

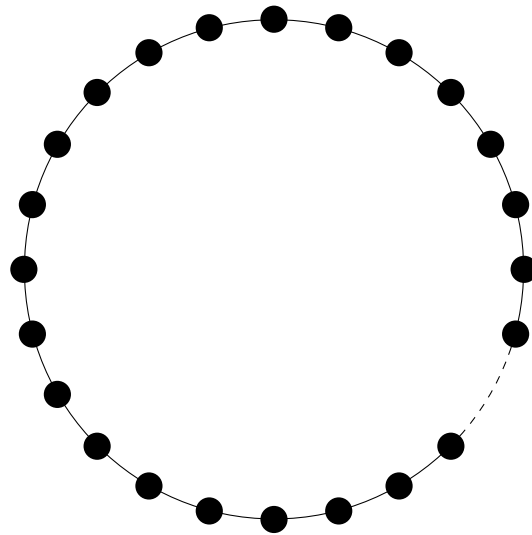
MSC PHYSICS AND ASTRONOMY  
THEORETICAL PHYSICS  
MASTER'S THESIS

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# Integrability, Bethe Ansatz and open quantum systems

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MATTHIJS WANROOIJ



First Examiner & Supervisor: Dr. Vladimir Gritsev  
Second Examiner: Prof. Dr. Jean-Sébastien Caux  
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Title: Integrability, Bethe Ansatz and open quantum systems  
Author: Matthijs (M.I.O.) Wanrooij, [mw112345@outlook.com](mailto:mw112345@outlook.com), 15250059  
Supervisor: Dr. V. Gritsev  
Second Examiner: Prof. Dr. J.-S. Caux  
Examination date: August 20, 2025

Institute of Physics  
University of Amsterdam  
Science Park 904, 1098XH Amsterdam  
<https://iop.uva.nl/>

# Abstract

Quantum integrable systems are characterized by a high degree of symmetry and a large number of conserved quantities. Frameworks such as Bethe Ansatz have proven extremely successful in solving quantum integrable systems, but the interpretation of quantum integrability has been plagued by inconsistencies and poor formulations. We discuss integrability in both the classical and quantum sense, and place its meaning in the context of chaos theory and ergodicity. We also study the core principles of algebraic Bethe Ansatz and its relation to Richardson-Gaudin models. The main results of this thesis are related to systems that are both quantum integrable and open. Open quantum systems have one or more dissipative channels that take the system out of isolation and enforce the exchange of information with an external environment (breaking unitary time evolution within the system of interest). Their dynamics is governed by the Lindblad superoperator, which generates a completely positive and trace-preserving (CPTP) map that evolves density matrices into density matrices. The Lieb-Liniger model for bosons with hard-core interactions in one dimension is a quantum integrable system that is tractable in the thermodynamic limit. We discuss the Lieb-Liniger model and perform a numerical study of the Lindbladian spectrum for a Lieb-Liniger system with dissipation. We also present efficient numerical methods for extracting the Bethe roots from a certain class of Richardson-Gaudin models with dissipation, such as the central spin model with a complex-valued coupling.

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# 1. Introduction

Integrability theory is one of those disciplines that seems to have benefited greatly from continuous and ongoing cross-pollination between physics and mathematics. Today, integrability can be found at the intersection of physics and pure mathematics, with applications as diverse as the triangulation of random surfaces, random matrices, vertex models, Lie algebraic structures and symmetric polynomials [34, 130, 85]. Quantum integrability has been at the heart of the quantum inverse scattering method, which has solved many systems in condensed matter theory, and has led to important advancements in mathematics, such as the formulation of quantum groups.

Despite its ubiquity, it is easy for most physicists to avoid learning about (quantum) integrability and to pass it off as pedantic, ‘something for mathematicians’, an insignificant detail or even a buzzword that is used to invigorate the abstract of a lousy paper. The following quote from Cristoph Sträter’s thesis [113] is funny, because the underlying statement is at least partially true:

Commonly among physicists, quantum integrability is regarded as highly involved mathematics that is neither *possible* nor *useful* to understand.

Reassuringly, he then goes on to say:

Understanding the basic concepts that are needed to solve many integrable systems in condensed matter physics, however, is certainly feasible for every physicist without a background on Hopf algebras or quantum groups.

In this thesis, we will take the latter approach, and look at integrability through the lens of condensed matter theory. It will be our aim to place integrability in its proper context, which we will do in Section 2, and to discuss examples of integrable systems and methods to solve them. The quantum integrable system featuring most prominently in this thesis is the Lieb-Liniger model for bosons in one dimension with Dirac delta interactions. Its description and solution methods will take up the bulk of Section 3, while Section 4 is devoted to more general and abstract approaches for solving a variety of quantum integrable systems: the algebraic Bethe Ansatz and Richardson-Gaudin frameworks.

We will also be concerned with quantum systems that are both integrable and open, in the sense that we will sacrifice Hermitian Hamiltonians and unitary time-evolution (in the system of interest) in favour of a description that allows for the effects of dissipation or gain. In the second part of Section 3, the Lieb-Liniger model is turned into an open quantum system by adding an imaginary part to its coupling, and we investigate the spectrum of the corresponding Lindbladian. Finally, Section 5 will introduce the so-called BA/ODE-correspondence and elaborate on a method for efficient computation of Bethe roots in some Richardson-Gaudin type systems with dissipation.

Regarding the form and style of the thesis, I feel like I owe the reader a small explanation. I wanted my thesis to be as self-contained as possible. Among other things, this philosophy has resulted in a very explicit writing style, an extensive appendix and the liberal use of examples and reminders (indicated by coloured boxes) that aim to refresh preliminary concepts or reinforce theoretical aspects. For some, this style of writing will be dull; but when I have to write up an extensive report, my aim is always to be in a position where I am able to recover what I understood quickly and effortlessly – also in 10 years from now, when the familiarity and aptitude for the subject that I possess at this moment will long have waned. A second consideration that led me to write my thesis in a pedagogical way is the paucity of entry-level sources for learning in particular the basics of Bethe Ansatz (if you are not a mathematician), Richardson-Gaudin models and quantum integrability. In some cases (especially regarding Section 2), availability of source material is not the primary concern, but rather the fact that various perspectives are not combined in the same way as we intend to do. A comprehensive writing style will then have the added advantage of being able to deliver a smooth introduction to other physics students with no background in the field. To whomever may read the thesis, I sincerely hope that you will find (parts of it) enlightening and a joyful read.

## 2. Integrability, chaos and ergodicity (and why we care)

This chapter is the result of a desire to understand the interplay between three disciplines: integrability, ergodicity and chaos. On topics such as these, most physicists will have, to various extents, a decent amount of intuition, which is maybe why a more comprehensive overview, with a focus on the interfaces, seems hard to come by. In papers where concepts of a related nature arise, they are frequently packaged in terms of keywords such as thermalization, mixing, scrambling and (dis)order, without precisely specifying the underlying meaning. Regrettably, while writing this chapter, I became increasingly aware that the topic at hand could easily be the subject of an entire thesis. This is the chapter that I started first and finished last, even though I can hardly call it finished, if it can ever be finished in the first place. As a consequence, I had to sacrifice depth in order to be more comprehensive, and I do not doubt that I might have overlooked things or that I might even be straight-out inaccurate on a handful of points. Nevertheless, I hope to raise awareness of some big ideas through a combination of heuristics and examples, and to bring on the right questions for anyone interested in the subject. In good faith, we start by discussing classical notions, before transitioning to quantum mechanical systems.

### 2.1. What does integrability tell us?

Why do we care at all about integrability? Integrable systems are systems with a high amount of symmetry. This often – but not always – makes them exactly solvable. And sometimes – but again not always – the exact solutions may even come in the form of closed-form expressions. As might be expected, the classical and quantum notions of integrability are completely different. The definition of classical integrability is very well agreed upon, whereas there is limited consensus on the meaning of quantum integrability. In this chapter, I will give a high level overview of both notions, explain the need for a different treatment, and elaborate on the characteristics they *do* have in common.

We mentioned in passing that integrability is connected with the important topic of solvability. Naturally, we will explore this statement in more depth throughout the thesis. However, anyone new to the field may rightfully ask if there are more concrete implications of integrability, and in particular, if they carry physical significance. The answer, reassuringly, is yes. Associated to integrable systems are, among others, the following statements [126]:

- The conserved quantities present in integrable systems prevent an isolated integrable system from relaxing to a thermal state.
- Empirical laws such as the Kubo law in linear response theory and Fourier’s law in thermal conduction have to be modified or generalized to hold for integrable systems.
- It is conjectured and has been verified on multiple occasions that energy level spacings in integrable systems are Poisson distributed (Berry-Tabor conjecture [81]), while energy levels in non-integrable systems generally follow a Wigner-Dyson distribution.

### 2.2. Liouville integrability

#### 2.2.1. Liouville-Arnold theorem

The **Liouville-Arnold theorem** is the cornerstone of classical integrability theory. It relates integrability to the presence of sufficiently many constants of motion. In this subsection, we work towards the statement of the theorem, following closely lecture notes of Dunajski [40] and Ott [92]. The proof has been relegated to Appendix A. Let us first recall some preliminary notions.

**Hamiltonian formalism** We work in a  $2n$ -dimensional phase space  $M$  to describe the motion of a system with  $n$  degrees of freedom. We define local coordinates  $(p_i, q_j)$ ,  $j = 1, 2, \dots, n$ . Dynamical variables are functions  $f : M \times \mathbb{R} \rightarrow \mathbb{R}$  such that  $f = f(p, q, t)$ .

Let  $f, g : M \times \mathbb{R} \rightarrow \mathbb{R}$ . We define the Poisson bracket of  $f, g$  to be a function

$$\{f, g\} = \sum_{k=1}^n \left[ \frac{\partial f}{\partial q_k} \frac{\partial g}{\partial p_k} - \frac{\partial f}{\partial p_k} \frac{\partial g}{\partial q_k} \right]. \quad (1)$$

Note in particular the following properties:

$$\begin{aligned} \{f, g\} &= -\{g, f\}, & (\text{anti-symmetry}) \\ \{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} &= 0. & (\text{Jacobi identity}) \end{aligned}$$

The coordinate functions<sup>1</sup>  $(p_j, q_k)$  satisfy the canonical commutation relations

$$\{p_j, p_k\} = 0, \quad \{q_j, q_k\} = 0, \quad \{q_j, p_k\} = \delta_{jk}.$$

Given a Hamiltonian  $H = H(p, q, t)$ , the on-shell dynamics is determined by the condition (we use the chain rule)

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \sum_{k=1}^n \left[ \frac{\partial f}{\partial q_k} \dot{q}_k + \frac{\partial f}{\partial p_k} \dot{p}_k \right] = \frac{\partial f}{\partial t} + \sum_{k=1}^n \left[ \frac{\partial f}{\partial q_k} \frac{\partial H}{\partial p_k} - \frac{\partial f}{\partial p_k} \frac{\partial H}{\partial q_k} \right] = \frac{\partial f}{\partial t} + \{f, H\}, \quad (2)$$

for any  $f = f(p, q, t)$ . Setting  $f = p_j$  or  $f = q_j$  yields Hamilton's equations of motion:

$$\boxed{\dot{p}_j = -\frac{\partial H}{\partial q_j}, \quad \dot{q}_j = \frac{\partial H}{\partial p_j}.} \quad (3)$$

Example

Setting  $f = p_j$  yields

$$\frac{dp_j}{dt} = \frac{\partial p_j}{\partial t} + \sum_{k=1}^n \left[ \frac{\partial p_j}{\partial q_k} \frac{\partial H}{\partial p_k} - \frac{\partial p_j}{\partial p_k} \frac{\partial H}{\partial q_k} \right] = -\sum_{k=1}^n \delta_{jk} \frac{\partial H}{\partial q_k} = -\frac{\partial H}{\partial q_j}.$$

Note that Hamiltonian systems are extremely restricted. The dynamics are completely specified by a single scalar function of  $p, q$  and possibly  $t$  (the Hamiltonian), while for a general dynamical system of the form

$$\frac{d\mathbf{x}}{dt} = \mathbf{F}(\mathbf{x}, t),$$

we need to specify all the components of the vector function  $\mathbf{F}(\mathbf{x}, t)$ .

The restricted nature of Hamiltonian systems finds an expression in the form of **Liouville's theorem** (not to be confused with the Liouville-Arnold theorem, that we are working towards). We define the *phase space distribution function*  $\rho(p, q)$  as the function that determines the probability that the system occupies the infinitesimal phase space volume  $d^n q d^n p$ . The Liouville equation governs the evolution of  $\rho(q, p; t)$  over time:

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \sum_{i=1}^n \left( \frac{\partial \rho}{\partial q_i} \dot{q}_i + \frac{\partial \rho}{\partial p_i} \dot{p}_i \right) = \frac{\partial \rho}{\partial t} + \{\rho, H\}. \quad (4)$$

Liouville's theorem now is the following:

**Theorem 2.1 (Liouville)** *For Hamiltonian systems, the distribution function  $\rho(p, q)$  is constant along any trajectory in phase space, that is:*

$$\frac{d\rho}{dt} = 0,$$

<sup>1</sup>Recall: A function is a map  $f : M \rightarrow \mathbb{R}$ , i.e. a map that assigns a real number to each point on the manifold.



along any such trajectory.

Note: The symplectic condition

A more fundamental principle than Liouville's theorem lies hidden in the symplectic structure of Hamilton's equations. To be more precise, it can be shown that for three orbits an infinitesimal distance apart,  $(p_i(t), q_i(t))$ ,  $(p_i(t) + \delta p_i(t), q_i(t) + \delta q_i(t))$  and  $(p_i(t) + \delta p'_i(t), q_i(t) + \delta q'_i(t))$ , the *differential symplectic area* is conserved:

$$\frac{d}{dt} \sum_i (\delta p_i \delta q'_i - \delta q_i \delta p'_i) = 0. \quad (5)$$

For a system with one degree of freedom, the condition (5) is identical to Liouville's theorem. For systems with more degrees of freedom, they are not the same, but the symplectic condition can be shown to imply volume conservation. The quantity within parentheses in eq. (5) is the differential form of Poincaré's integral invariant.

As a consequence of Liouville's theorem, Hamiltonian systems don't have attractors, since the image of the set of points in phase space belonging to the 'volume of influence' of the attractor would contract to the attractor under the flow, and this is forbidden.<sup>2</sup>

## Constants of motion

**Definition 2.1** A function  $f = f(p_j, q_j, t)$  that satisfies  $\dot{f} = 0$  when eqs. (3) hold is known as a first integral (integral of motion) or a constant of motion. It is equivalent to say that  $f(p(t), q(t), t) = \text{constant}$  if  $p(t)$ ,  $q(t)$  are solutions of (3).

Note that eq. (2) tells us that a constant of motion satisfies

$$\dot{f} = \frac{\partial f}{\partial t} + \{f, H\} = 0, \quad (6)$$

on shell.

**Corollary** In systems without explicit time dependence, the Hamiltonian (the energy) is a constant of motion.

**Remark** Sometimes, integrals of motion are defined as a subset of the constants of motion, in the sense that they are functions of only the phase-space coordinates (position and velocity/momentum) that are constant along an orbit, whereas constants of motion may also depend on time (as long as the total function, with all its dependencies, is constant along the trajectory). We will not uphold such a distinction.

Note that any (functionally independent) first integral can be used to eliminate one equation of motion. This motivates the claim that eq. (3) will be solvable, provided it has sufficiently many constants of motion. Geometrically, each independent conserved quantity imposes one relation among the phase-space variables, thereby confining trajectories to a hypersurface that is the intersection of all constraints in phase space. More precisely, each constant of motion defines a hypersurface of dimension  $2n - 1$  that contains the solution, and two such hypersurfaces intersect in a  $(2n - 2)$ -dimensional hypersurface. A general trajectory lies on a hypersurface of dimension  $2n - L$ , where  $L$  represents the number of (independent) constants of motion. If  $L = 2n - 1$ , the surface is a curve, and a solution to eq. (3). See also Figure 1.

How do we find first integrals?

<sup>2</sup>Some systems with a Hamiltonian formulation can settle into attractor-like behaviour, see for example the Bianchi IX model in the Mixmaster (Belinski-Khalatnikov-Lifshitz) regime. This solution to the Einstein field equations displays a curious interplay between Hamiltonian and chaotic behaviour, featuring among others a strange (i.e. fractal) 'attractor' (actually, it is a repeller, but let's just call it an attractor), but not in the usual sense as the consequence of genuine dissipation with the associated change in phase-space volume [29].

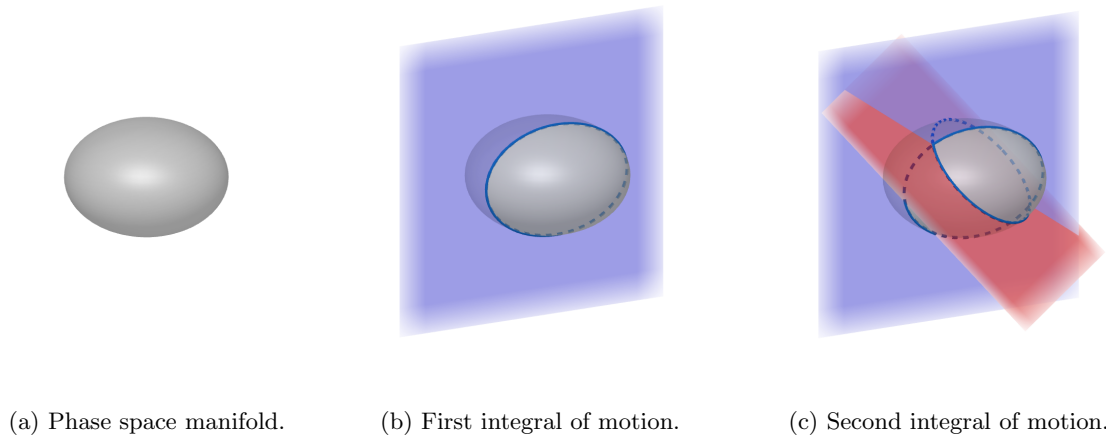


Figure 1: The phase space is a manifold of dimension  $2n$ . Each integral of motion defines a hypersurface of dimension  $2n - 1$ . The dynamics live on the intersection of these hypersurfaces with the phase space manifold. In the sketch, the dynamics take place on the curve intersecting the two discs in (c). Graphics generated with [GeoGebra](#).

- Noether's theorem gives some of them, corresponding to symmetries of eq. (3), but in general the first integrals found with Noether's theorem are not exhaustive;
- Let  $f, g$  be two first integrals, not explicitly depending on time (recall that first integrals, per the remark above, can depend on time) Then  $\{f, g\}$  will also be a first integral. To see this, note that

$$\{f, \{g, H\}\} + \{g, \{H, f\}\} + \{H, \{f, g\}\} = 0,$$

and hence  $\{H, \{f, g\}\} = 0$ , i.e.  $\{f, g\}$  is a constant of motion.

Energy always exists as a first integral for time-independent Hamiltonian systems, but quite often it is the only first integral.

**The Liouville-Arnold theorem** Before we state the Liouville-Arnold theorem, we need to define the notion of Liouville integrability and canonical transformations.

**Definition 2.2** (Liouville integrability [40]) *An integrable system consists of a  $2n$ -dimensional phase space  $M$  together with  $n$  independent functions (in a sense that that gradients  $\nabla f_j$  are linearly independent vectors on a tangent space to any point in  $M$ )  $f_1, \dots, f_n : M \rightarrow \mathbb{R}$  that are in involution:*

$$\{f_j, f_k\} = 0, \quad j, k = 1, \dots, n.$$

**Remark** *Note that the number of functionally independent conserved charges can never be larger than  $2n - 1$ . In a system with  $2n - 1$  functionally independent conserved charges, motion takes place on a one-dimensional curve in phase space; adding another charge would confine motion to a zero-dimensional (trivial) subspace.*

How can we square the definition of Liouville integrability with the intuition we developed about constants of motion? Obviously, something fishy is going on here. In the paragraph beneath Definition 2.1, we argued that, for a general system, we need  $2n - 1$  conserved quantities for the trajectories in phase space to be confined to curves and be a solution to Hamilton's equations of motion (3). Now, it seems, we only need  $n$  conserved quantities. What has changed? The answer lies in the severe restrictions that are imposed on the topology of the phase space by the requirement that the conserved quantities are in involution. We will return to this point shortly, but we need one more ingredient to fully appreciate the Liouville-Arnold theorem: canonical transformations.

What is the effect of canonical coordinate transformations on Hamilton's equations of motion (3)? A coordinate transformation of phase space from one set of coordinates  $p, q$  to a new set,

$$Q_k = Q_k(p, q), \quad P_k = P_k(p, q),$$

is called *canonical* if it preserves the Poisson bracket

$$\{f, g\}_{p,q} = \sum_{k=1}^n \left[ \frac{\partial f}{\partial q_k} \frac{\partial g}{\partial p_k} - \frac{\partial f}{\partial p_k} \frac{\partial g}{\partial q_k} \right] = \sum_{k=1}^n \left[ \frac{\partial f}{\partial Q_k} \frac{\partial g}{\partial P_k} - \frac{\partial f}{\partial P_k} \frac{\partial g}{\partial Q_k} \right] = \{f, g\}_{P,Q}. \quad (7)$$

for all  $f, g : M \rightarrow \mathbb{R}$ . Canonical transformations leave the form of the Hamilton's equations (3) invariant. Variables related through a canonical transformation are said to be *canonically conjugate*.

Note: Alternate definition of canonical variables

One can also define canonical variables as variables that satisfy the Poisson brackets

$$\{P_i, P_j\}_{p,q} = 0, \quad \{Q_i, Q_j\}_{p,q} = 0, \quad \{Q_i, P_j\}_{p,q} = \delta_{ij}$$

To see that this is an equivalent statement, use the chain rule to write

$$\begin{aligned} \frac{\partial f}{\partial q_i} &= \sum_{k=1}^n \left[ \frac{\partial f}{\partial Q_k} \frac{\partial Q_k}{\partial q_i} + \frac{\partial f}{\partial P_k} \frac{\partial P_k}{\partial q_i} \right], \\ \frac{\partial f}{\partial p_i} &= \sum_{k=1}^n \left[ \frac{\partial f}{\partial Q_k} \frac{\partial Q_k}{\partial p_i} + \frac{\partial f}{\partial P_k} \frac{\partial P_k}{\partial p_i} \right]. \end{aligned}$$

The Poisson bracket of  $f, g$  then is

$$\{f, g\}_{p,q} = \dots = \sum_{j,k=1}^n \left[ \frac{\partial f}{\partial Q_k} \frac{\partial g}{\partial P_j} \{Q_k, P_j\} - \frac{\partial f}{\partial P_k} \frac{\partial g}{\partial Q_j} \{Q_j, P_k\} + \frac{\partial f}{\partial Q_k} \frac{\partial g}{\partial Q_j} \{Q_k, Q_j\} + \frac{\partial f}{\partial P_k} \frac{\partial g}{\partial P_j} \{P_k, P_j\} \right].$$

Inserting the prescribed commutation relations, we arrive at eq. (7):

$$\{f, g\}_{p,q} = \sum_{j,k=1}^n \left[ \frac{\partial f}{\partial Q_k} \frac{\partial g}{\partial P_j} \delta_{jk} - \frac{\partial f}{\partial P_k} \frac{\partial g}{\partial Q_j} \delta_{jk} \right] = \sum_{k=1}^n \left[ \frac{\partial f}{\partial Q_k} \frac{\partial g}{\partial P_k} - \frac{\partial f}{\partial P_k} \frac{\partial g}{\partial Q_k} \right] = \{f, g\}_{P,Q}.$$

A canonical transformation can be implemented by means of a generating function,  $S(P, q, t)$ , which depends on the old position coordinates  $q$  and the new momentum coordinates  $P$ . In terms of the generating function, the change of variables is given implicitly through

$$Q_i = \frac{\partial S(P, q, t)}{\partial P_i}, \quad p_i = \frac{\partial S(P, q, t)}{\partial q_i}, \quad (8)$$

which can be solved to obtain  $P$  and  $Q$  in terms of  $p$  and  $q$ .

The principle underlying the Liouville-Arnold theorem is to find a canonical transformation such that, in the new variables,  $H = H(P_1, \dots, P_n)$ , and

$$P_k(t) = P_k(0) = \text{const}, \quad Q_k(t) = Q_k(0) + t \frac{\partial H}{\partial P_k}.$$

**Theorem 2.2** (Liouville-Arnold [40]) *Let  $(M, f_1, \dots, f_n)$  be an integrable system with Hamiltonian  $H = f_1$ , and let*

$$M_f \equiv \{(p, q) \in M; f_k(p, q) = c_k\}, \quad c_k = \text{const}, \quad k = 1, \dots, n,$$

be an  $n$ -dimensional level surface of first integrals  $f_k$ . Then

- If  $M_f$  is compact and connected, it is diffeomorphic to a torus

$$T^n \equiv S^1 \times S^1 \times \dots \times S^1,$$

and (in a neighbourhood of this torus in  $M$ ) one can introduce the action-angle coordinates

$$I_1, \dots, I_n, \phi_1, \dots, \phi_n, \quad 0 \leq \phi_k \leq 2\pi,$$

such that angles  $\phi_k$  are coordinates on  $M_f$  and actions  $I_k = I_k(f_1, \dots, f_n)$  are first integrals.

