Final report for the SNN 118028 bilateral research project „Thermalization in non-equilibrium quantum systems”

Overview

The SNN 118028 collaborative research started – with a slight delay – in 2016-2017, with a two day kick-off meeting and mini-workshop organized in Budapest, in October 2017. After this meeting, many visits took place from both sides over the years and amounted in several joint publications and collaborative – still ongoing – research projects as well as more informal collaborations yielding separate but not independent publications – without actual co-authorship. For the closing year, we planned a closing miniworkshop in Ljubljana (planned to be extended to a midsize conference), but this conference has unfortunately been ruined by the COVID situation.

Our research mainly focused on the investigation of the dynamics of correlated quantum systems such as ultracold atoms, nanostructures, and quantum computation-related architectures. In collaboration with the group of Tomaz Prosen, University Ljubljana, we developed theoretical methods which make it possible to access and study dynamics of correlated quantum systems at intermediate to long time scales. In our research, we applied these methods to uncover some fundamental properties of non-equilibrium quantum evolution and thermalization, and also used them to study experimentally relevant systems and models, sometimes in collaboration with leading experimental groups.

In this report, we focus exclusively on results from the Hungarian partner, but the Slovenian side of the project has been equally fruitful. Altogether, 33 publications resulted from this collaborative grant just on the Hungarian side, all published in highly ranked international journals: 22 appeared in Physical Review journals (8 out of them in the Physical Review Letters), one in Science Magazine, and the remaining publications – apart from a few preprints (one of the submitted to Nature) – appeared in journals such as JHEP, Journal of Statistical Physics, or Scientific Reports.

Most important results

Before giving a more detailed account of the results achieved, we would like to highlight a few of them, which we believe stand out in some regard.

Truncated Conformal Space Approach (TCSA). One of the specialties of our groups is to study non-equilibrium dynamics by perturbing exactly solvable conformal field theories. We have used this method to study a number of models and phenomena such as the so-called Kibble-Zurek mechanism, or the non-equilibrium Gibbs paradox, but maybe the most important application of this method was a study of coupled Bose-fluids, published in the Physical Review Letters, where we computed the time evolution of correlators after a quantum quench, directly accessible in experiments with ultracold atoms.

Semiclassical approach to quantum dynamics. In a series of papers, we have developed a generalized version of the semiclassical approach of Subir Sachdev, where we use semiclassical methods to describe the non-equilibrium quantum dynamics of correlated systems in terms of their elementary excitations and their collisions. This method allowed us to derive analytical non-equilibrium benchmark results (correlation functions, front profiles etc.) for fundamental systems such as the sine-Gordon model, or the O(n) sigma model, both describing many physical systems, and relevant for experiments. We tested these methods against “*ab initio”* (i.e. TEBD) methods at short time scales, and found excellent agreement.

Clarification of OTO. Out of Time Ordered (OTO) correlations triggered a lot of interest recently. We have studied OTO correlations in various integrable as well as non-integrable and long-ranged models.

We find for all the studied models that the OTO correlator detects the ground state (zero temperature) quantum phase transitions, but it also signals dynamical quantum phase transitions in models with long-ranged interaction. These findings, which are directly relevant for current experiments on trapped ions or Rydberg atoms, have placed the OTO correlator in a new perspective, and received a lot of attention.

Development of a NA-MPS *program package.* We have developed a non-Abelian Matrix Product State package, based on a novel mathematical structure of non-Abelian tensors, which allows us to perform Time Evolving Block Decimation and Density Matrix Renormalization Group computations with a radically decreased bond dimension and thus with high accuracy, even reachable on simple personal computers. The structures developed have a variety of application areas: they enable us to study efficiently quantum dynamics, quantum chemistry problems as well as nuclear models, and allow to investigate the dynamics of open quantum systems in a Matrix Product Operator approach, too. As a "side result", these efforts culminated in the observation and study of the Wigner crystal in carbon nanotubes, published in Science in 2019.

Detailed description of results

Semiclassical theory of quantum quenches and MPO-based methods

Currently the most efficient way to simulate quantum systems is to focus is to apply so-called Matrix Product State (PMS) or Matrix Product Operator (MPO) methods. The efficiency of these methods is, however limited by the finite information that can be stored in an MPS/MPO, and the fast growth of this with time evolution due to entanglement generation, therefore, even MPS/O methods break down after quite a short time way before the system reaches thermal equilibrium We combined two strategies to extend the extension of these simulations: (1) we developed MPS/MPO classes to exploit non-abelian symmetries as much as possible to condense information/storage (2) we combined this with an approximate semiclassical description, formulated in terms of (gapped) elementary excitations.

