Summary of research related to NKFIH grant K119442 entitled "Interaction, topology and dynamics in exotic quantum systems"

During the 5 project years, we have published, among many others, 8 Phys. Rev. Lett., 1 Nature Communications, 2 ACS Nano and 1 PRX Quantum papers. The following research has been carried out:

1 Spin relaxation

The nuclear spin relaxation rate of Weyl semimetals was investigated theoretically using a newly developed method, coined ab initio field theory. We have shown that $1/T_1T$, where T_1 and T are the relaxation rate and temperature, respectively, scales with the square of the maximum of the chemical potential and temperature, while naive expectations predicted a scaling with the fourth power. This unusual behaviour roots back to the anomalous hyperfine coupling in Weyl semimetals, which diverges with the inverse of energy upon approaching the Weyl point. This was published as Z. Okvátovity et al., Phys. Rev. B 94, 245141 (2016).

Then, using our theory, we teamed up with the experimental group of M. Baenitz in Dresden and analyzed the recent experimental data on the nuclear spin-lattice relaxation rate of the Weyl semimetal TaP and argued that its non-monotonic temperature dependence is explained by the temperature dependent chemical potential of Weyl fermions. We also developed the theory of the Knight shift in Weyl semimetals, which contains two counteracting terms. The diamagnetic term is always negative, while the paramagnetic one scales with the chemical potential and changes sign depending on the doping level. Altogether, the Knight shift was predicted to vanish or even change sign upon changing the doping or the temperature, making it a sensitive tool to identify Weyl points. We also calculated the Korringa relation for Weyl semimetals which shows an unusual energy dependence rather than being constant as expected for a non-interacting Fermi system. The results were published in Z. Okvátovity et al., Phys. Rev. B 99, 115107 (2019)

We have studied the fundamental theory of spin-relaxation in semiconductors in L. Szolnoki et al., Sci. Rep. 7, 9949 (2017). It was shown that the full "phase diagram" of spin-relaxation including momentum relaxation rate and spin-orbit coupling strength can be constructed using the combination of an analytic and Monte Carlo based technique. This can be used to investigate the spin relaxation rate of the parent compound of graphene, graphite.

We settled the long-standing problem, whether the two alternative descriptions of spin-relaxation in metals, namely the Elliott-Yafet and D'yakonov-Perel', can be unified on common physical grounds. This work was selected as Editors' Suggestion in Phys. Rev. B, published as L. Szolnoki et al., Phys. Rev. B 96, 245123 (2017).

We studied the generic phase diagram of spin relaxation in metals and semiconductors, published in G. Csősz et al., Phys. Rev. Research 2, 033058 (2020). We developed a numerical method to calculate spin relaxation times for cases when the analytic approaches break down and have also shown that the so-called Loschmidt echo can be introduced to tackle cases when the so-called reversible decoherence dominates and its effect can be reversed to yield the true spin-relaxation time.

2 Non-hermitian dynamics

Our initial results on the project inspired us to follow this unplanned direction of research and investigate non-hermitian dynamics. Our most important publication followed from this enterprise as B. Dóra et al., Nat. Commun. 10, 2254 (2019). We studied the extension of the Kibble-Zurek scaling to non-hermitian quantum systems. Exceptional points (EPs) are ubiquitous in non-hermitian systems, and represent the complex counterpart of critical points. By driving a system through a critical point at finite rate induces defects, described by the Kibble-Zurek mechanism, which finds applications in diverse fields of physics. We generalized this to a ramp across an EP. We found that adiabatic time evolution brings the system into an eigenstate of the final non-hermitian Hamiltonian and demonstrate that for a variety of drives through an EP, the defect density satisfies a universal scaling in terms of the equilibrium critical exponents. Defect production is suppressed compared to the conventional hermitian case as the defect state can decay back to the ground state close to the EP. We provided a physical picture for the studied dynamics through a mapping onto a Lindblad master equation with an additionally imposed continuous measurement.

