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

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Bethe Ansatz techniques

In this chapter we give a detailed introduction to the coordinate Bethe Ansatz for the Lieb-Liniger model and the spin-1/2 XXZ spin chain, and a brief review of the algebraic Bethe Ansatz. Special attention is given to the thermodynamic limit of the coordinate Bethe Ansatz, as this is essential for a careful derivation of the quench action approach in the next chapter. There exist many excellent introductions to Bethe Ansatz techniques, see e.g. Refs [11, 12, 13, 16, 93, 94]. We do not attempt to improve on this and we simply present all the necessary ingredients for a good understanding of the rest of the thesis. Readers familiar with Bethe Ansatz techniques can safely skip this chapter.

2.1 Bethe Ansatz for the Lieb-Liniger model

We here present the exact solution of the Lieb-Liniger model [63, 64, 65, 66], by which we mean an exact and analytic diagonalization of the fully interacting Lieb-Liniger Hamiltonian in Eq. (1.2). The method employed goes under the name of coordinate Bethe Ansatz and was first applied to a one-dimensional ferromagnet with contact interactions [10], or the isotropic Heisenberg chain.

The Lieb-Liniger model describes bosons in one dimension undergoing a two-body contact interaction in the form of a delta-function potential. For system size L, its Hamiltonian in second-quantized form is given by

$$\hat{H} = \int_0^L dx \left[\partial_x \hat{\Psi}^\dagger(x) \partial_x \hat{\Psi}(x) + c \hat{\Psi}^\dagger(x) \hat{\Psi}^\dagger(x) \hat{\Psi}(x) \hat{\Psi}(x) \right] , \tag{2.1}$$

where the Bose fields $\hat{\Psi}(x,t)$, $\hat{\Psi}^\dagger(x,t)$ obey the canonical equal-time commutation relation: $\left[\hat{\Psi}(x,t),\, \hat{\Psi}^\dagger(y,t)\right] = \delta(x-y)$. The time variable t will often be left implicit. Remember we used dimensions such that $\hbar = 2m = 1$. The bosons repel each other when the interaction parameter $c \in \mathbb{R}$ is positive, whereas for negative c the model is said to be in the attractive regime. At $c = 0$ one retrieves free bosons. We will impose a ring-like geometry, or periodic boundary conditions: $\hat{\Psi}(x+L) = \hat{\Psi}(x)$. For the Fourier transform [see Eqs (A.1)] of the

Bose field we adopt the convention

$$\hat{\Psi}_k^\dagger = \frac{1}{L}\int_0^L dx\, e^{ikx}\hat{\Psi}^\dagger(x)\,, \tag{2.2}$$

such that $\left[\hat{\Psi}_k, \hat{\Psi}_p^\dagger\right] = \frac{1}{L}\delta_{k,p}$.

The particle number and momentum operator, respectively defined as

$$\hat{N} = \int_0^L dx\, \hat{\Psi}^\dagger(x)\hat{\Psi}(x), \qquad \hat{P} = \frac{i}{2}\int_0^L dx\, \left[\partial_x\hat{\Psi}^\dagger(x)\hat{\Psi}(x) - \hat{\Psi}^\dagger(x)\partial_x\hat{\Psi}(x)\right], \tag{2.3}$$

are both conserved quantities: $\left[\hat{H},\hat{N}\right] = \left[\hat{H},\hat{P}\right] = 0$. We will consider N-particle states of the form

$$|\boldsymbol{\lambda}\rangle = |\psi_N(\boldsymbol{\lambda})\rangle \;=\; \frac{1}{\sqrt{N!}}\int_0^L d^N x\, \psi_N(\boldsymbol{x}|\boldsymbol{\lambda})\, \hat{\Psi}^\dagger(x_1)\dots\hat{\Psi}^\dagger(x_N)\,|0\rangle\,, \tag{2.4}$$

where the (in general complex) numbers $\boldsymbol{\lambda} = \{\lambda_j\}_{j=1}^N$ are quasi-momenta and called rapidities, $\psi_N(\boldsymbol{x}|\boldsymbol{\lambda})$ is the N-particle wave function and $|0\rangle$ is the vacuum state. One can easily show that applying the Hamiltonian in Eq. (2.1) to the state $|\boldsymbol{\lambda}\rangle$ is equivalent to applying the first-quantized Lieb-Liniger Hamiltonian, given in Eq. (1.2), to the N-particle wave function. The form of the first-quantized momentum is well known, $P = -i\sum_{j=1}^N \frac{\partial}{\partial x_j}$.

2.1.1 Diagonalization

To gain insight in what the eigenfunctions look like, let us begin with very few particles. For one particle there is obviously no interaction and the eigenfunctions are simply plane waves: $\psi_1(x|\lambda) = e^{i\lambda x}$. The rapidity corresponds to the momentum of the particle and the energy is given by $\omega_\lambda = \lambda^2$. In general, the eigenvalues of a Hamiltonian eigenstate $|\boldsymbol{\lambda}\rangle$ will be denoted by

$$\hat{H}|\boldsymbol{\lambda}\rangle = \omega_{\boldsymbol{\lambda}}|\boldsymbol{\lambda}\rangle\,, \qquad \hat{P}|\boldsymbol{\lambda}\rangle = P_{\boldsymbol{\lambda}}|\boldsymbol{\lambda}\rangle\,, \qquad \hat{N}|\boldsymbol{\lambda}\rangle = N|\boldsymbol{\lambda}\rangle\,. \tag{2.5}$$

Two particles

For $N = 2$ the most general wave function is symmetric under interchange of positions (we are dealing with indistinguishable particles with bosonic statistics),

$$\psi_2(\boldsymbol{x}|\boldsymbol{\lambda}) = f_2(x_1,x_2|\lambda_1,\lambda_2)\Theta(x_2-x_1) + f_2(x_2,x_1|\lambda_1,\lambda_2)\Theta(x_1-x_2)\,, \tag{2.6}$$

where Θ is the Heaviside step function. Let us focus on solving the eigenfunction equation in the fundamental domain, $x_1 \le x_2$. When the particles are not on top of each other, $x_1 < x_2$, they are free and the equation is solved by a product of plane waves. As the Schrödinger equation is a linear second-order differential equation, the most general solution for periodic boundary conditions is

$$f_2(x_1,x_2|\lambda_1,\lambda_2) = A_{\lambda_1\lambda_2}\, e^{i(\lambda_1 x_1+\lambda_2 x_2)} + A_{\lambda_2\lambda_1}\, e^{i(\lambda_2 x_1+\lambda_1 x_2)}\,, \tag{2.7}$$

where $A_{\lambda_1\lambda_2}$ are complex coefficients to be determined. Since the derivative of the step function is a Dirac delta function and using partial integration (as for any physical quantity the wave function is integrated over), one obtains

$$H\psi_2(\boldsymbol{x}|\boldsymbol{\lambda}) = (\lambda_1^2+\lambda_2^2)\psi_2(\boldsymbol{x}|\boldsymbol{\lambda}) \\ +2\,\delta(x_1-x_2)[c(A_{\lambda_1\lambda_2}+A_{\lambda_2\lambda_1}) - i(A_{\lambda_1\lambda_2}-A_{\lambda_2\lambda_1})(\lambda_1-\lambda_2)]\,e^{i(\lambda_1+\lambda_2)x_1}\,. \tag{2.8}$$

The wave function is an eigenfunction of the two-particle Lieb-Liniger Hamiltonian if

$$\frac{A_{\lambda_1\lambda_2}}{A_{\lambda_2\lambda_1}} = \frac{i(\lambda_1-\lambda_2)+c}{i(\lambda_1-\lambda_2)-c} = -\,e^{i\theta(\lambda_1-\lambda_2)}\,, \tag{2.9}$$

where the two-body phase shift is defined as $\theta(\lambda) = 2\arctan\left(\frac{\lambda}{c}\right)$ and the minus sign is customary. Note that we used the identity $2i\arctan(z) = \log(1+iz) - \log(1-iz)$. This solves the two-particle problem.

Another name for the two-body phase shift is scattering angle. Starting from a configuration where particle 1 is left of particle 2, $x_1 < x_2$, with associated rapidities $\lambda_1 > \lambda_2$, the particles will scatter around a delta-function potential and the scattering problem is solved by $\psi_2(\boldsymbol{x}|\boldsymbol{\lambda}) \sim e^{i(\lambda_1x_1+\lambda_2x_2)} - e^{-i\theta(\lambda_1-\lambda_2)}e^{i(\lambda_2x_1+\lambda_1x_2)}$, where θ is indeed called the scattering angle and given in Eq. (2.9). The scattering amplitude is only given by a phase shift and the particles only interchange their rapidities. As we will see, this phenomenon of 'what comes out' equals 'what goes in' [15] is highly nontrivial and particular for integrable models. Also note that translational invariance implies that θ only depends on the difference between rapidities and since the reverse scattering process should give the same wave function, the scattering angle is an antisymmetric function.

