Final report for the European INSTANS program

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From 12 January to 7 March, I spent eight weeks at the Department for Theoretical Physics at Oxford University in the group of Prof. Essler. This stay was made possible through financial funding from the INSTANS program, for which I am most grateful. In this report, I will give an overview over the activities that I undertook in Oxford.

In my research proposal for the INSTANS grant, I sketched two projects: Firstly, the study of excited states of the spin-1/2 Heisenberg chain both from the lattice and a field-theoretical point of view. Secondly, properties of impurities in two-dimensional dimerized spin systems. The first project could nearly be finished during my stay in Oxford. Work on the second project is still continuing. Additionally, many new ideas on different projects evolved which I will describe in the following.

The remainder of this report contains five sections. The next section deals with work on the excitation spectrum of a spin chain viewed from the lattice and the field-theoretical perspective, followed by a section on the influence of boundary conditions on the spectrum and density oscillations in a spin chain. After that, I will comment on a new project, namely research on a quantum quench. The last section summarizes work on ground state properties and non-equilibrium dynamics in the Gaudin model. The report ends with a paragraph on the scientific atmosphere in Oxford in general.

1 Lattice *vs* continuum theory for the spin-1/2 Heisenberg chain

One project that I was planning while writing the research proposal for the INSTANS grant was how to close the gap between two different approaches to study excited states in the spectrum of the periodic spin-1/2 XXZ Heisenberg chain: On the one hand, the Bethe Ansatz (BA) solution of this model is well known [1], and excited states are encoded by the distribution of the BA quantum numbers in the complex plane. On the other hand, low-energy excitations are described by an effective bosonic field theory [2]. As far as individual energy levels are concerned, this field-theory in the past was used to calculate asymptotic expansion of the ground state energy [2] and a few excited levels [3] for large system sizes. Within the BA approach, the calculation of even low-lying levels is generally plagued by complex BA roots [4] which can make a numerical evaluation for large system sizes very cumbersome.

In our work, a step towards closing this gap is made: We calculate the asymptotic expansions of individual energy levels for a large number of low-lying energies from the field-theoretical picture analytically, by taking into account non-linear corrections to the Gaussian model. We then compare these results to numerical data from the BA, in the cases where such data can be obtained without complex roots. We find that even for moderate chain lengths with $20 - 100$ sites, the relative deviation from the exact BA-data is of the order of less than a percent. However, our results are valid also in those cases where the evaluation of the BA equations is plagued by complex strings.

An important outcome of this work is the asymptotic expansion of the lattice eigenstates in terms of the field-theoretical states. This connection turns out to be important in order to understand the behaviour of correlation functions in excited states [5]. Since it is much easier to deal with the field-theoretical states than with the lattice eigenstates this offers the opportunity to calculates dynamical correlation functions for to calculate form factors for low-lying excitations [6].

This work will be published in the very near future.

2 Density fluctuations and spectral properties of the open spin-1/2 Heisenberg chain

Recent work on density oscillations in the Hubbard model [7], together with [8–11], rose the question in how far open boundary conditions, a boundary field included, may alter the spectrum compared to the periodic case, and in how far such a modification is visible in the wave vector of Friedel oscillations in the density.

In order to study the basic mechanism, we restricted ourselves to the Heisenberg model, where charge fluctuations are suppressed compared to the Hubbard model. Prof. Essler and me showed that open boundary conditions generally induce a shift of the conformal anomaly (except at zero boundary field and half filling), and that this shift can be related to a shift of the Fermi vector in the Friedel oscillations. In other words, it is possible to obtain information about an additional term in the conformal anomaly by measuring the wave vector of the Friedel oscillations to order $\mathcal{O}(1/N)$, where N is the number of lattice sites. In order to obtain this result, we performed a finite-size scaling of the ground state in the presence of boundary fields at different fillings on the level of the discrete BA equations. We then performed the continuum limit, with our focus being the surface contribution to the conformal anomaly. The connection to the wave vector of Friedel oscillations could be established by bosonization.

It seems as if this result can be generalized to the Hubbard model, which includes charge fluctuations, by standard techniques. This work may be published in the future.

3 Quantum quenches

During the last decade, it has become possible to control the interaction between particles in ultracold atomic gases with very high accuracy [12]. Thereby, the study of non-equilibrium quantum dynamical processes has come into experimental reach. Recent theoretical work on quantum quenches in field theories [13, 14] incited Prof. Essler and me to wonder in how far a field-theoretical description of a quantum quench can model even processes on a lattice realistically, given that the low energy properties are asymptotically equivalent, see section 1. Following this route, we calculated several correlation functions using two Gaussian theories, involving spin and charge degrees of freedom, given that this is the asymptotically leading low-energy theory of the Hubbard model. These calculations relied on the assumption that non-linear corrections to the Gaussian models, which always occur in a field-theoretical description of a lattice model, can safely be neglected.

However, a talk by Paul Wiegmann about his work on nonlinear dynamics in fermionic systems [15, 16] made it clear that our assumption is not valid generally. It seemed important to us to find a model which permits to calculate the dynamics after a quantum quench in its full generality, without any approximations. This led Prof. Essler to the idea of studying correlation functions after quenching one-dimensional non-interacting bosons to one-dimensional non-interacting fermions. Since bosonic and fermionic fields are related by a Jordan-Wigner-type transformation [17, 18], the behaviour of correlation functions following a sudden change from bosonic to fermionic statistics can be calculated exactly. This allowed us to find a closed expression for the single particle Green's function and the density-density-correlation function after the quench for N particles. These expressions involve N-fold integrals over determinants depending on the N particle momenta. We are now facing the task of deriving an exact expression at finite particle density for short and especially for long times. This project is still ongoing.

4 Ground state properties and non-equilibrium dynamics in the Gaudin model

Discussions with Prof. Essler have been very helpful in making progress to understand the spectrum of the central-spin, or Gaudin model. In this model, one spin interacts with N_b many bath spins via Heisenberg exchange, where the N_b many exchange parameters can be chosen arbitrarily. This model is being used widely to model the hyperfine interaction of a single electron spin with N_b nuclear spins in a quantum dot [19].

The electron in such a quantum dot can be viewed as the experimental realization of a quantum bit. For quantum storage purposes, it is crucial to know the process of decoherence of the central spin. That is the question how fast the electron spin loses its polarization when it has been in a pure up- or down-state initially.

The model is integrable and the Bethe-Ansatz solution is known [20, 21], and it is natural to ask what can be learnt from the exact solution about the decoherence process. First steps in this direction have been undertaken recently [22]. During the last two months, further progress was made. Especially, we found a systematic way to classify low-lying excitations in the different sectors of constant magnetization. This allows it to calculate the spin-spin correlation functions between the electron spin and the nuclear spins and therefore to make analytical prediction about the screening cloud in a quantum dot. This project is the subject of intense research at present and will result in a publication in the not too far future.

5 General remarks

Thanks to the financial support by the INSTANS network, it was possible for me not only to enjoy most fruitful discussions and the collaboration with Prof. Essler. This grant also put me in contact with academic staff members of the Department of Theoretical Physics in Oxford, whose experience, expertise and physical insight I benefitted a lot from. Among these are Prof. Cardy and Prof. Chalker, with whom I enjoyed very interesting discussions.

Furthermore, I learned about how science is taught at Oxford University, about the tutoring system, the Colleges, the very individual training of students. These experiences will be beneficiary to my own teaching activities.

Finally, the very short impression I got from Oxford University as a whole, together with the Colleges, was unique and often enough overwhelming. I thank INSTANS for having made this stay possible to me.

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