- The canonical equations of motion (3) become

$$\dot{I}_k = 0, \quad \dot{\phi}_k = \omega_k(I_1, \dots, I_n), \quad k = 1, \dots, n,$$

and so the integrable system is solvable by quadrature.<sup>a</sup>

---

<sup>a</sup>A finite number of algebraic operations and integrations of functions, even if these operations (integration, inversion) cannot be performed symbolically.

**Remark** Note that we assume that  $H$  has no explicit time dependence, and in practice, the majority of integrable systems satisfy this condition (in fact, the energy is often the only conserved quantity). However, some systems with a time-dependent Hamiltonian can be reformulated in a way that removes explicit time dependence in an extended phase space with time and its conjugate momentum added as new coordinates.

The Liouville-Arnold theorem tells us that the flow generated by the integrable Hamiltonian takes place on  $n$ -tori (parametrized by  $n$  angle variables) and never returns to the same point; this is known as *quasiperiodic motion*. A trajectory starting on one of these tori never leaves that torus, which is why we call the tori *invariant*. The submanifolds on which trajectories reside are not very complex, and this lies at the basis of the connection between integrability and ‘solvability’ [38].

What we are really doing then, is finding a suitable set of coordinates such that the dynamics essentially trivializes, instead of solving the partial differential equations associated with the equations of motion. The ability to do this is what sets integrable systems apart from non-integrable systems. To put it another way, we see that what distinguishes integrable from non-integrable systems is that for integrable systems with  $n$  degrees of freedom, we can take the Hamiltonian, and, under canonical transformation, transform it to a new Hamiltonian  $\bar{H}$  depending only on the action variables, i.e. on only *half* ( $n$  out of  $2n$  of) the phase space variables:

$$H(p, q) \xrightarrow{\text{can. transf.}} \bar{H}(I). \quad (\text{integrable})$$

Conversely, if, during the canonical transformation to action-angle variables, we cannot get rid of the angle variables, our system is non-integrable:

$$H(p, q) \xrightarrow{\text{can. transf.}} \bar{H}(I, \phi). \quad (\text{non-integrable})$$

Furthermore, the requirement that for integrable systems the  $n$  independent constants of motion be in involution, highly restricts the topology on which the trajectory lies: it is an  $n$ -parameter family of  $n$ -tori. That is, for each action variable  $I_i$  there is an  $n$ -torus that is parametrized by the angle variables  $(\phi_1, \dots, \phi_n)$ . This is why for integrable systems, we can do with  $n$  instead of  $2n - 1$  constants of motion to solve Hamilton’s equations of motion.

Example: A two-dimensional integrable system

In a two-dimensional integrable system, the trajectory is restricted to a 2-torus. Naively (without knowing anything about the Liouville-Arnold theorem), one would expect a 4-dimensional phase space.

In the literature on classical integrability, you will often hear the terms ‘superintegrable’ and ‘maximally superintegrable’. A classical system with  $n$  degrees of freedom is called *superintegrable* if it has more than  $n$

(but less than  $2n-1$ ) functionally independent conserved charges. If the system has exactly  $2n-1$  functionally independent conserved charges, it is said to be *maximally superintegrable*. Note that a system may never have more than  $2n-1$  functionally independent conserved charges; see the remark below Definition 2.2. The need for all conserved quantities to be in involution cannot be satisfied if the number is greater than  $n$  (involution of all charges would imply functional dependence), and hence it is not a requirement:

Type	# Conserved quantities	In involution
Liouville integrable	$n$	yes
Superintegrable	$> n, < 2n-1$	not all
Maximally superintegrable	$2n-1$	not all

(9)

A well-known example of a maximally superintegrable system is the classical Kepler problem for the motion of a particle subject to the gravitational attraction of a much heavier object such as a planet or a star. The problem possesses  $n = 3$  degrees of freedom (motion can take place in the  $x$ -,  $y$ - and  $z$ -direction). The conserved quantities are the energy  $E$ , three components of the angular momentum vector  $\mathbf{L}$ , and one component of the Laplace-Runge-Lenz vector  $\mathbf{A} = \mathbf{p} \times \mathbf{L} - m\mathbf{k}\mathbf{r}/r$  (the other two components are not independent of  $E$  and  $\mathbf{L}$ ). We therefore have  $5 = 2n-1$  integrals of motion.

### 2.2.2. The KAM-theorem and classical integrability beyond Liouville

How prevalent is integrability? At the extremes of the spectrum, we find two diametrically opposed views, that can be summarized as follows [92]:

1. Every system is integrable, if only we are able to find (possibly very complicated)  $n$  functionally independent constants of motion in involution.
2. Given an integrable Hamiltonian  $H_0(p, q)$ , the addition of an infinitesimal perturbation  $\epsilon H_1(p, q)$  such that  $H(p, q) = H_0(p, q) + \epsilon H_1(p, q)$ <sup>3</sup> immediately destroys any conserved charges except for the energy as soon as  $\epsilon \neq 0$ .

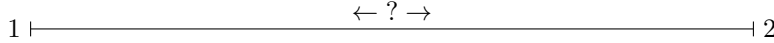


Figure 2: Where do we place integrability?

Position 2 would imply that for small  $\epsilon$ , trajectories would initially evolve close to the unperturbed  $n$ -tori of the Liouville-Arnold theorem, before straying off at later times.

A responsible view to take lies somewhere in the middle, and is motivated by the famous **KAM-theorem** (Kolmogorov-Arnold-Moser) [71, 86, 4]. The gist of the theorem is that, given quite general conditions, an integrable system remains integrable under small perturbations. In the phase space, small perturbations typically destroy the *resonant* (or *commensurate*)  $n$ -tori of the unperturbed system, which form a dense set in the unperturbed system, while most *non-resonant* (or *incommensurate*) tori are preserved. Non-resonant tori are those whose  $n$ -dimensional frequency vector  $\boldsymbol{\omega} \equiv \partial H(\mathbf{I})/\partial \mathbf{I}$  satisfies the criterion

$$|\mathbf{m} \cdot \boldsymbol{\omega}| > K(\boldsymbol{\omega})|\mathbf{m}|^{-n+1},$$

for all (except the zero) integer vectors  $\mathbf{m}$ , where  $|\cdot|$  is the L1-norm ( $|\mathbf{m}| = |m_1| + |m_2| + \dots + |m_n|$ ) and  $K(\boldsymbol{\omega}) > 0$  is a number independent of  $\mathbf{m}$ . The set of vectors  $\boldsymbol{\omega}$  that do not satisfy this criterion has zero Lebesgue measure in frequency-space, meaning that non-resonant tori abound. A highly simplified form of the KAM-theorem is the statement that under very general conditions, given a small perturbation  $\epsilon$  most (measure-wise, in phase space) of the tori associated with the unperturbed integrable Hamiltonian survive.<sup>4</sup> In other words, the KAM-theorem guarantees some sense of stability in the face of perturbations to integrable systems, which leads us to discard position 2 as a viable view.

<sup>3</sup>Or in action angle variables:  $H(I, \theta) = H_0(I) + \epsilon H_1(I, \theta)$ .

<sup>4</sup>Here, for a torus of the unperturbed system with frequency  $\boldsymbol{\omega}_0$  to ‘survive’ the perturbation means the following: there exists a torus of the perturbed system ( $\epsilon \neq 0$ ) with a frequency vector  $\boldsymbol{\omega}(\epsilon) = k(\epsilon)\boldsymbol{\omega}_0$  subject to the conditions that (1)  $k(\epsilon) \rightarrow 1$  as  $\epsilon \rightarrow 0$  and (2) the perturbed toroidal surface with frequency  $\boldsymbol{\omega}(\epsilon)$  deforms continuously into the unperturbed torus as  $\epsilon \rightarrow 0$ .

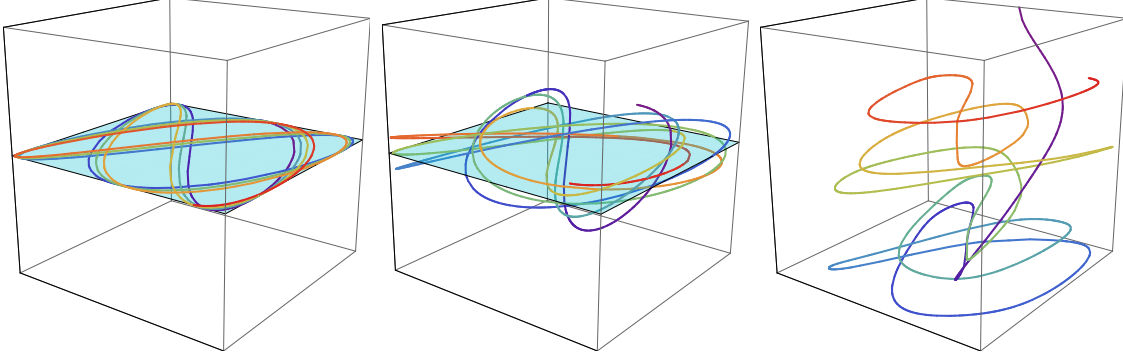


Figure 3: Illustration of the KAM-theorem. The first picture shows integrable motion confined to an equal-energy shell (blue plane) of the phase space (cube). In the next picture, the system's trajectories are subjected to small perturbations. Whether these perturbations grow or decline is the subject of the KAM-theorem: if they diminish, motion on the equal-energy shell is eventually restored, landing us back onto the first picture, whereas if they grow, trajectories will spread throughout the phase space and instead of integrable motion, we end up with the chaotic motion of the third picture. Figure taken from [87].

On a sidenote, while the KAM-theorem tells us that in systems close to integrable Hamiltonian systems many solutions persist forever under slight perturbations, the so-called *Nekoroshev estimates* [89] state that all solutions remain close to their integrable counterparts for an exponentially long time. Namely, given a nearly integrable Hamiltonian  $H_0(I) + \epsilon H_1(I, \theta)$  with  $n$  degrees of freedom (and sweeping technicalities under the carpet), we are guaranteed the bound [95]:

$$|I(t) - I(0)| < \epsilon^{1/(2n)}, \quad \text{for } |t| < \exp \left[ c \left( \frac{1}{\epsilon} \right)^{1/(2n)} \right],$$

with  $c$  some constant.

**Classical integrability beyond Liouville** Even though there seems to be broad consensus on interpreting Hamiltonian integrability in the Liouville sense, there has been exploration into alternative forms of integrability for non-Hamiltonian dynamical systems. One such interpretation worth mentioning is known as *broad integrability*, and contains Liouville integrability as a special case [131]. It was probably first written down coherently by Bogoyavlenskij [16].

**Definition 2.3** (broad integrability [131]) *A vector field  $X$  on a manifold  $M$  is said to be integrable of type  $(p, q)$ , where  $p \geq 1$ ,  $q \geq 0$ ,  $p + q = \dim(M)$ , if there exists  $p$  vector fields  $X_1 = X, X_2, \dots, X_p$  and  $q$  functions  $F_1, \dots, F_q$  on  $M$ , which satisfy the following conditions:*

- *The vector fields commute pairwise:*

$$[X_i, X_j] = 0 \quad \forall i, j.$$

- *The functions  $F_1, \dots, F_q$  are common first integrals of  $X_1, \dots, X_p$ :*

$$X_i(F_j) = 0 \quad \forall i, j.$$

- *$X_1 \wedge X_2 \wedge \dots \wedge X_p \neq 0$  and  $dF_1 \wedge \dots \wedge dF_q \neq 0$  almost everywhere.*

*Under the above conditions,  $(X_1, \dots, X_p, F_1, \dots, F_q)$  is said to be an integrable system of type  $(p, q)$ .*

**Corollary** *Liouville integrable Hamiltonian systems (those living on a symplectic  $2n$ -dimensional manifold) are also integrable of type  $(n, n)$ , in the sense that they have  $n$  commuting first integrals together with their  $n$  commuting Hamiltonian vector fields.*

As has been [pointed out](#), it is also important to agree that in the above we have been talking exclusively about global properties. This is because any Hamiltonian system is locally integrable, as a consequence of *Darboux's theorem* [31]. More precisely, let  $(M, \omega)$  be a  $2n$ -dimensional real symplectic manifold with globally defined Hamiltonian  $H : M \times [t_i, t_f] \rightarrow \mathbb{R}$ , and a time evolution governed by Hamilton's equations of motion.

1. The notion of complete/Liouville integrability means that there exist  $n$  independent globally defined real-valued functions  $I_i$ ,  $i \in \{1, \dots, n\}$  (the action variables) satisfying  $\{I_i, I_j\} = 0$ ,  $i, j \in \{1, \dots, n\}$ .
2. On the contrary, a local version of the first property exists. Namely, given a fixed point  $x^* \in M$ , under relatively lenient regularity assumptions, it is *always* possible to find locally<sup>5</sup> Hamilton's principal function  $S(q^1, \dots, q^n; I_1, \dots, I_n; t)$  – the  $n$ -parameter complete solution of the Hamilton-Jacobi equation ( $I_i$ ,  $i \in \{1, \dots, n\}$  are integration constants).

The *global* property 1 is rare, while the *local* property 2 is generic.

## 2.3. Classical ergodicity, chaos and integrability

Having introduced Liouville integrability, we redirect our focus to classical ergodic theory and chaos, before making an attempt at discerning their interdependence.

### 2.3.1. Classical ergodic theory

Classical ergodic theory is concerned with investigating  $\mathcal{P}$ , the phase space (or a region of the phase space, such as an energy shell in Hamiltonian systems) equipped with an operator  $\mathcal{T}^t : \mathcal{P} \rightarrow \mathcal{P}$  that evolves points in  $\mathcal{P}$  with time  $t$ . The main questions we are interested in are the following [120]:

- Starting from an initial point, which regions of  $\mathcal{P}$  are explored?
- How rapidly does a typical point explore these regions?

The analysis of such questions is facilitated when there exists a measure<sup>6</sup>  $\mu(A) \geq 0$ ,  $A \subseteq \mathcal{P}$ , that is preserved under the time evolution:  $\mu(\mathcal{T}^t A) = \mu(A)$ . We have seen already that the natural measure for Hamiltonian systems is given by the phase-space volume  $\int_A d^n q d^n p$  (Liouville's theorem). Dynamics are said to be [ergodic](#) in  $\mathcal{P}$  if almost all points explore every region of nonzero measure in  $\mathcal{P}$ .

An important concept that we will rely on in the subsequent treatment of quantum integrability is the connection between ergodicity and time-averaged correlation functions. Ergodicity in the sense of the previous paragraph has been shown (*Birkhoff's ergodic theorem* [28]) to be equivalent to time-averaged correlations becoming independent of the initial condition in the infinite time limit, up to exceptions of measure zero (isolated periodic orbits or other closed surfaces with lower dimension than  $\mathcal{P}$ ) [92]:

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T f(\tilde{\mathbf{x}}(t)) dt = \langle f(\tilde{\mathbf{x}}) \rangle. \quad (\text{ergodicity})$$

Here,  $f(\tilde{\mathbf{x}})$  is a smooth function of the phase space variable  $\tilde{\mathbf{x}}$ ,  $\tilde{\mathbf{x}}(t)$  is a trajectory in phase space and  $\langle f(\tilde{\mathbf{x}}(x)) \rangle$  is the phase-space average (weighted by the measure). In other words, in the infinite time limit, the presence of the system in a region  $B \subseteq \mathcal{P}$  cannot be traced back to the starting region  $A \subseteq \mathcal{P}$ :

$$\lim_{T \rightarrow \infty} \frac{1}{2T} \int_{-T}^T dt \mu[(\mathcal{T}^t A) \cap B] = \mu(A)\mu(B), \quad \forall A, B \subseteq \mathcal{P}.$$

One can, and frequently does, formulate the preceding statements in the following way: ergodicity means that long-time averages (for a single particle) and ensemble averages agree.<sup>7</sup>

The mechanism responsible for the decorrelation of time-averaged correlation functions over time is called *strong mixing* or just *mixing*. We call a system mixing if any ensemble  $A$  with sufficiently many neighbouring

<sup>5</sup>In a sufficiently small open Darboux neighbourhood of  $x^*$ .

<sup>6</sup>See Appendix B.1.

<sup>7</sup>In mnemonic form: 'time averages equal space averages.'



states (nonzero measure) in  $\mathcal{P}$  over time spreads out equally over every region of  $\mathcal{P}$ . For a two-element correlation function, the mixing condition translates into an independence condition on the measures:

$$\lim_{t \rightarrow \infty} \mu[(\mathcal{T}^t A) \cap B] = \mu(A)\mu(B), \quad A, B \subseteq \mathcal{P}. \quad (\text{strong mixing})$$

*Weak mixing* corresponds to the limit converging exactly except at a vanishing fraction of times:

$$\lim_{T \rightarrow \infty} \frac{1}{2T} \int_{-T}^T dt \left| [\mu(\mathcal{T}^t A) \cap B] - \mu(A)\mu(B) \right| = 0. \quad (\text{weak mixing})$$

*K-mixing* occurs when all higher order correlation functions also become uncorrelated, which is the case when its Kolmogorov-Sinai entropy is positive.

Mixing is a stronger requirement than ergodicity, because not only do we require that almost all points in the phase space explore every region of nonzero measure in  $\mathcal{P}$ , but also that all regions are visited more or less *uniformly*.

Note: Strong mixing explained with a cocktail [46]

J. W. Gibbs provided the following intuitive picture of strong mixing. Imagine adding a shot of scotch to a glass of water. We add a volume  $\mu(S)$  of scotch, and the total volume of the cocktail (scotch + water) is  $\mu(C)$ . Now we stir the cocktail for  $t$  units of time, which is represented by the time evolution operator  $\mathcal{T}^t$ . The cocktail is thoroughly mixed if the concentration of scotch equals  $\mu(S)/\mu(C)$  in any region  $V$  of the cocktail:

$$\frac{\mu[(\mathcal{T}^t S) \cap V]}{\mu(V)} = \frac{\mu(S)}{\mu(C)}, \quad \text{for any } V, \mu(V) \neq 0.$$

If, after an infinite time stirring, the cocktail is in this state, it is a strong mixing system:

$$\lim_{t \rightarrow \infty} \mu[\mathcal{T}^t S \cap V] = \mu(S)\mu(V),$$

where we have set  $\mu(C) = 1$  since we are free to choose units. This is eq. (strong mixing). Weak mixing corresponds to the situation where we allow some bubbles of either scotch or water to remain even after an infinite amount of stirring, but on average, these fluctuations even out as  $t \rightarrow \infty$ .

More levels of mixing may be considered, and this process naturally inspires a ‘hierarchy of randomness’, the *ergodic hierarchy*. Figure 4 displays a typical ergodic hierarchy, but bear in mind that additional levels are sometimes included. According to the classification, mere ergodicity is the lowest rung of random behavior in dynamical systems. Levels of the ergodic hierarchy are characterized in part by a *Lyapunov exponent*  $\lambda$ .

Note: Lyapunov exponents

Let  $\delta(t)$  describe the separation vector between two trajectories in phase space with initial (infinitesimal) separation  $\delta_0$ . The Lyapunov exponent  $\lambda$  is a measure for how quickly these trajectories diverge:

$$|\delta(t)| \approx e^{\lambda t} |\delta_0|.$$

In an  $n$ -dimensional phase space, there are  $n$  Lyapunov exponents. These can be identified with the axes of an ellipsoid that is created when a ‘ball of initial conditions’ with radius  $\delta_0$  around some starting point is stretched out and compressed under the flow of the system. The maximal Lyapunov exponent is defined as

$$\lambda = \lim_{t \rightarrow \infty} \lim_{|\delta_0| \rightarrow 0} \frac{1}{t} \ln \frac{|\delta(t)|}{|\delta_0|}.$$

Looking slightly ahead, Lyapunov exponents quantify what we mean by condition (i) for chaos (sensitive dependence on initial conditions); a positive maximal Lyapunov exponent is therefore generally taken as a feature of chaos, although there are examples which show that it is not a sufficient condition.



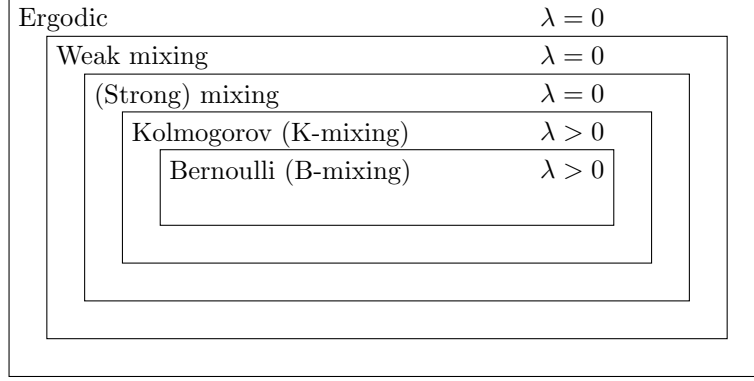


Figure 4: The ergodic hierarchy, Bernoulli  $\subset$  Kolmogorov  $\subset$  Strong mixing  $\subset$  Weak mixing  $\subset$  Ergodic, with  $\lambda$  indicating the Lyapunov exponent for each region. A system that is ergodic but not weak mixing, strong mixing etc. is called *merely ergodic*, and similarly for other levels. Some versions of the ergodic hierarchy feature additional levels. Adapted from [120].

### 2.3.2. Classical chaos

There is no universal agreement on what precisely is meant by chaos in the context of dynamical systems, but there are some characteristics that (nearly) all definitions seem to have in common. Heuristically, chaos may be thought of in the following manner:

**Definition 2.4** (Chaos, Strogatz [114]) *Chaos is aperiodic long-term behaviour in a deterministic system that exhibits sensitive dependence on initial conditions.*

1. ‘aperiodic long-term behaviour’ means that there are trajectories which do not settle down to fixed points, periodic orbits, or quasiperiodic orbits as  $t \rightarrow \infty$ . For practical reasons, we should require that such trajectories are not too rare. For instance, we could insist that there be an open set of initial conditions leading to aperiodic trajectories, or perhaps that such trajectories should occur with nonzero probability, given a random initial condition.
2. ‘deterministic’ means that the system has no random or noisy inputs or parameters. The irregular behaviour arises from the system’s nonlinearity, rather than from noisy driving forces.
3. ‘sensitive dependence on initial conditions’ means that nearby trajectories separate exponentially fast, i.e. the system has a positive Lyapunov exponent.

Example: An ‘almost’ chaotic system in the sense of Strogatz [114]

The system  $\dot{x} = x$  is obviously deterministic and it is not very hard to intuit that nearby trajectories separate exponentially. However, infinity acts like an attracting fixed point: trajectories fly off to infinity, without ever returning. Chaotic behaviour should be aperiodic, and therefore we cannot allow such fixed points.

Devaney [33] gives a slightly different but mathematically much more precise definition of a chaotic system, which he defines as a set  $V$  together with a map  $f$ , satisfying three conditions.

**Definition 2.5** (Chaotic map, Devaney) *Let  $V$  be a set. A map  $f : V \rightarrow V$  is said to be chaotic if*

- (i)  *$f$  has sensitive dependence on initial conditions.*
- (ii)  *$f$  is topologically transitive.*
- (iii) *Periodic points are dense in  $V$ .*

We will briefly point out how these three requirements make sense. Sensitive dependence on initial conditions (i) captures the idea that tiny uncertainties in the initial data eventually evolve into large differences between

final states (colloquially known as the ‘butterfly effect’).<sup>8</sup> Topological transitivity (ii) and density of periodic points in  $V$  (iii) are harder to relate to intuition, but suffice it to say that (ii) pinpoints the desire of a chaotic system to ‘spread out’ (any region of the space can eventually reach any other region; one can detect a signature of ergodicity here), while (iii) guarantees that periodic behaviour is everywhere and provides a skeleton of regularity within unpredictability (this hints at the fact that chaotic behaviour is still completely deterministic).

J. Banks, J. Brooks, G. Cairns, G. Davis and P. Stacey later proved in the short note [6] that (ii) and (iii) imply (i), but for pedagogical reasons it is convenient to explicitly separate the sensitive dependence on initial conditions.

Note: Some clarification on Definition 2.5 [33]

**Definition 2.6**  $f : J \rightarrow J$  is said to be topologically transitive if for any pair of open sets  $U, V \subset J$  there exists  $k > 0$  such that  $f^k(U) \cap V \neq \emptyset$ .

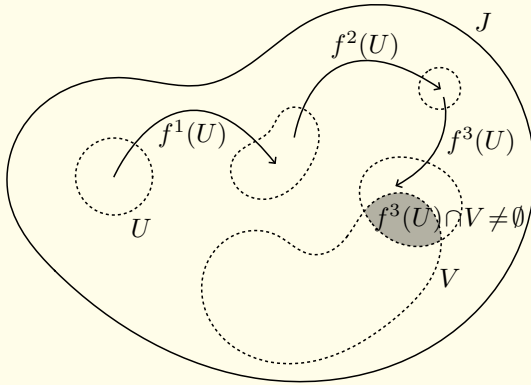


Figure 5: Topological transitivity.

**Definition 2.7**  $f : J \rightarrow J$  has sensitive dependence on initial conditions if there exists  $\delta > 0$  such that, for any  $x \in J$  and any neighbourhood  $N$  of  $x$ , there exists  $y \in N$  and  $n \geq 0$  such that  $|f^n(x) - f^n(y)| > \delta$ .