Three particles

The generalization of Eqs (2.6) and (2.7) to three particles is

$$\psi_3(\boldsymbol{x}|\boldsymbol{\lambda}) = \sum_{P\in S_3} f_3(\boldsymbol{x}_P|\boldsymbol{\lambda})\,\Theta(x_{P_3}-x_{P_2})\,\Theta(x_{P_2}-x_{P_1})\,, \tag{2.10}$$

where S_3 are all permutations of $(1,2,3)$ and $\boldsymbol{x}_P = (x_{P_1}, x_{P_2}, x_{P_3})$, and (in the fundamental domain $x_1 \le x_2 \le x_3$)

$$f_3(x_1,x_2,x_3|\lambda_1,\lambda_2,\lambda_3) = \sum_{P\in S_3} A_{\lambda_{P_1}\lambda_{P_2}\lambda_{P_3}}\,e^{i(\lambda_{P_1}x_1+\lambda_{P_2}x_2+\lambda_{P_3}x_2)}\,. \tag{2.11}$$

Demanding that the wave function is an eigenfunction leads to six conditions for the six unknown amplitudes $A_{\lambda_j\lambda_k\lambda_\ell}$. Three conditions come from the domain boundary $x_1 = x_2$ and three come from the boundary $x_2 = x_3$. The point

$x_1 = x_2 = x_3$ does not impose an extra condition. The conditions become

$$\frac{A_{\lambda_1\lambda_2\lambda_3}}{A_{\lambda_2\lambda_1\lambda_3}} = \frac{i(\lambda_1-\lambda_2)+c}{i(\lambda_1-\lambda_2)-c} = -e^{i\theta(\lambda_1-\lambda_2)}\,, \tag{2.12a}$$

$$\frac{A_{\lambda_1\lambda_2\lambda_3}}{A_{\lambda_1\lambda_3\lambda_2}} = \frac{i(\lambda_2-\lambda_3)+c}{i(\lambda_2-\lambda_3)-c} = -e^{i\theta(\lambda_2-\lambda_3)}\,, \tag{2.12b}$$

plus the cyclic permutations of $(\lambda_1, \lambda_2, \lambda_3)$. This solves the three-particle problem. Note that when two rapidities are interchanged, the relative amplitude is independent of the third rapidity. We will shortly come back to this.

N particles

Generalization to N particles of the conditions (2.12) is possible [11]. Their solution is of the form $A_{\lambda_P} \sim (-1)^{[P]} \prod_{j<k} \left(\lambda_{P_j} - \lambda_{P_k} + i\,c\right)$, where $[P]$ is the signature of the permutation $P \in S_N$. After some algebra one finds that the N-particle wave function (also called the Bethe wave function) is given by

$$\psi_N(\boldsymbol{x}|\boldsymbol{\lambda}) = \frac{(-i)^{N(N-1)/2}}{\sqrt{N!}} \prod_{j>k} \mathrm{sgn}(x_j - x_k)\ldots \tag{2.13a}$$

$$\ldots \sum_{P\in S_N} (-1)^{[P]}\, e^{i\sum_{\ell=1}^{N} \lambda_{P_\ell} x_\ell + \frac{i}{2}\sum_{j>k} \mathrm{sgn}(x_j-x_k)\theta(\lambda_{P_j}-\lambda_{P_k})}$$

$$= F_{\boldsymbol{\lambda}} \sum_{P\in S_N} \prod_{j>k}^{N} \left(1 - \frac{ic}{\lambda_{P_j}-\lambda_{P_k}} \mathrm{sgn}(x_j - x_k)\right) \prod_{\ell=1}^{N} e^{i\lambda_{P_\ell} x_\ell}, \tag{2.13b}$$

where sgn denotes the sign function and the normalization factor

$$F_{\boldsymbol{\lambda}} = \frac{\prod_{j>k=1}^{N} (\lambda_j - \lambda_k)}{\sqrt{N!\prod_{j>k=1}^{N}\left((\lambda_j-\lambda_k)^2 + c^2\right)}} \tag{2.13c}$$

is chosen for convenience, as will become clear shortly. This is the coordinate Bethe Ansatz. It is valid in all domains, i.e. $0 \le x_j < L$ for all $j = 1, \ldots, N$. Coordinates outside this interval must be shifted by a multiple of L. For example, $\psi_N(-\boldsymbol{x}|\boldsymbol{\lambda}) = \psi_N(L - \boldsymbol{x}|\boldsymbol{\lambda})$, where for the right-hand side one can use Eqs (2.13) if $0 \le x_j < L$ for all $j = 1, \ldots, N$.

Note that with these conventions the interchange of two rapidities causes a sign flip of the wave function. This prohibits two rapidities having the same value and we thus have a Pauli exclusion principle for a system of bosons. This is not a problem, since the relations between spin and statistics is not valid in $1+1$ spacetime dimensions. In what follows we will see that due to this Pauli principle the ground state of the Lieb-Liniger model is a Fermi sea. The energy and momentum eigenvalues of the N-particle Bethe wave function are given by

$$\omega_{\boldsymbol{\lambda}} \;=\; \sum_{j=1}^{N} \lambda_j^2\,, \qquad P_{\mathbf{e}} \;=\; \sum_{j=1}^{N} \lambda_j\,. \tag{2.14}$$

Cusp form of boundary condition

To gain insight in what the wave function looks like, note that after integration over an infinitesimal region of the boundary of the fundamental domain $x_1 \leq x_2 \leq \ldots \leq x_N$ the conditions on the wave function are as follows:

$$\left(\frac{\partial}{\partial x_{j+1}} - \frac{\partial}{\partial x_j} - c \right) \psi_N(\boldsymbol{x}|\boldsymbol{\lambda}) \bigg|_{x_{j+1}=x_j+0^+} = 0 \,, \tag{2.15}$$

for $j = 1, 2, \ldots, N-1$. This discontinuity of the first derivative of the wave function results in a cusp. So the wave function is a product of plane waves whenever all coordinates are different, and has cusps when two (or more) coordinates are equal. The cusp conditions are equivalent to the conditions in Eqs (2.9) and (2.12).

2.1.2 General discussion

Taking a closer look at the conditions on the scattering amplitudes, we see that any scattering process is decomposable in two-body scattering processes and that the order of these processes is irrelevant. Take for example three particles in the fundamental domain $x_1 \leq x_2 \leq x_3$ that come in and scatter such that particles 1 and 3 interchange rapidities. The scattering amplitudes obey the relations

$$\frac{A_{\lambda_3\lambda_2\lambda_1}}{A_{\lambda_1\lambda_2\lambda_3}} = \frac{A_{\lambda_3\lambda_2\lambda_1}}{A_{\lambda_3\lambda_1\lambda_2}} \frac{A_{\lambda_3\lambda_1\lambda_2}}{A_{\lambda_1\lambda_3\lambda_2}} \frac{A_{\lambda_1\lambda_3\lambda_2}}{A_{\lambda_1\lambda_2\lambda_3}} = \frac{A_{\lambda_3\lambda_2\lambda_1}}{A_{\lambda_2\lambda_3\lambda_1}} \frac{A_{\lambda_2\lambda_3\lambda_1}}{A_{\lambda_2\lambda_1\lambda_3}} \frac{A_{\lambda_2\lambda_1\lambda_3}}{A_{\lambda_1\lambda_2\lambda_3}} \,, \tag{2.16}$$

where the second equality is a consequence of the Yang-Baxter relation for scattering matrices. The validity of this relation is highly nontrivial and an important condition for a system to be quantum integrable.

The absence of independent three-body (or higher) scattering processes is called nondiffractive scattering and is intimately connected with the presence of higher conservation laws. Since in any scattering process outgoing rapidities equal ingoing rapidities, any symmetric function of the N rapidities $\boldsymbol{\lambda}$ is conserved in time. The operator whose eigenvalue is such a function, is automatically a conserved quantity. In Section 2.3 we will find an infinite set of local conserved charges $\{\hat{Q}_m\}_{m=1}^{\infty}$ whose respective eigenvalues are given by $\hat{Q}_m|\boldsymbol{\lambda}\rangle = \left[\sum_{j=1}^{N}(\lambda_j)^m\right]|\boldsymbol{\lambda}\rangle$ (see Ref. [95]). In Ref. [15] it is argued that this nondiffractive property is essential for a system to be quantum integrable.

Despite the above derivation of the Bethe wave function, it is a mistake to picture experimental realizations of the Lieb-Liniger gas as a collection of particles with definite measurable momentum equal to their associated rapidities and only undergoing two-particle collisions. At finite density N/L the gas exhibits collective excitations, wave packets of many different rapidity modes. The individual rapidity modes scatter in the clean way here described, but the scattering of collective excitations is messy. Furthermore, rapidities should not be confused with physical momenta since the particles in the Lieb-Liniger model are not free. The Bethe wave function is not an eigenfunction of single-particle momentum operators $-i\frac{\partial}{\partial x_j}$. Given the rapidities, the distribution of physical momenta can still be calculated however and corresponds for example to the measured particle momenta if the gas would suddenly be released from the optical trap [24]. As an exception, the sum of all rapidities does correspond to the total physical momentum of the state [see Eq. (2.14)].

Other examples of models that are exactly solvable by means of the coordinate Bethe Ansatz are the (anisotropic) Heisenberg chain [82, 84], which will be introduced in Section 2.2, the Hubbard model [16] for fermions on a lattice, the Kondo [96] and Anderson [96] impurity models and Richardson-Gaudin models [11]. These are all models with contact interactions. There are also models with long-range interactions. Notable examples are bosons in a one-dimensional Coulomb potential, whose scattering angle is a constant up to a sign function [97, 15], and the Haldane-Shastry model [98, 99], which is the long-range equivalent of the Heisenberg spin model.