The resulting semi-semiclassical algorithm allowed us to address non-equilibrium relaxation in one dimensional systems [Phys. Rev. Lett. 119, 100603 (2017)], where internal degrees of freedom of the quasiparticles are treated fully quantum-mechanically, while their orbital motion is captured semi-classically. We have applied this new approach to coupled Bose condensates and have shown that it is able to capture multistep thermalization processes of the soliton gas. We have also used a simpler version of this method to describe front propagation [Phys. Rev. E 98, 032105 (2018)] in the O(n) model. We have studied the propagation of magnetic fronts by means of analytical as well as Monte-Carlo methods, and demonstrated the existence of a second front, propagating slower than the 'sound velocity', and which broadens diffusively, while a local equilibrium is formed at the fast, propagating front.

To test our semiclassical method, we carried out TEBD computations with our novel NAMPS (non-Abelian MPS) code for the quench dynamics of the S=1 Heisenberg chain, and determined numerically the complete spin distribution of the chain cut into two [Werner et al, Phys. Rev. B 100, 035401 (2019)]. This distribution reflects the dynamics and collisions of the quasiparticles created by the quench. The results of the full quantum simulation were found to agree extremely well with the predictions of our approximate semi-semiclassical theory.

Although some details of our NAMPS method have been published already in our 2019 publication, we have also published a longer review of the method – together with the analysis of quench dynamics in the SU(3) Hubbard model [Phys. Rev. B 102, 155108 (2020)]. In this work we used the NAMPS class to perform NA-TEBD (non-Abelian Time Evolving Block Decimation) simulations, and demonstrate that our approach increases the speed and memory storage efficiency of matrix product state based computations by several orders of magnitudes, and makes large bond dimensions accessible even on simple desktop architectures. We have determined the time evolution of various local operators and

correlation functions in the SU(3) Hubbard model, and have shown that interactions turn algebraic charge relaxation into exponential, and suppress coherent quantum oscillations rapidly. We have also developed an NA-MPO (non-Abelian Matrix Product Operator) method, which allows us to make simulations on open quantum systems. The first review on this method is being prepared for publication.

The power of our methods has been demonstrated on a collaboration with the experimental group of Shahal Ilani (Weizmann), amounting in a Science publication [Science 364, 870 (2019)]. In this work we used more standard DMRG methods with symmetries in combination of a very non-trivial basis construction to describe the so-called Wigner necklace, a crystalline state of strongly interacting electrons on a carbon nanotube, imaged by Ilani's group in real-space. The comparison to theoretical modeling demonstrates the dominance of Coulomb interactions over kinetic energy and the weakness of exchange interactions in a quantum crystal, and – with the experiments – provided direct evidence for this long-sought electronic state.

Fundamental non-equilibrium concepts in solvable models

One of our goals was to study relatively simple models to address fundamental questions related to thermalization and quantum work. Luttinger liquids as well as models such as the transverse field Ising model or random matrix ensembles provide nice and tractable frameworks to investigate a variety of non-equilibrium concepts such as dynamical phase transitions, dissipation induced transitions, scrambling, and thermalization.

Out of time ordered correlation functions. 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. We have shown [Phys. Rev. Lett. 119, 026802 (2017)] that the latter feature shows up in a Luttinger liquid, whose density fluctuations we study at long and short wavelengths, both in equilibrium and after a quantum quench. We find rich behavior combining robustly universal and non-universal features. The OTO commutators display temperature- and initial-state independent behavior and grow as t^2 for short times. These results challenge the common interpretation of the OTO commutator in chaotic systems. We have also investigated information scrambling at an impurity quantum critical point [Phys. Rev. B 96, 155116 (2017)]. The out-of-time-ordered (OTO) commutator was suggested to characterize chaotic behavior in quantum mechanical systems. We have shown that the OTO commutator of the impurity spin reveals markedly distinct behavior depending on the low energy impurity state. In the Fermi liquid ground state, the OTO commutator vanishes for late times, while in the critical, two channel case, the impurity OTO commutator is completely temperature independent and saturates quickly to its upper bound 1/4.