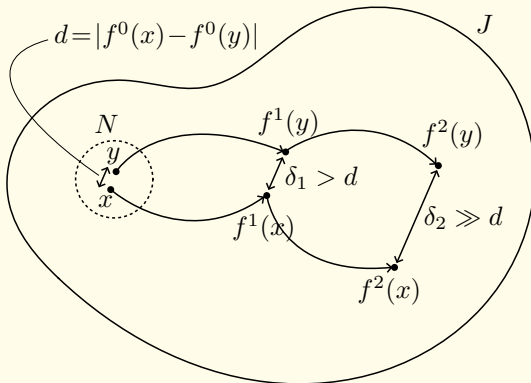


Figure 6: Sensitive dependence.

What this means is that under a topologically transitive map, points are moved from one arbitrarily small neighbourhood to any other, and hence it is impossible to decompose the system into two disjoint open sets which are invariant under the map.

#### Example

Rotating a circle is topologically transitive but not sensitive to initial conditions, because points don’t move relative to each other with each iteration.

Intuitively, a map possesses sensitive dependence on initial conditions if there exist at least one point close to  $x$  which, under repeated application, moves far enough (at least  $\delta$ ) way from it. The concept is essentially expressing the idea of the Lyapunov exponent.

#### Example

The logistic map  $f(x) = \mu x(1 - x)$  with  $\mu = 4$  ( $x \in [0, 1]$ ) has sensitive dependence on initial conditions (it is also topologically transitive and exhibits dense period orbits: it is chaotic).

<sup>8</sup>This quote ascribed to E. N. Lorenz elegantly gets the message across [30]: “Chaos: When the present determines the future but the approximate present does not approximately determine the future.” It captures both the sensitivity to initial conditions while also stressing that chaos is, given the initial conditions are known with infinite precision, completely deterministic.

**Definition 2.8** A subset  $A$  of a topological space  $X$  is said to be dense if every point in  $X$  either belongs to  $A$  or else is arbitrarily close to a member of  $A$ . (More precisely, A subset  $A \subset X$  is dense in  $X$  if the closure  $\bar{A}$  of  $A$  equals  $X$ , i.e.  $\bar{A} = X$ .)

There is not much to explain here as far as intuition goes: points in a dense subset are arbitrarily close to any point in the embedding set.

#### Example

The rational numbers  $\mathbb{Q}$  are a dense subset of the real numbers  $\mathbb{R}$  since every real number is either rational or has a rational number arbitrarily close to it (per the Diophantine approximation).

As a remark, we note that if  $J$  has no isolated points, then the statement that  $f$  is topologically transitive is guaranteed if there is a point  $x_0 \in J$  such that its orbit  $x_0, f(x_0), f^2(x_0), \dots$  is dense. The converse is also true, see Silverman [105].

Example: Chaotic maps in the sense of Devaney [33]

We present three chaotic maps:

- The map  $f : S^1 \rightarrow S^1$  given by  $f(\theta) = 2\theta$  is chaotic.
  - (i) is satisfied because the angular distance between points is doubled upon every iteration.
  - (ii) follows from the observation that any arc in  $S^1$  acted upon by  $f^k$  will eventually cover all of  $S^1$  and, in particular, any other arc in  $S^1$ .
  - (iii) can be seen by writing  $f^n(\theta) = 2^n\theta$ , such that  $f^n(\theta)$  is  $2\pi$ -periodic if and only if  $2^n\theta = \theta + 2k\pi$  for some integer  $k$ , i.e. if and only if  $\theta = 2k\pi/(2^n - 1)$  where  $0 \leq k \leq 2^n$  is an integer. This means that the periodic points of  $f$  are the  $(2^n - 1)^{\text{th}}$  roots of unity. The points of period  $n$ , being evenly spaced around the circle, partition the circle into arcs of length  $2\pi/(2^n - 1)$ . If we pick any two points  $x, y$  on the circle such that  $|x - y| = \epsilon > 0$ , then we may choose  $n$  sufficiently large to ensure that  $2\pi/(2^n - 1) < \epsilon$ . In other words, one of the endpoints of the arcs (that partition the circle) must lie between  $x$  and  $y$ , and hence a periodic point lies between  $x$  and  $y$ . Since we never made any assumptions on  $x$  and  $y$  (they are arbitrary points), there will always be at least one periodic point between them. Hence periodic points are dense in  $S^1$ .
- The logistic map  $F_\mu(x) = \mu x(1 - x)$  transitions to the fully chaotic regime on an invariant Cantor set for  $\mu > 2 + \sqrt{5}$  [33].
- The shift map  $\sigma : \Sigma_2 \rightarrow \Sigma_2$  on the sequence space  $\Sigma_2$  of zeros and ones, defined by  $\sigma(s_0 s_1 s_2 \dots) = s_1 s_2 s_3 \dots$ , is chaotic [14].

An important theorem that often comes up in the study of conservative systems bound to a finite volume and that has close connotations with chaos is the **Poincaré recurrence theorem**, which can be formulated in different ways:

**Theorem 2.3** (Poincaré recurrence theorem) Let  $(X, \Sigma, \mu)$  be a finite measure space (see Appendix B.1) and let  $f : X \rightarrow X$  be a measure-preserving transformation. Then for any  $\sigma \in \Sigma$ , the set of points  $x \in \sigma$  for which  $\exists N \in \mathbb{N}$  such that  $f^n(x) \notin \sigma \forall n > N$  has zero measure.

The proof of this theorem is relatively straightforward and can be found in most standard textbooks on dynamics or measure theory (see for example Petersen [94]). The gist of the theorem is that almost every point in  $\sigma$  returns to  $\sigma$  almost infinitely often, and exceptions make up only an infinitesimal part of  $\sigma$  (a part of zero measure). Exceptions could be isolated periodic orbits or other closed surfaces that have a dimension lower than  $\mathcal{P}$ , the phase space.

This means that discrete systems obeying the Poincaré recurrence theorem will eventually return to a state

that is exactly the same, while continuous systems will get arbitrarily close to any previously attained state. Terrence Tao illustrates the counter-intuitive implications of the theorem with the following consequence: if one burns a piece of paper in a box, then there exist arbitrarily small perturbations of the initial conditions such that the piece of paper will eventually reassemble (up to arbitrarily small error). Naturally, one might ask if such an occurrence would violate the second law of thermodynamics, but we can escape disaster by reasoning that the required time for reassembly to take place is extraordinarily large – much larger than the lifetime of the universe<sup>9</sup> [117].

At first sight, the relation between the Poincaré recurrence theorem and chaos (in the sense of sensitive dependence on initial conditions) seems to carry a degree of uneasiness: (assuming a continuous system) recurrence brings one back arbitrarily close to the same point in phase space over and over again, whereas chaotic motion seems to preclude such ‘regular’ patterns. Upon further thought however, the uneasiness is resolved by the insight that one will indeed return arbitrarily close to one’s starting point, but when this happens, the trajectory afterward will look nothing like what it did the first time around.

One might be interested to know that a similar ‘quantum recurrence’ theorem exists for time-independent systems with discrete energy eigenstates. Considering,  $|\psi(t)\rangle$ , the state vector of the system at time  $t$ , it states that for every  $\epsilon > 0$  and  $T_0 > 0$  there exists a time  $T > T_0$  such that  $\| |\psi(T)\rangle - |\psi(0)\rangle \| < \epsilon$  [15].

Before we return to classical integrability, we wish to point out a couple of things. First of all, two aspects of chaotic systems are often misrepresented:

- As asserted in requirement 2, chaotic systems are completely deterministic, which means that there is nothing random to be found. Sensitive dependence on initial conditions should *not* be conflated with randomness.
- Secondly, nothing about a chaotic system forbids exact solutions, see for example [51] or [115], where, given non-zero angular momentum, an exact (albeit not a closed-form) solution to the three-body problem is found in the form of an infinite Puiseux series.

Following the ergodic hierarchy, some authors have tried to embed chaotic behaviour into a *chaotic hierarchy* for classifying chaotic systems from weak to strong, with Bernoulli systems being the most chaotic. This is reflected in their positive Lyapunov exponent. (Strongly) mixing systems lack a positive Lyapunov exponent and therefore do not show exponentially diverging trajectories over time; however, they still possess a degree of irregularity which justifies their classification as weakly chaotic. Systems that are merely ergodic, on the other hand, do not necessarily show decaying time correlations, which does not make them chaotic at all.

The preceding argument also reveals an important connection between ergodicity and chaos: if a system is chaotic (at least in the sense discussed in this section), it also has to be ergodic:

$$\text{chaotic} \quad \Rightarrow \quad \text{ergodic}$$

The reverse implication is not necessarily true:

$$\text{chaotic} \quad \nLeftarrow \quad \text{ergodic}$$

This can be deduced, for example, from the fact that merely strong mixing systems (and all weaker categories) have zero Lyapunov exponent.

Example: Ergodic, but not chaotic

Without proof: A map that enacts an irrational rotation on a circle is globally ergodic (since eventually every point on the circle will be visited), but not at all chaotic, since nearby points will not separate under repeated application of the map.

<sup>9</sup>This is ultimately an expression of the fact that the recurrence time  $T_{rec}$  is inversely proportional to its measure, i.e. scales with  $1/\mu(E)$  (*Kac’s lemma* [62]), and  $\mu(E)$ , where  $E$  represents the configurations in which the piece of paper is nicely assembled, is tiny for a system on the order of  $N_A$  (Avogadro’s number) of particles. In fact, the volume of these low-entropy microstates will be exponentially small compared to the volume of the full energy surface in phase space:  $\mu(E) \sim \exp(-cN_A)$ . This means that  $T_{rec} \sim \exp(10^{23}) \gg$  lifetime of the universe.

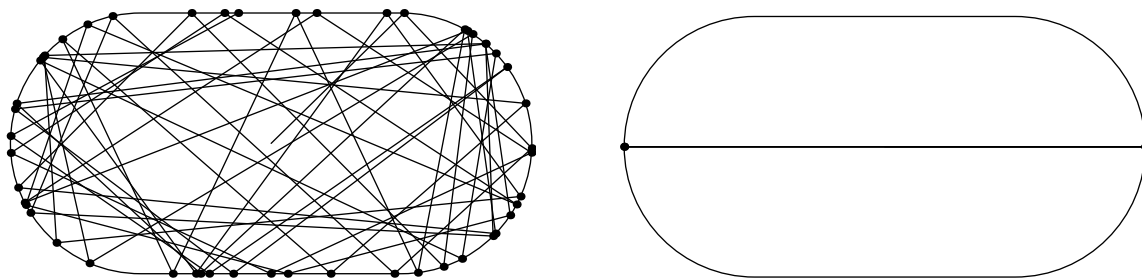


Figure 7: The Bunimovich stadium displays chaotic motion (left) or integrable motion (right), depending on initial conditions. Asymptote code adapted from [1].

Rather pedantically, we emphasize that any claims we have made concerning integrability, ergodicity and chaos apply to *global* properties. Many known systems are not globally ergodic or chaotic, and their analysis has to be performed by separately considering the various domains of phase space with qualitatively different behaviour. We give four examples:

- In systems that are not globally chaotic but display a mix of chaotic and regular domains, such as the Chirikov standard map [23, 22], one may find islands of stability that do not mix with other regions, and this trivially precludes global ergodicity.
- An even simpler example, to drive the point home, would be to artificially split a chaotic system into two subsystems by introducing some kind of barrier. The modified system would obviously not be globally ergodic.
- In systems that are not globally Liouville integrable, the phase space can be mixed, showing (quasi)-periodic motion for some initial conditions and chaotic motion for other initial conditions. This is the case in for example the Hénon-Heiles model for the motion of a star confined to a plane around a galactic center, with Hamiltonian  $H = \frac{1}{2}(x^2 + y^2) + \lambda(x^2y - y^3/3)$ . The only conserved quantity is the energy  $E$  (the Hamiltonian is not translation invariant, so there is no conservation of momentum). At low energies, motion is regular and confined to tori in phase space. At higher energies, regions of chaos emerge as nonlinear terms become more important [101].
- Some systems are known to be integrable for some initial conditions while displaying chaotic behaviour for others. In particular, this holds for a class of systems that goes by the name of *dynamical billiards*. A well-known instance of this class is the Bunimovich stadium. Assuming specular reflections<sup>10</sup> from the boundary, some initial conditions yield integrable motion while other trajectories are chaotic, see Figure 7.

### 2.3.3. Relation to classical integrability

Let us recap and contrast (Liouville) integrable and non-integrable systems by relating them to the key concepts of this chapter: constants of motion, ergodicity and chaos.

**Conserved charges** It should be clear that in integrable systems, there exists an extensive set of conserved charges (constants of motion), and that these charges should also be in involution. More precisely, Liouville-integrable systems with  $n$  degrees of freedom possess at least  $n$  functionally independent constants of motion in involution, and superintegrable systems possess up to  $2n - 1$  ones, although not all of them can be in involution. The presence of conserved charges constrains the dynamics of the system by forcing trajectories to live on simple submanifolds of the phase space, and this ultimately is what makes integrable dynamics ‘solvable’. In (globally) non-integrable systems, on the other hand, energy is often the only constant of motion, if there is any at all.

<sup>10</sup>Incident and reflected rays make the same angle on opposite sides of the surface normal.

**Chaos** In a chaotic system, neighbouring bundles of trajectories in phase space spread out exponentially with time. Trajectories can explore the phase space uniformly, or eventually settle onto an attractor, if there is one. These systems are non-integrable. In (globally) integrable systems, however, we have seen via the Liouville-Arnold theorem that trajectories do not exponentially diverge from each other. In fact, we found that all motion in Liouville integrable systems (under certain global conditions) is either (quasi-)periodic or static, and that the trajectories lie on very simple submanifolds:  $n$ -tori. These trajectories are not very complex, and enable us to ‘solve’ integrable systems. In addition, Hamiltonian systems – and therefore Liouville integrable systems – cannot have attractors because of phase space conservation. So Liouville integrability is at strict odds with chaos.

**Ergodicity** In an ergodic system, nearly all initial points are associated with trajectories that explore every region of nonzero measure in the phase space. In stronger levels of the ergodic hierarchy, there is even the requirement that all regions of phase space are visited more or less uniformly (mixing). In an ergodic system, long-time averages and ensemble averages agree. In the global sense, *integrable systems cannot be ergodic*. The presence of conserved charges in integrable system confines the dynamics to specific submanifolds of the phase space:  $n$ -tori.

When we make the transition to quantum integrability, we will do so by contrasting integrability with ergodicity (in the quantum sense). I wish to make the point that ergodicity is more fundamental to non-integrable systems than chaos is. A system that is (globally) non-integrable is always ergodic, but it does not have to be chaotic: it might for example not possess sensitive dependence on initial conditions, while still spreading out over the entire phase space. Having learned this, we will presently reframe the discussion of quantum integrability entirely in terms of the ergodic perspective.

We conclude the discussion on classical integrability, ergodicity and chaos with a categorization of classical dynamical systems in Figure 8, based on the preceding sections.

## 2.4. Quantum ergodicity and integrability

We started the section on classical integrability by discussing the relevance of constants of motion in the context of classical Hamiltonian systems. It is therefore natural that we also start the section on quantum integrability by discussing the consequences of symmetries in a quantum mechanical system. Concretely, let  $R$  be an operator representing a symmetry. Then

$$[H, R] = 0, \quad (10)$$

implying that we can diagonalize  $H$  in an eigenbasis of  $R$ , given by the eigenfunctions  $\{\phi_{n,a}\}$  satisfying  $R\phi_{n,a} = r_n\phi_{n,a}$ . Here, we assume all  $r_n$  to be different, and  $\alpha$  labels eigenfunctions  $\phi_{n,\alpha}$  belonging to the same  $r_n$ . In this basis, the commutator relation (10) can be written as

$$0 = \langle \phi_{n,\alpha} | RH - HR | \phi_{m,\beta} \rangle = (r_n - r_m) \langle \phi_{n,\alpha} | H | \phi_{m,\beta} \rangle.$$

Since all  $r_n$  were assumed to be different, we require

$$\langle \phi_{n,\alpha} | H | \phi_{m,\beta} \rangle = \delta_{nm} H_{\alpha\beta}^{(n)}, \quad \text{with } H_{\alpha\beta}^{(n)} = \langle \phi_{n,\alpha} | H | \phi_{n,\beta} \rangle.$$

What this means is that the matrix representation of  $H$  has been reduced to a block-diagonal form:

$$H = \begin{pmatrix} H^{(1)} & 0 & \cdots \\ 0 & H^{(2)} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix},$$

with  $H^{(n)} = H_{\alpha\beta}^{(n)} = \langle \phi_{n,\alpha} | H | \phi_{n,\beta} \rangle$ . The procedure can be repeated until all symmetries have been exhausted. Each additional symmetry makes  $H$  closer to a completely diagonal matrix, by cutting up the blocks into smaller and smaller units. It should therefore be clear that the presence of symmetries in a quantum mechanical system is also strongly connected to its solvability.

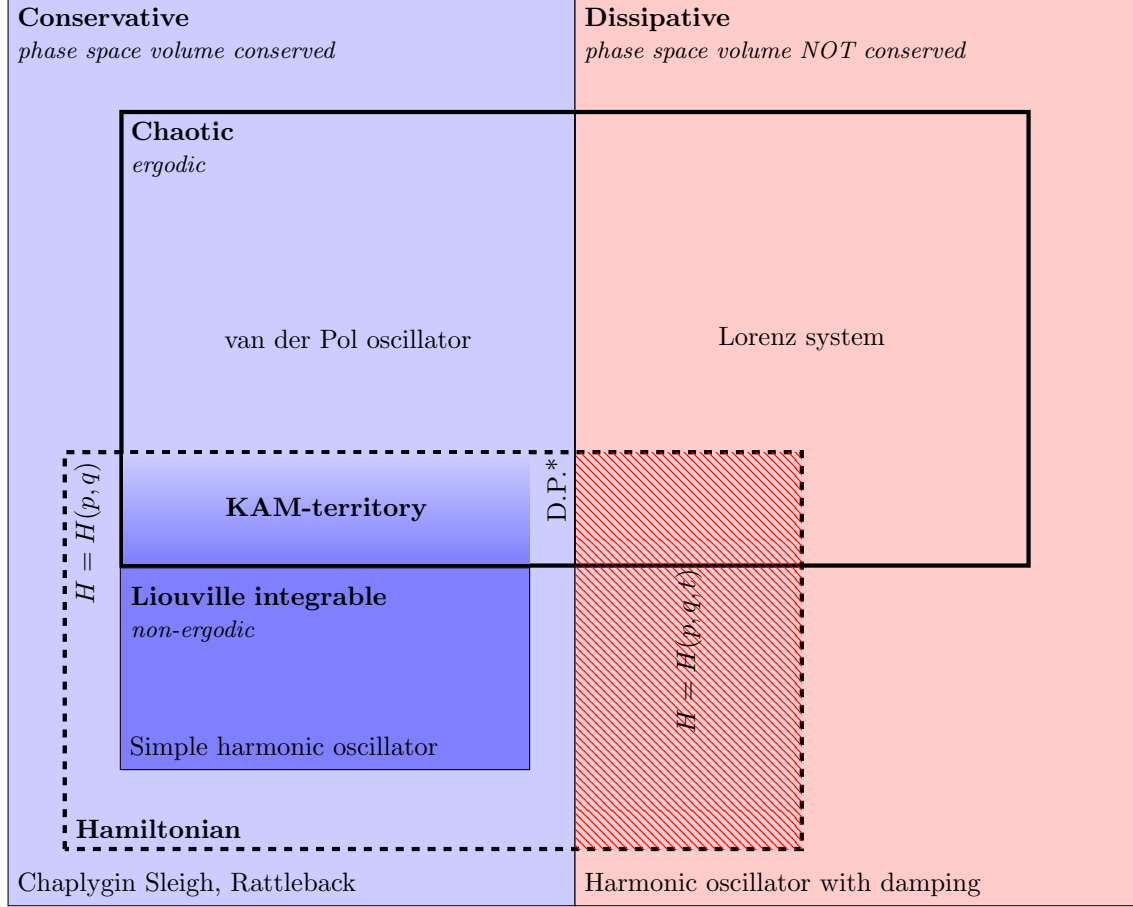


Figure 8: Classification of classical dynamical systems with examples and (global) ergodic properties. I chose to represent systems to which the KAM-theorem applies as interpolating between Liouville integrable and (Hamiltonian) chaotic, depending on the strenght of the perturbation. \*D.P. stands for double pendulum.

#### 2.4.1. Quantum ergodic theory

In the previous section, we discussed the meaning of chaos and ergodicity in the classical sense, and landed on the conclusion that integrable systems, while showing relations to chaos, are best described as the ‘opposite’ of ergodic systems. In this section, we will try to frame the discussion of quantum integrability in terms of the quantum analog of ergodicity.

Note: Quantum chaos

Having found ergodicity as a sufficient framework to explain integrability, we will not enter into a separate discourse on quantum chaos. However, many interesting developments have been made in this field, and concepts such as the Lyapunov exponent and sensitive dependence on initial conditions have been generalized to quantum systems, see for example the highly influential paper by Maldacena, Shenker, and Stanford [79]. A powerful tool in the study of quantum chaos is random matrix theory, which has been very succesful in capturing universal spectral statistics of chaotic quantum systems. A concise introduction to RMT is Chapter 3 of Stöckmann [111], and a more in-depth review can be found in the book by Mehta [84].

Interestingly, random matrix theory has proven very successful at providing a paradigm for level-spacing statistics in generic, non-integrable systems. These systems tend to exhibit level repulsion – it is very unlikely to find two energy levels near each other –, and their nearest-neighbour energy level



Table 1: The classical  $\rightarrow$  quantum map.

Classical mechanics	Quantum mechanics
Phase space, $M$ (manifold)	Hilbert space of states, $\mathcal{H}$
Observables are functions $f \in C^\infty(M)$	Observables are Hermitian operators on $\mathcal{H}$
Symplectic (or, more generally, Poisson) structure $\{\cdot, \cdot\} : C^\infty(M) \times C^\infty(M) \rightarrow C^\infty(M)$ , which is a biderivation that makes $C^\infty(M)$ into a Lie algebra	Analog of the Poisson bracket is the usual bracket of operators $[A, B] = AB - BA$
Motion is governed by a Hamiltonian $H \in C^\infty(M)$ , and the equations of motion are the Hamilton equations $\dot{y}_i = \{y_i, H\}$	Motion is governed by a Hamiltonian $H : \mathcal{H} \rightarrow \mathcal{H}$ , and the equation of motion is the Schrödinger equation, $\dot{\psi} = -iH\psi$
# of degrees of freedom equals # of pairs $(p, q)$ of conjugate phase space variables; degrees of freedom are additive	# of degrees of freedom is $\dim(\mathcal{H})$ ; degrees of freedom are not additive

spacings follow a Wigner-Dyson distribution. In integrable systems on the other hand, degeneracies in the energy levels are allowed due to the large number of conserved quantities that label the eigenstates. Therefore, levels do not repel, but are distributed independently of each other in the spectrum. The resulting level statistics are Poissonian, similar to what one would find in a non-interacting system.

In quantum mechanics, there are non-local features that render the phase space picture we developed obsolete: how does the phase space manifold of a system look like, if we cannot even properly localize a particle (its wavefunction being essentially all over the place, and there being an uncertainty on the ratio of its position and momentum)? Instead of a phase space manifold, we are dealing with a Hilbert space of states, and observables are no longer ordinary functions but Hermitian operators on the Hilbert space, see Table 1.

Isolated quantum states evolve according to unitary time evolution. That is, for a system that is initially (at  $t = 0$ ) in the state  $|\psi_0\rangle$ , the time evolution is given by

$$|\psi(t)\rangle = e^{-iHt} |\psi_0\rangle = \sum_n c_n |n\rangle e^{-iE_n t}, \quad (11)$$

where the coefficients  $c_n$  are the projection of  $|\psi_0\rangle$  onto a basis of energy eigenstates  $|n\rangle$ ,  $c_n = \langle n|\psi_0\rangle$ , and we assumed normalization of the coefficients:  $\sum_n |c_n|^2 = 1$ . We also work with finite systems, such that the spectrum is discrete.

Under unitary time evolution (11), the long-time average of the density matrix,  $\bar{\rho}$ , is

$$\bar{\rho} = \overline{|\psi(t)\rangle \langle \psi(t)|} = \sum_{\alpha, \beta} c_\alpha c_\beta^* \overline{e^{-i(E_\alpha - E_\beta)t}} |\psi_\alpha\rangle \langle \psi_\beta| \simeq \sum_\alpha |c_\alpha|^2 |\psi_\alpha\rangle \langle \psi_\alpha| + \sum_{\alpha \neq \beta} c_\alpha c_\beta^* |\psi_\beta\rangle \langle \psi_\alpha| \delta_{E_\beta, E_\alpha} + 0,$$

where the first term represents diagonal contributions, the second term represents off-diagonal contributions with degenerate energies and the third term represents all other off-diagonal contributions. Note that the third term vanishes because the rapidly oscillating complex exponentials cancel in the large time limit if  $E_\alpha$  and  $E_\beta$  are incommensurate,  $E_\alpha \neq E_\beta$ .<sup>11</sup> We will also neglect the second term, reasoning that any physically realizable system will have strong enough disorder and interactions to lift most degeneracies. The resulting ensemble is the *diagonal ensemble*.