Our results triggered the attention of P. Xue and her experimental group in Beijing. Together with them, we published a paper as L. Xiao et al., PRX Quantum 2, 020313 (2021) on the experimental confirmation of the non-hermitian Kibble-Zurek theory. By using single-photon interferometry, we simulated several ramp protocols around distinct exceptional points. In addition, we extended the scaling properties to the defect fluctuations, which enables us to extract the correlation length and dynamical exponents of the underlying the exceptional point (EP) and therefore to gain direct experimental information about the universality class of the EPs.

In two Phys. Rev. Lett. papers (B. Dóra et al., Phys. Rev. Lett. 124, 136802 (2020) and Á. Bácsi et al., Phys. Rev. Lett. 124, 136401 (2020)), we focused on non-hermitian Luttinger liquid (LL) physics. In particular, we analyzed the response of a non-interacting Fermi gas after quantum quenching to a PT-symmetric LL by focusing on the fermionic single particle density matrix. For short times, we demonstrated the emergence of unique phenomena, characteristic to non-hermitian systems, that correlations propagate faster than the conventional maximal speed, known as the Lieb-Robinson bound. These emergent supersonic modes travel with velocities that are multiples of the conventional light-cone velocity. This behaviour is argued to be generic for correlators in non-hermitian systems. Our analytical results are benchmarked by numerically exact methods. Additionally, we studied a one-dimensional Fermi gas in the presence of dissipative coupling to environment through the Lindblad equation. After switching on the dissipation, the system approaches a steady state, which is described by a generalized Gibbs ensemble. The fermionic single particle density matrix resembles deceivingly to that in a hermitian interaction quench. It decays inversely with the distance for short times due to the fermionic correlations in the initial state, which changes into a non-integer power law decay for late times, representing dissipation induced Luttinger liquid behaviour. However, the crossover between the two regions occurs due to dissipation induced damping, and is unrelated to the propagation of excitations

We investigated the stability of a Luttinger liquid, upon suddenly coupling it to a dissipative environment. Within the Lindblad equation, the environment couples to local currents and heats the quantum liquid up to infinite temperatures. The single particle density matrix reveals the fractionalization of fermionic excitations in the spatial correlations by retaining the initial non-integer power law exponents, accompanied by an exponential decay in time with interaction dependent rate. The early time dynamics is captured numerically by performing simulations on spinless interacting fermions, using several numerically exact methods. Our results could be tested experimentally in bosonic Luttinger liquids and were published in Á. Bácsi et al., Phys. Rev. Lett. 125, 266803 (2020).

3 Dynamics of information scrambling

We have published three Phys. Rev. Lett. papers addressing the fate of quantum information propagation and scrambling in B. Dóra et al., Phys. Rev. Lett. 119, 026802 (2017), M. Heyl et al., Phys. Rev. Lett. 121, 016801 (2018) and B. Dóra et al., Phys. Rev. Lett. 121, 056803 (2018), respectively . First, information scrambling and the butterfly effect in chaotic quantum systems can be diagnosed by out-of-time-ordered (OTO) commutators through an exponential growth and large late time value, proposed recently by Kitaev. We have shown that the latter feature shows up in a strongly correlated many-body system, a Luttinger liquid, whose density fluctuations we studied at long and short wavelengths, both in equilibrium and after a quantum quench. Therefore, the large late time value of the OTO commutator does not diagnose quantum chaos.

In a second work, we have calculated the out-of-time ordered correlator in transverse field Ising models with short and long range as well as integrable and non-integrable realizations. It was demonstrated that this quantity can be used to detect and locate equilibrium phase transitions by performing an out of equilibrium measurement after a quantum quench. This could be useful to determine equilibrium phase diagrams in a non-equilibrium setting. This turns out to be the most cited publication of the project with 53 independent citations from MTMT.

In a third paper, we focused on the properties of the center of mass coordinate of an interacting one dimensional Fermi gas. By combining numerics with bosonization, we demonstrate that the autocorrelation function of the center of mass coordinate is universal throughout the metallic phase. It exhibits persistent oscillations and its short time dynamics reveal important features of the quantum liquid, such as the Luttinger liquid parameter and the renormalized velocity. The full counting statistics of the center of mass follows a normal distribution already for small systems. Our results apply to non-integrable systems as well and are within experimental reach for e.g. carbon nanotubes and cold atomic gases.