Note that in the dilute limit every translationally invariant two-body interaction leads to nondiffractive scattering, regardless of the potential, since in this limit three-body scattering is suppressed because of low densities and conservation of momentum and energy ensure nondiffractiveness for two-particle scattering. In this thesis we will solely work in finite-density setups.

2.1.3 Quantization and the Bethe equations

So far the values of the rapidities were left unspecified. Imposing a finite ring-like geometry quantizes them and leads to a discrete spectrum. The periodicity conditions for the wave function are

$$\psi_N\left(x_1,\ldots,x_j,\ldots,x_N|\boldsymbol{\lambda}\right) = \psi_N\left(x_1,\ldots,x_j+L,\ldots,x_N|\boldsymbol{\lambda}\right)\,, \tag{2.17}$$

for all $j=1,\ldots,N$. This translates into conditions on the rapidities called Bethe equations:

$$e^{i\lambda_j L} \;=\; -\prod_{k=1}^{N}\frac{\lambda_j-\lambda_k+ic}{\lambda_j-\lambda_k-ic}, \qquad \text{for} \quad j=1,\ldots,N\,. \tag{2.18}$$

Taking the logarithm on both sides gives an alternative formulation of the Bethe equations,

$$\lambda_j \;=\; \frac{2\pi}{L}I_j-\frac{1}{L}\sum_{k=1}^{N}\theta\left(\lambda_j-\lambda_k\right), \qquad \text{for} \quad j=1,\ldots,N\,, \tag{2.19}$$

where $\theta(\lambda)=2\arctan\left(\frac{\lambda}{c}\right)$ is again the scattering angle. The quantum numbers $\boldsymbol{I}=\{I_j\}_{j=1}^{N}$, coming from the multi-valuedness of the logarithm, are integers when N is odd and half-odd integers when N is even. They can be chosen arbitrarily and as long as they are all different a nontrivial solution will exist and is unique [100]. They have to be different because of the Pauli exclusion principle, coming from the form of the wave function, and the fact that $I_j = I_k$ implies $\lambda_j = \lambda_k$. A state with rapidities that form a solution to the Bethe equations will be called a Bethe state and its rapidities are often called Bethe roots.

In the attractive regime $c < 0$ the solutions to the Bethe equations are in general complex numbers. In Ref. [101] it was proven that every solution is self-conjugate, i.e. $\bar{\boldsymbol{\lambda}} = \boldsymbol{\lambda}$. Complex rapidities can be interpreted as bound states of bosons with a factor in the wave function that falls off exponentially in the coordinates. For example, the ground state in the attractive regime is formed by a single bound state of N particles [65].

In this thesis we will focus on the repulsive regime instead, $c > 0$. In that case all Bethe roots are real, excluding the possibilities of bound states [100]. Monotonicity of the scattering angle implies that $\lambda_j > \lambda_k$ if $I_j > I_k$. From Eq. (2.14) it then follows that the quantum numbers of the N-particle ground state form a symmetric Fermi sea:

$$I_j^{\mathrm{GS}} \;=\; -\frac{N+1}{2} + j, \qquad \text{for} \quad j = 1, \dots, N\,. \tag{2.20}$$

Observe that the ground state of the free-boson gas ($c = 0$) has rapidities $\lambda_j = 0$ for all $j = 1, \dots, N$. This is consistent since the Pauli principle does not hold in this limit, as can be seen from Eq. (2.13c). The (unnormalized) wave function is a constant: $\lim_{c\to 0} \psi_N\big(\boldsymbol{x}|\boldsymbol{\lambda}^{\mathrm{GS}}\big) = \sqrt{N!}$.

Finally, the squared norm of a Bethe state wave function is given by a determinant, as hypothesized by Gaudin [11] and proved by Korepin [102]:

$$\|\boldsymbol{\lambda}\|^2 = \|\psi_N\left(\boldsymbol{x}|\boldsymbol{\lambda}\right)\|^2 = \int_0^L \mathrm{d}^N x \, |\psi_N\left(\boldsymbol{x}|\boldsymbol{\lambda}\right)|^2 \;=\; \det\left(G_{jk}\right)\,, \tag{2.21}$$

with the $N \times N$ Gaudin matrix defined by

$$G_{jk} = \delta_{jk}\Big(L + \sum_{l=1}^{N} K(\lambda_j - \lambda_l)\Big) - K(\lambda_j - \lambda_k)\,, \qquad K(\lambda) \;=\; \frac{2c}{\lambda^2 + c^2}\,. \tag{2.22}$$

The function K is related to the two-body phase shift, $K(\lambda) = \frac{d}{d\lambda}\theta(\lambda)$. Throughout this thesis we will often use implicitely normalized Bethe states, i.e. without writing the norm explicitely.

2.1.4 The Tonks-Girardeau gas

The interesting limit $c \to \infty$ brings the model into the Tonks-Girardeau (TG) regime [103, 67]. The Bethe wave function becomes

$$\begin{aligned}
\chi_N(\boldsymbol{x}|\boldsymbol{\lambda}) &= \lim_{c\to\infty} \psi_N(\boldsymbol{x}|\boldsymbol{\lambda}) && (2.23a)\\
&= \frac{1}{\sqrt{N!}} \left(\sum_P (-1)^{[P]} \prod_{j=1}^{N} e^{i\, x_j \lambda_{P_j}} \right) \prod_{1\le l<j\le N} \mathrm{sgn}(x_j - x_l) && (2.23b)\\
&= \frac{1}{\sqrt{N!}} \det\left[e^{i x_l \lambda_j}\right] \prod_{1\le l<j\le N} \mathrm{sgn}(x_j - x_l)\,, && (2.23c)
\end{aligned}$$

and has norm squared $\|\chi_N(\boldsymbol{x}|\boldsymbol{\lambda})\|^2 = L^N$. In Ref. [67] it was established that the theory has the spectrum of free spinless fermions and the Tonks-Girardeau wave function is, up to a symmetrization factor, given by the free-fermion Slater determinant. Most expectation values in the Tonks-Girardeau gas are the same as for free fermions, but (importantly) the momentum distribution functions are different.

The Bethe equations are trivial in the Tonks-Girardeau regime, the rapidities given by $\lambda_j = \frac{2\pi}{L} I_j$. The cusp condition on the wave function becomes $\psi_N(\ldots, x_j = x_{j+1}, x_{j+1}, \ldots) = 0$, meaning that particles are impenetrable to each other. They are hard-core bosons.

2.1.5 Observables and measurements

Here we briefly outline the observables in the Lieb-Liniger model that are of theoretical as well as experimental interest. The most basic observable is the local density of the Bose gas, $\hat{\rho}(x,t) = \hat{\Psi}^\dagger(x,t)\hat{\Psi}(x,t)$, which can be measured by preparing a gas in a trap and simply taking a picture with a CCD camera [104, 105]. For a certain parameter regime the observed density profile at finite temperature is in good agreement [71] with the thermodynamic Bethe Ansatz approach of Yang and Yang [100, 12, 13].

The operator that measures the (bosonic) momentum distribution is given by

$$\hat{n}_k = \hat{\Psi}_k^\dagger \hat{\Psi}_k = \frac{1}{L^2} \int_0^L dx\, dy\, e^{ik(x-y)} \hat{\Psi}^\dagger(x)\hat{\Psi}(y)\,, \tag{2.24}$$

where the momenta are quantized $k = \frac{2\pi}{L} m$, with $m \in \mathbb{Z}$. The operator on the right-hand side is the one-body reduced density matrix, $\hat{\Psi}^\dagger(x)\hat{\Psi}(y)$. In experiments the momentum distribution can be measured by releasing the trap, letting the gas expand as free particles and again taking a picture with a CCD camera. The positions of the particles is directly related to their momenta at the time of release. This is for example done in the famous Newton's cradle experiment [24]. An alternative method for measuring the momentum distribution is Bose-gas focusing [106, 71].

Another important physical quantity is the dynamic structure factor $S(x,t) = \langle \hat{\rho}(x,t)\hat{\rho}(0,0)\rangle$, where the operator is evaluated on either a generic pure state $|\psi\rangle$ or an ensemble. Note that we have assumed translational invariance here and generalization is needed for configurations with a broken translational symmetry. Also, we neglect singular terms by implicitely considering normal-ordered operators throughout this thesis. The unequal time density-density correlator measures how likely it is that a density fluctuation travels a distance x during a time t. Its Fourier transform (on a pure state, see Appendix A) does that for density waves with momenum k and energy ω,

$$S(k,\omega) = \int_0^L \mathrm{d}x \int_{-\infty}^{\infty} \mathrm{d}t\, e^{i(kx-\omega t)}\, S(x,t) \tag{2.25a}$$

$$= 2\pi L \sum_{\boldsymbol{\mu}} \frac{|\langle\psi|\,\hat{\rho}(0,0)\,|\boldsymbol{\mu}\rangle|^2}{\|\boldsymbol{\mu}\|^2}\, \delta(\omega - \omega_\psi + \omega_{\boldsymbol{\mu}})\, \delta_{k,P_{\boldsymbol{\mu}}-P_\psi}\,, \tag{2.25b}$$

where the last line is its Lehmann representation and we inserted a resolution of the identity in terms of normalized Bethe states. Similarly, the static structure factor is the equal-time density density correlator $S(x) = \langle \hat{\rho}(x,0)\hat{\rho}(0,0)\rangle$ and its Fourier transform is given by $S(k) = L\sum_{\boldsymbol{\mu}} |\langle\psi|\,\hat{\rho}_{-k}\,|\boldsymbol{\mu}\rangle|^2$.