The previous results lead us to study OTO at quantum critical points. We have studied OTO in different variants of transverse-field Ising models in one dimension, including the integrable one as well as nonintegrable and long-range extensions [Phys. Rev. Lett. 121, 016801 (2018)]. We find for all the studied models that the OTO correlator in ground states detects the quantum phase transition. After a quantum quench from a fully polarized state, for the short-range models we observe that the asymptotic long-time value of the OTO correlator signals still the equilibrium critical points and ordered phases, while for the long-range extension, the OTO correlator determines instead a dynamical quantum phase transition in the model. These findings could be observed in current experiments of trapped ions or Rydberg atoms.

We also studied spatially local spin correlation function i.e., the expectation value of spin commutators and the corresponding out of time ordered commutator (OTOC) of Dirac--Weyl systems in one, two, and three spatial dimensions [Phys. Rev. B 101, 245125 (2020)]. The OTOC reveals a universal temporal initial growth and late time decay, which are identified as a characteristic signatures or Dirac-Weyl fermions. These features remain present also at finite temperatures. Our results indicate that Dirac--Weyl systems are slow information scramblers.

Entanglement in momentum space. We have also studied the entanglement content of reduced thermal density matrices for momentum-space bipartitioning in Luttinger liquids using analytical and numerical methods [Phys. Rev. B 96, 085109 (2017)]. We have shown that the momentum-space entanglement Hamiltonian is as universal as the physical Hamiltonian. The low lying part of its spectrum contains an "entanglement gap", persisting up to temperatures comparable to the level spacing, while the momentum-space entanglement is carried by high energy modes (compared to temperature), featuring a completely flat spectrum.

Optimal control. In another work, we have determined the optimal protocol of the finite time interaction switch on of a Luttinger liquid by targeting a minimal final state energy or maximal final state overlap with a target final state [Bácsi et al, Phys. Rev. B99, 245110 (2019)]. In the limit of long protocol time, minimizing energy requires a smooth protocol while maximizing overlap requires a linear quench protocol.

Dissipative environment. We studied a one-dimensional interacting Fermi gas in the presence of dissipative coupling to the environment, as described by the Lindblad equation [Phys. Rev. Lett. 124, 136401 (2020)]. The fermionic single particle density matrix resembles deceivingly to that obtained in Hermitian interaction quenches. 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 behavior. The velocity of information spreading is set by the dissipative coupling, and differs significantly from the original sound velocity.

In an even more recent work [Phys. Rev. Lett., in print, (2021)], we studied heating effects as generated by a Lindbladian coupling. Within the Lindblad approach, 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 spectrum of the time evolved density matrix is gapped, which collapses gradually as −ln(t). The von Neumann entropy crosses over from the early time −tln(t) behavior to ln(t) growth for late times. 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.

Driven systems and quantum work. Although it has not been the main line of our research, we have also investigated extensively driven interacting and many-body systems, an extremely hard subject even in the absence of interactions. Our research focused here on various aspects of heating.

We developed a novel perturbative expansion based on the replica trick for the Floquet Hamiltonian governing the dynamics of periodically kicked systems where the kick strength is the small parameter [Phys. Rev. Lett. 120, 200607 (2018)]. The expansion is formally equivalent to an infinite resummation of the Baker-Campbell-Hausdorff series in the undriven (nonperturbed) Hamiltonian, while considering terms up to a finite order in the kick strength. As an application of the replica expansion, we analyze an Ising spin 1/2 chain periodically kicked with a magnetic field with a strength h, which has both longitudinal and transverse components. We demonstrate that even away from the regime of high frequency driving, if there is heating, its rate is nonperturbative in the kick strength, bounded from above by a stretched exponential: $e^{-cst \times h^{-1/2}}$. This guarantees the existence of a very long prethermal regime, where the dynamics is governed by the Floquet Hamiltonian obtained from the replica expansion.

We have constructed a random matrix theory to describe work statistics and work generation in generic fermionic systems. We have generalized Anderson's orthogonality determinant formula [Phys. Rev. Research 2, 023224 (2020)], and studied numerically the full distribution of work as a function of time. We find that absorbed energy increases linearly with time, while its variance exhibits a *superdiffusive* behavior due to Pauli's exclusion principle. The probability of adiabatic evolution decays as a stretched

exponential rather than exponential. Also, the diffusion constant in energy space depends on the random matrix ensemble studied.