Reaching a target quantum state from an initial state within a finite temporal window is a challenging problem due to non-adiabaticity. We study the optimal protocol for switching on interactions to reach the ground state of a weakly interacting Luttinger liquid within a finite time, starting from the non-interacting ground state. The protocol is optimized by minimizing the excess energy at the end of the quench, or by maximizing the overlap with the interacting ground state. For short quench durations, the optimal protocol exhibits fast oscillation and excites high energy modes. For long quench times, minimizing energy requires a smooth protocol while maximizing overlap requires a linear quench protocol. In this limit, the minimal energy and maximal overlap are both universal functions of the system size and the duration of the protocol. These are published in Á. Bácsi et al., Phys. Rev. B 99, 245110 (2019).

We investigated the behaviour of OTO commutators correlators in Dirac-Weyl systems, and identified the fingerprints of Dirac excitation on the long time behaviour. It reveals a universal t^2 initial growth and a t^{-2} late time decay. This latter feature is identified as a characteristic signature or Dirac-Weyl fermions, and remains present also at finite temperatures. Our results indicate that Dirac–Weyl systems are slow information scramblers. Our results were published in Z. Okvátovity et al., Phys. Rev. B 101, 245125 (2020).

4 Experimental results

We studied the fundamental electronic and magnetic properties of black phosphorus. The mono-layer black phosphorus or phosphorene has emerged as a structurally similar two-dimensional compound to graphene, however with a built-in charge gap and an affinity for charge doping. We presented a combined approach on black phosphorus including ^{31}P nuclear magnetic resonance experiment and lineshape modeling, microwave impedance measurements, and electron spin resonance experiments. This study may serve as an important reference for future studies on this material, published in B. G.

Márkus et al., Phys. Stat. Sol. B, 254, 1700232, (2017).

The 1st ASC Nano paper (B. Márkus et al., ACS Nano 14, 7492 (2020)), we synthesized a novel nanostructural material, Li and Na doped graphene. The high level of intercalation was proven using Raman and electron spin resonance spectroscopic methods. The ESR experiments evidence that an ultralong spin relaxation lifetime is present for the itinerant electrons. The measured magnitude of the spin relaxation time is comparable to that found for ultraclean, mechanically exfoliated graphene.

In the 2nd ACS Nano publication (J. Palotás et al., ACS Nano 14, 11254 (2020), we studied the light induced metastable excitations in single-wall carbon nanotubes, exciton, using a purpose-built optically detect magnetic resonance spectrometer. We have identified the signal of long lived triple exciton states and we have measured the magnetic resonance lifetimes of these triplet states. In addition, we measured the singlet-triplet energy gap which follows the inverse of the nanotube diameter, thus evidencing the effect of quantum confinement.

The density of states was studied in alkali atom doped single-wall carbon nanotubes (SWCNT). The Luttinger to Fermi-liquid crossover manifests in the emergence of an electron spin resonance signal of itinerant charge carriers. The study allowed to identify that SWCNTs behave as a weakly correlated Fermi liquid upon alkali atom doping. Isotope engineered single wall carbon nanotubes were synthesized inside host outer tubes from precursor fullerenes and small organic molecules. It was shown that the carbon isotopes show a remarkable clustering (i.e. little carbon atom diffusion takes place during the inner tube growth). The material may serve as an isotope engineered template for future quantum information processing, published in P. Szirmai et al., Phys. Rev. B 96, 075133, (2017).

A novel optically detecting magnetic resonance (ODMR) spectrometer was developed. The uniqueness of the spectrometer stems from the presence of a tunable laser source and analysis of the emitted light. The first successful wavelength resolved ODMR studies were presented on SWCNTs, published in M. Negyedi et al., Rev. Sci. Inst. 88, 013902, (2017)

We continued our investigation on the identifying the nature of the Raman spectrum in SWCNT. In particular, we showed that the Raman spectrum of isotope engineered SWCNTs can be explained by assuming small arrays of ^{13}C. This confirmed the absence of carbon diffusion during the process when inner nanotubes are grown inside host outer tubes. The results are published in J. Koltai et al., J. Phys. Chem. C 120, 29520, (2016) and Phys. Stat. Sol. B, 254, 1700217 (2017).