The density-density correlation function is experimentally accessible through Bragg spectroscopy (see e.g. Ref. [79]). A superposition of two laser beams induces a periodic potential coupling to the density of the gas,

$$\hat{V}_{\mathrm{B}} = A\int_0^L dx\cos(kx-\omega t)\,\hat{\rho}(x,t)\,, \tag{2.26}$$

where A is the intensity of the laser and k and ω can be varied. At finite temperature T, the total momentum and energy transferred into the system can be estimated via linear response theory [107],

$$\frac{dP_{\mathrm{tot}}}{dt} = \left(\frac{A}{2}\right)^2 kL\left(1-e^{-\omega/T}\right) S_T(k,\omega)\,, \tag{2.27a}$$

$$\frac{dE_{\mathrm{tot}}}{dt} = \left(\frac{A}{2}\right)^2 \omega L\left(1-e^{-\omega/T}\right) S_T(k,\omega)\,, \tag{2.27b}$$

where S_T is the finite-temperature dynamic structure factor ($k_B = 1$). The total momentum and energy can be measured via the momentum distribution after releasing the trap.

Over time the bosonic particles inevitably leak out of the one-dimensional trap due to three-body recombination. This renders them insensitive to the trapping potential and they will start falling down due to gravity. The loss was first described in Ref. [108] and is associated with the expectation value of the density cubed [109], $g_3 = \langle (L\,\hat{\rho}(0)/N)^3\rangle$.

Note that the matrix elements on Bethe states of the observables here described form a crucial ingredient in the theoretical study of the Lieb-Liniger model [12]. These form factors are known in determinant form as a consequence of Slavnov's theorem for scalar products of Bethe states [110]. A determinant representation of the field form factor is known as well [111, 112, 113].

2.1.6 The thermodynamic limit

As will be explained in Section 3.1, throughout this thesis we will be mainly concerned with Bethe Ansatz-solvable quantum models of infinite system size. In this thermodynamic limit (which we denote as $\lim_{\text{th}}$) both number of particles and system size are sent to infinity, $N, L \to \infty$, while particle density $n = N/L$ is kept fixed. We will now carefully specify what we mean with the thermodynamic limit in the case of the coordinate Bethe Ansatz for the Lieb-Liniger model.

Density distributions

For an N-particle Bethe state specified by quantum numbers $\boldsymbol{I}$ and rapidities $\boldsymbol{\lambda}$, the distance between rapidities can be estimated by

$$\frac{2\pi}{L}(I_j - I_k) \geq \lambda_j - \lambda_k \geq \frac{2\pi}{L}\frac{1}{1+\frac{2n}{c}}\,, \tag{2.28}$$

for all pairs $I_j > I_k$. Here we used Eqs (2.19) and the inequality

$$\theta(\lambda) - \theta(\mu) = \int_\mu^\lambda d\nu\, K(\nu) \leq \frac{2}{c}(\lambda - \mu)\,, \quad \lambda > \mu\,. \tag{2.29}$$

If the distance between consecutive quantum numbers does not scale with N, the distance between rapidities decreases with N^{-1}. In the thermodynamic limit the rapidities of a Bethe state lie dense on the real axis and can be characterized by a density ρ, such that in the interval $[\lambda, \lambda + d\lambda]$ the number of rapidities is $L\rho(\lambda)d\lambda$.

To derive the properties of this density function we define, given an N-particle Bethe state, a function $\lambda^{(N)}$ on the whole real axis by

$$\lambda^{(N)}(x) = 2\pi x - \frac{1}{L}\sum_{k=1}^{N}\theta\big(\lambda^{(N)}(x) - \lambda_k\big)\,. \tag{2.30}$$

The resemblance with the Bethe Eqs (2.19) is obvious and $\lambda_k = \lambda^{(N)}(I_k/L)$ for all $k = 1, \dots, N$. It can be shown that $\lambda^{(N)}$ exists and is a monotonically increasing, 1-to-1 function [12]. Its inverse, whose derivative is a measure for the density of rapidities of the Bethe state, will be denoted by $x^{(N)}$. Density functions of occupied and unoccupied quantum numbers on the space of quantum numbers are defined by

$$\rho^{(N)}(x) = \frac{1}{L}\sum_{n\in\boldsymbol{I}}\delta(x - n/L)\,, \qquad \rho_h^{(N)}(x) = \frac{1}{L}\sum_{n\in\mathbb{Z}\setminus\boldsymbol{I}}\delta(x - n/L)\,. \tag{2.31}$$

These functions are also called particle and hole densities, respectively. Note that the hole density is defined for odd N, since for even N the quantum numbers are half-odd integers and $\mathbb{Z}$ must be replaced by $\mathbb{Z}+1/2$. A density for the total number of vacancies, both occupied and unoccupied, is simply given by (N odd)

$$\rho_t^{(N)}(x) = \rho^{(N)}(x) + \rho_h^{(N)}(x) = \frac{1}{L}\sum_{n\in\mathbb{Z}} \delta(x - n/L)\,. \tag{2.32}$$

Generically, matrix elements of local observables in between Bethe states are expressible in terms of rapidities. We are therefore eventually interested in the densities of Bethe roots on the rapidity space. Using the properties of the Dirac delta function one can define the corresponding density functions,

$$\rho^{(N)}(\lambda) = \frac{1}{L}\sum_{k=1}^{N} \delta(\lambda - \lambda_k) = \rho^{(N)}\big(x^{(N)}(\lambda)\big)\,\frac{dx^{(N)}(\lambda)}{d\lambda}\,, \tag{2.33}$$

and similarly for the hole density and the total density.

Density functions and the thermodynamic Bethe equation

These are distributions at finite size. We would like to have density functions in the thermodynamic limit counting the density of occupied quantum numbers or rapidities. We are only interested in Bethe states for which the density function is continuously differentiable, possibly apart from a measure-zero set of points like for the ground state. Although it is in principle possible to come up with thermodynamic Bethe states that do not obey this condition, these states play no role in the equilibrium description after generic quantum quenches studied in this thesis. In accordance with the Euler-Maclaurin formula, the density function for quantum numbers should obey

$$\int_a^b dx\,\rho(x)\,f(x) = \lim{}_{\text{th}} \int_a^b dx\,\rho^{(N)}(x)\,f(x)\,, \tag{2.34}$$

for any continuously differentiable function f and any finite interval $[a,b]$. The hole occupation density $\rho_h(x)$ and the vacancy density $\rho_t(x)$ should obey similar relations, as well as the respective rapidity density functions $\rho(\lambda)$, $\rho_h(\lambda)$ and $\rho_t(\lambda)$. It is obvious from Eq. (2.32) that $\rho_t(x) = 1$.

To specify what is meant with the thermodynamic limit of a Bethe state and to give a rigorous definition of the density functions, it proves useful to introduce a third representation of Bethe states. A Bethe state of N rapidities is specified by which N quantum numbers are occupied in the space of (half-odd) integers. Now let us divide the space of quantum numbers in boxes of length ℓ_i, where i labels the different compartments. Let n_i be the number of occupied quantum numbers in box i. Within box i there are $\binom{\ell_i}{n_i}$ ways of distributing the occupied quantum numbers. The precise occupation is given by the quantity c_i. A Bethe state is then equivalently specified by the distribution over boxes $\mathbf{n} = \{n_i\}_i$ accompanied by the in-box distributions $\mathbf{c} = \{c_i\}_i$. We have equivalence of rapidities, quantum numbers and box distributions,

$$\boldsymbol{\lambda} \leftrightarrow \boldsymbol{I} \leftrightarrow (\mathbf{n}, \mathbf{c}) \,. \tag{2.35}$$

In the thermodynamic limit we demand the box sizes to blow up, $\lim_{\text{th}} \ell_i = \infty$, while $\lim_{\text{th}} \ell_i/N = 0$. This means that in x space the box sizes shrink to zero and the density $\rho(x)$ is insensitive to the in-box configurations $\mathbf{c}$.