In a bid to come up with a description of ergodicity in quantum mechanical systems, von Neumann [122] sets out on the premise that ergodicity is attained when all states come arbitrarily close to any other state on a given energy surface, with ‘sojourning times’ in each part of the state space proportional to the (generalized)

<sup>11</sup>This result probably appears familiar to those who have seen the stationary action principle in the path integral formalism.



volume of these areas. He proves that the aforementioned is realized if there are no resonances between the energy eigenvalues of the states:

$$E_\alpha - E_\beta \neq E_{\alpha'} - E_{\beta'}, \quad \text{unless} \quad \begin{cases} \text{either} & \alpha = \alpha' \text{ and } \beta = \beta', \\ \text{or} & \alpha = \beta \text{ and } \alpha' = \beta'. \end{cases}$$

In other words, if there are no degeneracies in energy differences. Furthermore, requiring that time- and micro-canonical averages of the state vector agree also makes necessary the absence of degeneracies between the energies themselves,  $E_\alpha \neq E_\beta$  for  $\alpha \neq \beta$ . von Neumann points out, however, that this condition is too stringent. After all, knowing all energy eigenvalues and specifying the energy surface amounts to complete and exact knowledge of the system, while the essence of an ergodic theorem should lie not in the knowledge of exact trajectories on an energy surface, but rather in the agreement between time-averages and ensemble averages (in line with classical notions). Until now, we have altogether neglected the role of the macroscopic.

We now adopt this viewpoint, and fall back onto the maxim ‘time averages equal space averages’ to state that *quantum ergodicity is realized when the long-time ( $t \rightarrow \infty$ ) average  $|\psi(t)\rangle \langle \psi(t)|$  equals the value predicted by the microcanonical ensemble*:

$$\boxed{|\psi(t)\rangle \langle \psi(t)| = \rho_{mc}}, \quad (\text{QE, states})$$

where  $\rho_{mc}$  is the microcanonical density matrix. This is a natural way to think about quantum ergodicity, because the notion of all microstates in a given energy shell occurring with equal probability maps onto the classical idea of spending equal amounts of time in all regions of the phase space.

(QE, states) holds naturally for wavefunctions with  $|c_\alpha|^2 = 1/D \forall \alpha$ , which obviously occupy a very niche position in the space of all possible wavefunctions. von Neumann [122] however proved in what became known as the **quantum ergodic theorem** (QET) that, in many cases, it is still true for *all* initial wavefunctions  $\psi_0$  with  $\|\psi_0\|^2 = 1$  that  $|\psi(t)\rangle \langle \psi(t)|$  is *macroscopically equivalent* to  $\rho_{mc}$ . By macroscopically equivalent, we mean equivalence after course-graining, i.e. after splitting the Hilbert space into subspaces that are large on the microscopic scale (contain many eigenvalues) but small on the macroscopic scale (different energies in the interval are not discriminated).

We will only state von Neumann’s ergodic theorem informally and clarify its meaning.

**Theorem 2.4** (QET, informal [50]) *Let  $\mathcal{H}$  be a Hilbert space of dimension  $D$  and let  $\mathcal{H} = \bigoplus_\nu \mathcal{H}_\nu$  be its decomposition into mutually orthogonal subspaces  $\mathcal{H}_\nu$  with  $d_\nu = \dim \mathcal{H}_\nu$  (such that  $D = \sum_\nu d_\nu$ ), so-called ‘macro-spaces’. Let  $P_\nu$  be the projector onto  $\mathcal{H}_\nu$ . We call a system normal if, for most times  $t$  in the long run,*

$$\|P_\nu \psi(t)\|^2 \approx \frac{d_\nu}{D}. \quad (12)$$

*For a finite-dimensional Hilbert space with no degeneracies and no resonances, provided the  $d_\nu$  are sufficiently large, most families  $\mathcal{D} = \{\mathcal{H}_\nu\}$  of mutually orthogonal subspaces of  $\mathcal{H}$  will satisfy (12) for every  $\nu$  and every wavefunction  $\psi_0 \in \mathcal{H}$  with  $\|\psi_0\| = 1$ .*

For a rigorous statement and proof of von Neumann’s QET, see von Neumann [122] or Goldstein et al. [50], particularly Section 5. Goldstein et al. [50] also eventually relax the assumption that  $d_\nu \ll D \forall \nu$  – a requirement that is implicit in Theorem 2.4, but features in the full version of the QET – and expand its range of validity to a stronger sense of normality.

Conceptually speaking, eq. (12) expresses what fraction of the total number of Hilbert space states  $D$  is found in one of the orthogonal subspaces, and it says that if we compute the probability of the late-time wavefunction to be in the subspace  $\mathcal{H}_\nu$  by projecting it onto this subspace and taking the square of its norm, we should approximately find this fraction. The connection with statistical physics and in particular with eq. (QE, states) lies in the fact that if the system is in a microcanonical ensemble, we expect to find the density matrix of a maximally mixed state, i.e.  $\rho_{mc} \propto \mathbb{1}$  with  $\rho_{mc}^{ii} = 1/D$ . After course-graining, we therefore expect the probability to find the system in a given subspace to be proportional to the dimension of the subspace, and this is what eq. (12) embodies.

To make progress, we change perspectives from states to observables, and formulate time evolution in terms of matrix elements of individual operators. This shift may seem quite remarkable, but it is not surprising from a historical perspective when considering that most of the substance leading up to von Neumann's QET is formulated in terms of matrix elements. As before, we consider (unitary) time evolution, but now applied to the expectation value of an observable  $O(x)$ :

$$\langle O(x, t) \rangle = \sum_{\alpha, \beta} c_{\alpha}^* c_{\beta} \langle \alpha | O(x) | \beta \rangle e^{i(E_{\alpha} - E_{\beta})t},$$

The time average of this expectation value in the large time ( $t \rightarrow \infty$ ) limit is:

$$\overline{\langle O(x) \rangle} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle O(x, t) \rangle dt \simeq \sum_{\alpha} |c_{\alpha}|^2 \langle \alpha | O(x) | \alpha \rangle + \sum_{\alpha \neq \beta} c_{\alpha}^* c_{\beta} \langle \alpha | O(x) | \beta \rangle \delta_{E_{\alpha}, E_{\beta}} + 0,$$

where we keep the same terms for the same reasons.

Assuming the distribution of the  $|c_{\alpha}|^2$  is sufficiently narrow in energy – such that we can coarse-grain the spectrum on energy shells of width  $\Delta E$  that are small on macroscopic scales but sufficiently large to contain many states, we can come up with a counterpart to (QE, states), and ask ourselves the question under what conditions the following equality holds:

$$\boxed{\sum_{\alpha} |c_{\alpha}|^2 \langle \alpha | O(x) | \alpha \rangle \stackrel{?}{=} \sum_{E \leq E_{\alpha} < E + \Delta} \frac{1}{\mathcal{N}} \langle \alpha | O(x) | \alpha \rangle}, \quad (\text{QE, observables})$$

where  $\mathcal{N}$  is the number of states in the energy-shell  $[E, E + \Delta)$ . Mossel [87] and Rigol, Dunjko, and Olshanii [98] formulate three scenarios that satisfy (QE, observables):

1. As before, it could be that the coefficients  $c_n$  are constant for equal energies within the band, namely  $|c_{\alpha}|^2 = 1/\mathcal{N}$ .
2. The expectation values  $\langle \alpha | O(x) | \alpha \rangle$  are approximately constant in the shell  $[E, E + \Delta)$ .
3. The fluctuations in the coefficients  $c_{\alpha}$  and expectation values  $\langle \alpha | O(x) | \alpha \rangle$  are uncorrelated.

It is quite clear that the first scenario applies only to a narrow subset of initial states, and it is therefore disfavored to explain the thermalization of an arbitrary initial state.

The third scenario corresponds to a broad range of physical states in which the coefficients  $c_n$  exhibit large fluctuations between eigenstates. The summation then amounts to what is effectively an unbiased sampling of the matrix elements  $\langle \alpha | O(x) | \alpha \rangle$  over the energy band, since the coefficients and the  $\langle \alpha | O(x) | \alpha \rangle$  are uncorrelated by assumption. If the system is large enough, one obtains a value close to the true mean of the expectation value, in agreement with the prediction of the microcanonical ensemble. This approach has been verified to provide an alternative path to thermalization for certain initial states of one-dimensional lattice systems with hard-core bosons and spinless fermions that – crucially – obey the required conditions imposed by scenario 2 before a quantum quench is performed [99]. Yet again, however, it does not account for the thermalization of arbitrary initial states.

The second scenario, which goes by the name of the **eigenstate thermalization hypothesis** (ETH) [110, 32], turns out to be much better equipped to deal with arbitrary initial states. In fact, it deals with all initial states narrow in energy. The required conditions for the ETH to hold can be refined as follows [99]:

- The diagonal matrix elements  $\langle \alpha | O(x) | \alpha \rangle$  should vary smoothly with energy, and the difference between neighbouring values,  $\langle \alpha + 1 | O(x) | \alpha + 1 \rangle - \langle \alpha | O(x) | \alpha \rangle$  should vanish exponentially with system size.
- Off-diagonal matrix elements  $\langle \alpha | O(x) | \beta \rangle$  with  $\alpha \neq \beta$  should be much smaller than diagonal matrix elements, and should themselves vanish exponentially with system size.

To appreciate why these conditions apply to a significantly broader class of initial states, Rigol, Dunjko, and Olshanii [98] argue that any initial state is in fact a superposition of thermal states, but that coherences between the thermal states obscure its thermal nature. Given enough time, dephasing (the suppression of the non-diagonal elements) gets rid of the coherences and reveals the thermal state, see Figure 9. If theoretical conjecture does not convince you, it will help to know that the ETH has been experimentally verified to hold for a large number of physical systems. In addition, rigorous proofs have been provided in special limits, for example in the semiclassical limit of certain quantum systems whose classical counterparts are chaotic [104, 123].

#### Note: Quantum coherences

Quantum coherence is a term that is often mentioned but is rarely defined. The intuition behind quantum coherence comes from classical wave mechanics: a constant phase shift between waves. It refers to a constant phase shift between two states. In quantum mechanics, a coherent superposition of two states,  $\psi_1$  and  $\psi_2$ , is represented by a global state

$$\Psi = A(\psi_1 + Be^{i\phi}\psi_2),$$

where  $A \in \mathbb{C}$  and  $B \in \mathbb{R}$ ,  $B > 0$ . The difference in phase between  $\psi_1$  and  $\psi_2$  in this superposition is  $\phi$ . This is a coherent superposition, *even if  $\phi$  is not constant in time*. The density matrix of  $\Psi$  has off-diagonal elements. Decoherence erases the off-diagonals.

#### Example

Consider two basis states  $|0\rangle$  and  $|1\rangle$ , and the state  $|c\rangle = \frac{1}{\sqrt{2}}(|0\rangle + e^{i\phi}|1\rangle)$ .  $|c\rangle$  is a (normalized) coherent state as long as the phase  $\phi$  is constant everywhere. The density matrix is

$$\rho = \frac{1}{2} \begin{pmatrix} 1 & e^{i\phi} \\ e^{-i\phi} & 1 \end{pmatrix}.$$

Now suppose the phase  $\phi$  is random, so the mean expectation value of  $e^{i\phi}$  is zero, and the off-diagonal elements vanish. The new density matrix does not represent a coherent state anymore.

Note that the density matrix depends on the choice of basis, and that every density matrix can be diagonalized. When we say ‘coherence between (orthogonal) states  $|\alpha\rangle$  and  $|\beta\rangle$ ’, it means that we are looking at the density matrix in a basis containing these two vectors. In other words, the coherence between  $|\alpha\rangle$  and  $|\beta\rangle$  is the matrix element

$$\langle\alpha|\rho|\beta\rangle.$$

Confusingly enough, a *coherent state* carries the meaning of a state that closely resembles the specific quantum state of the quantum harmonic oscillator, and therefore does not relate directly to the considerations outlined here.

Note that the ETH only makes statements about specific observables, and does so on a case-by-case basis; it does not purport to apply to every observable in a system, unlike the context in which we discussed classical ergodicity – at the global/system level. Indeed, one can always trivially construct operators that (dis)obey the ETH by writing down a matrix in which the elements explicitly (dis)obey the requirements set out by the ETH. However, one should of course bear in mind the physical relevance of such operators. Typically, the ETH is applied to few-body (but not necessarily local) operators [99].

Another fundamental difference between ergodicity at the quantum level and classical ergodicity is the fact that quantum ergodicity really only makes sense in the infinite size (thermodynamic) limit, where the system’s spectrum becomes continuous. In a finite-size system (with a discrete spectrum), the quantum analogue of the Poincaré recurrence theorem dictates that an observable eventually returns arbitrarily close

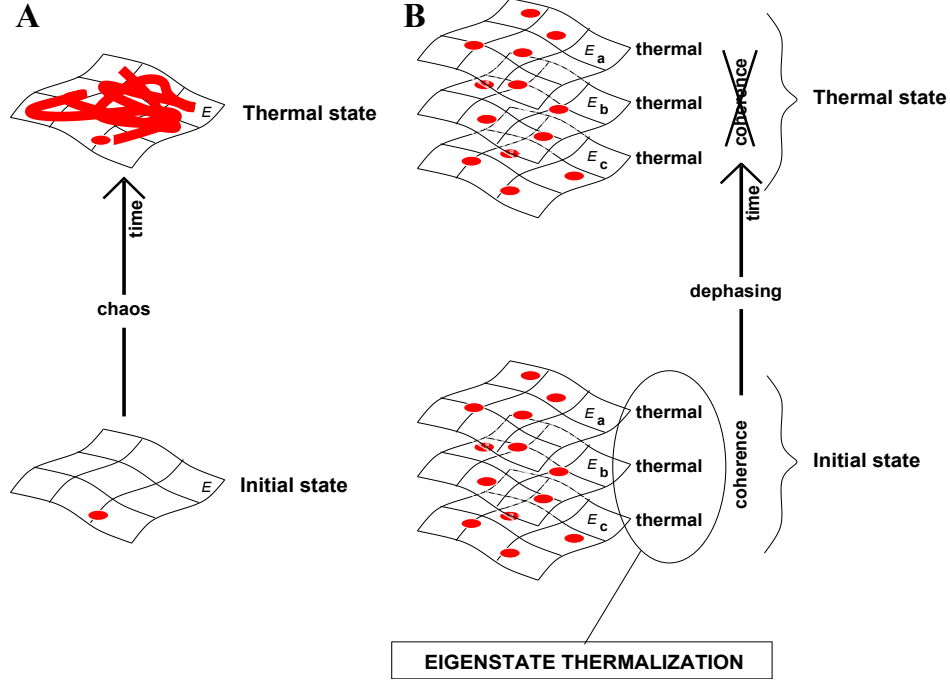


Figure 9: Illustration of the conjectured mechanism underlying the eigenstate thermalization hypothesis. In classical mechanics (left), an initial state thermalizes over time because of chaotic dynamics. In quantum mechanics (right) every eigenstate of the Hamiltonian is a superposition of thermal states that are initially not distinguishable as such because of coherences. Time evolution destroys these coherences and reveals the thermal nature. Figure taken from [98].

to its initial state, and this messes up the smooth correspondence between time-averages and ensemble averages for every observable. The ETH, although experimentally verified in finite-size systems, also has the clearest interpretation in the  $N \rightarrow \infty$  limit: we have seen that off-diagonal elements vanish exponentially with system size. In other words, the ETH becomes an exact statement in the thermodynamic limit.

Interestingly, quantum systems with a large number of conserved charges, which, for the time being, we will take as meaning quantum integrable, are known to violate the ETH for the intuitive reason that the presence of many conserved charges restrains the dynamics to the extent that relaxation to a thermal state is impossible. Instead, it has been suggested that integrable systems reach a state described by a *generalized Gibbs ensemble* (GGE) – this is sometimes called the ‘generalized ETH’, and has been experimentally confirmed in various integrable systems [100, 60, 124].

#### Why is it called thermalization?

The ETH puts forth restrictions on the matrix elements of observables under which the long-time average value of the observable will equal the value predicted by the *microcanonical ensemble*. Yet in the context (and in the name) of the ETH, we speak about *thermalization*, which in textbook interpretations means progressing towards a state that is accurately described by the *canonical ensemble*. The resolution is simple: the ETH deals with closed, isolated quantum systems evolving under unitary dynamics. In such a system, there is no isolated heat bath or energy exchange, and the relevant statistical ensemble is therefore the microcanonical ensemble (which is really just the limiting case of the canonical ensemble at fixed energy).

### 2.4.2. A better definition of quantum integrability

We already explained how the lack of a phase-space structure in quantum mechanics makes a straightforward translation of classical to quantum ergodicity impossible. Without a clear phase space structure, it should be obvious that Liouville integrability will not survive the classical to quantum transition. If this is not bad enough for you yet, consider a consequence of the Hilbert space structure of quantum mechanics that further complicates matters: unlike classical degrees of freedom, which are additive, the Hilbert space structure of quantum mechanics demands that quantum mechanical degrees of freedom in composite systems be combined through the tensor product of individual Hilbert spaces. In all but the most simple quantum systems, we can therefore not count degrees of freedom in the same way as we would for an arbitrarily complicated classical system. This should be the final nail in the coffin for any attempt at a naive translation of Liouville integrability to quantum mechanics.

In spite of these concerns, many authors – even today – seek to define quantum integrability by simply extending the definition of classical integrability to the quantum domain, replacing Poisson brackets with commutators and promoting the conserved charges to operators. The definition will state something like this:

**Definition 2.9 (Naive QI!)** *A system is quantum integrable if it has a maximal set of independent commuting conserved charges  $\mathcal{Q}_\alpha$ ,  $\alpha = 1, \dots, \dim(\mathcal{H})$ .*

This definition has no predictive power whatsoever, as can be seen from a very simple argument:

- The spectral theorem tells us that any (Hermitian) Hamiltonian is diagonalizable;
- We can then find  $\dim(\mathcal{H})$  orthogonal state vectors  $|\Psi_\alpha\rangle$  (where  $\mathcal{H}$  denotes the Hilbert space) and build the projectors  $\mathcal{Q}_\alpha = |\Psi_\alpha\rangle\langle\Psi_\alpha|$ ;
- This constitutes a maximal commuting set;
- We found that all quantum models with  $\dim(\mathcal{H}) < \infty$  are integrable!

The problem with this approach to integrability is that construction of  $\dim(\mathcal{H})$  conserved charges defies the philosophy underlying what an integrable system should be. From an information theory perspective, the ‘fundamental merit of integrability’ should be that it enables us to completely specify the system with *less* information than is necessary to fully specify a generic, ‘unstructured’ system, which has a Hilbert space that scales exponentially with system size:  $\dim(\mathcal{H}) \propto \exp(N)$ . If we adopt the approach above, *there would be nothing special about an integrable system whatsoever*: there is no requirement for additional structure that – from an information theory point of view – could allow us to specify the system with an amount of information that scales subexponentially with system size. As we want to somehow incorporate the fundamental merit of integrability, we will need our definition to be far more restrictive. In particular, it is imperative to impose conditions on the *structure* and the *counting* of the charges.

Note: Local vs. global charges and maximality

In literature, quantum integrability is often phrased as having a ‘maximal set of local charges’. Local charges can be expressed as a sum (or integral) of spatially localized densities. The ‘degree of locality’ of the charge can be deduced from the number of summations necessary to specify it; e.g., a Hamiltonian with nearest neighbour interactions involves a single summation over sites of simple operator combinations. The reason for considering local and not global charges is that local charges are far more restrictive and more plentiful than the (often few) available global charges. Global charges, which are those that are effectively taken care of by the global symmetries of the model (Noether’s theorem), only provide information about the state of the system as a whole; they do not restrict intricate local interactions and scattering processes in the same manner as do local charges. A system can have a few globally conserved quantities and still exhibit ergodic behaviour. In other words, global charges are too coarse-grained to ‘tame’ the complexity of many-body quantum physics. On a related note, Caux and Mossel [21] argue that the the notion of locality and maximality (or

completeness) are contradictory, since enforcing locality restricts the number of conserved charges to be far smaller than the required number for maximality,  $\dim(\mathcal{H})$ . It is mentioned that the misconception probably arose from integrable quantum field theory literature, where sometimes an infinite set of conserved charges is confused with a maximal one.

Following Caux and Mossel [21], we can channel this spirit into the following set of requirements that any definition of quantum integrability should satisfy:

1. It should be unambiguous;
2. It should partition the set of all possible quantum models into distinct classes;
3. It should make different classes of models display distinguishable physical behaviour.

The definition of quantum integrability proposed by Caux and Mossel [21] is subject to the following preliminary constructs:

- A size sequence is defined as an infinite sequence of strictly increasing integers, i.e.  $(N_1, N_2, N_3, \dots)$  with  $N_1 < N_2 < N_3 < \dots$
- A Hilbert space  $\mathcal{H}^{(N_a)}$  is associated to each size  $N_a$  in the sequence. This Hilbert space is constructed by tensoring  $N_a$  elemental Hilbert spaces  $\mathcal{H}_j$ ,  $j = 1, \dots, N_a$ , which are all assumed to be finite-dimensional,  $\dim(\mathcal{H}_j) \equiv d_j < \infty$ . As a consequence,  $\dim(\mathcal{H}^{(N_a)}) = \prod_{j=1}^{N_a} d_j \equiv d^{(N_a)}$  is also finite.
- Operators in the Hilbert space  $\mathcal{H}_j$  can be represented by Hermitian matrices of size  $d_j \times d_j$ . These can be decomposed in a basis  $\mathbf{e}_j^i$ ,  $i = 1, \dots, d_j^2$ . Likewise, operators  $\mathcal{Q}^{(N_a)}$  in  $\mathcal{H}^{(N_a)}$  can be decomposed in the  $(d^{(N_a)})^2$  basis matrices  $\mathbf{e}^{i_1 \dots i_{N_a}} \equiv \otimes_{j=1}^{N_a} \mathbf{e}_j^{i_j}$  (the *preferred basis*),  $\mathcal{Q}^{(N_a)} = \sum_{i_1, \dots, i_{N_a}} \mathcal{Q}_{i_1 \dots i_{N_a}}^{(N_a)}$ .
- Given an operator  $\mathcal{Q}$  in a preferred basis  $\mathbf{e}^{i_1 \dots i_{N_a}}$ , the number of nonzero entries  $\mathcal{Q}_{i_1 \dots i_{N_a}}^{(N_a)}$  is denoted as  $N_e(\mathcal{Q}^{(N_a)})$ . The *density character* for a size sequence of operators  $(\mathcal{Q}^{(N_1)}, \mathcal{Q}^{(N_2)}, \dots)$ , is defined as the nature<sup>12</sup> of the minimal function  $f(N_a)$  that at each size of the size sequence is bounded from below by the number of nonzero entries, i.e.  $N_e(\mathcal{Q}^{(N_a)}) < f(N_a) \forall a$ .
- Starting from the Hilbert spaces  $\mathcal{H}^{(N_a)}$ , through some simple and meaningful<sup>13</sup> algorithm  $\mathcal{A} : \mathcal{H}^{(N_a)} \rightarrow \mathcal{H}^{(N_a)}$ , a corresponding size sequence of Hermitian operators  $(H^{(N_1)}, H^{(N_2)}, \dots)$  is defined, which have the interpretation of Hamiltonians. Furthermore, the Hamiltonians are restricted to the polynomial density character class, i.e. Hamiltonians which can be expressed in terms of a finite number of sums over elemental labels.
- Each Hamiltonian  $H^{(N_a)}$ , being Hermitian and finite, obeys the spectral theorem. This implies the existence of a maximal set of conserved charges  $\{\mathcal{Q}_\alpha^{(N_a)}\}$ ,  $\alpha = 1, \dots, d^{(N_a)}$  in involution. The labeling of the charges is chosen in such a way to create meaningful finite size sequences  $(\mathcal{Q}_\alpha^{(N_a)}, \mathcal{Q}_\alpha^{(N_a+1)}, \dots)$ , for all individual  $\mathcal{Q}_\alpha^{(N_a)}$  with  $\alpha = 1, \dots, \alpha_{max} \leq d^{(N_a)}$ .

These preliminary constructs have been organized in Figure 10.

<sup>12</sup>Linear, polynomial, exponential, etc.

<sup>13</sup>I am not sure if I fully understood the implications of ‘simple and meaningful’, but the way I interpret the statement is that the algorithm should preserve essential physics as the system size changes. For example, interactions should retain their character, coupling constants should be independent of system size and the algorithm should ensure that the sequence of Hamiltonians converges to a well-defined and physically sensible model in the thermodynamic limit.

