we consider how a weak breaking of the additional symmetry affects the surface band, employing first-order perturbation theory and a quasiclassical approximation. We find that the surface states still persist for a weak breaking of the additional symmetry but that the band does not remain perfectly flat. The broadening of the band strongly depends on the deviation of the spin-orbit-coupling vector from its unperturbed direction as well as on the spin-orbit-coupling strength and the triplet-pairing amplitude.

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The Superconducting Symmetries of CeRh₂As₂

Fabian Jakubczyk, TU Dresden, Germany

P4

Multiphase unconventional superconductivity is a rare phenomenon, which has recently been discovered in the tetragonal but locally noncentrosymmetric heavy-fermion compound CeRh₂As₂. Here, the transition between two distinct superconducting phases occurs as a function of magnetic field applied along the *c* axis ($H||c$) and the formation of superconductivity takes place around $T_{SCI} \approx 0.3$ K. At $\mu_0 H^* \approx 4$ T the superconductor changes from a low-field to a high-field state with a large critical field of $\mu_0 H_{c2} \approx 14$ T. However, for in-plane fields ($H||ab$) only the low-field phase appears, with $\mu_0 H_{c2} \approx 2$ T. Recent As-NQR & -NMR experiments revealed additional intriguing phenomena in this material, for they detected the onset of antiferromagnetism within the superconducting low-field phase, i.e., at $T_N < T_{SCI}$. In order to study the coexistence and interplay of the potential superconducting and magnetic phases, as well as the effect of an external magnetic field, we conduct a symmetry analysis complemented by a Landau free energy expansion. Thereby we can give a statement about the probable symmetries of the superconducting states and their intrinsic connection to magnetism in this material.

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Observation of Zero Energy States of 1D Gadolinium Chains on Nb(110) Superconducting Surface

P5

Yu Wang, JMU Würzburg, Germany

Transition metal adatoms act as magnetic impurities that cause Yu-Shiba-Rusinov (YSR) bound states to form within the energy gap of conventional s-wave superconductors. These bound states are localized at the impurity sites and can assemble into one dimensional (1D) YSR chains that display zero-energy edge states that could be topologically trivial or non-trivial. This study focuses on investigating the impact of rare-earth-metallic species (REMs), specifically Gadolinium atoms as magnetic impurities on Nb(110). The research has revealed the presence of zero-energy states at the edges of chains as short as 5Gd, which may signify the first time that topologically non-trivial zero-energy edge states have been generated from REMs. This discovery could have significant implications for the development of new superconducting materials and the design of future quantum devices.

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Intermixing-Driven Surface and Bulk Ferromagnetism in the Quantum Anomalous Hall Candidate $\text{MnBi}_6\text{Te}_{10}$

P6

Abdul-Vakhab Tcakaev, JMU Würzburg, Germany

The recent realizations of the quantum anomalous Hall effect (QAHE) in MnBi_2Te_4 and MnBi_4Te_7 benchmark the $(\text{MnBi}_2\text{Te}_4)(\text{Bi}_2\text{Te}_3)_n$ family as a promising hotbed for further QAHE improvements. The family owes its potential to its ferromagnetically (FM) ordered MnBi_2Te_4 septuple layers (SLs). However, the QAHE realization is complicated in MnBi_2Te_4 and MnBi_4Te_7 due to the substantial antiferromagnetic (AFM) coupling between the SLs. An FM state, advantageous for the QAHE, can be stabilized by interlacing the SLs with an increasing number n of Bi_2Te_3 quintuple layers (QLs). However, the mechanisms driving the FM state and the number of necessary QLs are not understood, and the surface magnetism remains obscure. Here, robust FM properties in $\text{MnBi}_6\text{Te}_{10}$ ($n = 2$) with $T_C = 12$ K are demonstrated and their origin is established in the Mn/Bi intermixing phenomenon by a combined experimental and theoretical study. The measurements reveal a magnetically intact surface with a significant magnetic moment and FM properties similar to the bulk. This investigation thus consolidates the $\text{MnBi}_6\text{Te}_{10}$ system as a perspective for the QAHE at elevated temperatures.

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Magnetic Warping in Topological Insulators

Gabriele Naselli, IFW Dresden, Germany

P7

We analyze the electronic structure of topological surface states in the family of magnetic topological insulators $\text{MnBi}_{2n}\text{Te}_{3n+1}$. We show that, at natural-cleavage surfaces, the Dirac cone warping changes its symmetry from hexagonal to trigonal at the magnetic ordering temperature. In particular, an energy splitting develops between the surface states of the same band index but opposite surface momenta upon formation of the long-range magnetic order. As a consequence, measurements of such energy splittings constitute a simple protocol to detect the magnetic ordering via the surface electronic structure, alternative to the detection of the surface magnetic gap. Interestingly, while the latter signals a nonzero surface magnetization, the trigonal warping predicted here is, in addition, sensitive to the direction of the surface magnetic flux. Our results may be particularly useful when the Dirac point is buried in the projection of the bulk states, caused by certain terminations of the crystal or in hole-doped systems, since in both situations the surface magnetic gap itself is not accessible in photoemission experiments.

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Direct Observation of Mn Anti-Site Sublattice Coupling and its Distinct Ordering Transition in Magnetic Topological Insulator Candidates

P8

Manaswini Sahoo, IFW Dresden, Germany

The magnetic topological insulator candidates promise a new era of novel quantum phenomena and their application in spin-based technologies. MnBi_2Te_4 , through antiferromagnetic, is the most promising among all, providing tunable magnetic and electronic order by different means. One of them is intermixing where cationic intermixing plays an important role in stabilizing a net magnetization. Here we studied through sensitive local probe techniques like Nuclear magnetic resonance and muon spin relaxation, the role and impact of intermixing on the magnetic properties of all the MnBi_2Te_4 (Bi_2Te_3) $_n$, $n = 0, 1, 2$ family and MnSb_2Te_4 powder samples, revealing opposite coupling of the magnetic sites at the ground state and effective decoupling at above certain temperatures. This result opens a new path towards controlling the intermixing as a probe to realize the much anticipated ferromagnetic topological insulators.