Let us assume the box size grows like $\ell_i \sim N^\alpha$ with system size, for some arbitrary value $0 < \alpha < 1$. Other dependencies, for example $\ell_i \sim \log N$, can be treated similarly. The density of occupied quantum numbers for a Bethe state in the thermodynamic limit is then given by

$$\rho(x) = \lim_{\text{th}} \left. \frac{n_i}{\ell_i} \right|_{i \sim x L^{1-\alpha}} \,. \tag{2.36}$$

With this definition the condition in Eq. (2.34) is automatically satisfied and $L\rho(x)dx$ is the number of occupied quantum numbers is the interval $[x, x + dx]$. The hole and the (trivial) vacancy occupation densities are given by

$$\rho_h(x) = \lim_{\text{th}} \left. \frac{\ell_i - n_i}{\ell_i} \right|_{i \sim x L^{1-\alpha}} \,, \qquad \rho_t(x) = \lim_{\text{th}} \left. \frac{\ell_i}{\ell_i} \right|_{i \sim x L^{1-\alpha}} = 1 \,. \tag{2.37}$$

The densities of Bethe roots in the thermodynamic are now given by

$$\rho(\lambda) = \rho(x) \frac{dx(\lambda)}{d\lambda} \,, \qquad \rho_h(\lambda) = \rho_h(x) \frac{dx(\lambda)}{d\lambda} \,, \qquad \rho_t(\lambda) = \frac{dx(\lambda)}{d\lambda} \,, \tag{2.38}$$

where $x(\lambda) = \lim_{\text{th}} x^{(N)}(\lambda)$ and obeys the integral equation

$$\lambda = 2\pi \, x(\lambda) - \int_{-\infty}^{\infty} d\mu \, \rho(\mu) \, \theta(\lambda - \mu) \,, \tag{2.39}$$

which is the thermodynamic limit of Eq. (2.30). Differentiating this equation with respect to λ gives the thermodynamic version of the Bethe equations,

$$\rho_t(\lambda) = \frac{1}{2\pi} + \frac{1}{2\pi} \int_{-\infty}^{\infty} d\mu \, \rho(\mu) \, K(\lambda - \mu) \,. \tag{2.40}$$

Remember $K(\nu) = 2c/(\nu^2 + c^2)$. The thermodynamic Bethe equation is an integral equation relating ρ and ρ_h nontrivially. This should be contrasted with the trivial relation for the quantum-number densities, $\rho(x) + \rho_h(x) = 1$. To understand this, note that the distance between quantum-number vacancies is constant while the distance between 'vacant rapidities' is not constant and depends on the Bethe state.

Yang-Yang entropy

This description of a Bethe state in the thermodynamic limit in terms of ρ and ρ_h neglects the specific in-box configuration of quantum numbers. It can be viewed as a macroscopic description of an ensemble of Bethe states, whose microscopics are specified by their in-box distribution. At finite size the number of microstates, associated with an out-box distribution $\mathbf{n}$, is given by

$$\exp\left(S_{\mathrm{YY},\mathbf{n}}\right) = \prod_i \binom{\ell_i}{n_i} . \tag{2.41}$$

The number of in-box configurations grows exponentially with system size and $S_{\mathrm{YY},\mathbf{n}}$ is at leading order extensive in system size. In the thermodynamic limit, its extensive part only depends on the root densities ρ and ρ_h and is given by

$$\begin{aligned}
s_{\mathrm{YY}}[\rho] &= \lim\nolimits_{\mathrm{th}} \frac{1}{L} S_{\mathrm{YY},\mathbf{n}} &\text{(2.42a)}\\
&= \lim\nolimits_{\mathrm{th}} \frac{1}{L} \sum_i \left[n_i \log\left(\frac{\ell_i}{n_i} - 1\right) - \ell_i \log\left(1 - \frac{n_i}{\ell_i}\right)\right] &\text{(2.42b)}\\
&= \int_{-\infty}^{\infty} dx \, \left[\rho(x)\log\left(\frac{1}{\rho(x)} - 1\right) - \log\left(1-\rho(x)\right)\right] &\text{(2.42c)}\\
&= \int_{-\infty}^{\infty} d\lambda \left[\rho_t(\lambda)\log\rho_t(\lambda) - \rho(\lambda)\log\rho(\lambda) - \rho_h(\lambda)\log\rho_h(\lambda)\right] &\text{(2.42d)}\\
&=: \int_{-\infty}^{\infty} d\lambda \, s_{\mathrm{YY}}[\rho,\lambda] \, . &\text{(2.42e)}
\end{aligned}$$

To conclude, the root densities ρ and ρ_h describe an ensemble of Bethe states with Yang-Yang entropy [100] (hence the subscript)

$$S_{\mathrm{YY}}[\rho] = L \int_{-\infty}^{\infty} d\lambda \left[\rho_t(\lambda)\log\rho_t(\lambda) - \rho(\lambda)\log\rho(\lambda) - \rho_h(\lambda)\log\rho_h(\lambda)\right] . \tag{2.43}$$

Representative state

It is useful to introduce the notion of a representative state for a distribution ρ. It is defined as a Bethe state $|\boldsymbol{\lambda}\rangle$ for large finite system size N such that we have for any smooth (local) observable $\hat{\mathcal{O}}$

$$\langle\boldsymbol{\lambda}|\hat{\mathcal{O}}|\boldsymbol{\lambda}\rangle = \langle\rho|\hat{\mathcal{O}}|\rho\rangle\left[1 + O(N^{-1})\right] , \tag{2.44}$$

where the quantity $\langle\rho|\hat{\mathcal{O}}|\rho\rangle$ is a functional of the root density ρ. Given a density ρ, there is (approximately) a number $e^{S_{YY}[\rho]}$, exponentially growing with system size, of possible choices for a representative state [12]. In Eq. (2.44) and in the following we denote operators by the same symbol $\hat{\mathcal{O}}$ both for finite system size and in the thermodynamic limit. It is clear from the context which one is meant.

2.1.7 Excitations

In the time-evolution of the quench action description particle-hole excitations on thermodynamic Bethe state will play a crucial role. To describe them, let us start with a finite-size Bethe state and make a distinction between regular rapidities and hole rapidities,

$$|\boldsymbol{\lambda}\rangle = \left|\{\lambda_j\}_{j=1}^{N-m} \cup \{\lambda_k^h\}_{k=1}^{m}\right\rangle , \tag{2.45}$$

where $m < N$ denotes the number of hole rapidities. The N rapidities obey the usual Bethe equations (2.19). Now consider a different state where the quantum numbers associated with hole rapidities $\{\lambda_j^h\}_{j=1}^m$ become unoccupied whereas previously unoccupied quantum numbers associated with particle rapidities $\{\lambda_j^p\}_{j=1}^m$ become occupied. We denote the particle-hole excitations by $\mathbf{e} = \{\lambda_j^h \to \lambda_j^p\}_{j=1}^m$, which despite the notation are to be understood in terms of replacing occupied quantum numbers. The excited Bethe state is denoted by

$$|\boldsymbol{\lambda}, \mathbf{e}\rangle = \left|\{\lambda_j\}_{j=1}^{N-m} \cup \{\lambda_k^h \to \lambda_k^p\}_{k=1}^{m}\right\rangle = \left|\{\tilde\lambda_j\}_{j=1}^{N-m} \cup \{\tilde\lambda_k^p\}_{k=1}^{m}\right\rangle = |\tilde{\boldsymbol{\lambda}}\rangle\,, \tag{2.46}$$

where the new rapidities $\tilde{\boldsymbol{\lambda}} = \{\tilde\lambda_j\}_{j=1}^{N-m} \cup \{\tilde\lambda_k^p\}_{k=1}^{m}$ again obey the usual Bethe equations.

In the thermodynamic limit with the number of particle-hole excitations subleading in system size, $\lim_{\text{th}} \frac{m}{N} = 0$, the shift regular rapidities is of order $1/N$ and is given by (using Eqs (2.19))

$$L(\tilde\lambda_j - \lambda_j)\left[1 + \frac{1}{L}\sum_{k=1}^{N-m} K(\lambda_j - \lambda_k)\right] \tag{2.47}$$

$$= \sum_{k=1}^{N-m} (\tilde\lambda_k - \lambda_k) K(\lambda_j - \lambda_k) - \sum_{k=1}^{m}\left[\theta\big(\lambda_j - \tilde\lambda_k^p\big) - \theta\big(\lambda_j - \tilde\lambda_k^h\big)\right] + O(N^{-1})\,.$$

These shifts are parametrized by the back-flow or shift function F, which is defined by [12]

$$F(\lambda_j) = -\frac{1}{2\pi}\lim_{\text{th}} L(\tilde\lambda_j - \lambda_j)\left[1 + \frac{1}{L}\sum_{k=1}^{N-m} K(\lambda_j - \lambda_k)\right] \tag{2.48}$$

and obeys the integral equation

$$2\pi F(\lambda) = \sum_{k=1}^{m}\left[\theta\left(\lambda - \tilde\lambda_k^p\right) - \theta\left(\lambda - \tilde\lambda_k^h\right)\right] + \int_{-\infty}^{\infty} d\mu\, \frac{\rho(\mu)}{\rho_t(\mu)} K(\lambda - \mu) F(\mu). \tag{2.49}$$

Due to linearity of the integral equation the total back flow is the sum of back-flow functions for the individual particle-hole pairs, each obeying its ows integral equation. The shifts of the regular rapidities are $\tilde\lambda_j - \lambda_j = -F(\lambda_j)/[L\rho_t(\lambda_j)] +$

$\mathcal{O}(N^{-2})$. The momentum of a Bethe state is extensive in system size, but the change in momentum due to particle-hole excitations is finite and given by

$$\delta P_{\mathbf{e}}[\rho] = \lim\nolimits_{\mathrm{th}} \left[P_{(\boldsymbol{\lambda},\mathbf{e})} - P_{\boldsymbol{\lambda}}\right] = \sum_{k=1}^{m} \left(\tilde{\lambda}_k^p - \tilde{\lambda}_k^h\right) - \int_{-\infty}^{\infty} d\mu\, \frac{\rho(\mu)}{\rho_t(\mu)} F(\mu)\,. \quad (2.50)$$

It is important to note that the momentum shift is independent of in-box configurations and therefore a functional of the root density ρ. Similarly, the energy of the Bethe state changes by

$$\delta\omega_{\mathbf{e}}[\rho] = \sum_{k=1}^{m} \left((\tilde{\lambda}_k^p)^2 - (\tilde{\lambda}_k^h)\right) - \int_{-\infty}^{\infty} d\mu\, \mu \frac{\rho(\mu)}{\rho_t(\mu)} F(\mu)\,. \quad (2.51)$$

The entropy of the thermodynamic Bethe state, which is also an extensive quantity, shifts by [114]

$$\delta S_{\mathrm{YY},\mathbf{e}}[\rho] = \int_{-\infty}^{\infty} d\mu\, s_{\mathrm{YY}}[\rho,\mu] \frac{\partial}{\partial\mu} \left(\frac{F(\mu)}{\rho_t(\mu)}\right)\,, \quad (2.52)$$

where s_{YY} is defined in Eq. (2.42e).