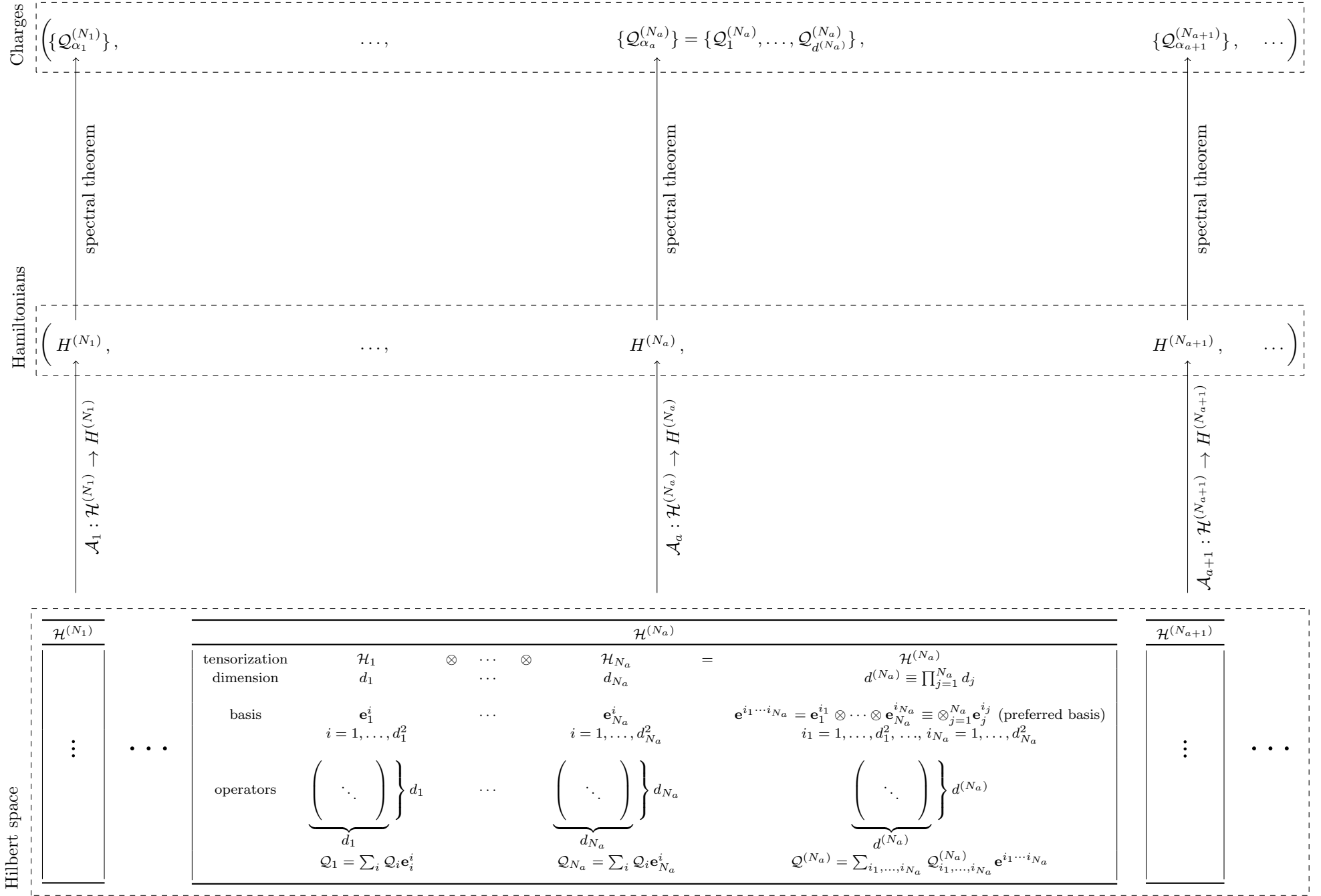


Figure 10: Preliminary constructs leading up to the definition of quantum integrability proposed by Caux and Mossel [21].



The new definition is formulated as follows:

**Definition 2.10** (Quantum integrability) *A Hamiltonian  $H$  is called  $O(f(N))$  quantum integrable if it is a member of a sequence  $(H^{(N_1)}, H^{(N_2)}, \dots)$  of operators having  $O(f(N))$  density character in the preferred basis, for which it is possible to define a sequence of sets of operators  $(\{\mathcal{Q}^{(N_1)}\}, \{\mathcal{Q}^{(N_2)}\}, \dots)$  such that*

- *all operators  $\mathcal{Q}_\alpha^{(N_a)}$  in  $\{\mathcal{Q}^{(N_a)}\}$  commute with each other and with their Hamiltonian  $H^{(N_a)}$ ;*
- *the operators in  $\{\mathcal{Q}^{(N_a)}\}$  are algebraically independent;*
- *the cardinality  $\mathcal{C}^{(N_a)}$  of the set  $\{\mathcal{Q}^{(N_a)}\}$  becomes unbounded in the infinite size limit;*
- *each member  $\mathcal{Q}_\alpha^{(N_a)}$ ,  $\alpha = 1, \dots, \mathcal{C}^{(N_a)}$  can be embedded within a sequence of operators  $(\mathcal{Q}_\alpha^{(N_1)}, \mathcal{Q}_\alpha^{(N_2)}, \dots)$  with  $O(f(N))$  density character in the preferred basis.*

The **first** requirement also features in the naive definition and is the analogue of involution from Liouville integrability in classical systems. Note that algebraic (and not linear) independence is put forth as a **second** requirement. The underlying reason is subtle but consequential, and to illustrate it we revert to the projectors: projectors  $\{P_i\}$  onto eigenstates, while linearly independent, are not algebraically independent since  $P_i P_j = 0$  for  $i \neq j$ . We want a notion more like functional independence, e.g. maybe the operators should not have low-degree polynomial relations. The **third** requirement is put in place to strongly constrain the dynamics even in the thermodynamic limit, where the presence of only a handful (any finite number) of conserved charges would not be sufficiently restrictive.

One of the key merits of this definition is that it does away with the binary notion of quantum integrability and replaces it with a classification based on the density character of the sequence of operators its Hamiltonian is embedded in, which is reflected in the **fourth** requirement.<sup>14</sup> Note that *any* model fulfilling the naive definition of quantum integrability can be found in some integrability class, and generically the charges will have exponential density character. It is therefore understood that a model is quantum integrable if it is at least subexponentially integrable, and otherwise we call it non-integrable.

**Physical interpretation** Caux and Mossel [21] make physical sense of the Definition 2.10 by making contact with ergodic properties, and in particular through *Mazur's inequality*: consider the operator  $A$  and the canonical average  $\langle \Delta A(0) \Delta A(t) \rangle$ , where  $\Delta A = A - \langle A \rangle$ . If  $\{\bar{\mathcal{Q}}_\alpha\}$ ,  $\alpha = 1, \dots, N_{\bar{\mathcal{Q}}}$  is a set of constants of motion, the long-time average obeys

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \langle \Delta A(0) \Delta A(t) \rangle \geq \sum_{\alpha=1}^{N_{\bar{\mathcal{Q}}}} \frac{|\langle (\Delta A) \bar{\mathcal{Q}}_\alpha \rangle|^2}{\langle \bar{\mathcal{Q}}_\alpha^2 \rangle}. \quad (13)$$

Here, the charges are defined to be ‘orthogonal’ for the chosen form of averaging (hence the notation with the bar, to set them apart from the charges we previously encountered, which are not constrained by this requirement):

$$\langle \bar{\mathcal{Q}}_\alpha \bar{\mathcal{Q}}_\beta \rangle = \delta_{\alpha\beta} \langle \bar{\mathcal{Q}}_\alpha^2 \rangle, \quad (14)$$

and equality is obtained if the set of charges is maximal.

#### Heuristic derivation

Since it seems that Mazur’s inequality is relatively unknown and certainly not within the scope of many standard textbooks, we will outline the arguments that underpin it, based on the original paper by Mazur from 1969 [82]. The inequality is derived for classical systems but generalizes to quantum mechanical systems in a straightforward manner.

We consider a dynamical function of canonical variables  $q_i, p_i$ ,  $i \in \{1, \dots, n\}$ :

$$X(t) = X(q_1(t), \dots, q_n(t), p_1(t), \dots, p_n(t)),$$

described by the Hamiltonian  $H(q_1, \dots, p_n)$ . We assume, without loss of generality, that

<sup>14</sup>J.-S. Caux tried to make this clear to me with the following quote: “All regularizable quantum models are integrable, but some are more integrable than others.”



- The canonical average of  $X$  is zero:  $\langle X \rangle = \frac{1}{Z(\beta)} \int d\Gamma e^{-\beta H} X = 0$ , where  $d\Gamma = dq_1 \cdots dq_n dp_1 \cdots dp_n$  is the phase space volume element and  $Z(\beta) = \int d\Gamma e^{-\beta H}$  is the partition function;
- $X^2$  is normalized to one:  $\langle X^2 \rangle = 1$ .

We denote by  $\langle X \rangle_{mc}$  the microcanonical average of  $X$ :

$$\langle X \rangle_{mc} \equiv \bar{X}(E) = \frac{1}{\Omega(E)} \int d\Gamma \delta(H - E) X,$$

where  $\Omega(E) = \int d\Gamma \delta(H - E)$  is the structure function of the system. It follows, from the assumption that  $\langle X \rangle = 0$ , that

$$\begin{aligned} \langle X \rangle &= \frac{1}{Z(\beta)} \int dE e^{-\beta E} \int d\Gamma \delta(H - E) X \\ &= \frac{1}{Z(\beta)} \int e^{-\beta E} \Omega(E) \bar{X}(E) dE = \int P(E) \bar{X}(E) dE = \langle \bar{X}(E) \rangle = 0, \end{aligned} \quad (15)$$

where  $P(E) = Z(\beta)^{-1} e^{-\beta E} \Omega(E)$  is the energy frequency distribution in the canonical ensemble, with  $\int dE P(E) = 1$ .

The derivation of Mazur's inequality is based on two theorems by Khinchine [65, 66]:

**Theorem 2.5** *Let  $Y(t)$  be an arbitrary dynamical function.*

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle Y(0) Y(t) \rangle dt = F(0^+) - F(0^-) \geq 0, \quad (16)$$

where  $F(\omega)$  is the spectrum of  $Y(t)$ , defined through the Fourier-Stieltjes representation of the autocorrelation function  $\langle Y(0) Y(t) \rangle$ :  $F(\omega) = \int_{-\infty}^{+\infty} e^{it\omega} d\langle Y(0) Y(t) \rangle$ .

A small point of attention: since the autocorrelation function  $\langle Y(0) Y(t) \rangle$  is positive definite, and we furthermore assume it is continuous in  $t$ , Bochner's theorem guarantees the existence of a non-negative measure to be identified with  $dF(\omega)$ , which in turn guarantees that the spectral function  $F(\omega)$  is non-decreasing; because  $F(\omega)$  is furthermore finite, it is of bounded variation. This is enough to proof existence of the Fourier-Stieltjes representation.

**Theorem 2.6** *Let  $Y(t) = X(t) - \bar{X}(E)$ . For almost all initial conditions on the surface of constant energy  $E$ , we have*

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle Y(0) Y(t) \rangle_{mc} dt = 0 \iff \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T Y(t) dt = 0, \quad (17)$$

such that the variable  $X(t)$  is ergodic in the sense of Section 2.3.1 (equality of ensemble averages and microcanonical prediction in the long-time limit):

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T X(t) dt = \bar{X}(E).$$

Note that this means that we can consider the condition on the lhs of (17) for the vanishing of the long-time average of the autocorrelation function in the microcanonical ensemble as another sufficient condition for ergodicity.

The autocorrelation obeys

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle X(0) X(t) \rangle dt = \int dE P(E) \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle X(0) X(t) \rangle_{mc} dt = \langle \bar{X}^2(E) \rangle, \quad (18)$$

where the physical justification for the first equality is to consider the expectation values in the micro-canonical ensemble (at fixed energy) and then to integrate over all possible energies with appropriate weight given by the distribution  $P(E)$ . The second equality follows from (17) when we realize that, written out, it says that

$$\begin{aligned} \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle Y(0)Y(t) \rangle_{mc} dt &= \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle (X(0) - \bar{X}(E))(X(t) - \bar{X}(E)) \rangle_{mc} dt \\ &= \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \left[ \langle X(0)X(t) \rangle_{mc} + \langle -X(0)\bar{X}(E) - \bar{X}(E)X(t) \rangle_{mc} + \langle \bar{X}^2(E) \rangle_{mc} \right] dt = 0. \end{aligned}$$

The term  $\langle -X(0)\bar{X}(E) - \bar{X}(E)X(t) \rangle_{mc}$  can be seen to vanish if integrated over  $E$  weighted by  $P(E)$  because of (15), which leaves us with the required relation between  $\langle X(0)X(t) \rangle_{mc}$  and  $\langle \bar{X}^2(E) \rangle_{mc}$  (up to a sign).

Furthermore, the quantity  $\langle \bar{X}(E) \rangle$  obeys the inequality<sup>a</sup>

$$\left\langle \left[ \bar{X}(E) - \frac{\langle X \Delta H \rangle}{\langle (\Delta H)^2 \rangle} \Delta H \right]^2 \right\rangle \geq 0, \quad \Delta H = H - \langle H \rangle,$$

which justifies the Schwartz inequality:

$$\langle \bar{X}^2(E) \rangle \geq -\frac{\langle X \Delta H \rangle^2}{\langle (\Delta H)^2 \rangle^2} \langle (\Delta H)^2 \rangle + 2 \frac{\langle X \Delta H \rangle}{\langle (\Delta H)^2 \rangle} \langle \bar{X}(E) \Delta H \rangle \geq \frac{\langle X \Delta H \rangle^2}{\langle (\Delta H)^2 \rangle},$$

since  $\langle \bar{X}(E) \Delta H \rangle = \bar{X}(E) \langle H - \langle H \rangle \rangle = 0$ . It can be shown that this is in fact an *equality*:

$$\langle \bar{X}^2(E) \rangle = \frac{\langle X \Delta H \rangle^2}{\langle (\Delta H)^2 \rangle},$$

which means that we can write (18) as

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle X(0)X(t) \rangle dt = \frac{\langle X \Delta H \rangle^2}{\langle (\Delta H)^2 \rangle}.$$

The lower bound on the time-average of the autocorrelation function is derived schematically as follows:

- Assume the existence of a set of constants of motion, including the Hamiltonian,  $A_1(q_1, \dots, p_n), \dots, A_m(q_1, \dots, p_n)$ , where we take  $A_1 = \Delta H$  and  $\langle A_i \rangle = 0, i = 1, \dots, m$ ;
- Rewrite the autocorrelation function in terms of a dynamical function of the constants of motion,  $Z(q_1, \dots, p_n) = X(q_1, \dots, p_n) - \sum_k c_k A_k(q_1, \dots, p_n) = X - \mathbf{c} \cdot \mathbf{A}$ , where  $\mathbf{c}$  is a vector of constants;
- By virtue of (16), we see that

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle Z(0)Z(t) \rangle dt = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle (X(0) - \mathbf{c} \cdot \mathbf{A})(X(t) - \mathbf{c} \cdot \mathbf{A}) \rangle dt \geq 0,$$

and this implies

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle X(0)X(t) \rangle dt \geq -\mathbf{c} \cdot \langle \mathbf{A} \mathbf{A} \rangle \cdot \mathbf{c} + 2\mathbf{c} \cdot \langle X \mathbf{A} \rangle.$$

- After maximizing the rhs and applying a linear transformation  $\mathbf{A}' = S \cdot \mathbf{A}$  to the functions  $A_1, \dots, A_m$ , choosing  $S$  such that  $A'_1 = A_1 = \Delta H$  and  $\langle A'_i A'_j \rangle = \langle A_i^2 \rangle \delta_{ij}$ , we arrive at the desired inequality:

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle X(0)X(t) \rangle dt \geq \sum_{k=1}^m \frac{\langle X A'_k \rangle^2}{\langle A_k'^2 \rangle} \geq \frac{\langle X \Delta H \rangle^2}{\langle (\Delta H)^2 \rangle}.$$

<sup>a</sup>For the trivial reason that it represents the expectation value of the square of a difference of numbers.

The operator  $A$  is called *ergodic* (in the Mazur sense)<sup>15</sup> if

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \langle \Delta A(0) \Delta A(t) \rangle = 0, \quad (19)$$

i.e. if long-time correlations average out. In light of the bound (13), this means that  $A$  is orthogonal to *all* the conserved charges – since even a slight overlap would result in a nonzero right hand side and hence the long-time average correlation would have to be at least this large.

If we generalize the canonical average  $\langle \cdot \rangle$  to a generic energy-diagonal expectation value  $\langle \cdot \rangle_{\mathbf{f}} \equiv \frac{1}{Z_{\mathbf{f}}} \sum_{\alpha} f_{\alpha} \langle \alpha | \cdot | \alpha \rangle$ , with the partition function a sum of specified real-valued parameters,  $Z_{\mathbf{f}} \equiv \sum_{\alpha} f_{\alpha}$ , we can consider physically meaningful operators (expressed in the preferred basis)  $A = \sum_{i_1, \dots, i_N} A_{i_1 \dots i_N} \mathbf{e}^{i_1 \dots i_N}$  and consider building the terms  $|\langle (\Delta A) \bar{Q}_{\alpha} \rangle_{\mathbf{f}}|$  on the right-hand side of Mazur’s inequality (13). For an orthogonal set of charges obeying eq. (14) it is possible to write

$$A = \sum_{\alpha} a_{\alpha} \bar{Q}_{\alpha} + A', \quad \text{with } a_{\alpha} = \frac{\langle (\Delta A) \bar{Q}_{\alpha} \rangle_{\mathbf{f}}}{\langle \bar{Q}_{\alpha}^2 \rangle_{\mathbf{f}}},$$

with  $A'$  an off-diagonal operator (in the energy basis) which therefore does not contribute to eq. (13). The overlap coefficients  $a_{\alpha}$  are then simply related to the right-hand side of Mazur’s inequality. This is enough to come full circle and relate the definition of quantum integrability according to Caux and Mossel [21] to ergodicity in the Mazur sense:

- In a generic non-integrable model, the charges  $Q_{\alpha}$  have exponential density character. Any such charge  $Q_{\alpha_1}$  can be used as a basis for the set  $\bar{Q}_{\alpha}$  of orthogonal charges, and will have an exponentially small overlap coefficient  $a_{\alpha_1}$ . A second charge  $\bar{Q}_{\alpha_2}$  that has been orthogonalized w.r.t.  $\bar{Q}_{\alpha_1}$  in order to satisfy eq. (14) will then have vanishing overlap  $a_{\alpha_2}$  with the operator of interest  $A$ . Following the same argument, all other charges  $\bar{Q}_{\alpha_3}, \bar{Q}_{\alpha_4}, \dots$  will have vanishing overlaps  $a_{\alpha_3}, a_{\alpha_4}, \dots$ , and the operator  $A$  will be ergodic in the Mazur sense.
- In a linearly integrable model, the charges  $Q_{\alpha}$  can be written as single summations of local operator products, and an orthogonalization procedure does not change this, such that we may expect finite overlap coefficients. The same logic holds for any other subexponentially integrable model.

#### Note

For the interested reader, the remainder of the paper offers a second physical explanation of the proposed definition, based on the quantum quench procedure rather than the ergodic perspective. The idea of a quantum quench is to prepare a system in an eigenstate of  $H_{\lambda}$ , followed by instantaneously changing  $\lambda \rightarrow \lambda'$ . If  $[H_{\lambda}, H_{\lambda'}] \neq 0$ , one expects complicated non-equilibrium dynamics to ensue.

**Final remark** The defects that are inherent to the naive definition of quantum integrability, Definition 2.9, should be apparent by now. While its lack of physical grounding and its nondiscriminatory applicability has been rightfully addressed, I want to dedicate the final remark of this section to underline the pragmatical value of its contents for solving many ‘hands-on’ physics problems, when an obvious non-trivial choice for the conserved charges presents itself, and when the connection to the underlying physics is of minor importance.

The redeeming feature of the involution (commutation) requirement is that it *does* place strong constraints on the charges in all but the most contrived situations. Hence, the requirement that (a reasonable) set of charges be in involution has far-reaching consequences on its own, even if all the subtleties surrounding the further classification of the physical system are discarded, and for a typical setting this is often enough. An example of what I call a ‘typical setting’ is Dima and Faribault [35]. A set of charges with certain freedom in their parametrization presents itself naturally throughout the problem (here, it forms the starting point for the problem), and then Definition 2.9 is invoked to further constrain the charges by fixing the values

<sup>15</sup>Please note that ergodicity in the Mazur sense is declared at the level of *individual operators* (not at the system level) in the infinite size limit, as was also pointed out and motivated in the section on the ETH.

of the free parameters. Such ‘naive use of the naive definition’ seems legitimate to me if one’s interest is limited to these practical aspects, although it would probably be better to drop the name ‘integrability’ (and all the deeper associations it carries) in favour of something closer to the true meaning, such as ‘imposing involution’.

## 2.5. Truths and misconceptions about integrability

If there is one heuristic to remember from the previous assortment of definitions, facts and comments, let it be that conserved quantities put restrictions on the dynamics of a system, and that integrability means that the number of such conserved quantities is sufficiently plentiful for the system to behave in a ‘well-mannered’ way which lends itself to the application of analytical tools. In other words, it is as if the presence of the conserved quantities limits the wiggle room that the system has. In literature, there are many ways in which the notion of integrability is misrepreseted or used carelessly. To end our discussion, let us address some misconceptions, and also distill what we think to be true based on the contents of this section.

### Misconceptions about integrability

1. *“Integrability equals (exact) solvability.”* The statement is wrong in both directions. Complete integrability is far stronger than solvability of the initial value problem, since it implies the absence of chaotic orbits. More precisely, all bounded orbits in integrable systems are quasiperiodic: they lie on invariant tori. In light of the claim that complete integrability is far stronger than solvability, it comes as no surprise that the opposite direction (solvability implies integrability) does not hold either. For example, the simple harmonic oscillator with damping is perfectly solvable, but not Liouville integrable due to dissipation.
2. *“Integrability means being able to find a closed-form solution.”* This is categorically not true, and examples abound. As we will see in Section 3, the solution of the Lieb Liniger model, which is integrable by all reasonable definitions (linearly integrable in the sense discussed above), takes the form of a set of integral equations in the thermodynamic limit, that have to be solved numerically.
3. *“Integrability just means having a very large (infinite) number of conserved charges.”* While integrable systems are characterized by an extensive number of conserved charges, this requirement alone is not enough. As we have seen, every system in the thermodynamic limit admits an infinite number of conserved quantities in involution, namely the projectors constructed from eigenstates. One needs some more stringent restrictions on the conserved charges, such as those put forth by Caux and Mossel [21].

### Truths about integrability

1. *“Integrability is kind of the opposite of chaos.”* The underlying idea is that if we have an extensive number of conserved charges, we can describe macroscopic observables in terms of these unchanging entities, and the dynamics remain heavily constrained. This intuitively contradicts the notion of thermalization and chaos.
2. *“Non-integrable systems are ergodic.”* In the global sense, integrable systems cannot be ergodic. In quantum systems, the statement holds in the thermodynamic limit for physical operators, in the Mazur sense.

### 3. Lieb-Liniger model and open quantum systems

In this section, we study the Lieb-Liniger model: a system of bosons with hard-core interactions in one dimension. We discuss its repulsive and attractive regimes, and work towards a description of the model out of isolation, in an environment with dissipation or gain (an open quantum system). Open quantum systems are represented by non-Hermitian Hamiltonians, and we will construct such a Hamiltonian by adding a small imaginary part to the coupling of the Lieb-Liniger Hamiltonian. We will eventually use numerical methods to find eigenvalues of the Lindbladian superoperator for the Lieb-Liniger model with a simple, double-field dissipation term, using both the well-studied Coordinate Bethe Ansatz as well as relatively recent insights into the spectral structure of a certain class of open quantum systems.

**Why we care about  $1 + 1$  dimensions** All of the systems that we explore to some depth in this thesis have one spatial dimension. While ‘life on the line’ inevitably sacrifices some of the richness that comes only to higher dimensional systems – think topological order, spontaneous symmetry breaking and long-range order, and, in the context of field theories, non-trivial gauge field configurations like monopoles –, there are plenty of features that make up for the loss. An obvious advantage is the relative ease of working in lower dimensions as opposed to working in higher ones. Besides having fewer indices to run over and more generally less of a clutter when doing computations, toy models in  $1 + 1$  dimension often permit a non-perturbative treatment, which allows phenomena such as renormalization and asymptotic freedom to be described exactly [42]. In fact, some features occur exclusively in  $1 + 1$  dimension, such as the detachment from strict bosonic and fermionic behaviour that we will observe in the Lieb-Liniger model. Lastly, it is worth mentioning that systems in  $1 + 1$  dimension have found concrete experimental applications. The one-dimensional bosonic gas, for instance, has occupied a prominent place in experiments involving cold atoms. Efforts to back theoretical predictions related to the one-dimensional bosonic gas with experimental findings have been set in motion by D. Weiss et al. (2004) through the observation of a one-dimensional Tonks-Girardeau gas [68], and have since branched out to include such measurements as momentum-distribution profiles [93], quantum correlations [67], Yang-Yang thermodynamics [119] and dark solitons [63]. Common (ultra)cold atoms used in these experiments are  $^{87}\text{Rb}$ ,  $^{39}\text{K}$  and  $\text{Cs}$  [61], and it is typically possible to realize a wide range of interaction strengths via Feshbach resonances.