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Bismuth-Rich Intermetallic Rods

Maria Herz, TU Dresden, Germany

Black needle-shaped crystals of the bismuth-rich mixed halogenide $\text{Bi}_{21}\text{Rh}_4\text{Cl}_6\text{I}_7$ showcase an orthorhombic structure that consists of infinite intermetallic rods $_{\text{inf}^1}[\text{Bi}_9\text{Rh}_2]^{3+}$ and discrete anionic groups $[\text{Bi}_2^{\text{II}}\text{Cl}_2\text{I}_5]^{3-}$ and $[\text{Bi}^{\text{III}}\text{Cl}_4\text{I}_2]^{3-}$. The rods consist of Rh-centered $[\text{RhBi}_8]$ polyhedra that alternately share triangular and rectangular faces. Using traditional electron counting rules, the rod can be interpreted as a covalent polymer with Rh_2 dumbbells bonded to molecular Bi_2 and Bi_5 units, while a quantum-chemical bonding analysis shows that the bonds involving Rh atoms are largely diffuse, while two-center bonds dominate in the bismuth units. Initial resistivity measurements indicate a temperature-independent resistance and this, along with the strong spin-orbit coupling inherent to this bismuth-rich compound, makes it a candidate for a topological insulator.

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Insights Into the Electronic Properties of Doped Topological Insulators: Bi_2Se_3 and Bi_2Te_3

P10

Shailja Sharma, IFW Dresden, Germany

Topological insulators (TI) are one of the most exciting and studied systems in condensed matter physics [1]. TI are characterized by the gapless topological surface states that are located inside the bulk band gap [2]. Bi_2Se_3 and Bi_2Te_3 are the typical three-dimensional TI and their surface states have been extensively studied through transport and spectroscopy experiments [3,4]. Here, I will present the detailed electronic transport properties and high-resolution angle-resolved photoemission spectroscopy (ARPES) studies on Ag-doped Bi_2Se_3 and Pd-doped Bi_2Te_3 . The Dirac cone-like surface states in ARPES confirm that $\text{Ag}_x\text{Bi}_2\text{Se}_3$ and $\text{Pd}_x\text{Bi}_2\text{Te}_3$ retain their topological properties even upon doping [5,6].

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Efficient THz Third Harmonic Generation in Topological HgTe Quantum Wells

Tatiana Aureliia Uaman Svetikova, HZDR Dresden-Rossendorf, Germany

P11

High harmonic generation (HHG) has applications in various fields, including ultra-short pulse measurements, material characterization, and imaging microscopy. Strong THz nonlinearity and efficient third harmonic generation (THG) have been demonstrated in graphene [1], therefore it is natural to assume the presence of the same effect in other Dirac materials, such as topological insulators (TI) [2,3]. In particular, topological states can be found in HgTe quantum wells with a thickness of more than 6.3 nm [4]. This study presents the third harmonic generation (THG) in an 8 nm-thick HgTe quantum well in the THz spectrum range at different temperatures and THz powers. The fundamental frequency is 0.5 THz, and the efficiency of the THG process approaches 1% in the electric field. Furthermore, we perform a two-color pump-probe experiment with a pump in the range of 20 THz to 28 THz and a broadband THz probe (0.3 THz - 2.5 THz). The free electron laser (FEL) source with intense pulses and a high repetition rate of 13 MHz is used as a pump. Using the intense FEL radiation, we selectively excite Dirac electrons in the surface state of HgTe without affecting the substrate and the buffer layers and probe their relaxation processes. The two-color pump-probe experiment is used to extract the scattering time and conductivity in the framework of the Drude model. We then apply the acceleration model [5] we generalised for arbitrary band dispersion using the experimentally obtained parameters to simulate the observed THG in the HgTe samples. We observe a remarkably good agreement between the experiment and the acceleration model predictions. Our experiments provide insight into the physical mechanisms leading to a giant THz nonlinearity in HgTe-based 2D topological insulators.

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Triple-Q Order in $\text{Na}_2\text{Co}_2\text{TeO}_6$ from Proximity to Hidden-SU(2)-Symmetric Point

P12

Wilhelm Krüger, TU Dresden, Germany

In extended Heisenberg-Kitaev-Gamma-type spin models, hidden-SU(2)-symmetric points are isolated points in parameter space that can be mapped to pure Heisenberg models via nontrivial duality transformations. Such points generically feature quantum degeneracy between conventional single-Q and exotic multi-Q states. We argue that recent single-crystal inelastic neutron scattering data place the honeycomb magnet $\text{Na}_2\text{Co}_2\text{TeO}_6$ in proximity to such a hidden-SU(2)-symmetric point. The low-temperature order is identified as a triple-Q state arising from the Néel antiferromagnet with staggered magnetization in the out-of-plane direction via a 4-sublattice duality transformation. This state naturally explains various distinctive features of the magnetic excitation spectrum, including its surprisingly high symmetry and the dispersive low-energy and flat high-energy bands. Our result demonstrates the importance of bond-dependent exchange interactions in cobaltates, and illustrates the intriguing magnetic behavior resulting from them.

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Entropically-Driven Spin-Liquid to Spin-Liquid Thermal Crossover in a Pyrochlore Magnet

P13

Daniel Lozano-Gómez, TU Dresden, Germany

One of the foremost goals in the study of pyrochlore magnetism is the search for spin-liquid phases composed of highly-disordered yet strongly correlated states. These phases are usually found in Hamiltonians possessing a highly degenerate ground state manifold preventing the onset of long-range order. In this work, we present a spin model on the pyrochlore lattice that realizes a novel classical spin-liquid at intermediate temperatures, collapsing into another spin-liquid phase at low temperatures. We demonstrate that the spin-liquid phase at intermediate temperatures is described by an emerging long-wavelength theory involving both vector and tensor fields, leading to the observation of twofold and fourfold pinch points, as well as, pinch-line singularities in the spin correlation functions. On the other hand, for the low-temperature spin-liquid, an effective long-wavelength theory describing a Coulomb phase is obtained. We demonstrate that the crossover between both phases has an entropic origin, providing the first realization of an entropically-driven selection of a spin-liquid.

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Research Data Management Services for All of **P14** ct.qmat

Jonas Schwab, JMU Würzburg, Germany

We present Research Data Management services provided to all members of ct.qmat. These include the electronic lab notebook eLabFTW, a community edition of Overleaf, a GitLab instance for collaborative source code management and beyond, the Research Data repository NOMAD Oasis and a JupyterHub.