In our discussion of excitations we focused on particle-hole pairs of rapidities. The creation or annihilation of a denumerable set of single rapidities can be treated likewise.

2.2 Bethe Anatz for the spin-1/2 XXZ chain

The one-dimensional antiferromagnetic spin-1/2 XXZ chain is a model for 1D spins with nearest-neighbor interactions. Setting external magnetic fields to zero, it is described by the Hamiltonian

$$\hat{H} = \frac{J}{4} \sum_{j=1}^{N} \left[\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta(\sigma_j^z \sigma_{j+1}^z - 1)\right]\,, \quad (2.53)$$

where the Pauli matrices σ_j^α ($\alpha = x, y, z$) represent the spin-1/2 degrees of freedom at lattice sites $j = 1, 2, \ldots, N$. The spin operators $\hat{S}_j^\alpha = \frac{1}{2}\sigma_j^\alpha$ obey the usual commutation relations, $[\hat{S}_j^\alpha, \hat{S}_k^\beta] = i\delta_{j,k}\epsilon^{\alpha\beta\gamma}\hat{S}_j^\gamma$. We assume periodic boundary conditions $\hat{S}_{N+1}^\alpha = \hat{S}_1^\alpha$. The exchange coupling $J > 0$ sets the energy scale and $\Delta \in \mathbb{R}$ parametrizes the anisotropy of the nearest-neighbor spin-spin coupling. The ground state is antiferromagnetic if $\Delta > 0$ and we will restrict our analysis to this regime. Note that if $\Delta = 0$, called the XY model, a Jordan-Wigner transformation reduces the theory to free spinless fermions. The Ising limit is obtained by sending $\Delta \to \infty$.

In this thesis we mainly focus on the gapped antiferromagnetic regime $\Delta > 1$. In this regime the antiferromagnetism is in the z direction and the ground state has a discrete $\mathbb{Z}_2$ symmetry in the thermodynamic limit, hence the gap. Unless stated otherwise, we will be working in this regime. When $0 < \Delta < 1$ the ground-state spins are strongly antiferromagnetically correlated in the xy plane. The $U(1)$ rotational symmetry around the z axis leads to gapless excitations. At the isotropic point $\Delta = 1$ the total-spin operators obey a global $SU(2)$ symmetry.

The isotropic spin chain was first conceived by Heisenberg [82] and is called the Heisenberg spin chain or spin-1/2 XXX chain. The anistropic generalization was first given in [83].

2.2.1 Bethe Ansatz solution

The XXZ Hamiltonian can be diagonalized by Bethe Ansatz [10, 84]. A derivation is analogous to the coordinate Bethe Ansatz for the Lieb-Liniger model and again hinges on the nondiffractiveness of scattering processes (see Section 2.1). Here, only the results of the coordinate Bethe Ansatz are stated. We choose the ferromagnetic state $|\uparrow\uparrow\ldots\uparrow\rangle = |\uparrow\rangle^{\otimes N}$ with all spins up as a reference state and construct interacting spin waves as excitations on this state. A state with M down spins falls in the magnetization sector $\langle\sigma^z_{\text{tot}}\rangle/2 = N/2 - M$ and is completely characterized by a set of complex quasimomenta $\boldsymbol{\lambda} = \{\lambda_j\}_{j=1}^M$, which are called rapidities. It is given by

$$|\boldsymbol{\lambda}\rangle = \sum_{\boldsymbol{x}} \psi_M(\boldsymbol{x}|\boldsymbol{\lambda})\ \sigma^-_{x_1}\ldots\sigma^-_{x_M}|\uparrow\uparrow\ldots\uparrow\rangle\ , \tag{2.54a}$$

where the positions of the down spins are denoted by the coordinates $\boldsymbol{x} = \{x_j\}_{j=1}^M \subset \{1,\ldots,N\}$, and we assume $x_j < x_k$ for $j < k$. The explicit wave function in coordinate space takes a Bethe Ansatz form,

$$\psi_M(\boldsymbol{x}|\boldsymbol{\lambda}) = \sum_{Q\in S_M} (-1)^{[Q]} \exp\left\{ -i\sum_{j=1}^M x_j\, p(\lambda_{Q_j}) - \frac{i}{2}\sum_{\substack{j,k=1\\k>j}}^M \theta_2(\lambda_{Q_k} - \lambda_{Q_j}) \right\} . \tag{2.54b}$$

The sum runs over the set of all permutations of integers $1,\ldots,M$, denoted by S_M, and $(-1)^{[Q]}$ is the parity of the permutation $Q \in S_M$. The total momentum of the state (2.54) is given by

$$P_{\boldsymbol{\lambda}} = \sum_{j=1}^M p(\lambda_j)\ , \quad \text{where} \quad p(\lambda) = -i\log\left[\frac{\sin(\lambda + \frac{i\eta}{2})}{\sin(\lambda - \frac{i\eta}{2})}\right] \tag{2.55}$$

is the momentum associated with a rapidity λ. The parameter $\eta > 0$ is determined by the anisotropy $\Delta = \cosh(\eta) > 1$ (the limit $\eta \to 0$ is considered in Section 5.8). Throughout the paper we choose the branch $-\pi/2 \le \mathrm{Re}(\lambda) < \pi/2$. Furthermore, θ_2 is the scattering phase shift defined by

$$\theta_2(\lambda) = 2\arctan\left(\frac{\tan(\lambda)}{\tanh(\eta)}\right)\ . \tag{2.56}$$

The state (2.54) is called Bethe state if the rapidities $\boldsymbol{\lambda}$ satisfy the Bethe equations,

$$\left[\frac{\sin(\lambda_j + \frac{i\eta}{2})}{\sin(\lambda_j - \frac{i\eta}{2})}\right]^N = -\prod_{k=1}^{M} \frac{\sin(\lambda_j - \lambda_k + i\eta)}{\sin(\lambda_j - \lambda_k - i\eta)} , \tag{2.57}$$

for $j = 1, \dots, M$. Rapidities obeying these equations are called Bethe roots. A Bethe state is an eigenstate of the XXZ Hamiltonian (2.53) with energy

$$\omega_{\boldsymbol{\lambda}} = J \sum_{j=1}^{M} \{\cos[p(\lambda_j)] - \cosh(\eta)\} = -J \sum_{j=1}^{M} \frac{\sinh^2(\eta)}{\cosh(\eta) - \cos(2\lambda_j)} . \tag{2.58}$$

Bethe states are orthogonal and their norm is given by $\| \, |\boldsymbol{\lambda}\rangle \, \| = \sqrt{\langle \boldsymbol{\lambda} | \boldsymbol{\lambda} \rangle}$ with [115, 102]

$$\langle \boldsymbol{\lambda} | \boldsymbol{\lambda} \rangle = \sinh^M(\eta) \prod_{\substack{j,k=1 \\ j \neq k}}^{M} \frac{\sin(\lambda_j - \lambda_k + i\eta)}{\sin(\lambda_j - \lambda_k)} \det\nolimits_M(G) , \tag{2.59a}$$

$$G_{jk} = \delta_{jk} \left(N K_{\eta/2}(\lambda_j) - \sum_{l=1}^{M} K_\eta(\lambda_j - \lambda_l) \right) + K_\eta(\lambda_j - \lambda_k) , \tag{2.59b}$$

where $K_\eta(\lambda) = \sinh(2\eta)/[\sin(\lambda + i\eta)\sin(\lambda - i\eta)]$ is the derivative of the scattering phase shift θ_2.

The spin-1/2 XXX chain

The isotropic case $\Delta = 1$ can be obtained from the XXZ case by taking the limit $\eta \to 0$. One must scale all rapidities by η, $\lambda \to \eta\lambda$, and subsequently take the XXX limit $\eta \to 0$. All the above equations then lead to their XXX equivalents. For more details, see Section 5.8. It should be noted that the interval of the real part of the rapidities is infinite now, $-\infty \leq \mathrm{Re}(\lambda) \leq \infty$. Solving the XXX Bethe equations for finite rapidities therefore does not give you all states in the Hilbert space. Instead, it only gives you the heighest weight states in terms of the global $SU(2)$ symmetry for the isotropic spin chain, i.e. states for which $S^z_{\mathrm{tot}} = S_{\mathrm{tot}}$. More on this can be found in Appendix D.