#### 3.1. Lieb-Liniger model

The Lieb-Liniger model describes a one-dimensional Bose gas with hard-core (Dirac delta) interactions. It provides fertile ground for exploring many of the unique features of  $1 + 1$ -dimensional systems, while maintaining a relatively simple character. In addition, the model is integrable and lends itself both to a coordinate Bethe Ansatz and algebraic Bethe Ansatz approach. The study of a one-dimensional gas of impenetrable, point-like bosons was initiated in 1960 by M. Girardeau, who at the same time recognized the correspondence to noninteracting fermions [49]. The repulsive case was subsequently analyzed in detail by E. H. Lieb and W. Liniger in 1963 [75, 74].<sup>16</sup> The emergence of bound states (so-called ‘strings’) in the attractive case was studied by M. Takahashi in the 1990s [116]. We will first introduce the model on the basis of two particles. This will reveal the structure of the coordinate Bethe Ansatz, after which the generalization to  $N$  particles is straightforward. Hereafter, we impose quantization and obtain the renowned Bethe equations of the system. Going to the thermodynamic limit, the defining equations of the model can be reformulated as integral equations over densities, and this naturally leads us to a discussion of excitations. Finally, we remark on the presence of bound states in the complex-coupling regime. The contents of this section relating to the repulsive Lieb-Liniger gas are mainly inspired by [45, 20, 72, 70, 102], while the discussion of bound states draws from [17, 116].

**Two-particle case** We start by considering two bosons with contact interactions, for which the Hamiltonian is

$$H = -\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} + 2c\delta(x_1 - x_2), \quad (20)$$

---

<sup>16</sup>Professor Lieb, who is 93 years old at the time of writing and still active in physics, apparently has no active recollection of Liniger at all.

with  $c \in \mathbb{R}$  (for now). The interaction can be attractive ( $c < 0$ ) or repulsive ( $c > 0$ ). One can divide up a generic eigenstate into configurations for  $x_1 < x_2$  and  $x_1 > x_2$ :

$$\Psi(x_1, x_2) = f(x_1, x_2)\theta_H(x_2 - x_1) + f(x_2, x_1)\theta_H(x_1 - x_2),$$

where

$$\theta_H(x) = \begin{cases} 1, & x > 0, \\ 0, & x < 0, \end{cases}$$

is the Heaviside step function. Note that  $\Psi(x_1, x_2)$  is symmetric in  $x_1$  and  $x_2$ , as we desire for bosons. The Schrödinger equation for the Hamiltonian eq. (20) is

$$\left[ -\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} + 2c\delta(x_1 - x_2) \right] \Psi(x_1, x_2) = E\Psi(x_1, x_2),$$

which can be solved by the usual superposition of plane waves:

$$\begin{aligned} f(x_1, x_2) &\equiv A(k_1, k_2)e^{i(k_1x_1 + k_2x_2)} + A(k_2, k_1)e^{i(k_2x_1 + k_1x_2)} \\ &= A_{12}e^{i(k_1x_1 + k_2x_2)} + A_{21}e^{i(k_2x_1 + k_1x_2)}. \end{aligned} \quad (21)$$

Upon insertion into the Schrödinger equation, and after using the identities  $\partial_x \theta_H(x) = \delta(x)$  and  $f(x)\partial_x \delta(x) \simeq -\partial_x f(x)\delta(x)$ , which is valid under the integral), we obtain:

$$H\Psi = (k_1^2 + k_2^2)\Psi + 2\delta(x_1 - x_2)[c(A_{12} + A_{21}) + i(A_{12} - A_{21})(k_1 - k_2)]e^{i(k_1 + k_2)x_1}.$$

The eigenvalue equation is satisfied if the off-diagonal terms vanish, which in turn is fulfilled if

$$\frac{A_{12}}{A_{21}} = \frac{i(k_1 - k_2) - c}{i(k_1 - k_2) + c}.$$

Note that the fraction, being of the form  $(a + ib)/(a - ib)$  with  $a, b \in \mathbb{R}$ , has unit modulus, and is therefore a pure phase term:

$$\frac{i(k_1 - k_2) - c}{i(k_1 - k_2) + c} = e^{i\tilde{\theta}(k_1 - k_2)}. \quad (22)$$

This can be rewritten as

$$\frac{i}{2} \ln \left( \frac{1 - i\frac{-c}{k_1 - k_2}}{1 + i\frac{-c}{k_1 - k_2}} \right) = -\frac{1}{2}\tilde{\theta}(k_1 - k_2),$$

and by invoking the identities  $\arctan(x) = \frac{i}{2} \ln((1 - ix)/(1 + ix))$ ,  $\arctan(x) + \arctan(1/x) = -\pi/2$  and  $\arctan(-x) = -\arctan(x)$ , we may write

$$\tilde{\theta}(k_1 - k_2) = -2 \arctan \left( \frac{k_1 - k_2}{c} \right) + \pi.$$

In conclusion, we have found that

$$\frac{A_{12}}{A_{21}} = e^{i\tilde{\theta}(k_1 - k_2)}, \quad \text{with} \quad \tilde{\theta}(k) = -2 \arctan \frac{k}{c} + \pi. \quad (23)$$

This is the phase-shift due to the contact interaction. It is a unique signature of the potential: each integrable model is characterized by a phase-shift function.

Before we attempt an  $N$ -particle generalization, there are two things to note (see Figure 11):

- In the limit  $c \rightarrow \infty$ , the scattering phase becomes that of free fermions:  $\pi$ .
- For vanishing quasi-momentum,  $k_1 \rightarrow k_2$ , eq. (21) vanishes, since  $\tilde{\theta}(k) \rightarrow \pi$  and hence  $A_{12} = -A_{21}$ . So in this limit, the wavefunction behaves as if it were fermionic and not bosonic. It is customary to factor out this fermionic statistical phase and define the scattering phase as an odd function of its argument that vanishes for  $k = 0$ . Thus, we redefine  $\theta(k) \equiv \tilde{\theta}(k) + \pi$ , with

$$\theta(k) \equiv -2 \arctan(k/c).$$

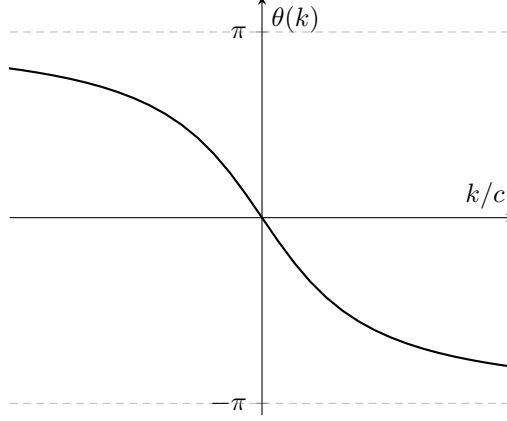


Figure 11: Graph of  $\theta(k) = -2 \arctan(k/c)$ .

**$N$ -particle generalization** Now, consider a system of  $N$  particles. The Hamiltonian in second quantized form is:

$$H_{LL} = \int dx [\partial_x \Psi^\dagger(x) \partial_x \Psi(x) + c \Psi^\dagger(x) \Psi^\dagger(x) \Psi(x) \Psi(x)]. \quad (24)$$

The corresponding equation of motion is known as the **nonlinear Schrödinger equation** (NLS):

$$i\partial_t \Psi = -\partial_x^2 \Psi + 2c \Psi^\dagger(x) \Psi(x) \Psi(x). \quad (25)$$

The quantum field theoretic problem can be converted to a quantum mechanical problem with Hamiltonian:

$$H_{LL} = -\sum_{j=1}^N \frac{\partial^2}{\partial x_j^2} + 2c \sum_{j<l} \delta(x_j - x_l). \quad (26)$$

Note: A little more detail

The rewriting from QFT  $\rightarrow$  QM is realized by acting with the field-theoretic operators on a generic bosonic eigenstate

$$|\psi_N(k_1, k_2, \dots, k_N)\rangle = \frac{1}{\sqrt{N!}} \int d^N x \chi_N(x_1, x_2, \dots, x_N; k_1, k_2, \dots, k_N) \Psi^\dagger(x_1) \Psi^\dagger(x_2) \cdots \Psi^\dagger(x_N) |0\rangle, \quad (27)$$

where  $\chi_N(x_1, x_2, \dots, x_N; k_1, k_2, \dots, k_N)$  is a symmetric function of the positions  $x_j$ . Acting for example with the field-theoretic momentum operator

$$\hat{P} = -\frac{i}{2} \int (\Psi^\dagger(x) \partial_x \Psi(x) - [\partial_x \Psi^\dagger(x)] \Psi(x)) dx$$

on  $|\psi_N\rangle$ , one can, using bosonic commutation relations and integration by parts, write down

$$\begin{aligned} \hat{P} |\psi_N(k_1, k_2, \dots, k_N)\rangle \\ = \frac{1}{\sqrt{N!}} \int d^N x \left( -i \sum_{j=1}^N \frac{\partial}{\partial x_j} \chi_N(x_1, x_2, \dots, x_N; k_1, k_2, \dots, k_N) \right) \Psi^\dagger(x_1) \cdots \Psi^\dagger(x_N) |0\rangle, \end{aligned}$$

which makes it manifestly clear that the action of  $P$  on  $|\psi_N\rangle$  is equivalent to the action of the quantum mechanical momentum operator  $\hat{K} = -i \sum_{j=1}^N \partial/\partial x_j$ . The quantum mechanical Hamiltonian is revealed in a similar way.

Note: Bosons and fermions in 1D

In the book authored by Korepin, Bogoliubov, and Izergin [72], the symmetric function  $\chi_N$  popping up in eq. (27) is shown to take the form

$$\chi_N = \frac{\prod_{j>l}(k_j - k_l)}{\sqrt{N! \prod_{j>l}[(k_j - k_l)^2 + c^2]}} \sum_{\mathcal{P}} \exp \left[ i \sum_{n=1}^N x_n k_{\mathcal{P}_n} \right] \times \prod_{j>l} \left[ 1 - \frac{ic\epsilon(x_j - x_l)}{k_{\mathcal{P}_j} - k_{\mathcal{P}_l}} \right], \quad (28)$$

where  $\epsilon(x_j)$  is the sign function. The thing to notice here is that  $\chi_N$  is *symmetric* with respect to the exchange of any two coordinates  $x_i \leftrightarrow x_j$  (bosonic symmetry),<sup>a</sup> while it is *anti-symmetric* with respect to the exchange of two quasi-momenta  $k_i \leftrightarrow k_j$  (fermionic anti-symmetry). This remarkable property of one-dimensional bosonic systems is sometimes referred to as the *Pauli principle for bosons*, and it is exemplary of the rather blurry nature of spin-statistics in 1 + 1 dimension. It also means that we can understand the Lieb-Liniger model from both the bosonic and the fermionic perspective, which opens up the possibility of a dual description regarding the (qualitative) behaviour of the system. Such a description is especially insightful when dealing with the limiting cases of the coupling strength  $c$ .

<sup>a</sup>This may be a little hard to infer directly from the form of  $\chi_N$ , but the minus sign that is picked up by the sign function under particle exchange is compensated by the reordering of indices in the product over  $j > k$ , such that the whole adjusts consistently. It will be clear if you write out the expression for small  $N$ .

The **Coordinate Bethe Ansatz** (CBA) for the wavefunction is a linear superposition of plane waves of the form

$$\Psi(x_1, \dots, x_N; \mathcal{Q}) = \sum_{\mathcal{P}} A_{\mathcal{P}}(\mathcal{Q}) e^{i \sum_j k_{\mathcal{P}_j} x_j}, \quad (29)$$

where  $\mathcal{P}$  is a permutation of the **rapidities** (quasi-momenta)  $\{k_j\}$ ,<sup>17</sup> while  $\mathcal{Q}$  is the permutation that specifies the particle order (*simplex*). Knowing the wavefunction in one simplex, for example in the *fundamental domain*  $x_1 < x_2 < \dots < x_N$ , fixes the solution completely, since we know the properties of the wavefunction under particle exchange. Therefore, we drop the explicit dependence on the coordinate permutation  $\mathcal{Q}$  and assume henceforth that we operate in the fundamental domain. Note that eq. (29) reduces to eq. (21) for  $N = 2$ , as we should demand.

All permutations can be generated by a sequence of two-body permutations. Exchanging two indices at a time is equivalent to the two-particle scattering problem, as considered before. Hence,

$$\frac{A_{\mathcal{P}}}{A_{\mathcal{P}'}} = -e^{i\theta(k-k')},$$

where  $k, k'$  are the quasi-momenta interchanged between permutation  $\mathcal{P}$  and  $\mathcal{P}'$ , and (as before) the scattering phase is  $\theta(k) = -2 \arctan(k/c)$ . Note that the wavefunction vanishes if two quasi-momenta coincide. The energy and momentum eigenvalues associated with eq. (29) are

$$E = \sum_{j=1}^N k_j^2, \quad K = \sum_{j=1}^N k_j, \quad (30)$$

with momentum operator  $\hat{K} \equiv -i \sum_{j=1}^N \partial / \partial x_j$ .

**Bethe equations** Now we quantize the system: we put it in a box of finite length  $L$  (which we can take to infinity at the end), and impose periodic boundary conditions on the box:

$$\Psi(x_1, x_2, \dots, x_j + L, \dots, x_N) = \Psi(x_1, x_2, \dots, x_j, \dots, x_N), \quad j = 1, \dots, N.$$

The pbc relate a given simplex with a simplex where one of the particles has been moved to the ‘end’; this can be realized by a sequence of two-body permutations. In taking a particle around the circle, it acquires a

<sup>17</sup>Rapidities represent the asymptotic momentum of the particle after a scattering event, in contrast to the actual momentum.



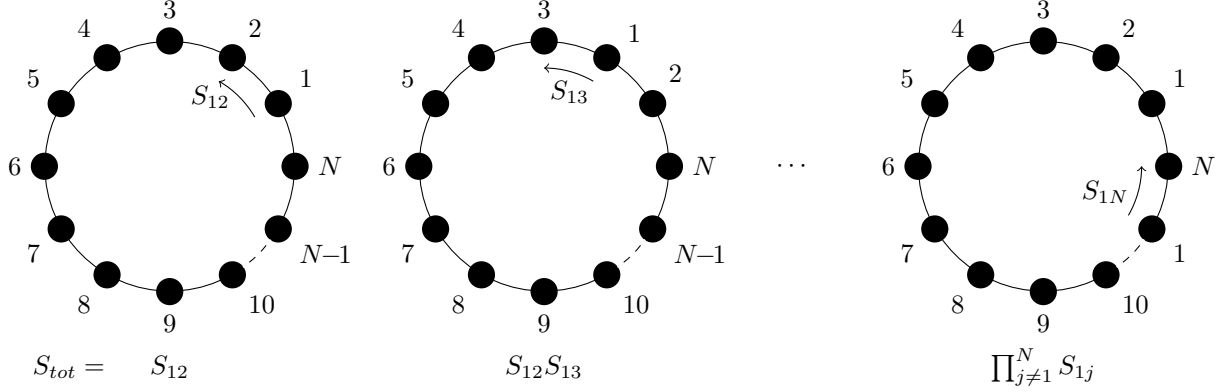


Figure 12: The total phase shift  $S_{tot}$  after scattering particle 1 with all other particles is the product of relative phase shifts:  $S_{tot} = \prod_{j \neq 1}^N S_{1j}$ . The relative phase shifts are  $S_{1j} = -e^{i\theta(k_1 - k_j)}$ . Demanding single-valuedness of the wavefunction (and therefore  $2\pi$ -periodicity in  $k_j$ ) then leads to the consistency equation  $e^{iLk_1} \prod_{j \neq 1}^N S_{1j} = 1 = e^{2\pi i n}$ ,  $n \in \mathbb{Z}$  (the total phase shift, being the product of the total scattering phase shift and the kinematic phase shift that is accumulated when transporting particle 1 one fully – a distance  $L$  – around the circle, should amount to 1, i.e. after ‘going full round’ the single-valuedness of the wavefunction dictates that we find the same value of the wavefunction at the starting position). Taking the log of both sides leads to the Bethe equations  $2\pi I_1 + \sum_{j \neq 1}^N \theta(k_1 - k_j) = Lk_1$  for the first particle, and the same procedure yields the full set of Bethe equations for all particles.

phase equal to all the scattering phase shifts associated with each scattering event, plus the kinematic phase accumulated because of the motion. To satisfy the pbc, the product of these quantities needs to add up to an integer multiple of  $2\pi$ , as explained in Figure 12.

This argument leads to the following set of equations:

$$e^{ik_j L} = \prod_{l \neq j} \left( \frac{k_j - k_l + ic}{k_j - k_l - ic} \right) = (-1)^{N-1} \prod_{l=1}^N e^{i\theta(k_j - k_l)}, \quad j = 1, \dots, N, \quad (31)$$

which relate the kinematic phase (lhs) to the scattering phase (rhs). Taking the logarithm, we get:

$$\begin{aligned} k_j L &= 2\pi \tilde{I}_j + (N-1)\pi - 2 \sum_{l=1}^N \arctan \left( \frac{k_j - k_l}{c} \right) \\ &= 2\pi I_j + \sum_{l=1}^N \theta(k_j - k_l), \end{aligned} \quad (32)$$

where the  $I_j$  are a set of (integer) quantum numbers which define the state (the **Bethe numbers**). Eqs. (31) or (32) are called the **Bethe equations**.

We again make some observations:

- The ground-state distribution of Bethe numbers is given by  $I_j = -(N+1)/2 + j$  with  $j = 1, \dots, N$ , i.e. a symmetric distribution around zero (like a Fermi sea).
- If two quantum numbers are equal,  $I_j = I_l$ , then their quasi-momenta coincide,  $k_j = k_l$ . In such cases the Bethe wavefunction (29) vanishes. So only sets of distinct Bethe numbers correspond to physical solutions. Furthermore, each choice of quantum numbers yields an eigenstate, provided that all Bethe numbers are different. These facts are consistent with the observation we have made in the note surrounding eq. (28), and we clearly see reflected the fermionic nature of the solution in quasi-momentum space, while the system is bosonic in real space.

- The limit  $c \rightarrow \infty$  is called the **Tonks-Girardeau regime** and can be understood equivalently in terms of hardcore bosons with  $\theta(k) \rightarrow 0$  and  $k_j = 2\pi I_j/L$  or in terms of free fermions. When we decrease  $c$  from infinity, we slowly turn on the scattering phase.

On top of these comments, let us state three important theorems pertaining to the solutions of the Bethe equations (32) for the repulsive Lieb-Liniger gas. The theorems, together with their proofs, can be found in Korepin, Bogoliubov, and Izergin [72].

**Theorem 3.1** *Solutions to the Bethe equations exist and can be uniquely parametrized by a set of integer (half-integer) numbers  $I_j$ , the Bethe numbers.*

**Theorem 3.2** *All the solutions  $k_j$  of the Bethe equations [with  $c < 0$ ] are real numbers.*

**Theorem 3.3** *If  $I_j > I_k$ , then  $k_j > k_k$ . If  $I_j = I_k$ , then  $k_j = k_k$ .*

**Thermodynamic limit** The Bethe equations (32) are a set of  $N$  coupled algebraic equations in  $N$  unknowns, the rapidities  $k_j$ . Obviously, for any  $N$  larger than, say,  $N = 3$ , we cannot hope to solve these equations analytically. However, if we let the number of particles go to infinity,  $N \rightarrow \infty$  (the thermodynamic limit), it turns out that we can actually make exact statements owing to the possibilities we gain by replacing sums over individual rapidities by integrals over densities. To enjoy these benefits, it is obligatory that we keep the density ratio  $N/L$  fixed and finite in order to guarantee that intensive properties like the energy per particle remain meaningful, and that the density itself is well-defined.

The first step towards the thermodynamic limit is to rewrite the Bethe equations (32) as

$$k_j - \frac{1}{L} \sum_{l=1}^N \theta(k_j - k_l) = y(k_j),$$

by arranging the  $I_j$ 's in increasing order. The ‘counting function’  $y(k)$  is defined by  $y(k_j) \equiv 2\pi I_j/L$  and monotonicity. Therefore, by definition,

$$y(k_j) - y(k_l) = \frac{2\pi}{L} (I_j - I_l). \quad (33)$$

In the limit  $N, L \rightarrow \infty$  with  $N/L$  fixed and finite we can introduce a density of quasi-momenta  $\rho(k_j)$  and replace sums over rapidities by integrals, as

$$\rho(k_j) = \lim_{N, L \rightarrow \infty} \frac{1}{L(k_{j+1} - k_j)} > 0, \quad \sum_j \rightarrow L \int \rho(k) dk. \quad (34)$$

Note that the factor  $L$  before the integral is needed to compensate for the extra dimensions of  $1/\text{length}$  that are introduced by the integration measure. The derivative, using eq. (33), is

$$y'(k_j) = \lim_{N, L \rightarrow \infty} \frac{y(k_j) - y(k_{j-1})}{k_j - k_{j-1}} = \lim_{N, L \rightarrow \infty} \frac{2\pi}{L(k_j - k_{j-1})} = 2\pi\rho(k_j), \quad (35)$$

and hence

$$\frac{1}{2\pi} y(k) = \int_{k_{min}}^k \rho(k') dk'.$$

We have therefore established a direct relation between the distribution of integers and the distribution of quasi-momenta. With these definitions, we proceed to write the thermodynamic limit of eq. (32) as an integral equation involving the counting function and quasi-momentum distribution. In particular, in the continuum limit, we replace  $2\pi I_j \rightarrow Ly(k)$  and  $\sum_{l=1}^N \theta(k_j - k_l) \rightarrow L \int_{k_{min}}^{k_{max}} \rho(k') \theta(k - k') dk'$ , such that

$$y(k) = k - \int_{k_{min}}^{k_{max}} \theta(k - k') \rho(k') dk'.$$

Taking the derivative with respect to  $k$ , using eq. (35), we find:

$$\rho(k) = \frac{1}{2\pi} - \frac{1}{2\pi} \int_{k_{min}}^{k_{max}} \theta'(k - k') \rho(k') dk' \equiv \boxed{\frac{1}{2\pi} - \frac{1}{2\pi} \int_{k_{min}}^{k_{max}} \mathcal{K}(k - k') \rho(k') dk'}, \quad (36)$$

Here, we introduced a kernel of integration<sup>18</sup> defined as the derivative of the scattering phase:

$$\mathcal{K}(k) = \frac{d}{dk} \theta(k) = -\frac{2c}{c^2 + k^2}. \quad (37)$$

The integral equation (36) with this particular kernel is known as the **Lieb-Liniger equation** (Lieb equation). It is a Fredholm-type linear integral equation that determines the distribution of the quasi-momenta. Note that the support of the kernel depends on the choice for the Bethe numbers, since they determine the limits of integration  $k_{min}$  and  $k_{max}$ .

Note: How to deal with integral equations [45]

Eq. (36) is a Fredholm equation of the second kind. It has the structure

$$\rho + \frac{1}{2\pi} \hat{\mathcal{K}}_q \rho = \left( \hat{\mathcal{I}} + \frac{1}{2\pi} \hat{\mathcal{K}}_q \right) \rho = \frac{1}{2\pi}, \quad (38)$$

where the integral operator  $\hat{\mathcal{K}}_q$  with support  $(-q, q)$  and positive kernel  $\mathcal{K}(k, k')$  is defined as

$$\left( \hat{\mathcal{K}}_q \rho \right)(k) \equiv \int_{-q}^{+q} \mathcal{K}(k, k') \rho(k') dk', \quad (39)$$

and  $(\hat{\mathcal{I}}\rho)(k) = \int_{-\infty}^{+\infty} \delta(k - k') \rho(k') dk'$  (it has the Dirac delta as its kernel). To perform formal manipulations and derive analytic expression, it is often convenient to write  $\rho(k)$  in terms of its resolvent or Green's function.

- Define the *resolvent*  $\hat{\mathcal{L}}_q$  of  $\hat{\mathcal{K}}_q$  as the operator that formally satisfies

$$\begin{aligned} \left( \hat{\mathcal{I}} - \hat{\mathcal{L}}_q \right) \left( \hat{\mathcal{I}} + \frac{1}{2\pi} \hat{\mathcal{K}}_q \right) &= \hat{\mathcal{I}}, \\ \left( \hat{\mathcal{I}} - \hat{\mathcal{L}}_q \right) \hat{\mathcal{K}}_q &= 2\pi \hat{\mathcal{L}}_q. \end{aligned}$$

- Moreover, one can introduce the Green's function associated to a linear operator as the function (symmetric in  $k$  and  $k'$ ) satisfying

$$\mathcal{U}_q(k, k') + \frac{1}{2\pi} \int_{-q}^{+q} \mathcal{K}(k, k'') \mathcal{U}_q(k'', k') dk'' = \delta(k - k'). \quad (40)$$

Using eq. (39), this is equivalent to

$$\left( \hat{\mathcal{I}} + \frac{1}{2\pi} \hat{\mathcal{K}}_q \right) \hat{\mathcal{U}}_q = \hat{\mathcal{I}}.$$

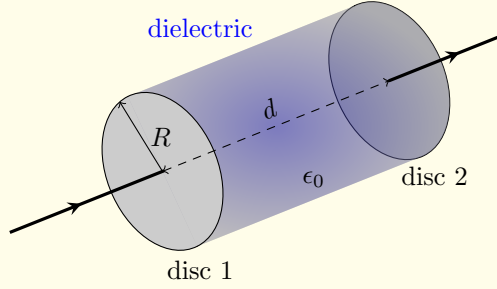
If either  $\hat{\mathcal{L}}_q$  or  $\mathcal{U}_q$  is known, the density can be written as

$$\rho(k) = \frac{1}{2\pi} \int_{-q}^q \mathcal{U}_q(k, k') dk' = \frac{1}{2\pi} - \frac{1}{2\pi} \int_{-q}^q \mathcal{L}_q(k, k') dk'. \quad (41)$$

This is easy to see: If we identify  $\hat{\mathcal{K}}(k, k') \rho(k') = \hat{\mathcal{L}}_q(k, k')$ , we get  $\rho(k) = \frac{1}{2\pi} - \frac{1}{2\pi} \int_{-q}^q \hat{\mathcal{K}}(k, k') \rho(k') dk' = \frac{1}{2\pi} - \frac{1}{2\pi} (\hat{\mathcal{K}}_q \rho)(k)$ , which is exactly eq. (38).