Integrable systems and truncated conformal space approach

We used the truncated conformal space approach (TCSA) as well as Bethe Ansatz methods to study a number of dynamical phenomena. For comparison, we often compared these with other numerical methods such as truncated Wigner methods, semiclassical approaches, or TEBD to describe the dynamics of exactly solvable models or models perturbed around integrable fixed points.

Quench and dynamics in the sine-Gordon model.

In one of our collaborative works [Phys. Rev. Lett. 121, 110402 (2018)], we computed correlation functions of the quantum sine-Gordon model, and found that correlations of excited states are markedly different from those of the thermal case, which can be explained by the integrability of the system. We also study dynamics after a quench, observing the effects of the interaction on the time evolution of correlation functions, their spatial dependence, and their non-Gaussianity as measured by the kurtosis. In another work [Phys. Rev. A 100, 013613 (2019)] we have studied the non-equilibrium time evolution of the phase field in the sine-Gordon model using two complementary approaches, and concluded that the phase-locking observed in recent experiments on coupled one dimensional Bose condensates cannot be explained in terms of homogeneous sine-Gordon dynamics. Our study hints at the role of other degrees of freedom or inhomogeneity in the experimental system.

We also implemented the recently developed generalized hydrodynamics (GHD) approach in the quantum sine-Gordon model [Phys. Rev. B 100, 035108 (2019)] and used it to study the non-equilibrium dynamics starting from inhomogeneous initial states. We compared the results with the predictions of the semiclassical approach and identified two different limits (a non-relativistic and a low temperature one) in which the semiclassical predictions are analytically recovered from GHD but found qualitative differences away from these limits.

We have shown that in the presence of topological excitations, correlations can develop outside of horizon and even between infinitely distant points after a global quantum quench [JHEP 2020, 224 (2020)]. We pointed out that, besides the maximum velocity bound implied by relativistic invariance, clustering of initial correlations is required to establish the “horizon effect”. In particular, quenches in the sine-Gordon model have an interesting property: despite the fact that the initial states have exponentially decaying correlations and cluster in terms of the bosonic fields, they violate the clustering condition for the soliton fields, which is argued to be related to the non-trivial field topology.

Ising and XXZ results.

We investigated the propagation of entanglement after quantum quenches in the non-integrable paramagnetic quantum Ising spin chain, observing a sudden increase in the entanglement production rate, related to the appearance of new quasiparticle excitations in the post-quench spectrum [Phys. Rev. A 98, 053610 (2018)]. We have argued that the phenomenon is the non-equilibrium version of the well-known Gibbs paradox related to mixing entropy.

We compared numerically simulated time evolution in the Ising field theory to two different analytic predictions based on form factor expansions in the pre-quench and post-quench basis, clarifying the domain of validity of these expansions and suggest directions for further improvement. We construct quench overlap functions and show that for quenches in the E8 model that the initial state is not of the integrable pair state form [SciPost Phys. 5, 027 (2018)]. Finally, we derived a new multiple integral formula for the propagator of the XXZ spin chain, using Bethe Ansatz and Quantum Transfer Matrix techniques [SciPost Phys. 6, 063 (2019)].

We also studied homogeneous quenches in integrable quantum field theories in the case where the initial state contained zero-momentum particles, and demonstrated that the two-particle pair amplitude necessarily has a singularity at the two-particle threshold [JHEP 08, 170 (2018)]. Constructing the explicit time dependence of one-point functions we find that the secular contribution normally linear in time is modified by a t ln t term, and encounter a novel type of secular contribution which is shown to be related to parametric resonance.

We constructed perturbative expansions of quench overlaps in quantum field theories, where either the pre-quench or the post-quench Hamiltonian is integrable [JHEP 2019, 47 (2019)]. Using the E8 Ising field theory for concrete computations, we gave explicit expressions for the overlaps up to second order in the quench size, and verified our results against numerical results obtained using the Truncated Conformal Space Approach. We demonstrated that the expansion using the post-quench basis is very effective, but found some serious limitations for the alternative approach using the pre-quench basis.

The Generalized Gibbs Ensemble (GGE) became one of the most fundamental concepts to describe prethermalized states of integrable systems. We clarified the status of GGE within the SU(3) symmetric chain [SciPost Phys. 8, 034 (2020)], where we showed that the set of conserved charges contains just enough information to completely fix the GGE and thus all physical properties of the equilibrated steady states.