2.2.2 String hypothesis

Contrary to the Lieb-Liniger model in the repulsive regime, Bethe roots are generically complex numbers now. For large system size N, the question of how the rapidities organize themselves is addressed by the string hypothesis [10, 116]. Rapidities of a Bethe state get grouped in strings,

$$\lambda_\alpha^{n,a} = \lambda_\alpha^n + \tfrac{i\eta}{2}(n + 1 - 2a) + i\delta_\alpha^{n,a} , \tag{2.60}$$

for $a = 1, \ldots, n$, where n is the length of the string and the deviations $\delta_\alpha^{n,a}$ vanish (typically) exponentially in system size. A more detailed discussion can be found in Section 5.8.8.

In the gapped regime ($\Delta > 1$) the string centers λ_α^n are real and lie in the interval $[-\pi/2, \pi/2)$. The physical interpretation of such an n-string is a bound state of n magnons, which becomes in the Ising limit $\Delta \to \infty$ a block of n adjacent down spins. Let M_n be the total number of n-strings of a Bethe state, then $\alpha = 1, 2, \ldots, M_n$ labels the n-strings and $\sum_{n=1}^{\infty} n\, M_n = M$. It is not always true that the full Hilbert is reproduced by states obeying the string hypothesis. Already for two down spins, $M = 2$, there are Bethe states that are not string states [117, 118]. However, in Ref. [96] it is argued that the string hypothesis is valid if temperature and/or magnetization are nonzero. Since our analysis will only involve Bethe states in the thermodynamic limit that are far from the ground state, we will assume throughout the thesis that the string hypothesis reproduces the full Hilbert space.

Under the string hypothesis and for vanishing deviations a state is solely characterized by its string centers λ_α^n. Neglecting the string deviations, the logarithmic form of the Bethe Eqs (2.57) can be recast into the Bethe-Gaudin-Takahashi (BGT) equations for string centers [116, 119, 11],

$$\theta_n\left(\lambda_\alpha^n\right) = \frac{2\pi}{N} I_\alpha^n + \frac{1}{N} \sum_{\substack{(m,\beta)\neq \\ (n,\alpha)}} \theta_{nm}\left(\lambda_\alpha^n - \lambda_\beta^m\right) \tag{2.61a}$$

for $n \geq 1$ and $\alpha = 1, 2, \ldots, M_n$. Here,

$$\theta_{nm}(\lambda) = (1-\delta_{nm})\theta_{|n-m|}(\lambda) + 2\theta_{|n-m|+2}(\lambda) + \ldots + 2\theta_{n+m-2}(\lambda) + \theta_{n+m}(\lambda) \tag{2.61b}$$

and

$$\theta_n(\lambda) = 2\arctan\left(\frac{\tan(\lambda)}{\tanh(\frac{n\eta}{2})}\right) . \tag{2.61c}$$

Note that the function θ_2 is the scattering phase shift (2.56). The quantum numbers I_α^n are integers (half-odd integers) if $N - M_n$ is odd (even).

As an example, in terms of string rapidities and quantum numbers the energy and momentum are given by

$$\omega_{\boldsymbol{\lambda}} = -\pi J \sinh(\eta) \sum_{n=1}^{\infty} \sum_{\alpha=1}^{M_n} a_n(\lambda_\alpha^n) , \qquad P_{\boldsymbol{\lambda}} = \frac{2\pi}{N} \sum_{n=1}^{\infty} \sum_{\alpha=1}^{M_n} I_\alpha^n , \tag{2.62}$$

where a_n will be defined in Eq. (2.64c).

2.2.3 Observables and measurements

In Section 1 we explained that neutron scattering can be used to probe effective 1D magnetic degrees of freedom in specific 3D crystals. Scattering neutrons exchange energy and momentum with the 1D magnet, which can be measured in an experimental setting. The differential cross section is given by [120]

$$\frac{d^2\sigma}{d\Omega\, d\omega} \sim \frac{k'}{k} \sum_{\alpha,\beta=x,y,z} \left(\delta_{\alpha,\beta} - \frac{k_\alpha\, k_\beta}{|k|^2}\right) S^{\alpha\beta}(k-k', E-E')\,, \tag{2.63}$$

where k is the incoming momentum, E the energy of the incoming neutron and the primed quantities are the outcoming momentum and energy. $S^{\alpha\beta}$ is called the dynamical structure factor and is defined as the Fourier transform of the dynamical spin-spin correlators $\langle \hat{S}^\alpha_j(t)\hat{S}^\beta_{j'}(0)\rangle$.

2.2.4 The thermodynamic limit

By thermodynamic limit we mean the limit of infinite system size, $N \to \infty$, while keeping the fraction of down spins M/N fixed. We will denote it by $\lim_{\mathrm{th}}$. In this limit Bethe states are characterized by distributions of string centers. The density of n-strings is given by the function ρ_n, such that $N\rho_n(\lambda)\,\mathrm{d}\lambda$ is the number of n-strings in the interval $[\lambda, \lambda + \mathrm{d}\lambda]$.

In the thermodynamic limit, the BGT Eqs (2.61) become a set of integral equations for the density distributions [116, 119, 11],

$$\rho_{n,t}(\lambda) \;=\; a_n(\lambda) - \sum_{m=1}^{\infty} (a_{nm} * \rho_m)(\lambda) \tag{2.64a}$$

for $n \geq 1$, where $\rho_{n,t}(\lambda) = \rho_n(\lambda) + \rho_{n,h}(\lambda)$ and $\rho_{n,h}$ is the hole density of n-strings. Further,

$$a_{nm}(\lambda) = (1-\delta_{nm})a_{|n-m|}(\lambda) + 2a_{|n-m|+2}(\lambda) + \ldots + 2a_{n+m-2}(\lambda) + a_{n+m}(\lambda) \tag{2.64b}$$

with

$$a_n(\lambda) = \frac{1}{2\pi}\frac{\mathrm{d}}{\mathrm{d}\lambda}\theta_n(\lambda) = \frac{1}{\pi}\frac{\sinh(n\eta)}{\cosh(n\eta) - \cos(2\lambda)}\,. \tag{2.64c}$$

The convolution is defined by

$$(f * g)\,(\lambda) = \int_{-\pi/2}^{\pi/2} \mathrm{d}\mu\, f(\lambda-\mu)\, g(\mu)\,. \tag{2.65}$$

For both numerical and analytical evaluation of the integral equations, it is often convenient to get rid of the infinite sum over string types and to work with the "partially decoupled" set of equations. The partially decoupled form of the thermodynamic BGT equations can be derived [13],

$$\rho_n(1+\eta_n) = s * (\eta_{n-1}\rho_{n-1} + \eta_{n+1}\rho_{n+1}) \tag{2.66a}$$

for $n \geq 1$, where the λ-dependence is left implicit and we use the conventions $\eta_0(\lambda) = 1$ and $\rho_0(\lambda) = \delta(\lambda)$. The kernel in Eqs (2.66a) reads

$$s(\lambda) = \frac{1}{2\pi} \sum_{k\in\mathbb{Z}} \frac{e^{-2ik\lambda}}{\cosh(k\eta)} \,. \tag{2.66b}$$

The set of positive, smooth functions $\boldsymbol{\rho} = \{\rho_n\}_{n=1}^{\infty}$ represents an ensemble of states with Yang-Yang entropy

$$S_{\rm YY}[\boldsymbol{\rho}] = N\sum_{n=1}^{\infty}\int_{-\pi/2}^{\pi/2} \mathrm{d}\lambda\, [\rho_{n,t}(\lambda)\log\rho_{n,t}(\lambda) - \rho_n(\lambda)\log\rho_n(\lambda) - \rho_{n,h}(\lambda)\log\rho_{n,h}(\lambda)]. \tag{2.67}$$

2.3 The algebraic Bethe Ansatz

The algebraic Bethe Ansatz, first developed in Refs [121, 122], is a very powerful and general method to handle many aspects of quantum integrable models. In essence, it is a second-quantized form of the coordinate Bethe Ansatz. There exists vast amount of excellent introductions to this method (see, for example, Refs [12, 16, 93, 36, 94]). We therefore take the freedom to quickly discuss its main points and to state the results that are important in this thesis, in particular the eigenvalues of local conserved charges.

Without reference to specific models a scattering matrix (scattering between an auxiliary and a physical degree of freedom, the R-matrix) is defined and nondiffractiveness is imposed by means of the Yang-Baxter equation. In a way, the latter is the generalization of the conditions in Eqs (2.9) and (2.12) on the scattering amplitudes. After some algebra, a transfer matrix $\hat{\tau}(\lambda)$ is constructed. This operator acts on the full physical Hilbert space and $\lambda \in \mathbb{C}$ is the spectral parameter, which can be viewed as a remnant of the auxiliary space. The crucial property of the transfer matrix is that it commutes for any pair of spectral parameters λ and λ', $[\hat{\tau}(\lambda), \hat{\tau}(\lambda')] = 0$.