<sup>18</sup>Note here the possible confusion about the use of the word 'kernel'. In linear algebra, it refers to all elements that are mapped to the zero element, whereas in this context it just means 'whatever is inside the integral'.

There exists an exact mapping between the Lieb-Liniger model and the problem of a circular disk condenser (capacitor) in classical physics (electrostatics).



The capacitance of a condenser made of two circular discs of radius  $R$  separated by a vacuum gap (the dielectric) of length  $d$  with permittivity  $\epsilon_0$  is known to be [18]

$$C(\alpha, \lambda) = 2\epsilon_0 R \int_{-1}^{+1} dz g(z; \alpha, \lambda), \quad (42)$$

where  $\alpha = d/R$ ,  $\lambda$  is the ratio of disc charges and  $g$  is the solution of the *Love equation*,

$$g(z; \alpha, \lambda) = 1 + \frac{\lambda\alpha}{\pi} \int_{-1}^{+1} dy \frac{g(y; \alpha, \lambda)}{\alpha^2 + (y - z)^2}, \quad -1 \leq z \leq 1. \quad (43)$$

Note that this expression has the form of the Lieb-Liniger equation if we identify  $\alpha = c$ ,  $y = k'$  and  $\lambda = 1$  (equally charged plates). Let us now consider the limits  $\alpha \ll 1$  (small gap) and  $\alpha \rightarrow \infty$  (infinite separation), which correspond to the weak-coupling and Tonks-Girardeau limit, respectively.

- $\alpha \ll 1$ : It is known that the Lieb equation in this regime can be written as [54]:

$$g(z; \alpha) \simeq \frac{\sqrt{1 - z^2}}{\alpha},$$

and hence we obtain the capacitance

$$C(\alpha) \simeq 2\epsilon_0 R \int_{-1}^{+1} dz \frac{\sqrt{1 - z^2}}{\alpha} = \frac{\pi\epsilon_0 R}{\alpha} = \frac{\epsilon_0 A}{d}, \quad (44)$$

where we recognized the integral over  $\sqrt{1 - z^2}$  with bounds  $[-1, +1]$  as comprising half the surface area of a disk with unit radius, i.e.  $\pi/2$ . This result will look familiar!

- $\alpha \rightarrow \infty$ : The Lieb equation takes on the simple form

$$g(z; \infty) = 1,$$

and hence

$$C(\alpha) \simeq 4\epsilon_0 R.$$

For the ground state, the limits of integration are symmetric (to minimize the momentum). We find for the momentum and energy per unit length:

$$p = \frac{K}{L} = \int_{-q}^q k \rho(k) dk = 0, \quad e = \frac{E}{L} = \int_{-q}^q k^2 \rho(k) dk, \quad (45)$$

where we used that  $\rho(-k) = \rho(k)$ , i.e.  $\rho(k)$  is even. Note that in taking the thermodynamic limit, we have traded exact knowledge of the solution to the Bethe equations and thus of the eigenstates for a better understanding of macroscopic properties of the system, such as eq. (45).

The limits of integration in eq. (45) are determined implicitly by the particle number  $N$ :  $N = \int_{-q}^q \rho(k) dk$ . We want to eliminate the  $q$ -dependence. To do this, we perform the rescaling

$$k \equiv qx, \quad c \equiv qg,$$

such that  $(\tilde{\rho}(x) \equiv \rho(qx))$ . Then the Lieb equation becomes

$$\tilde{\rho}(x) = \frac{1}{2\pi} + \frac{1}{\pi} \int_{-1}^{+1} \frac{g}{g^2 + (x-y)^2} \tilde{\rho}(y) dy, \quad (46)$$

$$n \equiv \frac{N}{L} = qG(g), \quad e \equiv \frac{E}{L} = q^3 F(g), \quad (47)$$

with

$$G(g) \equiv \int_{-1}^{+1} \tilde{\rho}(x) dx, \quad F(g) \equiv \int_{-1}^{+1} x^2 \tilde{\rho}(x) dx. \quad (48)$$

Now we eliminate the  $q$ -dependence by taking the ratios

$$\frac{e}{n^3} = \frac{F(g)}{G^3(g)}, \quad \gamma \equiv \frac{c}{n} = \frac{g}{G(g)} \equiv \tilde{G}(g), \quad (49)$$

where we defined the *dimensionless coupling*  $\gamma$ . This dimensionless coupling characterizes the 1D Bose physics entirely.

The ground state energy  $e$  (in terms of  $\gamma$ ) is then given by

$$e = n^3 u(\gamma), \quad u(\gamma) \equiv \frac{F(\tilde{G}^{-1}(\gamma))}{G^3(\tilde{G}^{-1}(\gamma))}.$$

This leads to the following approach for computing macroscopic properties:

1. Solve the (rescaled) Lieb equation, eq. (46);
2. Compute  $G(g)$  and  $F(g)$  from eq. (48);
3. Finally, find  $e$  and  $\gamma$  from eq. (49).

Let us briefly touch upon the following regimes:

- Strong repulsion: In the Tonks-Girardeau regime ( $g \rightarrow \infty$  or equivalently  $c \rightarrow \infty$ ), the system behaves like free fermions. The kernel  $\mathcal{K}$  vanishes and we find for the quasi-momenta distribution:

$$\tilde{\rho}(x) = \begin{cases} 1/2\pi, & |x| \leq 1, \\ 0, & |x| > 1. \end{cases} \quad \Rightarrow \quad \rho(k) = \begin{cases} 1/2\pi, & |k| \leq q, \\ 0, & |k| > q. \end{cases}$$

Corrections for large but finite  $g$  can be calculated perturbatively, leading to

$$u(\gamma) = \frac{\pi^2}{3} \left[ 1 - \frac{4}{\gamma} + \frac{12}{\gamma^2} + \mathcal{O}\left(\frac{1}{\gamma^3}\right) \right].$$

- Weak interaction: The  $g \rightarrow 0$  limit is technically involved, but was solved in the context of the Love equation for circular disk condensers. The asymptotic analysis yields:

$$\tilde{\rho}(x) = \frac{1}{2\pi g} \sqrt{1-x^2} + \frac{1}{4\pi^2} \frac{1}{\sqrt{1-x^2}} \left[ x \ln \left( \frac{1-x}{1+x} \right) + \ln \left( \frac{16\pi e}{g} \right) \right] + \mathcal{O}(1),$$

$$u(\gamma) = \gamma - \frac{4}{3\pi} \gamma^{3/2} + \left( \frac{1}{6} - \frac{1}{\pi^2} \right) \gamma^2 + \mathcal{O}(\gamma^{5/2}).$$

**Elementary excitations** We consider two types of elementary excitations (still at zero temperature):

- **Type I** excitations add a new particle with momentum  $|k_p| > q$ .
- **Type II** excitations remove a particle and create a hole with  $|k_h| \leq q$ .

We could also define a type III excitation as moving one of the momenta inside the Fermi sea  $|k| \leq q$  and above the  $q$ -treshold, but this can be realized as a combination of a type I & II excitation. In general, low energy excitations can all be constructed from type I and type II excitations, so we will focus on these types.

- **Type I:** Let's say  $N$  is odd. Recall that the distribution of Bethe numbers in the ground state is then given by

$$\{I_j\} = \left\{ -\frac{N-1}{2}, -\frac{N-3}{2}, \dots, \frac{N-1}{2} \right\}.$$

An excitation that adds a single particle (with momentum  $k_p$ ) will take the particle number  $N \rightarrow N+1$ , so the Bethe numbers in the new ground state with  $N+1$  particles will be

$$\{I'_j\} = \left\{ -\frac{N}{2}, -\frac{N}{2} + 1, \dots, \frac{N}{2} - 1, \frac{N}{2} + m \right\},$$

with  $m > 0$ . The total momentum of the configuration, previously 0 (in the ground state), will however not increase by the *bare momentum*  $k_p$  of the excited particle, but it is given by the *dressed momentum* that takes into account reconfigurations of all the other particles in response to adding the new particle.<sup>19</sup>

$$K = \frac{2\pi}{L} m. \quad (50)$$

We now set out to calculate the response of the system to the addition of the extra particle. We start by evaluating  $\Delta k_j = k'_j - k_j$ , which we obtain by subtracting the Bethe equations for the two configurations:

$$\Delta k_j L = \pi + \sum_{l=1}^N [\theta(k'_j - k'_l) - \theta(k_j - k_l)] + \theta(k'_j - k_p).$$

The  $\pi$ -term comes about because the Bethe numbers shift from integers to half-integers (or vice versa) when an extra particle is included.  $\Delta k_j \sim \mathcal{O}(L^{-1})$ , so we can expand the rhs to the same order in the system size  $L$ :

$$\begin{aligned} \Delta k_j L &\simeq \pi + \sum_{l=1}^N \mathcal{K}(k_j - k_l) (\Delta k_j - \Delta k_l) + \theta(k_j - k_p), \\ \Delta k_j \left[ 1 - \frac{1}{L} \sum_{l=1}^N \mathcal{K}(k_j - k_l) \right] &= \frac{1}{L} [\pi + \theta(k_j - k_p)] - \frac{1}{L} \sum_{l=1}^N \mathcal{K}(k_j - k_l) \Delta k_j, \end{aligned}$$

where we used the definition of the kernel, eq. (37), and performed the expansion

$$\begin{aligned} \mathcal{K}(k_j - k_l) &\equiv \frac{d}{dk} \theta(k_j - k_l) \\ &= \frac{\theta(k_j - k_l + \overbrace{(k'_j - k'_l - k_j + k_l)}^h) - \theta(k_j - k_l)}{k'_j - k'_l - k_j + k_l} + \mathcal{O}(h) \\ &= \frac{\theta(k'_j - k'_l) - \theta(k_j - k_l)}{\Delta k_j - \Delta k_l} + \mathcal{O}(h) \end{aligned}$$

<sup>19</sup>As Franchini [45] remarks: “This is a sign of the intrinsic non-local nature of a one-dimensional system excitation and provides a concrete example of the concept that one-dimensional systems are intrinsically strongly interacting, regardless of the actual strength of the coupling constant.”

in the first line. Note that  $h \propto 1/L$ . Now go to the thermodynamic limit, using eq. (36) to rewrite the lhs as a factor directly proportional to  $\rho(k)$ :

$$2\pi\Delta k\rho(k) = \frac{1}{L}[\pi + \theta(k - k_p)] - \int_{-q}^q \mathcal{K}(k - k')\Delta k'\rho(k')dk'. \quad (51)$$

We then define the *back-flow* (or *shift function*)

$$J(k|k_p) \equiv L\Delta k\rho(k) = \lim_{k \rightarrow k_j} \lim_{N, L \rightarrow \infty} \frac{k_j - k'_j}{k_{j+1} - k_j}, \quad (52)$$

in terms of which the equation above can be rewritten as:

$$J(k|k_p) + \frac{1}{2\pi} \int_{-q}^q \mathcal{K}(k - k')J(k'|k_p)dk' = \frac{1}{2\pi} \tilde{\theta}(k - k_p).$$

Here we used the definition of the phase-shift eq. (23) to absorb the  $\pi$  into  $\tilde{\theta}$ . This equation has a solution in terms of a Green's function  $\mathcal{U}_q$ , see eq. (40):

$$J(k|k_p) = \frac{1}{2\pi} \int_{-q}^q \mathcal{U}_q(k, k')\tilde{\theta}(k' - k_p)dk'. \quad (53)$$

The shift function is convenient for calculating the *dressed* momentum and energy upon adding a particle with *bare* momentum and energy  $k_p \leq |q|$  and  $k_p^2$ , respectively:

$$\begin{aligned} \Delta K(k_p) &= \frac{2\pi}{L}m = k_p + \sum_{j=1}^N \Delta k_j \stackrel{N \rightarrow \infty, (52)}{=} k_p + \int_{-q}^q J(k|k_p)dk \\ &\stackrel{(53)}{=} k_p + \frac{1}{2\pi} \int_{-q}^q dk \int_{-q}^q dk' \mathcal{U}_q(k, k')\tilde{\theta}(k' - k_p) \stackrel{(41)}{=} k_p + \int_{-q}^q \rho(k)\tilde{\theta}(k - k_p)dk, \\ \Delta e(k_p) &= k_p^2 + \sum_{j=1}^N [k_j'^2 - k_j^2] = k_p^2 + \sum_{j=1}^N [2k_j\Delta k_j + (\Delta k_j)^2] \simeq k_p^2 + \int_{-q}^q \rho(k)\tilde{\theta}(k - k_p)dk, \end{aligned}$$

where we used that the term  $(\Delta k_j)^2$  is suppressed like  $1/N$  relative to the leading term.

- **Type II:** An excitation that removes a single particle from the Fermi sea (and creates a hole) takes the particle number  $N \rightarrow N - 1$ , such that the new quantum numbers become

$$\{I''_j\} = \left\{ -\frac{N}{2} - 1, -\frac{N}{2} + 2, \dots, \frac{N}{2} - m - 1, \frac{N}{2} - m + 1, \dots, \frac{N}{2} \right\},$$

giving this state a positive momentum of  $K = \frac{2\pi}{L}m$ . We can proceed in the same way, and find that the back-flow satisfies the integral equation

$$J(k|k_h) + \frac{1}{2\pi} \int_{-q}^q \mathcal{K}(k - k')J(k'|k_h)dk' = -\frac{1}{2\pi} \tilde{\theta}(k - k_h).$$

The resulting dressed momentum and energy are

$$\begin{aligned} \Delta K(k_h) &= -k_h - \int_{-q}^q J(k|k_h)dk = -k_h - \int_{-q}^q \rho(k)\tilde{\theta}(k - k_h)dk, \\ \Delta e(k_h) &= -k_h^2 + \int_{-q}^q 2kJ(k|k_h)dk. \end{aligned}$$

In hindsight, we can conclude that the fact that all low-energy states can be built up from type I & II excitations is the consequence of the back-flow functions being linear integral equations. In particular, moving a particle from the Fermi sea to an excited is the combination of a type II (hole) and a type I (particle) excitation.

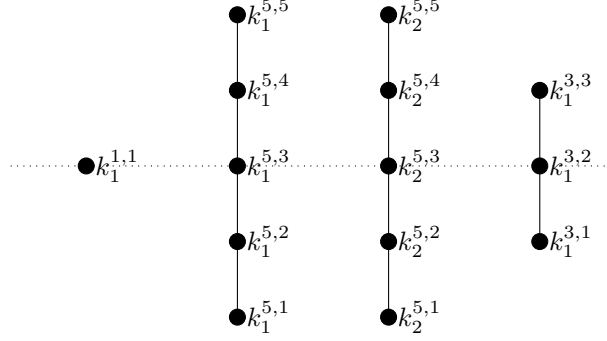


Figure 13: Configuration featuring a 1-string, two 5-strings and one 3-string, and the corresponding labelling of the rapidities  $k_\alpha^{j,a}$ . String centers lie on the dotted line.

**Bound states** ( $c > 0$ ) We have seen that for  $c > 0$  (repulsive regime), there exists a solution for the set of rapidities  $\{k\}$  and it is unique. Furthermore,  $\{k\}$  is real.

For  $c < 0$  (attractive regime), the situation is completely different. Define  $\bar{c} = -c > 0$ , and write the Bethe equations as

$$e^{ik_\alpha L} = \prod_{\beta \neq \alpha} \frac{k_\alpha - k_\beta - i\bar{c}}{k_\alpha - k_\beta + i\bar{c}}, \quad \alpha = 1, \dots, N. \quad (54)$$

Consider now a complex rapidity  $k_\alpha = k + i\eta$ , such that the Bethe equations for this rapidity are

$$e^{ik_\alpha L} = e^{ikL - \eta L} = \prod_{\beta \neq \alpha} \frac{k_\alpha - k_\beta - i\bar{c}}{k_\alpha - k_\beta + i\bar{c}} = \prod_{\beta \neq \alpha} \frac{k + i\eta - k_\beta + i\bar{c}}{k + i\eta - k_\beta + i\bar{c}}. \quad (55)$$

Let's consider finite  $N$  and  $L \rightarrow \infty$ .

- If  $\eta > 0$ ,  $e^{-\eta L} \rightarrow 0$ . Looking at the right hand side, there must be a rapidity  $k_\alpha$  such that  $k_\alpha = k_\beta + i\bar{c} + \mathcal{O}(e^{-\eta L})$ .
- On the other hand, if  $\eta < 0$ , we have  $e^{-\eta L} \rightarrow \infty$  and hence there must be a rapidity  $k_\alpha$  such that  $k_\alpha = k_\beta - i\bar{c} + \mathcal{O}(e^{-|\eta|L})$ .

The rapidities thus like to arrange themselves into clusters, the elements of each cluster being evenly spaced by  $\bar{c}$  in the imaginary direction. Such clusters represent bound states, and are often referred to as **strings**.

For given  $N$ , we can construct eigenstates with fixed string content by partitioning  $N$  into strings of length  $j$ , denoting the total number of strings by  $N_s$ . We will parametrize the string rapidities as

$$k_\alpha^{j,a} = k_\alpha^j + i\frac{\bar{c}}{2}(j+1-2a) + i\delta_\alpha^{j,a}, \quad (56)$$

with exponentially small deviations  $\delta \sim e^{-(cst)L}$ , provided  $N_s/L \rightarrow 0$ . Note that here,  $a = 1, \dots, j$  labels the rapidities within the string, while  $\alpha = 1, \dots, N_j$  labels strings of given length. See Figure 13 for an example with two 5-strings, one 3-string and one 1-string. We call  $k_\alpha^j$  the *string center*. The structure of eq. (56), where the deviations decay exponentially with the system size  $L$ , is referred to as the **string hypothesis** [116]. It is common to many integrable many-body systems, and even though there are known cases of non-exponentially vanishing deviations [121, 55], in general it is believed that their contribution to relevant quantities in the thermodynamic limit vanishes. Perfect strings have  $\delta_i = 0 \forall i$ , and they are exact eigenstates in the limit  $L \rightarrow \infty$  with  $N_s/L \rightarrow 0$  for arbitrary  $N$ .

Note that strong correlations of the particles in the string persist even if  $L \rightarrow \infty$ , for any particle number  $N$ . Compare this with the repulsive ( $c < 0$ ) case where, in the thermodynamic limit, we have to take  $N, L \rightarrow \infty$  such that the density  $\rho$  remains fixed, in order to retain strong interactions (for any finite  $N$ , we would instead obtain a dilute gas of bosons that spreads out uniformly).



The bound states behave as individual particles of mass  $j$ , with the energy and momentum of the string concentrated in  $k_\alpha^j$  given by. The energy and momentum of a string follow in a straightforward way from eq. (30):

$$\begin{aligned}
E_{(j,\alpha)} &= \sum_{a=1}^j |k_\alpha^{j,a}|^2 \\
&= \sum_{a=1}^j (k_\alpha^j + i\frac{\bar{c}}{2}(j+1-2a))(k_\alpha^j - i\frac{\bar{c}}{2}(j+1-2a)) \\
&= j(k_\alpha^j)^2 + \frac{\bar{c}^2}{4} \sum_{a=1}^j (j+1-2a)^2 \\
&= j(k_\alpha^j)^2 + \frac{\bar{c}^2}{4} (j^3 + 2j^2 + j) + \frac{\bar{c}^2}{4} \sum_{a=1}^j (-4aj - 4a + 4a^2) \\
&= j(k_\alpha^j)^2 + \frac{\bar{c}^2}{4} (j^3 + 2j^2 + j - 2j^2(j+1) - 2j(j+1) + \frac{2}{3}j(j+1)(2j+1)) \\
&= j(k_\alpha^j)^2 - \frac{\bar{c}^2}{12} j(j^2 - 1), \tag{57}
\end{aligned}$$

$$P_{(j,\alpha)} = jk_\alpha^j, \tag{58}$$

where in the second line we did not write deviations, because we work in the limit  $L \rightarrow \infty$ . The lowest energy state is a bound state with all  $N$  particles centered around 0, i.e. by choosing rapidities as:

$$k^{N,a} = i\frac{\bar{c}}{2}(N+1-2a) + \mathcal{O}(\delta),$$

with corresponding energy

$$E_{GS} = \sum_a (k^{N,a})^2 = -\frac{\bar{c}^2}{4} \sum_{a=1}^N (N+1-2a)^2 = -\frac{\bar{c}^2}{12} N(N^2 - 1). \tag{59}$$

An important remark is that  $E_{GS} \propto N^3$ , i.e. it is extensive, unlike the repulsive case. In particular, for a large number of particles, the energy can grow arbitrarily negative. Since, for the thermodynamic limit to exist, the energy should scale at most linearly in  $N$ , the attractive Lieb-Liniger model is unstable in the thermodynamic limit.

The fact that the deviations are exponentially small in the system size  $L$  allows us to significantly simplify the Bethe equations to involve only the string centers  $k_\alpha^j$ . In fact, from the original Bethe equations (31) it can be seen that string solutions in the limit  $L \rightarrow \infty$  correspond to purely imaginary rapidities. For example, the Bethe equation for the rapidity  $k_1^{2,1}$  in a single 2-string reads

$$e^{ik_1^{2,1}L} = \frac{k_1^{2,1} - k_1^{2,2} - i\bar{c}}{k_1^{2,1} - k_1^{2,2} + i\bar{c}} = \frac{(k_1^2 + i\frac{\bar{c}}{2}(2+1-2)) - (k_1^2 + i\frac{\bar{c}}{2}(2+1-4)) - i\bar{c}^2}{(k_1^2 + i\frac{\bar{c}}{2}(2+1-2)) - (k_1^2 + i\frac{\bar{c}}{2}(2+1-4)) + i\bar{c}^2} = \frac{0}{2i\bar{c}},$$

which is only satisfied if  $\text{Re}\{k_1^{2,1}\} = 0$  and  $\text{Im}\{k_1^{2,1}\} > 0$ .

The analogue of the Tonks-Girardeau regime in the attractive Lieb-Liniger model with  $c \rightarrow -\infty$  is the **super Tonks-Girardeau regime**. Interestingly, rapidities in the super Tonks-Girardeau regime are real-valued, and the system can be understood equivalently as a collection of strongly attractive bosons or as repulsive fermions with long-range interactions.

**Bound states with complex coupling** A recurring theme in this thesis is the addition of imaginary parts to the coupling constants of integrable quantum systems. We will start the exploration of such systems right here, by considering bound states in the Lieb-Liniger model with complex-valued  $c$ . Regrettably, our

endeavors in this direction are limited in scope and did not turn out to be very fruitful. We will only show that, in fact, the complexified Lieb-Liniger model also allows for the formation of bound states, by following almost step-by-step the derivation of the Bethe-Takahashi equations outlined in Appendix A of Calabrese and Caux [17]. More interesting results for the Lieb-Liniger model with complex-valued coupling (without a focus on the bound states) and the spectrum of its Lindbladian will be presented in Section 3.3.