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Thermal Transport in Weakly Coupled Spin-1/2 Heisenberg Ladders

P15

Anja Wenger, JMU Würzburg, Germany

This project aims to comprehend the quantum and thermal properties of the anti-ferromagnetic weakly coupled spin-1/2 Heisenberg ladder exposed to a magnetic field in the low energy limit. By utilizing fermionization and bosonization, we transform the interacting spin ladder into a solvable free boson theory, aligning with the Tomonaga-Luttinger model. We have successfully derived an analytical expression for the Luttinger parameters v_F (Fermi velocity) and K , thereby solving the model based on ladder parameters. The introduction of temperature into our theoretical framework allows for a description of thermodynamic quantities. The primary focus of this poster is to investigate the conformal anomaly and how it influences thermal transport. Of note is our observation that thermal transport defies classical theories, implying that, within our model, it is caused by quantum effects exclusively.

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Effect of (Non)-Magnetic Disorder in Quasi-1D Singlet Superconductors

P16

Morpurgo Giacomo, University of Geneva, Switzerland

We investigate the effects of the combination of interactions and disorder in a quasi 1D system. In this case, the critical temperature of superconductivity is an interesting observable for this purpose. Anderson's theorem indeed states that BCS-type superconductivity is resistant to non-magnetic disorder because time-reversal invariance is still preserved. In quasi 1D systems, since there the effect of disorder and interactions is more important than in higher dimensional systems, the Anderson theorem is generally not respected. We here study the competition between disorder and interactions in such systems by considering forward scattering disorder, both for magnetic and non-magnetic impurities. Using a field theory representation and renormalization, we show that non magnetic disorder preserves T_c in agreement with Anderson theorem. However, for the magnetic disorder, we find a reduction of the spin-gap and compute the reduction of T_c . We investigate the consequences for systems made of fermionic tubes with attractive interactions.

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Metal-Assisted Mechanical Exfoliation of 2D Material Monolayers

P17

Jiang Qu, IFW Dresden, Germany

A single MoS₂ monolayer (1L-MoS₂) with a large size of up to 2 mm was exfoliated and transferred on a silicon substrate with an ultra-flat gold film. Compared with the MoS₂ bulk, the 1L-MoS₂ shows a blue shift for E_{2g}¹ and a red shift for A_{1g} modes in Raman. The photoluminescence (PL) spectroscopy results also confirm the transition from an indirect (MoS₂ bulk) to a direct (1L-MoS₂) band gap material after exfoliation. A single peak at ~670 nm (~1.86 eV) was observed due to the generation of an A exciton from the direct excitonic transition at the Brillouin zone K-point in the 1L-MoS₂. Both Raman and PL confirmed the successful exfoliation of the 1L-MoS₂. Moreover, the Raman and PL of 1L-MoS₂ on the ultra-flat gold film were recorded. Gold-sulfur (Au-S) bond at the interface of 1L-MoS₂ and ultra-flat gold surfaces was observed, confirming the ultra-high yielding of monolayer MoS₂ of gold metal is because of the strong Au-MoS₂ interaction.

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Unstable Energy Level Alignment at Organic/Transition Metal Dichalcogenide Interfaces

P18

Hibiki Orio, JMU Würzburg, Germany

The hybrid interface of organic molecules and transition metal dichalcogenides (TMDCs) is weakly bounded by Van-der-Waals interaction. In this weak-interacted system, the interfacial energy level alignment is not in equilibrium and can be modulated by external perturbations. We investigated the electronic structure of copper phthalocyanine (CuPc) monolayer on different layered materials (graphite, TiSe₂, and WSe₂) by means of ultraviolet and x-ray photoelectron spectroscopy. Depending on the substrate, CuPc states show a different characteristic upon three hours of x-ray irradiation. The HOMO level is stable in CuPc/graphite case. However, for TiSe₂ and WSe₂, we find that the HOMO level shifts by 140 meV and 70 meV, respectively, upon x-ray illumination. Changes in film morphology and beam damages are subtle and insufficient to explain these different time evolution.

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Light-Matter Interaction of TMDCs in an Open Cavity

P19

Shiyu Huang, JMU Würzburg, Germany

With the discovery of graphene, two dimensional materials have attracted wide attention because of their fascinating properties, and transition metal dichalcogenides (TMDCs) have been considered as promising candidates. Excitons in monolayer TMDCs and their heterostructures can strongly couple to electromagnetic fields and are thus ideally suitable for integration in optical microcavities [1,2]. Monolayer of TMDCs shows direct bandgap and tightly-bound exciton with binding energy of few 100s meV [7]. Tungsten-based dichalcogenides presents a very large oscillator strength and high PL emission efficiency, so monolayer WS₂ is a fascinating active medium for forming exciton-polaritons at room temperature and studying hybrid light-matter states [3,4,5,6]. Moiré superlattices is formed by stacking two monolayers of TMDCs with a twist angle or a different lattice constant, which is promising to study optics controlling, excitonic landscapes, and towards exciton topology [8,9,10,11]. Here, we report the light-matter coupling of TMDCs in an open cavity, which is employed to confine the photonic field by two distributed Bragg reflectors (DBR). With the reducing of cavity length, the number of cavity modes reduces, and excitons in the TMDCs interact with the confined optical field. The geometry has the potential to achieve strong light-matter coupling and study polariton physics as well as interaction of excitons and exciton-polaritons [5]. Furthermore, it paves the way to future integration of Moiré heterostructures in tailored high-Q microcavities, with possibilities for electric control, low temperatures, and high magnetic field. Among many exciting properties, exciton Moiré lattices hold the potential for topologically non-trivial excitonic bands at the reconstructed domain boundaries [9].

