Theoretical study of disordered and correlated quantum systems

PhD thesis booklet

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1. Introduction

Understanding and describing quantum systems of many particles kept challenging many researchers for the last century. Often motivated by new experimental techniques, many different quantum systems have been investigated in the last century. Thanks to the rapid development of ultracold atomic techniques in the last decades, it is now possible to study the stationary states and dynamics of isolated quantum systems experimentally. These experiments have raised a considerable interest in the theoretical description of the ground states and dynamics of the corresponding quantum models. In addition, the explosion-like development of digital computers made detailed simulations of moderate-sized quantum systems possible. Although the potential of classical computers is strongly limited if we use them for the description of quantum systems [Feynman, 1982], many classical algorithms have been invented in the last decades which are able to simulate quantum systems in special cases efficiently. In my PhD research, I have used such algorithms to study disordered models and correlated one-dimensional quantum systems.

The experimental techniques in ultracold atomic systems enable us to create and quantum-simulate basic quantum models, which play fundamental role in theoretical condensed matter physics. For example, the discrete translational invariance of crystals can be emulated by optical lattices [Bloch, 2005], and static disorder can be modeled by laser speckles [Billy et al., 2008]. These two methods – combined with tunable interactions [Chin et al., 2010] – made it possible to experimentally demonstrate Anderson localization in one and three dimensions [Billy et al., 2008, Jendrzejewski et al., 2012]. These experiments demonstrated the existence of localized states deep in the localized regime. The critical states that appear on the phase boundary of localized and metallic regimes are, however, much harder to investigate experimentally. While the multifractal properties of the critical state are well known from numerical simulations, there are no experimental results on critical multifractality that are consistent with the numerics. In the second chapter of my thesis, I perform numerical simulations to study an experimental system of ultracold bosons, in which the critical state can be precisely excited and its multifractal spectrum can be measured.

In the second part of my thesis, I investigate one-dimensional interacting quantum systems numerically. Such one-dimensional systems can also be realized by ultracold atoms using strongly anisotropic traps [Parades et al., 2004]. These isolated one-dimensional systems are very popular in the theoretical community because many theoretical methods (Bethe ansatz, bosonization, conformal field theory) can be applied only for one-dimensional systems. The effect of interactions is also much stronger in one dimension, therefore the emerging quantum states often contain strong and exotic correlations. Quantum states of one dimensional systems can be well described by so-called matrix product states (MPS), that make algorithms like density matrix renormalization group (DMRG) [Schollwöck, 2011] or time evolving block decimation(TEBD) [Vidal, 2004] very efficient. The theoretical and analytical tools that are listed above enable us to study fundamental questions of statistical, particle, and condensed matter physics in one dimension, that are forming the basis of our intuitive physical picture also in higher dimensions.

2. Objectives

As a first objective, I investigated a disordered ultracold bosonic system in which the critical state of Anderson localization could be excited. In the proposed experimental setup, the critical correlations and multifractality could be measured by high resolution imaging of the excited cloud. The universal multifractal spectrum of the critical state was well known from numerical simulations [Rodriguez et al., 2009], but the results of former experiments performed in disordered semiconductors [Richardella et al., 2009] or with classical ultrasound [Faez et al., 2009] differed strongly from numerical predictions, and matched the theoretical expectations only qualitatively. Our goal was to give a proposal of an experperiment in which the universal multifractal spectrum could be precisely determined, and which could be realized by techniques already available. According to our initial expectations, we tried to find traces of multifractality in the so-called time-of-flight images, but this research direction did not prove succesful. Therefore, we slightly modified our goal, and searched multifractality in the projected real-space image of the three-dimensional cloud. We studied the experimental setup in detail by the accurate solution of a two-component disordered Gross-Pitaevskii equation, where the atom-atom interactions were treated at the mean field level.

Other objectives of my thesis were related to one-dimensional strongly correlated systems. First we developed a software based on matrix product states (MPS) in which one exploits flexibly the Abelian and non-Abelian symmetries of the system. In this code, one can perform ground state DMRG calculations and dynamical TEBD simulations. While most open-source MPS-based codes enable us to use Abelian quantum numbers, exploiting non-Abelian symmetries is a much harder task. On the other hand, by exploiting non-Abelian symmetries one can spare orders of magnitudes in required numerical resources.

As a the third objective of my work, I studied dynamics and relaxation of one-dimensional spin chains after quantum quenches. By using symmetry-exploiting TEBD simulations, we studied the question of thermalization in the integrable XXZ spin chain. This was a field of great interest, because the long-time stationary (equilibrium) state – due to the integrability of the model – was expected to be very different from the usual thermodynamic state [Rigol et al., 2007]. This expectation, however, has not been verified by simulations in a genuinely interacting system earlier. Furthermore, there was a disturbing contradiction between two competing approaches – the Generalized Gibbs Ensemble (GGE) based on infinite number of conserved local charges [Rigol et al., 2007], and the quench action formalism [Caux et al., 2013] – which we wanted to resolve by microscopic simulations.