We studied the dynamical aspect of quantum phase transitions in the Ising field theory, where the critical point can be crossed from different directions in the two-dimensional coupling space, leading to different scaling laws [SciPost Phys. 9, 055 (2020)]. We used the TCSA method to investigate the microscopic details of the Kibble-Zurek mechanism in this genuinely interacting field theory, and demonstrated dynamical scaling in the non-adiabatic time window. We also provided analytical as well as numerical evidence for specific scaling properties of various quantities, including higher cumulants of the excess heat.

In a recent work, we combined analytic and numerical techniques to precisely characterize the spectrum of the Heisenberg-Ising spin ladder in the regime of confinement [J. Stat. Mech. 9, 093106 (2020)]. We find two kinds of particles, intrachain and interchain mesons. The two types of mesons interpolate either between the same vacuum (intrachain) or between the two different ones (interchain). While the intrachain were previously known, the interchain ones are novel and represent general features of spin ladders with confinement.

Finally, in a work submitted to Nature [arXiv:2005.13302] we collaborated with a Chinese group of experimentalists to demonstrate that in the quasi-1D antiferromagnetic material $BaCo_2V_2O_8$ excitations are precisely described by the exceptional E8 Lie algebra. The large separation between the masked 1D and 3D quantum critical points of the system allows us to identify, for the first time, the full 8 single-particle E8 excitations as well as various multi-particle states in the spin excitation spectrum. This work opens new experimental route for exploring the dynamics of quantum integrable systems and physics beyond integrability, and thus bridge key physics in condensed matter and statistical field theory.

Dynamics of ultracold atoms

In addition to the works already accounted under the previous sections, we have also investigated various aspects of dynamics in ultracold atomic systems.

We studied several aspects of Time of Flight (ToF) images, a quench method broadly used to investigate correlated states of ultracold atoms. We studied numerically the momentum correlations in a two

dimensional, harmonically trapped interacting Bose system at T = 0 temperature, by developing a particle number preserving Bogoliubov approximation [PRA 95, 023625 (2017)]. We found that, quite surprisingly, the interaction induced coherent quantum fluctuations of the condensate manifest in *an anti-correlation dip* between short wave numbers k and -k. In contrast, for larger wave numbers, a weak positive correlation is found between particles of wave numbers k and -k, in accordance with the Bogoliubov result for homogeneous interacting systems.

In a subsequent work, we introduced *time of flight full counting statistics*, a novel characterization scheme of quantum states. Benchmarking this method on an interacting one dimensional Bose gas, we have shown that there the time of flight image displays several universal regimes, and provides detailed information on the quantum fluctuations of the quasi-condensate [PRA 95, 053621 (2017)]. We also demonstrated that time of flight full counting statistics captures (pre-)thermalization processes after a quantum quench, and can be useful for characterizing exotic quantum states.

In yet another work, we have investigated entropy production in coupled single-mode Bose-Einstein condensates. We have shown that the coherent oscillations of the condensates result in entropy oscillations on the top of a linear entropy generation at short time scales, while the long time limit of the entropy reflects the semiclassical dynamics of the system. In spite of the lack of equilibration, the entropy eventually saturates to a stationary value, well approximated by the prediction of a classical microcanonical ensemble [Phys. Rev. A 96, 023615 (2017)].

Together with Alain Aspect and Eugene Demler, we have also proposed an experiment to investigate the critical states of the Andreson localization transition, and the corresponding multifractal structure [Scientific Reports 8, 3641 (2018)]. We proposed to use two-component condensates with one of the components subject to disorder, and trigger transitions by crossed focused laser beams. Solving numerically the Gross-Pitaevskii equation on a lattice, we demonstrated that this method enables one to access critical multifractal properties. We have also explored the role of quantum geometrical tensor at the Anderson transition [Phys. Rev. Lett. 122, 106601 (2019)]. We have determined the finite size scaling of the quantum geometric tensor near the Anderson localization transitions of the orthogonal and unitary universality classes. We have revealed the two parameter crossover between the two universality classes that appears in low magnetic fields. We have determined the critical distributions of the geometric tensor, and have found it to show a remarkable isotropy.

Quantum simulating the Kondo-model is a very hard task. We also proposed a realization using alkali-earth elements and dynamical Floquet engineering [Kanász-Nagy, Phys. Rev. B 97, 155156 (2018)]. The dressed alkali atoms realize the anisotropic Kondo model, where the phase transition from the ferromagnetic to the antiferromagnetic state should take place. This setup provides a platform where non-equilibrium dynamical correlations can also be tested.