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Electronic and Transport Properties of Strained SrNbO₃ Thin Films on SrTiO₃(001)

P20

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The realization of quantum materials (QMs) with both electron correlations and topology is currently under active investigation. In this context, 4d transition metal oxides (TMOs) are excellent candidates, as they offer a good balance between electron-electron correlations and spin-orbit coupling (SOC), and recently good progress has been made in their thin-film synthesis and device fabrication. Recently, a topological band structure was predicted for an orthorhombic phase of SrNbO₃ with $a^0a^0c^-$ type octahedral rotation [1]. In an experimental study, it has been demonstrated that epitaxial strain can control octahedral rotations in SrNbO₃/SrTiO₃(001) (SNO/STO) films breaking the cubic symmetry, which in turn generates a novel Dirac semimetallic phase with extremely high mobility and Berry phase that make it promising for quantum materials applications [2]. In addition, a thickness dependent linear magnetoresistance of up to 150,000% and mobilities as high as 80,000 cm²/(V·s) have also recently been reported in SNO/STO heterostructures [3]. The understanding of these observations in the context of unique properties of oxides relies mostly on theoretical descriptions of the SNO electronic structure. Until now, only a few experimental studies exist to explore and understand the electronic properties. Although the synthesis of pristine SNO thin films is challenging due to the metastable nature of the Nb⁴⁺ cation with a d^1 configuration, metastable SNO can be preserved by capping films with an alternative oxide with greater atmospheric stability. In this study, we have grown epitaxial SNO/STO thin films of various thickness using pulsed laser deposition. To protect the surface of the SNO layer from over-oxidation, we passivated the films with an epitaxial STO capping layer. X-ray diffraction has been used to characterize the structure and measure the strain. Transport measurements show a metallic nature of the SNO thin films and high linear magnetoresistance for the strained films in agreement with literature. We have also investigated the role of strain on the electronic properties of the SNO/STO(001) thin films and the buried interfaces by angle dependent x-ray photoemission. Nb 3d core level spectra reveal mixed valence states of Nb⁵⁺, Nb⁴⁺ and Nb³⁺. We also discuss the systematic change in the Nb 4d states in the region near the Fermi energy with increasing SNO film thickness.

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Disorder Operator and Rényi Entanglement Entropy of Symmetric Mass Generation

P21

Zihong Liu, JMU Würzburg, Germany

In recent years a consensus has gradually been reached that the previously proposed deconfined quantum critical point (DQCP) for spin-1/2 systems, an archetypal example of quantum phase transition beyond the classic Landau paradigm, actually does not correspond to a true unitary conformal field theory (CFT). In this work we carefully investigate another type of quantum phase transition supposedly beyond the similar classic paradigm, the so called asymmetric mass generation (SMG) transition proposed in recent years. We employ the sharp diagnosis including the scaling of disorder operator and Rényi entanglement entropy in large-scale lattice model quantum Monte Carlo simulations. Our results strongly suggest that the SMG transition is indeed an unconventional quantum phase transition and it should correspond to a true $(2 + 1)d$ unitary CFT.

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A Toy Model to Investigate the Role of Topology in Quantum Phase Transitions

P22

Gabriel Rein, JMU Würzburg, Germany

Topology is believed to play a cardinal role in explaining quantum phase transitions as one can identify topological terms in the action of respective field theories. In this project, we formulate an $SU(N)$ -invariant version of the Liu-Wang model, a previous model where a QSH mass term is dynamically generated [1], by incorporating electronic flavor degrees of freedom. This generalization not only retains the previously identified semi-metal, quantum spin-Hall insulator and s-wave superconducting phases, but also reveals an emergent valence bond solid phase. Remarkably, for $N=2$ this rich phase diagram features both a continuous transition corresponding to deconfined quantum criticality and a first-order phase transition driven by interaction strength, both of which can be governed by topological terms. Among these terms is a theta-term, which enables control over their relevance by adjusting the number of electron flavors, N . This is in analogy to the distinction between integer and half-integer spin chains. By enhancing the symmetry, our approach offers a direct means to investigate the influence of topological effects on quantum phase transitions and to systematically explore their impact.

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Interaction-driven Boundary Effects in Hydrodynamic Flow of Electrons in Finite Sized Graphene Sheets

P23

Adrien Reingruber, JMU Würzburg, Germany

We present results of QMC simulations of finite sized graphene sheets with zigzag and armchair edges in one direction and periodic boundary conditions in the other direction. We compute the double occupancy, spin-spin and current-current correlations in order to understand the relation between different boundary conditions and the electric flow in hydrodynamic regime. In particular we study the spin ordering and possible appearance of the edge magnetism and its influence on the current flow along the edge and in the bulk.

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Non-Hermiticity and Parity-Time Symmetry at X-Ray Wavelengths

P24

Fabian Richter, JMU Würzburg, Germany

A certain class of Hamiltonians which are non-Hermitian but obey parity-time (PT) symmetry exhibit real spectra thus mimicking Hermitian properties. This theoretical concept has recently found fertile ground in optics and photonics where non-Hermitian eigenstates can be created and superposed through optical gain and loss. So far, these concepts have been mostly discussed in the optical regime. Similar control of x-rays is desirable due to their superior penetration power, high focusability and detection efficiency. Here, we investigate theoretically non-Hermitian x-ray photonics based on PT symmetry in a thin-film cavity setup containing Mössbauer nuclei resonant to the x-ray radiation. These cavities present loss which is modelled by a Lindblad term in the master equation. The presence of an external magnetic field introduces PT-symmetry breaking which could be used to control the properties of x-ray scattering.

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Superfluid Density of Non-Hermitian Superconductors

Helene Müller, JMU Würzburg, Germany



P25

A non-Hermitian description usually corresponds to non-equilibrium or open systems. Thus, non-Hermitian superconductors can occur under certain external influence. For example, due to modification of elastic properties of the material via spatiotemporal modulation, pump and/or decay of quasiparticles or light-induced effects. Here, we study whether a non-Hermitian description conserves one of the main properties of a superconducting material: the Meissner effect. This effect occurs in conventional superconductors due to the Cooper condensate, that is characterised by the superfluid density (or stiffness). Thus, we study how the superfluid density changes under different external conditions in a non-Hermitian formalism.

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Origin of Ferromagnetism in the Copper(II) Triangle $\text{NMe}_4[\text{Cu}_3(\mu_3\text{-F})(\text{TFA})_6(\text{Py})_3]$

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P26

The new copper(II) triangle $\text{NMe}_4[\text{Cu}_3(\mu_3\text{-F})(\text{TFA})_6(\text{Py})_3]$ [1] was studied using magnetic susceptibility and high-field electron paramagnetic resonance (HF-EPR) experiments, as well as numerically by ab-initio methods. The magnetization and susceptibility data reveal dominant ferromagnetic spin-spin exchange as well as the importance of anisotropy in the system. An Anderson Impurity Model based on LDA-DFT calculations elucidates that the ferromagnetic interactions originate from super-exchange via the central fluorine. For the superexchange interaction, not only the fluorine's 2p shell but also the 2s shell needs to be considered. In the HF-EPR data a substantial curvature of the resonance branches is observed and explained within the model by mixing between excited $S_z \approx 1/2$ and $S_z \approx -1/2$ states. The model also suggests that the spins are not parallel to each other in the ferromagnetic ground state but rather arranged in a chiral manner which is given by the molecular structure.