We showed in G. Csősz et al., Sci. Rep. 8, 11480, (2018) that the microwave absorption can be larger than in the normal state in the mixed state of type-II superconductors. Although this effect can be explained by the standard model of vortex absorption, still the effect had not been observed prior to our work. A study on fine powders of type two superconductors, MgB_2 and K_3C_{60} was key for this result. A detailed theoretical modeling was able to quantitatively account for the effect. Somewhat surprisingly and counterintuitively, the enhanced microwave absorption is the result of the superconducting condensate strength as it extends to finite frequencies when a DC magnetic field is applied, i.e. the effect is a direct consequence of the so-called Glover-Tinkham sum rule.

We studied the microwave cavity perturbation method, which is used to determine material parameters (electric permittivity and magnetic permeability) at high frequencies. We presented a method to determine the Q-factor and resonance frequency of microwave resonators which is conceptually simple but provides a sensitivity for these parameters which overcomes those of existing methods by an order of magnitude. We compared existing methods for this type of measurement to explain the sensitivity of the present technique, and we also made a prediction for the ultimate accuracy for the resonator Q and f(0) determination. This was published in B. Gyüre-Garami et al., Rev. Sci. Inst. 89, 113903, (2018)

We showed that absorbed power of nanoparticles during magnetic hyperthermia can be well determined from changes in the quality factor (Q factor) of a resonator in which the radiofrequency absorbent is placed. We presented an order of magnitude improvement in the Q factor measurement accuracy over conventional methods by studying the switch-on and off transient signals of the resonators. We found that a nuclear magnetic resonance console is ideally suited to acquire the transient signals and it also allows to employ the so-called pulse phase-cycling to remove transient artifacts. The improved determination of the absorbed power was demonstrated on various resonators in the 1-30 MHz range, including standard solenoids and also a birdcage resonator. These results were published in I. Gresits et al., Sci. Rep. 8, 12667, (2018) and J. Phys. D: Appl. Phys. 52, 375401, (2019).

The anomalous heat capacity peak and thermal conductivity of $BaVS_3$ near the metal-insulator transition present at 69 K was studied. The present study evidenced the entropy increase during the structural transition and it was shown that the additional entropy is caused by enhanced electron scattering as a result of the structural reorientation of the nuclei. Within the model it was possible to explain quantitatively the observed peak alike structure in the heat capacity and in heat conductivity. This is published as F. Márkus et al., Entropy 23, 1350 (2021).

5 Strongly interacting quantum systems

We focused on the attractive $SU(N)$ Anderson impurity model. We found that the phase diagram features mild N dependence and the ground state is always a Fermi liquid, in the attractive case a Kosterlitz-Thouless charge localization phase transition is revealed for $N > 2$. Beyond a critical value of attractive interaction an abrupt jump appears in the number of particles at the impurity site, and a singular Fermi liquid state emerges. Our work was published in C. P. Moca et al., Phys. Rev. Lett. 123, 136803 (2019).

In C. P. Moca et al., Phys. Rev. Lett. 125, 056401 (2020) publication, we elaborated on semiconducting nanotubes, displaying topologically protected end states of multiple degeneracies. We demonstrated numerically that the presence of Coulomb interactions induces the formation of massive end spins. These are the close analogues of ferromagnetic edge states emerging in graphene nanoribbon. The interaction between the two ends is sensitive to the length of the nanotube, its dielectric constant, as well as the size of the end spins. The effective interaction between end spins can be controlled by changing the dielectric constant of the environment, thereby providing a possible platform for two-spin quantum manipulations.

We proposed an all-electrical spectroscopic probe sensitive to the spin inversion at the topological transition in a superconductor. Our proposal relies on the indirect coupling of a time-dependent electric field to the electronic spin due to the strong Rashba spin-orbit coupling in the semiconductor. We analyze within linear response theory the dynamical correlation functions and demonstrate that some components of the susceptibility can be used to detect the nontrivial topological phases. Our results were published in D. Sticlet et al., Phys. Rev. B 102, 075437 (2020).