Finally, as a fourth objective, I studied the post-quench dynamics of gapped non-intagrable spin chains. Non-equilibrium dynamics in these models can be efficiently simulated by the so-called semiclassical and hybrid semi-semiclassical algorithms, in which the post-quench state is approximated by a dilute gas of quasiparticles [Kormos et al., 2016, Moca et al., 2017]. The simple semiclassical and the hybrid theory treat collisions differently: while in the semiclassical theory every collision is approximated by total reflection, in the hybrid approach the two-particle S-matrix is applied at each collision. While these uncontrolled approximations are very efficient, their predictions have not been compared to microscopic simulations earlier. The accurate microscopic test of these approximations has been therefore an important goal of our work. To do so, we have investigated the post-quench dynamics of the S=1 Heisenberg chain, and monitored the transport of quasiparticles by the distribution of the total spin of half of the chain. This distribution can be extracted easily both from non-Abelian TEBD simulations and the semiclassical methods.

3. New scientific results

1. I proposed an experiment that could be performed by a two-component ultracold Bose-Einstein condensate and in which the critical state of Anderson-localization could be excited and imaged. I showed that – similarly to the three-dimensional wave function – the projection of critical state contained critical correlations and multifractal fluctuations. I showed that the critical correlations and the multifractal spectrum could be extracted from the wave function of the interacting condensate. [W1]

2. I simulated the post-quench dynamics of the XXZ spin chain by the infinite chain TEBD algorithm, and I showed that the short-range spin-spin correlations relaxed to the values predicted by the quench action formalism, while the Generalized Gibbs Ensemble built on local charges failed. [W2, W3]

3. I constructed a generalization of matrix product states (MPS) in which arbitrary Abelian and non-Abelian symmetries could be exploited. Based on the introduced non-Abelian MPS (NA-MPS) I developed an efficient, symmetry-exploiting variant of the time evolving block decimation (TEBD) and density matrix renormalization group (DMRG) algorithms. [unpublished]

4. I simulated by SU(2) symmetric TEBD simulations the dynamics of the S=1 Heisenberg spin chain after a quantum quench induced by turning off the nearest-neighbor biquadratic coupling. I extracted the time dependent distribution of the total spin of the half-chain. I determined the same distribution by using semiclassical and hybrid semi-semiclassical theories, and I showed that the spin distribution predicted by the hybrid theory agrees with the TEBD simulations very accurately, while the semiclassical description turns out to be insufficient. [W4]

5. I constructed a relativistic minimal model for the description of quantum quenches in the S=1 spin chain. I determined the quasiparticle density and the momentum distribution by perturbation theory, and I extracted from these the energy density and the so called collision time. I compared the predicted values of the product of the energy density and the collision time by the values measured in the SU(2) symmetric TEBD simulations, and I found a surprisingly good agreement for slow quenches. [W4]

4. References

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5. Publications related to thesis points

[W1] Miklós Antal Werner, Eugene Demler, Alain Aspect, and Gergely Zaránd, *Selective state spectroscopy and multifractality in disordered Bose-Einstein condensates: a numerical study*, Scientific Reports **8**, 3641 (2018).

[W2] Balázs Pozsgay, Márton Mestyán, Miklós Antal Werner, Márton Kormos, Gergely Zaránd, and Gábor Takács, *Correlations after Quantum Quenches in the XXZ Spin Chain: Failure of the Generalized Gibbs Ensemble*, Physical Review Letters **113**, 117203 (2014).

[W3] Márton Mestyán, Balázs Pozsgay, Gábor Takács, and Miklós Antal Werner, *Quenching the XXZ spin chain: quench action approach versus generalized Gibbs ensemble*, Journal of Statistical Mechanics: Theory and Experiment 2015 (4) P04001.

[W4] Miklós Antal Werner, Cătălin Paşcu Moca, Örs Legeza, Márton Kormos, and Gergely Zaránd, *Spin fluctuations after quantum quenches in the $S = 1$ Haldane chain: numerical validation of the semi-semiclassical theory*, Physical Review B **100**, 035401 (2019).

6. Further publications

[W5] Miklós Antal Werner, Arne Brataas, Felix von Oppen, and Gergely Zaránd, *Anderson localization and quantum Hall effect: Numerical observation of two-parameter scaling*, Physical Review B **91**, 125418 (2015).

[W6] Balázs Pozsgay, Eric Vernier, Miklós Antal Werner, *On Generalized Gibbs Ensembles with an infinite set of conserved charges*, Journal of Statistical Mechanics: Theory and Experiment 2017 (9), 093103.

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[W8] Miklós Antal Werner, Arne Brataas, Felix von Oppen, and Gergely Zaránd, *Universal Scaling Theory of the Boundary Geometric Tensor in Disordered Metals*, Physical Review Letters **122**, 106601 (2019).