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Multi-Layer Laser-Structured Dielectric Systems for Photonic Transport

P27

Jakob Lindenthal, TU Dresden, Germany

Photonic crystals and waveguide arrays are attracting significant research attention in topological phenomena in solid-state physics. Especially for miniaturised photonic arrays in the visible and NIR wavelength range, high refractive index contrasts and precise fabrication are required. Commonly used lithography processes can often satisfy the experimental demands, but prototyping and experimental progress are hindered by long lead times, high processing complexity and high cost. The need for quickly deployable, adaptable, and sufficiently precise structuring processes can be met by femtosecond laser structuring techniques. We present simulation results and experimental approaches characterising the fabrication performance of laser-structured dielectric systems. The results include FDTD simulations of chiral waveguides and topological photonic crystal interfaces at a sub-micrometre feature resolution and experimentally realised systems to underline the feasibility of rapid prototyping in nano-photonics by femtosecond laser structuring. We showcase experimental approaches to use structured multi-layer stacks to induce properties such as chirality in photonic crystals while maintaining a high refractive index contrast allowing the miniaturisation of these systems. The fabrication results are complemented by preliminary optical characterisation results of the fabricated systems, pointing out new pathways for easily accessible, quickly adaptable nano-photonics experimental techniques.

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Exceptional Points in Strongly Correlated Materials: Spontaneous Symmetry Breaking and Charge Response

P28

Lorenzo Crippa, JMU Würzburg, Germany

Strongly correlated electronic materials offer one of the standard platforms to detect and classify non-hermitian topological features. These are generally a consequence of the many-body interaction terms, which entail a non-hermitian self-energy and a nontrivial form for two-particle correlation functions. We show how both effects can stabilize a peculiar type of non-hermitian degeneracies known as Exceptional Points. At the 1-particle level, we assess their presence at the onset of spontaneous symmetry-breaking, for systems whose noninteracting Hamiltonian features an un-protected Dirac dispersion. At the 2-particle level, we observe the emergence of Exceptional Points in the eigenvalue spectrum of generalized local charge susceptibilities in the simple Hubbard model, establishing a link between non-hermitian topology and phase instability of the electronic system.

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Intensity Asymmetries in Photoemission

Jakub Schusser, JMU Würzburg, Germany

Angle-resolved photoemission spectroscopy can provide complex information about the electronic wave functions in the momentum space or real space of crystalline solids. The orbital and spin textures are particularly relevant in providing information about the electronic wave functions in the momentum space of crystalline solids and topological semimetals [1]. Recent studies have discussed how the relative ratio between the strength of spin-orbit coupling in comparison to the energy scale of the inversion-symmetry-breaking potential plays a distinct role in determining the symmetry of linear dichroism (LD) and that both LD and circular dichroism (CD) can thus allow for a better understanding of the photoelectron spin polarization signal and its relation to the spin and orbital nature of the initial states [2,3]. We have extended these studies by introducing intrinsic dichroic observables time-reversal dichroism in angular distribution (TRDAD) [4] and intrinsic linear dichroism in angular distribution (iLDAD) [5] that may provide even more direct access to the electronic initial-state properties. Here we further expand our studies of TRDAD in soft X-ray regime and show its independence on photon energy and geometry as well as discuss how TRDAD can be extracted using circularly polarized light.

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Topological Quantum Optics in Atomic Emitter Arrays

P30

Jonathan Sturm, JMU Würzburg, Germany

Atomic emitter arrays with subwavelength spacing have proven themselves as powerful platforms for the implementation of topological lattice models. Edge states have been shown to allow for robust, emission-free, and directional photon transport due to topological protection. We study the quantum optics of semimetallic lattices and Chern insulators, the latter opening the possibility to realize fractional quantum Hall states in these systems. Furthermore, we investigate whether this approach can be extended to x-ray wavelengths.

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Effect of Gallium and Copper Doping on Structural and Transport Properties of the Topological Insulator Bi_2Se_3 by Molecular Beam Epitaxy

Daniel Brito, International Iberian Nanotechnology Laboratory, Portugal

P31

Three-dimensional topological insulators (TIs) are described by massless Dirac surface states and reduced carrier scattering, due to strong spin-orbit coupling and the time-reversal symmetry (TRS). Bi_2Se_3 is one of the most promising TI due to its relatively large bandgap (0.3 eV), which makes it the most suitable to work at room temperature. Recently, this material has been used to design materials exhibiting quantum anomalous Hall effect and topological superconductivity, which are keys for the future of quantum computing. These topological properties can be achieved by doping with specific elements, such as Cu or Sr however, studies with other elements are scarce. Here, we use a molecular beam epitaxy (MBE) to grow high-quality single-crystal thin films of gallium-doped Bi_2Se_3 . Gallium addition expands the crystal lattice as demonstrated in the shifts to lower angles in the X-ray diffraction (XRD) and redshifts in the Raman spectrum. Transport properties were analyzed by a Hall effect and weak antilocalization effect (WAL) at low-temperature and show that the Ga doping maintains the n-type semiconductor character but increases the bulk concentration from $8.6 \times 10^{18} \text{ cm}^{-3}$ to $6 \times 10^{19} \text{ cm}^{-3}$ at low temperature. Doping the material deteriorates the topological channels observed by WAL, two surface states are still observed at low Ga concentrations as in undoped Bi_2Se_3 . Our Ga-doped Bi_2Se_3 did not show superconductivity, even though, both the high electron concentration and the expansion of the crystal lattice are also observed in the topological superconductivity in Cu and Sr doped Bi_2Se_3 .

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First-Order Effect of Electron-Electron Interactions on the Anomalous Hall Conductivity of Massive Dirac Fermions

Alexandra-Daria Dumitriu-Iovanescu, University of Manchester, United Kingdom



P32

The influence of electron-electron interactions on the behaviour of two-dimensional Dirac fermion systems has been a subject of a longstanding debate. In this study, we investigate the first-order corrections to the anomalous Hall conductivity of massive Dirac fermions arising from contact interactions. Our calculations are performed using linear response theory at finite temperature and chemical potential using Matsubara Green's functions and diagrammatic perturbation theory. Notably, the presence of these interactions induces renormalisations of the gap, chemical potential, and Fermi velocity. In order to preserve both particle-hole symmetry and the Ward identity, we employ a non-trivial regularisation method for the contact interaction. Remarkably, in the limit of zero temperature and zero chemical potential, we find that the first-order corrections vanish, in accordance with the Coleman–Hill theorem, implying the absence of perturbative corrections to the topological Hall conductivity. Our findings shed light on the potentially crucial role of electron-electron interactions in shaping the transport properties of two-dimensional Dirac fermion systems.

