The quench action approach to out-of-equilibrium quantum integrable models

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Contributions to publications

The author would like to stress the importance of the collaborations from which the work in this thesis and the original publications stem. Many of the conceptual and technical advancements came into being through countless hours of discussions and intense teamwork. This process is sometimes chaotic, often unfruitful and always uncertain, but indispensable for scientific progress. At a more discernible level, the author contributed to the following aspects of the publications:

- [1] *Solution for an interaction quench in the Lieb-Liniger Bose gas*
  Numerical checks of the overlap formula; preliminary results towards analytic solution GTBA equations; computation of static density moments; computation of density-density matrix elements.
- [2] *A Gaudin-like determinant for overlaps of Néel and XXZ Bethe states*
  Developing the initial research question; obtaining preliminary results; finite-size checks of end result.
- [3] *Néel-XXZ state overlaps: odd particle numbers and Lieb-Liniger scaling limit*
  Minor contributions to technical details.
- [4] *Quenching the Anisotropic Heisenberg Chain: Exact Solution and Generalized Gibbs Ensemble Predictions*
  Derivation and numerical solution of GTBA equations; large-Δ expansion of densities and nearest-neighbor correlator; failure of the GGE.
- [5] *Quench action approach for releasing the Néel state into the spin-1/2 XXZ chain*
  Derivation and numerical solution of GTBA equations; large-Δ expansion of densities and nearest-neighbor correlator; results for quench to isotropic point.
- [6] *Separation of relaxation timescales in a quantum Newton's cradle*
  Initial derivation overlaps from combinatorial approach; quench action analysis; GGE analysis; asymmetric pulse; finite-temperature pulse; minor contributions to Fermi-Bose mapping.
- [7] *A transfer-matrix description for postquench density matrices*
  Derivation density matrix Lieb-Liniger model; numerical analysis Lieb-Liniger model; GTBA equations and numerical analysis for transfer matrix XXZ chain.

Summary

THE QUENCH ACTION APPROACH
TO OUT-OF-EQUILIBRIUM
QUANTUM INTEGRABLE MODELS

In part motivated by the spectacular advances in realizing cold-atom experiments, the study of relaxation in isolated many-body quantum systems has attracted much theoretical interest during the past decade. The two basic questions concern the dynamics and equilibration after a system is brought far out of equilibrium. What are efficient ways of describing the time evolution of physical observables and what does this tell us about the underlying physics? Do isolated out-of-equilibrium quantum systems evolve towards an equilibrium and, if so, what determines this equilibrium?

This thesis addresses these questions from the perspective of quantum integrable systems in one dimension. In particular, it aims to describe a new, powerful method, coined the quench action (QA) approach, that purports to give an exact description of the time evolution and the equilibrium of local observables in infinitely large systems after a so-called quantum quench. We present a detailed introduction to the method, its first successful implementations for interacting models and the interesting fundamental questions their results have initiated.

For more than half a century the subject of quantum integrable systems has been a very active field of research, in particular by means of the Bethe Ansatz. The exact knowledge of the full spectrum and Slavnov's formula for overlaps makes it a very powerful theoretical tool. Furthermore, current experimental realizations are in good approximation described by quantum integrable models. Important topics were (and still are) the properties of the spectra of integrable models, the structure of the ground state and low-energy excitations, the computation of matrix elements of physical observables and the limit of large system size. Examples of integrable models are the Lieb-Liniger model, the (an)isotropic Heisenberg spin chain, the Hubbard model, the Kondo and Anderson impurity models and the class of Richardson-Gaudin models.

Triggered by a number of seminal experimental and theoretical findings, during the past decade the study of these models has somewhat shifted towards their out-of-equilibrium properties. In the renowned experiment of the quantum Newton's cradle an integrability-broken one-dimensional Bose gas out of equilibrium is found not to thermalize. This surprising phenomenon is often attributed to integrability, though a full theoretical understanding is still lacking. Not unrelated is the theoretical concept of a generalized Gibbs ensemble (GGE). The extra local conserved charges in a quantum integrable model are thought to deform the thermal Gibbs ensemble and thereby alter the equilibrium expectation values of local observables. There is ample evidence that the GGE works for free theories and recently a first experimental observation of the GGE came from the Schmiedmayer group.

The important concept of a global quantum quench, where a quantum system in a Hamiltonian eigenstate is brought out of equilibrium by suddenly changing one or more parameters of the model, has proved to be the ideal vehicle to study out-of-equilibrium phenomena in quantum integrable models. However, problems involving the postquench time evolution of observables generally remain hard nuts to crack. The main reason is that brute-force computations encounter a double sum over the Hilbert space, whose number of terms grows exponentially with system size. Furthermore, until recently applications of the GGE to truly interacting systems had been limited, rendering stringent tests of its conjecture absent.