For certain choices of the R-matrix the operator $\frac{d}{d\lambda}\log[\hat{\tau}(\lambda)]\big|_{\lambda=\xi}$ is proportional to the Hamiltonian of a well-known integrable model, where ξ is a model-dependent complex number. For example, the transfer matrix associated to the spin-1/2 XXZ chain is given by

$$\hat{\tau}(\lambda) = \mathrm{Tr}_V\left[\hat{L}_N(\lambda) \otimes_{\mathcal{H}} \hat{L}_{N-1}(\lambda) \otimes_{\mathcal{H}} \ldots \otimes_{\mathcal{H}} \hat{L}_1(\lambda)\right] , \tag{2.68a}$$

where $\hat{L}_j(\lambda)$ is the Lax operator for lattice site j. This is an operator-valued (2×2)-matrix acting on an auxiliary space $V = \mathbb{C}^2$ and it is given by

$$\hat{L}_j(\lambda) = \frac{1}{\sin(\lambda + \frac{i\eta}{2})} \begin{pmatrix} \sin\left(\lambda + \frac{i\eta}{2}\sigma_j^z\right) & \sin(i\eta)\sigma_j^- \\ \sin(i\eta)\sigma_j^+ & \sin\left(\lambda - \frac{i\eta}{2}\sigma_j^z\right) \end{pmatrix} . \tag{2.68b}$$

Note that the trace is over auxiliary space only, whereas the $\otimes_{\mathcal{H}}$ are tensor products with respect to Hilbert space and matrix multiplication in auxiliary space. The XXZ Hamiltonian is obtained for $\xi = \frac{i\eta}{2}$.

Any operator constructed from the transfer matrix is automatically a conserved quantity of the model at hand. Although most constructions lead to very nonlocal charges, the charges

$$\hat{Q}_{m+1} \sim \frac{\partial^m}{\partial\lambda^m} \log[\hat{\tau}(\lambda)]\bigg|_{\lambda=\xi} , \qquad \text{for} \quad m = 0, 1, 2, \ldots , \tag{2.69}$$

are in fact local charges. In the case of spin chains, this means that each term in the operator has nontrivial support on a finite number of adjacent spins. For the Lieb-Liniger model local operators in second-quantized form can be written as single integrals over a finite number of field operators with a finite number of derivatives acting on them. Locality of the charges is proven using so-called trace identities for the logarithm of a product of Lax operators. As we will see in Chapter 3 the local charges play an important role in equilibration after a quantum quench.

A Bethe basis in second-quantized form is then constructed in terms of raising and lowering operators whose commutation relations with the transfer matrix are known. Demanding that the states are eigenstates of the transfer matrix (tantamount to diagonalizing the Hamiltionian) leads to the Bethe equations.

Important results that were derived from the algebraic Bethe Ansatz are a determinant formula for the overlap between a Bethe state and a Bethe wave function whose rapidities do not obey Bethe equations (Slavnov's theorem, see Ref. [110]) and the Gaudin norms of Bethe states [115, 11, 102]. Also determinant expressions for form factors of local operators can be derived, using the quantum inverse scattering method and Slavnov's theorem (see Ref. [12] and references therein).

2.3.1 Local conserved charges for the spin-1/2 XXZ chain

By construction, the transfer matrix $t(\lambda)$ is diagonal on the basis of Bethe states. On a state $|\boldsymbol{\lambda}\rangle$ is has eigenvalue

$$\tau(\lambda) = \prod_{k=1}^{M} \frac{\sin(\lambda - \lambda_k - i\eta)}{\sin(\lambda - \lambda_k)} + \left[\frac{\sin(\lambda - \frac{i\eta}{2})}{\sin(\lambda + \frac{i\eta}{2})}\right]^N \prod_{k=1}^{M} \frac{\sin(\lambda - \lambda_k + i\eta)}{\sin(\lambda - \lambda_k)} . \tag{2.70}$$

The conserved charges are defined via the coefficients of the operator expansion of the logarithm of the transfer matrix around the point $\lambda = i\eta/2$,

$$\hat{Q}_{m+1} = i\frac{\sinh^m(\eta)}{2^m}\frac{\partial^m}{\partial\lambda^m}\log[\hat{\tau}(\lambda)]\bigg|_{\lambda=i\eta/2}, \quad m \geq 0\,. \tag{2.71}$$

They commute by construction. Note that $\hat{P} = -\hat{Q}_1$ and $\hat{H} = J\hat{Q}_2$. The first nontrivial conserved charge, $\hat{Q}_3$, is proportional to the energy current [123]. The range of the charge $\hat{Q}_m$ is m (where we assume $m < N$). This means that each element $\hat{Q}_j^{(m)}$ in the decomposition $\hat{Q}_m = \sum_{j=1}^N \hat{Q}_j^{(m)}$ acts only nontrivially on a block of m adjacent sites.

In the thermodynamic limit the charges $\{\hat{Q}_m\}_{m=1}^\infty$ form an infinite set of local conserved charges. Acting on a representative state $|\boldsymbol{\lambda}\rangle$, the eigenvalue of charge $\hat{Q}_{m+1}$ is given by

$$\lim_{\text{th}}\langle\boldsymbol{\lambda}|\frac{\hat{Q}_{m+1}}{N}|\boldsymbol{\lambda}\rangle = \sum_{n=1}^{\infty}\int_{-\pi/2}^{\pi/2}\mathrm{d}\lambda\,\rho_n(\lambda)\,c_{m+1}^{(n)}(\lambda)\,, \quad m \geq 0\,, \tag{2.72a}$$

where

$$c_{m+1}^{(n)}(\lambda) = i(-1)^m\frac{\sinh^m(\eta)}{2^m}\frac{\partial^m}{\partial\lambda^m}\log\left[\frac{\sin(\lambda + \frac{i\eta}{2}n)}{\sin(\lambda - \frac{i\eta}{2}n)}\right]. \tag{2.72b}$$

To see this, note that an n-string (2.60) with string center λ_α^n and with neglected deviations $\delta_\alpha^{n,a}$ contributes a factor

$$\frac{\sin[\lambda - \lambda_\alpha^n - \frac{i\eta}{2}(n+1)]}{\sin[\lambda - \lambda_\alpha^n + \frac{i\eta}{2}(n-1)]} \tag{2.73}$$

to the first term of the transfer-matrix eigenvalue (2.70). As long as $m < N$, the second term of Eq. (2.70) does not contribute to the expectation value of charge Q_{m+1}. In the thermodynamic limit this is the case for any finite m.

2.3.2 Local conserved charges for the Lieb-Liniger model

For the Lieb-Liniger model similar results are known. Despite the simplicity of the form of the eigenvalues of the local conserved charges in terms of rapidities, one can construct them within the formalism of the algebraic Bethe Ansatz as well. The eigenvalue of the transfer matrix of the Lieb-Liniger model on a Bethe state $|\boldsymbol{\lambda}\rangle$ is

$$\tau(\mu) = \exp\left(-\frac{i\mu L}{2}\right)\prod_{j=1}^{N}\frac{\mu - \lambda_j + ic}{\mu - \lambda_j} + \exp\left(\frac{i\mu L}{2}\right)\prod_{j=1}^{N}\frac{\mu - \lambda_j - ic}{\mu - \lambda_j}\,. \tag{2.74}$$

The local conserved charges are defined as an expansion around the point $\mu = i\infty$:

$$\log\left[e^{i\mu L/2}\,\tau(\mu,\boldsymbol{\lambda})\right] \underset{\mu\to i\infty}{=} \sum_{j=1}^{N}\log\left[1+\frac{ic}{\mu-\lambda_j}\right] \tag{2.75a}$$

$$= \frac{ic}{\mu}\sum_{m=0}^{\infty}\frac{1}{\mu^m}\left[\sum_{j=1}^{N}\lambda_j^m+\sum_{k=0}^{m-1}\left(a_{m,k}\sum_{j=1}^{N}\lambda_j^k\right)\right], \tag{2.75b}$$

where the polynomial coefficients $a_{m,k}$ can easily be determined [12]. They are the expansion coefficients of the logarithm of the transfer matrix:

$$\log\left[e^{i\mu L/2}\,\hat{\tau}(\mu)\right] \underset{\mu\to i\infty}{=} \frac{ic}{\mu}\sum_{m=0}^{\infty}\frac{1}{\mu^m}\left[\hat{Q}_m+\sum_{k=0}^{m-1}a_{m,k}\,\hat{Q}_k\right]. \tag{2.76}$$

From this definition one could derive expressions for the charges in first or second quantized form. This is done in [95] up to $\hat{Q}_4$. For example,

$$\hat{Q}_3 = i\int_0^L dx\left[\hat{\Psi}^\dagger(x)\,\partial_x^3\hat{\Psi}(x) - 3c\hat{\Psi}^\dagger(x)\hat{\Psi}^\dagger(x)\hat{\Psi}(x)\,\partial_x\hat{\Psi}(x)\right]. \tag{2.77}$$

More important is that the charges are defined such that on a Bethe state $|\boldsymbol{\lambda}\rangle$ their eigenvalues are

$$\hat{Q}_m|\boldsymbol{\lambda}\rangle = \left[\sum_{j=1}^{N}(\lambda_j)^m\right]|\boldsymbol{\lambda}\rangle\,, \tag{2.78}$$

which is easily extended to the thermodynamic limit. Note that $\hat{Q}_0$ is the particle number operator $\hat{N}$, $\hat{Q}_1 = \hat{P}$ and $\hat{Q}_2 = \hat{H}$.