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One-Step Model Photoemission Calculations of Type-II Dirac Semimetal PtTe₂

P33

Muthu Prasath Thirugnanasambandam Masilamani, JMU Würzburg, Germany

Among the transition metal dichalcogenides (TMDC) class, PtTe₂ with trigonal structure belongs to type-II Dirac semimetals and attracted extensive research due to the Dirac points appearing at the band touching points of electron and hole pockets. Here we have studied photoelectrons from the surface and bulk states of PtTe₂ using a state-of-the-art ARPES experiment and one-step photoemission model within the spin-polarized relativistic Korringa-Kohn-Rostoker (SPR-KKR) Green's function method [1,2]. Our model quantitatively reproduces most of the features in the band structure mapped by experimental ARPES. It can differentiate surface and bulk states using the surface barrier potential and determinant criterion within the SPR-KKR package [3]. Previously, it was claimed that the topological surface state (TSS) at ~ 1 eV below the Fermi level in 1T-PdTe₂, a sister compound of 1T-PtTe₂, has surface character [4]. Our calculations, however, confirm that this state has bulk character. Moreover, our theoretical model of 1T-PtTe₂ will serve as the basis for future studies of asymmetries in measured spin texture which are induced by the experimental geometry [5] and the spin-orbital texture mapping from the spin- and angle-resolved photoemission.

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Electron Spin Resonance and Magnetic Phase Diagram of the Kitaev Candidate Material $\text{Na}_2\text{Co}_2\text{TeO}_6$

P34

Luca Bischof, KIP Heidelberg University, Germany

We report high-frequency high-field Electron Spin Resonance (ESR) measurements down to low temperatures on the Kitaev candidate material $\text{Na}_2\text{Co}_2\text{TeO}_6$. For in-plane ($B \perp c$) and out-of-plane ($B \parallel c$) magnetic fields up to 16 T, we observed several resonance modes in the ordered phase below $T_N \simeq 27$ K. They indicate magnetic phase transitions which are in agreement with the magnetic phase diagram constructed from our magnetization and dilatometric studies on $\text{Na}_2\text{Co}_2\text{TeO}_6$.

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Electronic Structure Evolution of Magnetic Weyl Semimetal $\text{Co}_3\text{Sn}_2\text{S}_2$ by Doping and Temperature

P35

Himanshu Lohani, JMU Würzburg, Germany

$\text{Co}_3\text{Sn}_2\text{S}_2$ is one of the member of kagome family which has been established as a prototype of magnetic Weyl semimetal with an attractive feature of Weyl points (WPs) proximity to Fermi level. We investigate tuning of the WPs across the Fermi level by different doping within the kagome network (Fe and Ni doping at Co site) and out of the kagome network (In substitution at Sn site). We observe clear shifts of selected bands, which are due both to doping and to the reduction of the magnetic splitting by doping. We discriminate between the two by studying the temperature evolution from ferromagnetic to paramagnetic state. We discuss these shifts with the help of DFT calculations using the Virtual Crystal Approximation.

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Emergence of Surface States on the Topologically Dark Surface of a Layered Weak 3D Topological Insulator

P36

Johannes Heßdörfer, JMU Würzburg, Germany

Weak 3D topological insulators (TI) can be considered as a stack of two-dimensional (2D) TI layers and can be distinguished from strong 3D TIs according to the behavior of their respective surface states [1]. In weak TI, there are topologically non-trivial as well as trivial surfaces (i.e. "dark surfaces") perpendicular and parallel to the layers, respectively. Here, the dark surface of a weak TI $\text{Bi}_{12}\text{Rh}_3\text{Ag}_6\text{I}_9$ is investigated using scanning tunneling microscopy, angle-resolved and X-ray photoelectron spectroscopy (ARPES and XPS), as well as density functional theory band structure calculations. In particular, the influence of surface preparation on surface termination is highlighted and the emergence of surface states within the 3D bulk band gap is demonstrated.

[1] Fu et al. Phys. Rev. Lett. 98, (2007)

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STM Growth Studies of 5,14-ol-5,14-diborapentacyclo on Low-Index Coinage Metal Surfaces

Wun-Chang Pan, JMU Würzburg, Germany

P37

In recent studies [1, 2], heteroatom-doped precursors have frequently been used to polymerize graphene nanoribbons with a large variety of structures or dopant heteroatoms. Using cryogenic scanning tunneling microscopy, we investigated the structure of self-assembled 5,14-ol-5,14-diborapentacyclo (CM218) on Cu(110), Cu(111), and Ag(111). While the order is relatively poor on Cu(110) where only few molecular chains can be observed for the second molecular layer, much better ordered molecular clusters and two-dimensional islands are found on Cu(111) at very low and medium sub-monolayer coverage, respectively. The main focus of our study, though, is on CM218 on Ag(111), where we find that molecular clusters and chains coexist with molecular islands. Topographic images of these honeycomb structures display a pronounced bias dependence. Molecule-functionalized tips allow for high-resolution images of these structures for which we suggest structural models. We investigate the electronic properties by scanning tunneling spectroscopy and differential conductance mapping.

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The Molecular Nanoprobe Ballistic Transport With Atomic Precision

P38

Markus Leisegang, JMU Würzburg, Germany

Low-loss charge carrier transport is of great interest for the realization of efficient and small electronic components. Improvements would minimize heat generation and reduce energy consumption at the same time. However, individual scattering processes that determine the loss in charge carrier transport occur on length scales from nanometers to micrometers. To study these in detail, measurement methods with high temporal or spatial resolution are required. For the latter, few established experiments exist, often based on scanning tunneling microscopy, which are however subject to various limitations. In order to get real space access to charge carrier transport at distances of the mean free path and thus in the ballistic regime, we developed and established the molecular nanoprobe (MONA) technique [1,2]. Hereby, we use a single molecule as a detector for charge carriers, which are injected into the substrate under investigation by the STM tip a few nanometers away from the molecule. The high spatial resolution of MONA combined with the small size of the molecular detector allows atomic control of transport paths down to the single nanometer level. In several publications, we have proven the capabilities of this novel technique, ranging from the influence of artificial [1,2] and natural occurring atomic structures [3] to the propagation of spin-polarized charge carriers in a Rashba-split surface state [5, 6]. Our plan is to extend these measurements to novel QSH materials where transport in low dimension states can shed light on hidden properties of these novel materials.