The logic of the QA approach is completely different from conventional numerical or GGE methods. Contrary to for example the GGE, it is a method based on first principles. It predicts the exact postquench expectation values of typical physical operators at any time after a global quantum quench to a Bethe Ansatz solvable model in the strict thermodynamic limit. The problem of the exponentially large number of terms in the Hilbert space sums is overcome by means of a saddle-point approximation. The basic input of the method are the overlaps between the initial state and the eigenstates of the postquench Hamiltonian. Due to an interplay between overlaps and entropy, a single eigenstate effectively dominates the postquench equilibrium of typical physical operators while all other states are suppressed exponentially in system size. Expectation values long after the quench are computed on this representative state, while the full time evolution is recovered via summation solely over excitations in the vicinity of the representative state. Note that this logic is fundamentally different from the usual description in terms of a statistical ensemble, where a mixed state specified by a density matrix predicts all macroscopic properties of the postquench equilibrium.

In this thesis we derived the QA approach from first principles and specified validity conditions for observables and overlaps. Interaction quenches from the free boson gas to the repulsive Lieb-Liniger model and from the Néel state to the spin-1/2 XXZ chain were solved exactly in the thermodynamic limit. Without the QA approach, strict thermodynamic and infinite-time limits for quenches to truly interacting systems generally remain unattainable. We also used the QA method to model the Bragg pulse on hard-core bosons.

The main achievements of the results presented in this thesis are as follows. Through our work we have established the broad applicability of the QA approach to quench problems in quantum integrable models. This mainly depends on the availability of overlaps and of their scaling towards the thermodynamic limit. Considering the universal features of the overlaps presented in this thesis, there is good hope that more general classes of quenches can be studied in the near future. The extension of the QA approach to the time evolution of simple correlators in spin chains is another pressing open problem. Second, we found a failure of the GGE based on all known local charges for the Néel-to-XXZ quench. Even the simplest nearest-neighbor correlators are predicted wrongly by the GGE and depending on the initial state the error can become of order one. A deeper understanding is still lacking, but will likely give us more insights into the physics of relaxation in quantum integrable systems. Third, we have seen a separation of relaxation timescales in the quantum Newton's cradle for a gas of hard-core bosons. After a Bragg pulse there is a short phase of rapid relaxation towards a temporary steady state that is governed by the GGE, followed by the oscillation in the trap at much longer timescales. Extensions of our methods to longer pulses and finite interaction parameter could provide key insights in the underlying physics of the absence of thermalization in the quantum cradle experiment.

Samenvatting

The Quench Action Approach
to Out-of-Equilibrium
Quantum Integrable Models

Gemotiveerd door de spectaculaire vooruitgang in de realisatie van experimenten met koude atomen, heeft de theoretische bestudering van geïsoleerde kwantumsystemen met veel deeltjes een hoge vlucht genomen gedurende de afgelopen tien jaar. De twee hoofdvragen betreffen de dynamica en equilibratie nadat een systeem ver uit evenwicht is gebracht. Hoe beschrijf je efficiënt de tijdsevolutie van fysische observabelen en wat zegt dit over de onderliggende fysica? Evolueren geïsoleerde buiten-evenwicht kwantumsystemen naar een nieuw evenwicht en zo ja, hoe wordt dit evenwicht bepaald?

Dit proefschrift benadert deze vragen vanuit het perspectief van kwantumintegreerbare systemen in één dimensie. In het bijzonder beschrijft het een nieuwe, krachtige methode, genaamd de quench actie (QA) methode, die een exacte beschrijving geeft van de tijdsevolutie en het evenwicht van lokale observabelen in oneindig grote systemen na een zogenaamde kwantumquench. We presenteren een gedetailleerde inleiding tot de methode, haar eerste succesvolle toepassingen en de interessante fundamentele vragen die hieruit zijn voortgekomen.

Al meer dan een halve eeuw vindt er zeer actief onderzoek plaats naar kwantumintegreerbare systemen, met name met behulp van de Bethe Ansatz. De exacte kennis van het volledige spectrum en Slavnov's formule voor inproducten maakt het een krachtig theoretisch middel. Bovendien worden huidige experimentele realisaties bij goede benadering beschreven door deze modellen. Belangrijke onderwerpen waren (en zijn nog steeds) de eigenschappen van spectra van integreerbare systemen, de structuur van de grondtoestand en excitaties met lage energie, de berekening van matrixelementen en de limiet van grote systemen. Voorbeelden van integreerbare systemen zijn het Lieb-Liniger model, de (an)isotrope Heisenberg spinketen, het Hubbard model, de Kondo- en Anderson-onzuiverheidsmodellen en de klasse van Richardson-Gaudin modellen.