- [1] J. Kügel et al., *Nano Lett.* 17, 5106 (2017)
- [2] M. Leisegang et al., *Nano Lett.* 18, 2165 (2018)
- [3] M. Leisegang et al., *Phys. Rev. Lett.* 126, 144601 (2021)
- [4] M. Leisegang et al., *J. Phys. Chem. C* 127, 592 (2023)
- [5] P. Härtl et al., *Nat. Comm.*, under consideration (2023)
- [6] P. Härtl et al., arXiv:2303.00393 (2023)

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Anisotropic Coupling of Individual Vibrational Modes to a Cu(110) Substrate

P39

Andreas Christ, JMU Würzburg, Germany

Vibrational modes are an inherent property of molecules where the inter-atomic distances of the atomic constituents oscillate around the equilibrium position. As simple as this motion may appear, it can influence the optical, chemical, and electronic properties of molecules. In some cases, the excitation of specific modes can even induce a structural change of the molecule in form of a tautomerization [1]. This causality is used in the MOlecular NANoprobe (MONA) technique to study a remote excitation of such vibrational modes by ballistic charge carriers with an STM [2]. Here, we present a study on the excitation behavior of porphycene adsorbed on a Cu(110) surface. We measured the anisotropic tautomerization rate for different charge carrier energies in the range between $-850 \text{ meV} < E < 850 \text{ meV}$. Our data display a clear inversion at the onset of the N-H stretching mode at $|E| = 376 \text{ meV}$. Below this energy, when the N-H bending mode is excited, the excitation probability exhibits maxima perpendicular to the rows of the copper substrate and minima along them. Above this energy the tautomerization process is dominated by the excitation of the N-H stretching mode. Here, the excitation probability is maximal along the rows and constant otherwise. This inversion reflects the orthogonality between the N-H bending and stretching mode. Additionally, we observed an energy-dependent asymmetry in the propagation direction of charge carriers injected into the Cu(110) surface state. This demonstrates the effect of an anisotropic band structure on the tunneling probability into energetically degenerated electronic states.

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[2] M. Leisegang et al., *Nano Letters* 18, 2165-2171 (2018)

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Ballistic Transport of Dirac Fermions in 3D Topological Insulator Quantum Wires

Titouan Charvin, IFW Dresden, Germany



P40

Dirac Fermions are describing the Topological Surface States (TSS) of a 3D Topological Insulator (3DTI). When brought to the 1D limit, the TSS are quantized by quantum confinement. The Dirac cone is hence decomposed in 1D subband. The zero-energy mode exhibit a linear, photon-like dispersion, characterized by a dissipationless electronic transport, coined Perfectly Transmitted Mode (PTM) [1]. However, the study of this mode is limited by the intrinsic disorder found in 3DTI systems, leading to an increased number of transport mode. [2] A solution to tackle this limit is to tune the Fermi Level by mixing 3DTI binary crystals with different natures of disorder. [3,4] Our approach consists in studying ternary $(\text{Bi}_x\text{Sb}_{1-x})_2\text{Te}_3$ and quaternary $(\text{Bi}_x\text{Sb}_{1-x})_2(\text{Te}_y\text{Se}_{1-y})_3$, grown with a catalyst-free, vapor transport method. [5] Studying quantum corrections to the transport, we identify the subband contributions to the transport with the aim to detect ballistic features of the PTM

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Kondo Screening and Coherence on the Kagome Lattice

Christos Kourris, TU Dresden, Germany



P41

The formation of a heavy Fermi liquid in metals with local moments is characterized by multiple energy and temperature scales, most prominently the Kondo temperature and the coherence temperature, characterizing the onset of Kondo screening and the emergence of Fermi-liquid coherence, respectively. In the standard setting of a wide conduction band, both scales depend exponentially on the Kondo coupling. Here we discuss how the presence of a flat, i.e., dispersionless, conduction band modifies this situation. The Kagome Kondo-lattice model, due to its rich band structure, leads to a plethora of non-conventional Kondo behaviour emerging at different fillings. We utilize a parton mean-field approach to determine both the Kondo temperature and the coherence temperature as function of the conduction-band filling, both numerically and analytically. For filling values corresponding to the flat conduction band, we show that the exponential is replaced by linear and quadratic dependences for the Kondo and coherence temperature respectively, while a cubic power law emerges in the coherence temperature at filling corresponding to the band edge between the flat and dispersive bands.

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Kagome Compounds

Avdhesh Kumar Sharma, TU Dresden, Germany

P42

In Solid materials, non-trivial topology, strong electron correlations and magnetism are main ingredients for realizing quantum properties, also unconventional superconductivity, charge and spin density waves, and quantum spin liquids. The kagome lattice, made up of corner sharing triangular lattice to hexagons are potential platform for these properties to observe. Their electronic band structure includes Von Hove singularities, Flat band and Dirac cone. In this poster, I introduce the fundamental properties of the Kagome lattice as well as discuss the complex observed phenomena seen in several kagome materials such as CDW (Charge Density wave) and SC (Superconductivity), modulation of magnetism and topology in some kagome magnets. I also highlight many open questions in the field as well as future research directions of Kagome systems.

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Study of Magnetic Properties of the Quantum Spin Liquid $\text{SrCu}(\text{OH})_3\text{Cl}$ Using Electron Spin Resonance