Aangespoord door een aantal cruciale experimentele en theoretische bevindingen is de bestudering van deze modellen de afgelopen tien jaar enigzins verschoven richting buiten-evenwicht eigenschappen. In het beroemde experiment van Newtons kwantumwieg werd ontdekt dat een 1D Bose gas met gebroken integrabiliteit eenmaal buiten evenwicht niet thermaliseert. Dit verrassende fenomeen wordt vaak toegedicht aan integrabiliteit, hoewel een volledig theoretisch begrip ervan nog steeds ontbreekt. Gerelateerd is het theoretische concept van een gegeneraliseerd Gibbs ensemble (GGE). De gedachte is dat de extra behouden ladingen van integreerbaarheid het thermische Gibbs ensemble vervormen en daarbij de evenwichtsverwachtingswaarden van lokale observabelen beïnvloeden. Er is overvloedig bewijs dat de GGE werkt voor vrije theorieën en recentelijk is een eerste experimentele observatie van de GGE wereldkundig gemaakt.

Het belangrijke concept van een globale kwantumquench, waarbij een kwantumsysteem in een eigentoestand buiten evenwicht wordt gebracht door plotseling een of meer parameter(s) van het model te veranderen, heeft zich bewezen als een ideale techniek om buiten-evenwicht fenomenen in kwantumintegreerbare modellen te bestuderen. In het algemeen is het echter lastig om vat te krijgen op de tijdsevolutie van observabelen na de quench. De hoofdreden is dat directe methoden stuiten op een dubbele som over de Hilbertruimte en het aantal termen van die sommen neemt exponentieel toe met systeemgrootte. Bovendien waren toepassingen van de GGE tot werkelijk interagerende systemen tot voor kort beperkt en waren serieuze tests van het GGE-vermoeden afwezig.

De logica van de QA methode is totaal anders dan die van de gebruikelijke numerieke methoden en de GGE. Zo gaat deze methode, in tegenstelling tot de GGE, louter uit van basisprincipes. Het voorspelt de exacte verwachtingswaarden van typische fysische observabelen op iedere tijd na een globale kwantumquench naar een model dat oplosbaar is met de Bethe Ansatz, en wel in de strikte thermodynamische limiet. Het probleem van het exponentieel grote aantal termen in de sommen over de Hilbertruimte wordt opgelost door een zadelpuntsbenadering. Cruciaal voor de methode zijn de inproducten van de initiële toestand met de eigentoestanden van de Hamiltoniaan na de quench. Een samenspel van de inproducten en de entropie selecteert een unieke eigentoestand. Deze domineert effectief het evenwicht van typische fysische observabelen, terwijl alle andere toestanden exponentieel in systeemgrootte onderdrukt worden. Verwachtingswaardes lang na de quench worden berekend op deze representatieve toestand, en de volledige tijdsevolutie wordt verkregen via sommatie over excitaties uitsluitend in de nabijheid van de zadelpuntstoestand. Merk op dat deze logica fundamenteel verschilt van de gebruikelijke beschrijving in termen van een statistisch ensemble, waarbij een gemengde toestand alle macroscopische eigenschappen van het evenwicht na de quench voorspelt.

In dit proefschrift is de QA methode afgeleid vanuit basisprincipes en zijn de toepasbaarheidscondities voor observabelen en inproducten bepaald. Interactiequenches van het vrije Bose gas naar het afstotende Lieb-Liniger model en van de Néel toestand naar de spin-1/2 XXZ keten werden opgelost in de thermodynamische limiet. Over het algemeen zijn de strikte limieten van oneindige systeemgrootte en tijd voor werkelijk interagerende systemen onbereikbaar zonder de QA methode. Ook hebben we de QA methode gebruikt om de Braggpuls voor bosonen met een harde kern te modelleren.

De belangrijkste resultaten in dit proefschrift zijn als volgt. Ons werk toont de brede toepasbaarheid aan van de QA methode voor quenches in kwantumintegreerbare modellen. Dit hangt hoofdzakelijk af van de beschikbaarheid van inproducten en hun schaling in de thermodynamische limiet. Gezien de universele structuur van de inproducten die in dit proefschrift worden besproken, is er goede hoop dat ook meer algemene klassen van quenches in de nabije toekomst bestudeerd kunnen worden. De uitbreiding van de QA methode naar de tijdsevolutie van simpele correlatoren in spinketens is een ander belangrijk open probleem. Ten tweede hebben we een falen van de GGE gebaseerd op alle lokale ladingen voor de Néel-naar-XXZ-quench gevonden. Zelfs de eenvoudigste naaste-buur correlatoren worden verkeerd voorspeld door de GGE en afhankelijk van de begintoestand kan de grootte van de fout van orde één zijn. Een beter begrip ontbreekt nog steeds, maar zal ons hoogstwaarschijnlijk een dieper inzicht geven in de fysica van relaxatie in kwantumintegreerbare systemen. Ten derde hebben we een scheiding van relaxatietijden waargenomen voor Newtons kwantumwieg voor ondoordringbare bosonen. Na een Braggpuls is er een korte fase van snelle relaxatie naar een tijdelijk stationaire toestand die wordt beschreven door de GGE, gevolgd door een oscillatie in de harmonische potentiaal voor veel grotere tijdschalen. Uitbreiding van onze methodes naar langere pulsen en eindige interactieparameter kan belangrijke inzichten opleveren in de onderliggende fysica van de afwezigheid van thermalisatie in het experiment van de kwantumwieg.