Sudip Pal, University of Stuttgart, Germany

P43

We have investigated the magnetic properties of the quantum spin liquid candidate $\text{SrCu}(\text{OH})_3\text{Cl}$ using electron spin resonance (ESR) spectroscopy at the X-band frequency ($\nu = 9.4 \text{ GHz}$) down to temperature $T = 1.8 \text{ K}$. Recently much attention has been focused on the understanding of spin $S = 1/2$ located on a triangular lattice after a perfect triangular lattice was proposed as a putative quantum spin liquid candidate. In this context, the compound $\text{SrCu}(\text{OH})_3\text{Cl}$ offers a unique playground. It crystallizes in orthorhombic crystal structure, and this structure can be derived by breaking the planar cuprate layer to form isolated, non-planar triangular copper trimers which are connected by strontium coordination spheres. Because of the special atomic arrangement, the copper trimers form planes in which three spins form a perfect triangular structure. Importantly, each copper triangle is isolated from the others, providing an opportunity to study the magnetic ground state of isolated perfect triangular lattice. The ESR spectra of single crystal of $\text{SrCu}(\text{OH})_3\text{Cl}$ can be well described by a single Lorentzian line shape. The ESR intensity which is proportional to the static magnetic susceptibility can be described by a Curie-Weiss function at high temperatures. However, the inverse susceptibility deviates from the expected linear behavior at lower temperatures. The ESR linewidth shows a non-monotonic behavior as a function of temperature. It gradually decreases as the temperature is lowered, which is followed by a sharp increase at further lower temperatures. On the other hand, although the ESR g-factor increases monotonically with decreasing temperature, it changes rather rapidly at lower temperatures concomitant with the strong temperature dependence of the linewidth. Our ESR results indicate that the title compound does not exhibit long range magnetic ordering down to $T = 1.8 \text{ K}$, but a short-range magnetic correlation begins to build up at low temperatures

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First-Principles Study of Thermoelectric Properties of NaN

Darius-Alexandru Deaconu, University of Manchester, United Kingdom



P44

Van der Waals materials have become an essential playground for studying quantum phenomena, such as quantum confinement and low-dimensional physics. Based on ab-initio calculations we propose that alkali nitrides (AN) are a new category of materials that could serve as promising platforms for thermoelectric applications. These materials exhibit properties similar to graphene-like materials, while also displaying the polymorphism present in TMDs. In order to highlight their thermoelectric properties, NaN was chosen as a prototypical system for this family, which is a Dirac semi-metal. Using the semiclassical Boltzmann transport theory under the constant relaxation time approximation, we have analysed the variation of Seebeck coefficients for a range of dopings around the Dirac crossings present in the electronic band structure.

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Engineering Organic Molecules with Long-Lived Quantum Coherence

Burak Gurlek, MPI Structure and Dynamics of Matter, Germany



P45

Single organic molecules in the solid-state are one of the promising optical platforms for realizing quantum networks owing to their remarkable coherent properties and flexibility in their chemical synthesis. However, the molecular excited states associated with the strong Fourier-limited zero-phonon lines of these systems decay within nanoseconds, posing a challenge for practical applications in quantum technologies. In this theoretical work, we propose a new molecular system with quantum coherences up to millisecond time scales. Here, we exploit the inherent optomechanical character of organic molecules in a solid organic crystal. The proposed scheme consists of a single organic molecule in a host matrix with a structured phononic environment. By suppressing phononic decay channels, we realize and exploit long optomechanical coherence times up to milliseconds for storing and retrieving information. We show that the resulting long-lived vibrational states facilitate reaching the strong optomechanical regime at the single photon level. The proposed system shows the promise of organic molecules for achieving unexplored optomechanical phenomena and long-lived quantum memories.

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Critical Properties of a Quantum Loop Model on a Zig-Zag Ladder

Bowy La Riviere, TU Delft, The Netherlands



P46

Motivated by recent discovery of the non-magnetic Ising transition, at which the energy gap of magnetic excitations remains open, we search for other types of non-magnetic phase transitions that can be realized in quantum spin chains. In this work we focus on a new chiral transition recently reported in the context Rydberg atoms between the period-four and disorder phase. To explore whether chiral transitions can also be realized in quantum spin chains, we look at the quantum loop model, i.e. an effective model of spin-1 ladder with a constrained Hilbert space limited to the singlet sector only. We use extensive density-matrix renormalization group simulations to show the presence of chiral perturbations and to unveil how these affect the nature of the quantum phase transitions between the plaquette (period-four) and the next-nearest-neighbor Haldane (disordered) phases.

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Dimensional Crossover in Weakly-Coupled Interacting Chains

Lorenzo Pizzino, University of Geneva, Switzerland



P47

In our work we study a system made of 1D chains (interacting particles) weakly-coupled along the transverse direction. Our aim is to study the interplay between interactions and the (weak) transverse coupling between the chains. By means of field-theory (Bosonization technique) and Renormalization group, we perturbatively study the gap that opens in the spectrum and the crossover temperature above which the chains behave as if they were uncoupled. We benchmark our findings with numerical simulations (DMRG) and show how it can drastically improve the computational time.

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Kibble Zurek Mechanism and Finite-Time Scaling in Rydberg Arrays

Jose Soto, TU Delft, The Netherlands



P48

Rydberg atoms have become an ideal platform for studying isolated quantum many-body systems. By controlling the laser detuning and the inter-atomic distance, one can investigate diverse critical phenomena, in particular, the commensurate-incommensurate quantum phase transitions. Our approach involves numerical simulation of critical real-time dynamics within non-equilibrium chains of Rydberg atoms. Utilizing the time-evolving block decimation algorithm, we decode the intricacies of the commensurate-incommensurate phase transition via the application of the Kibble-Zurek mechanism and Finite-Time Scaling. We study the isolated conformal points surrounded by the new chiral quantum phase transition types with an effective blockade model where a constraint of no double occupancy replaces the short-distance repulsions. Combining the Kibble-Zurek mechanism with the Finite-Time Scaling theory, we extract all major critical exponents ν , z and β . The implications of the finite-size effect will be briefly discussed.

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Z_n Effect in Adiabatic Winding-Up Quantum Spin Helices

Anshuman Tripathi, University of Hamburg, Germany



P49

When manipulating quantum systems cyclically with slowly changing external fields, topologically and geometrically nontrivial quantum systems generally do not return to the initial state after one cycle. This is especially the case for topological quasiparticles, e.g., the 4π Josephson effect of Majoranas, and more exotic anyonic effects with higher order of periodicity. Here, we study the winding-up of easy-plane quantum spin helices in spin-1/2 chains by twisting the boundary fields. At Heisenberg anisotropy $\Delta = J/2$, the ground state evolve to helical state and system returns to the ground state after n cycles of the adiabatic time evolution, where n increases linearly in dependence on the chain length. This unification of various periodicities in a single system is a unique feature and the winding-up is analogous to adiabatically pumping a helical quantum spin quasiparticle. Extrapolation of our results to large spin systems reveals a universal scaling for the winding-up process, whose exponent we determine. We also observe that the adiabatic process connects phantom helices with spin-current maximizing helices, which both have been recently shown to exhibit an increased stability against external perturbations.

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