We consider a configuration of  $N$  particles, with  $N_j$  strings of length  $j$ . The Bethe equations are

$$e^{ik_j L} = \prod_{l \neq j} \frac{k_j - k_l + ic}{k_j - k_l - ic}.$$

Substitute in the string hypothesis, eq. (56):

$$\begin{aligned} e^{ik_\alpha^{j,a} L} &= \prod_{(l,\beta,b) \neq (j,\alpha,a)} \frac{k_\alpha^{j,a} - k_\beta^{l,b} - i\bar{c}}{k_\alpha^{j,a} - k_\beta^{l,b} + i\bar{c}} \\ &= \prod_{(l,\beta,b) \neq (j,\alpha,a)} \frac{k_\alpha^j - k_\beta^l + \frac{i\bar{c}}{2}(j+1-2a+i\delta_\alpha^{j,a}-l-1+2b-i\delta_\beta^{l,b}) - i\bar{c}}{k_\alpha^j - k_\beta^l + \frac{i\bar{c}}{2}(j+1-2a+i\delta_\alpha^{j,a}-l-1+2b-i\delta_\beta^{l,b}) + i\bar{c}} \\ &= \prod_{(l,\beta,b) \neq (j,\alpha,a)} \frac{k_\alpha^j - k_\beta^l + i\bar{c}(\frac{j-l}{2} - a + b - 1) + i\delta_\alpha^{j,a} - i\delta_\beta^{l,b}}{k_\alpha^j - k_\beta^l + i\bar{c}(\frac{j-l}{2} - a + b + 1) + i\delta_\alpha^{j,a} - i\delta_\beta^{l,b}}, \end{aligned}$$

where the indices run as follows:

$$a = 1, \dots, j, \quad \alpha = 1, \dots, N_j, \quad b = 1, \dots, k, \quad \beta = 1, \dots, N_k.$$

Note that the condition on the terms is that  $(k, \beta, b) \neq (j, \alpha, a)$ , i.e. not all three indices can take on the same value simultaneously. This allows us to split the product in a term where  $(l, \beta) \neq (j, \alpha)$  while  $a$  can be equal to  $b$ , and a term where  $b \neq a$ , while  $j = l$  and  $\alpha = \beta$ :

$$e^{ik_\alpha^{j,a} L} = \underbrace{\prod_{(l,\beta) \neq (j,\alpha)} \prod_{b=1}^l \frac{k_\alpha^j - k_\beta^l + i\bar{c}(\frac{j-l}{2} - a + b - 1) + i\delta_\alpha^{j,a} - i\delta_\beta^{l,b}}{k_\alpha^j - k_\beta^l + i\bar{c}(\frac{j-l}{2} - a + b + 1) + i\delta_\alpha^{j,a} - i\delta_\beta^{l,b}}}_{\text{inter-string}} \underbrace{\prod_{b \neq a, j=l, \alpha=\beta} \frac{i\bar{c}(-a+b-1) + i\delta_\alpha^{j,(a,b)}}{i\bar{c}(-a+b+1) + i\delta_\alpha^{j,(a,b)}}}_{\text{intra-string}}.$$

In the process, we split up the product into inter- and intra-string parts,<sup>20</sup> and defined  $i\delta_\alpha^{j,a} - i\delta_\alpha^{j,b} \equiv \delta_\alpha^{j,(a,b)}$ . We may also throw away all string deviations for inter-string factors, since these involve rapidities that are well-separated:

$$e^{ik_\alpha^{j,a} L} = \prod_{(l,\beta) \neq (j,\alpha)} \prod_{b=1}^l \frac{k_\alpha^j - k_\beta^b + i\bar{c}(\frac{j-l}{2} - a + b - 1)}{k_\alpha^j - k_\beta^b + i\bar{c}(\frac{j-l}{2} - a + b + 1)} \prod_{b \neq a, j=l, \alpha=\beta} \frac{i\bar{c}(-a+b-1) + i\delta_\alpha^{j,(a,b)}}{i\bar{c}(-a+b+1) + i\delta_\alpha^{j,(a,b)}}.$$

Now, take the product of these equations within the string under consideration.

- The left hand side becomes:

$$\prod_{a=1}^j e^{ik_\alpha^{j,a} L} = e^{i \sum_{a=1}^j k_\alpha^{j,a} L} = e^{ij k_\alpha^j L}$$

(since the imaginary parts of  $k_\alpha^{j,a}$  cancel).

- The intra-string part on the right hand side becomes:

$$\prod_{a=1}^j \prod_{b \neq a} \frac{\bar{c}(-a+b-1) + \delta_\alpha^{j,(a,b)}}{\bar{c}(-a+b+1) + \delta_\alpha^{j,(a,b)}} = (-1)^{j(j+1)} = 1.$$

---

<sup>20</sup>Intra-string because we multiply over the  $a, b$  indices, which label rapidities within the string, while  $\alpha, \beta$  are fixed.

- The inter-string part becomes:

$$\begin{aligned}
& \prod_{a=1}^j \prod_{b=1}^l \frac{k + i\bar{c}\left(\frac{j-l}{2} - a + b - 1\right)}{k + i\bar{c}\left(\frac{j-l}{2} - a + b + 1\right)} \\
&= \left(\frac{k - i\bar{c}|j-l|/2}{k + i\bar{c}|j-l|/2}\right) \left(\frac{k - i\bar{c}(|j-l|+2)/2}{k + i\bar{c}(|j-l|+2)/2}\right)^2 \cdots \left(\frac{k - i\bar{c}(j+l-2)/2}{k + i\bar{c}(j+l-2)/2}\right)^2 \left(\frac{k - i\bar{c}(j+l)/2}{k + i\bar{c}(j+l)/2}\right) \\
&\equiv e_{|j-l|}(k) e_{|j-l|+2}^2(k) e_{|j-l|+4}^2(k) \cdots e_{j+l-2}^2(k) e_{j+l}(k) \\
&\equiv E_{jl}(k),
\end{aligned}$$

where we have introduced the notation

$$e_j(k) \equiv \frac{k - i\bar{c}j/2}{k + i\bar{c}j/2},$$

and wrote  $k \equiv k_\alpha^j - k_\beta^k$ . Writing out the product for a few values of  $a, b$  will help to reveal how the structure on the second line emerged. For example, taking  $j = k = 2$ ,

$$\begin{aligned}
\prod_{a=1}^2 \prod_{b=1}^2 \frac{k + i\bar{c}(-a + b - 1)}{k + i\bar{c}(-a + b + 1)} &= \underbrace{\left(\frac{k - i\bar{c}}{k + i\bar{c}}\right)}_{a=1, b=1} \underbrace{\left(\frac{k}{k + 2i\bar{c}}\right)}_{a=1, b=2} \underbrace{\left(\frac{k - 2i\bar{c}}{k}\right)}_{a=2, b=1} \underbrace{\left(\frac{k - i\bar{c}}{k + i\bar{c}}\right)}_{a=2, b=2} \\
&= 1 \cdot \left(\frac{k - i\bar{c}}{k + i\bar{c}}\right)^2 \left(\frac{k - 2i\bar{c}}{k + 2i\bar{c}}\right),
\end{aligned}$$

which is indeed consistent with the second line.

Putting all terms together, we obtain

$$e^{ij k_\alpha^j L} = \prod_{(l, \beta) \neq (j, \alpha)} E_{jl}(k_\alpha^j - k_\beta^l).$$

Taking the natural log and defining  $\phi_j(k) = 2 \arctan(2k/\bar{c}j)$  such that  $-i \log(-e_j(k)) = \phi_j(k)$  gives us the **Bethe-Takahashi equations** [116],

$$jk_\alpha^j L - \sum_{(l, \beta)} \Phi_{jl}(k_\alpha^j - k_\beta^l) = 2\pi I_\alpha^j, \quad (60)$$

with scattering phase shifts

$$\Phi_{jl}(k) = (1 - \delta_{jl})\phi_{|j-l|}(k) + 2\phi_{|j-l|+2}(l) + \cdots + 2\phi_{j+l-2}(k) + \phi_{j+l}(k).$$

Now again consider a complex rapidity  $k_\alpha = k + i\eta$ , but complexify the coupling,  $c = \gamma + i\omega$  with  $\gamma, \omega \in \mathbb{R}$ . The Bethe equations for this rapidity are

$$e^{ik_\alpha L} = e^{ikL - \eta L} = \prod_{\beta \neq \alpha} \frac{k_\alpha - k_\beta - i\gamma - \omega}{k_\alpha - k_\beta - i\gamma + \omega} = \prod_{\beta \neq \alpha} \frac{k - k_\beta + i(\gamma + \eta) - \omega}{k - k_\beta - i(\gamma - \eta) + \omega}.$$

Again consider finite  $N$  and  $L \rightarrow \infty$ .

- If  $\eta > 0$ ,  $e^{-\eta L} \rightarrow 0$ , and there must be a rapidity  $k_\beta$  such that  $k_\beta = k + i(\gamma + \eta) - \omega + \mathcal{O}(e^{-\eta L})$ .
- If  $\eta < 0$ ,  $e^{-\eta L} \rightarrow \infty$ , and hence there must be a rapidity  $k_\beta$  such that  $k_\beta = k - i(\gamma - \eta) + \omega + \mathcal{O}(e^{-|\eta|L})$ .

This motivates a string hypothesis in which the clusters are evenly spaced in *both* the real and the imaginary direction around the string center  $\lambda_\alpha^j$ :

$$k_\alpha^{j,a} = k_\alpha^j + \frac{\omega}{2}(j+1-2a) - i\frac{\gamma}{2}(j+1-2a). \quad (61)$$

Obviously, this reduces to the ordinary string hypothesis eq. (56) for  $\omega = 0$ . One can repeat the derivation leading up to eq. (60) and find that it does not break down anywhere. So for complex-valued couplings, we can use the Bethe-Takahashi equations with  $\bar{c} \rightarrow -i\omega - \gamma$  to calculate the string centers  $\lambda_\alpha^j$ , and then plug these into the new string hypothesis eq. (61) to obtain the  $k_\alpha^{j,a}$ .

Note: Choosing the Bethe numbers

Unlike in the repulsive case, where the ground state distribution of Bethe numbers is always given by  $I_j = -(N+1)/2 + j$ , with  $j = 1, \dots, N$ , choosing the Bethe numbers in the attractive Lieb-Liniger model is not as straightforward. Finding the distribution that minimizes the energy is only possible after the string content has been specified, i.e. a choice has been made for the number of 1-strings, 2-strings, etc. The *global* ground state however will always take the form of a bound state of all  $N$  particles into a single string centered at zero,

$$k^{N,a} = i \frac{\bar{c}}{2} (N+1-2a) + \mathcal{O}(\delta),$$

with energy  $E_{gs} = -\frac{\bar{c}^2}{12} N(N^2-1)$ , as derived concluded in eq. (59). This is intuitively clear from the cubic scaling with  $N$ , but it has also been demonstrated that the  $N$ -particle bound state has lower energy than any combination of smaller bound states or free particles, see McGuire [83].

Comment

Back in the first few months of my thesis, when I was exploring the Lieb-Liniger model and string solutions, I wrote a Jupyter Notebook that solves the Bethe-Takahashi equations for both real- and complex-valued couplings, given the string content (number of strings and their lengths). The script is nothing spectacular and isn't terribly hard to code up yourself, but if anyone in the future reads this and wants to save some time, do not hesitate to contact me at [mw112345@outlook.com](mailto:mw112345@outlook.com).

**Lieb-Liniger: Final remarks** We end this section with some remarks about the Lieb-Liniger model that I found interesting, but that are of no further importance to the thesis.

- In the repulsive regime, the connection between rapidities and the norm of the corresponding eigenstate is given by the *Gaudin-Korepin formula*. For string states, an analogous expression can be derived, see Calabrese and Caux [17]. The connection to correlation functions is made through dynamical structure factors, which are the Fourier transforms of correlation functions. Such DSF's are commonly expressed in terms of 'form factors'. See again Calabrese and Caux [17], where dynamical correlation functions pertaining to the density- and field operators are calculated between the ground state and an arbitrary excited state of the attractive Lieb-Liniger gas.
- We considered the Lieb-Liniger model at zero temperature. To go to finite temperatures, we need to consider general excited states. In broad terms, one defines the finite-temperature partition function as a sum over the Bethe numbers  $\{I_j\}$  that parametrize a state, and then rewrites the partition function in terms of the (macroscopic) particle and hole densities. Finally, one can go to the thermodynamic limit and perform a saddle-point approximation to find the most relevant contribution to the partition function. The resulting equation is called the *Yang-Yang equation*, and its solution gives the dressed energy per particle excitation as a function of the temperature. It is the key to computing thermodynamic quantities of the Lieb-Liniger model. The Yang-Yang equation is the first version of what has become known as the *Thermodynamic Bethe Ansatz* (TBA). For a detailed analysis, see Franchini [45] Section 2.9 or Korepin, Bogoliubov, and Izergin [72] Sections 1.5-1.7.
- The main limitation of the coordinate Bethe Ansatz is its form as a superposition of terms that grows exponentially with the number of particles  $N$ . Knowledge of eigenfunctions is only implicit, and the calculation of objects of interest (correlation functions) very quickly becomes cumbersome or impossible. Some numerical approaches which are not restricted to integrable systems do a more

Table 2: Comparison between the repulsive and attractive Lieb-Liniger model.

	repulsive	attractive
coupling	$c > 0$	$c < 0$
rapidities	real	complex-valued
eqs. for rapidities	Bethe, eq. (32)	Bethe-Takahashi, eq. (60)
bound states	no	yes
ground state	equally spaced particles	single string centered at 0
limit $ c  \rightarrow \infty$	Tonks-Girardeau	super Tonks-Girardeau <sup>22</sup>
bosonic description	hard-core	strongly attractive
fermionic description	free	repulsive, long-range interactions
thermodynamic limit	$N \rightarrow \infty, \rho = N/L$ fixed	unstable

efficient job at calculating correlation functions than methods based on the CBA. Algebraic Bethe Ansatz methods (Section 4) provide a cleaner expression for eigenstates, because they are essentially a second quantized form of CBA in which eigenstates are formed by repeated application of a creation operator on a vacuum state  $|0\rangle$ .

- In the regime of small (repulsive) interaction  $c \ll \rho$ , the bosonic field will not completely condense, since the formation of long-range order at any finite temperature is forbidden in one dimension.<sup>21</sup> A large fraction of the particles will however still be in the zero momentum state and form a ‘quasi-condensate’. Under such assumptions, we can treat the Lieb-Liniger Hamiltonian with chemical potential,

$$H_{LL} = \int dx [\partial_x \Psi^\dagger(x) \partial_x \Psi(x) + c \Psi^\dagger(x) \Psi^\dagger(x) \Psi(x) \Psi(x) - h \Psi^\dagger(x) \Psi(x)],$$

semi-classically and handle  $\Psi(x)$  as a classical, complex-valued field. The Euler-Lagrange equation for this Hamiltonian is

$$i\Psi_t = -\Psi_{xx} - h\Psi + 2c\Psi^\dagger\Psi, \quad (62)$$

which is called the one-dimensional *Gross-Pitaevskii* equation, and can be recognized as the non-linear Schrödinger equation (with chemical potential) that we mentioned before.

- For a summary of the different properties of the attractive and repulsive Lieb-Liniger model, refer to Table 2.

### 3.2. Open quantum systems and Lindbladians

The Lindblad master equation is a Markovian master equation that governs the time-evolution of open quantum systems. A master equation describes the evolution of a system that is at any given time in a probabilistic combination of states. The Lindblad master equation in particular generalizes the Schrödinger equation to open quantum systems. Open quantum systems comprise a broad spectrum of systems whose characteristic property is that they should not be considered in isolation, but rather in contact with their surroundings, see Figure 14. These systems carry particular physical interest for the simple reason that *any system* is to some extent interacting with its environment, and the isolated quantum systems we encounter in textbook quantum mechanics are no more than idealizations of systems where such interactions are negligible. A striking feature of open quantum systems is that their dynamics is no longer unitary. Of course, the dynamics of the total system (system of interest + environment) *will* be unitary, but we are interested in a description of the system of interest and are prepared to sacrifice unitarity in this *effective* description, by modeling interactions with the environment as dissipation or gain in the subsystem.

We start this section with a general discussion of the Lindblad master equation. The generator of the dynamics in open quantum systems and the central object in the Lindblad master equation is the Lindbladian

<sup>21</sup>(Hohenberg-)Mermin-Wagner theorem.

<sup>22</sup>In this limit, the rapidities are real-valued.

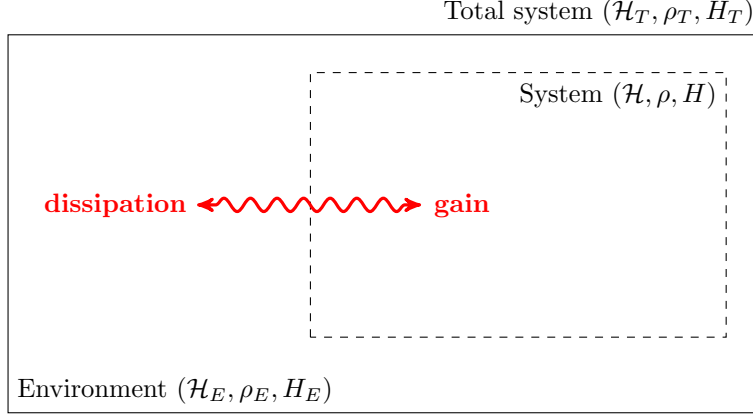


Figure 14: An open quantum system can be modeled as an environment interacting with the system of interest. The Lindblad equation is an effective motion equation for the system of interest.

$\mathcal{L}$ . We will prove that the real part of the eigenvalues of  $\mathcal{L}$  are non-positive, a property that we will employ to verify the numerical results in Section 3.3.

The Lindbladian  $\mathcal{L}$  is a *superoperator*, in the sense that it maps density operators on  $\mathcal{H}$  to density operators, instead of mapping state vectors to state vectors (as a regular operator would):

$$\mathcal{L} : \rho(\mathcal{H}) \rightarrow \rho(\mathcal{H}).$$

The motivation for such an object is best illustrated by the familiar **von Neumann equation** for the time-evolution of density matrices:

$$\dot{\rho} = \frac{1}{i\hbar} [H, \rho] \equiv \mathcal{L}' \rho, \quad (63)$$

i.e. we can write the von Neumann equation as the action of a superoperator  $\mathcal{L}'$  on the generic density matrix  $\rho$ . Just as the Schrödinger equation describes how pure states evolve in time, the von-Neumann equation describes how a density operator evolves, and the Lindbladian generates this time evolution to open quantum systems.

Note: Derivation of the von Neumann equation

The von Neumann equation can be derived by differentiating the expression for the density matrix  $\rho = \sum_i p_i |\Psi_i\rangle \langle \Psi_i|$ , with respect to time:

$$\frac{d\rho}{dt} = \dot{\rho} = \sum_i p_i \left( \frac{d}{dt} |\Psi_i\rangle \langle \Psi_i| + |\Psi_i\rangle \frac{d}{dt} \langle \Psi_i| \right).$$

By substituting the Schrödinger equation  $i\hbar \frac{d}{dt} |\Psi\rangle = H |\Psi\rangle$ , we obtain

$$\dot{\rho} = \frac{1}{i\hbar} \sum_i p_i (H |\Psi_i\rangle \langle \Psi_i| - |\Psi_i\rangle \langle \Psi_i| H) = \frac{1}{i\hbar} (H\rho - \rho H) = \frac{1}{i\hbar} [H, \rho].$$

When one does computations with superoperators, it is convenient to work in **Fock-Liouville space**. The idea is that some linear combinations of density matrices (namely those that preserve  $\text{Tr} = 1$  and positivity) are again valid density matrices, implying that we can create a Hilbert space of density matrices by defining a scalar product on the space. In this way, one forms a linear space of matrices, in which the matrices can be interpreted as vectors ( $\rho \rightarrow |\rho\rangle\rangle$ ). The usual definition of the scalar product of matrices  $\phi$  and  $\rho$  is

$$\langle\langle \phi | \rho \rangle\rangle \equiv \text{Tr} [\phi^\dagger \rho]. \quad (64)$$

The **Lindblad master equation** for open quantum systems – the object of interest for this section – is given by

$$\mathcal{L}(\hat{\rho}) \equiv \partial_t \hat{\rho} = \frac{1}{i\hbar} [\hat{H}, \hat{\rho}] + \sum_{k=1}^K \left( \hat{L}_k \hat{\rho} \hat{L}_k^\dagger - \frac{1}{2} \{ \hat{L}_k^\dagger \hat{L}_k, \hat{\rho} \} \right). \quad (65)$$

The first (commutator) term is just the von Neumann equation, eq. (63). The additional terms represent so-called ‘jump operators’, and they encode the dissipative part of the dynamics.

A couple of remarks concerning the jargon of open quantum systems are in place. The Lindblad master equation (65) also goes by the name of *Gorini-Kossakowski-Sudarshan-Lindblad equation* (GKSL equation). The superoperator  $\mathcal{L}$  is called either the **Lindbladian** or *Liouvillian*, although the term ‘Liouvillian’ seems to refer more generally to the generator of an arbitrary master equation, whereas ‘Lindbladian’ is found specifically in the context of open quantum systems (all apples are fruit, but not all fruits are apples).

Manzano [80] provides an excellent first introduction to the Lindblad master equation and constructs a derivation from two angles: from microscopic dynamics, and as the most general way of mapping density matrices onto density matrices. There are in fact many derivations in existence, each starting from a different set of assumptions. Other common derivations of the Lindblad equation, as well as other Markovian master equations, can be found in for example Alicki and Lendi [2] and references therein.

It can be proven that the real part of the eigenvalues of the Liouvillian superoperator are all non-negative. In the following, let  $B(\mathcal{H})$  denote the space of bounded operators acting on a Hilbert space  $\mathcal{H}$ , i.e.  $B : \mathcal{H} \rightarrow \mathcal{H}$ .

**Definition 3.1** (Positive operator) *A  $\in B(\mathcal{H})$  is called a positive operator ( $A > 0$ ) if and only if  $\langle \phi | A | \phi \rangle \geq 0$ ,  $\forall |\phi\rangle \in \mathcal{H}$ .*

**Definition 3.2** (Positive map) *A linear map  $\Phi : B(\mathcal{H}) \rightarrow B(\mathcal{H})$  is positive iff  $\Phi(A)$  is positive for all positive  $A \in \mathbb{C}^{n \times n}$ .*

**Definition 3.3** (Completely positive map) *A linear map  $\Phi : B(\mathcal{H}) \rightarrow B(\mathcal{H})$  is completely positive iff  $\Phi \otimes \mathbb{1}_p$  is positive for all positive integers  $p$ .*

In simple words, complete positivity means that the map is not only positive for the system  $S$  that it acts on, but also for any enlarged system that has  $S$  as a subsystem.

Next, we will state an important theorem that provides a necessary and sufficient condition for a map to be completely positive. For a proof, we refer to the original paper by Choi [24].

**Theorem 3.4** (Choi-Kraus [24]) *A linear map  $\Phi : \mathbb{C}^{n \times n} \rightarrow \mathbb{C}^{m \times m}$  is completely positive if and only if  $\Phi$  admits a so-called Kraus form,  $\Phi(A) = \sum_i V_i^\dagger A V_i$ , for all  $A$  in  $\mathbb{C}^{n \times n}$ , where  $V_i$  are  $n \times m$ -matrices.*

The theorem, in its original form, has been formulated for matrix operators, but it holds more generally, for bounded, linear operators. With these preliminary constructs in place, we can prove that the Liouvillian generates maps that are completely positive and trace-preserving, and that the trace distance between operators can only diminish (contract) under the flow of such a map. The proofs of the following two lemmas follows Zhang and Barthel [129], with some clarifications from Nielsen and Chuang [90].

**Lemma 3.1** (CPTP-property) *Every Liouvillian generates a completely positive trace-preserving (CPTP) map.*

*Proof.* Let  $\mathcal{E}_t = e^{\mathcal{L}t}$ . We prove the completely positive and trace-preserving properties separately.

- completely positive: Decompose

$$\mathcal{L} = \mathcal{L}^{(0)} + \sum_{k=1}^K \mathcal{L}^{(k)},$$

with  $\mathcal{L}^{(0)} = -i[\hat{H}, \hat{\rho}] - \frac{1}{2} \sum_{k=1}^K \{\hat{L}_k^\dagger \hat{L}_k, \hat{\rho}\}$  and  $\mathcal{L}^{(k)} = \hat{L}_k \hat{\rho} \hat{L}_k^\dagger$ , for  $k \geq 1$ . Now use the Lie-Trotter product formula to write

$$\mathcal{E}_t = \lim_{N \rightarrow \infty} (e^{\mathcal{L}^{(0)} \Delta t} e^{\mathcal{L}^{(1)} \Delta t} \dots e^{\mathcal{L}^{(K)} \Delta t} + \mathcal{O}(\Delta t^2))^N, \quad \text{with } \Delta t = t/N.$$

By neglecting terms of order  $\mathcal{O}(\Delta t^2)$  and comparison with the decomposition of the Lindbladian, we can write

$$e^{\mathcal{L}^{(0)} \Delta t}(\hat{\rho}) = \hat{V} \hat{\rho} \hat{V}^\dagger, \quad \text{with } \hat{V} \equiv e^{-i\hat{H}\Delta t - \frac{1}{2} \sum_k \hat{L}_k^\dagger \hat{L}_k \Delta t},$$

and, by means of a Taylor expansion,

$$e^{\mathcal{L}^{(k)} \Delta t}(\hat{\rho}) = \sum_{m=0}^{\infty} \frac{\Delta t^m}{m!} \hat{L}_k^m \hat{\rho} \hat{L}_k^{\dagger m},$$

for  $k \geq 1$ . These maps are both manifestly completely positive, since they are in Kraus form.

- trace-preserving: It follows immediately that

$$\partial_t \text{Tr } \mathcal{E}_t(\hat{\rho}) = \text{Tr } \mathcal{L}(\mathcal{E}_t(\hat{\rho})) = 0, \quad (66)$$

since  $\text{Tr } \mathcal{L}(\hat{\sigma}) = 0$  for all operators  $\hat{\sigma}$  in the Fock-Liouville space.<sup>23</sup>

□

Instinctively, the trace-preserving property of  $\mathcal{E}_t$  is required because of that fact that diagonal entries of the density matrix represent the probabilities of the system to be in the corresponding basis states, and these need to sum to 1, also at later times. Positivity is natural when one remembers that the entries of the density matrix represent probabilities. Note that CPTP-maps in the context of open quantum systems are sometimes called *quantum channels*.

**Definition 3.4** (Trace norm & trace distance) *The trace norm of an operator  $\hat{\rho}$  is defined as*

$$\|\hat{\rho}\|_1 \equiv \text{Tr} \left[ \sqrt{\hat{\rho}^\dagger \hat{\rho}} \right].$$

*The trace distance  $T(\hat{\rho}, \hat{\rho}')$  of two operators  $\hat{\rho}$  and  $\hat{\rho}'$  is defined as half the trace norm of the difference between  $\hat{\rho}$  and  $\hat{\rho}'$ ,*

$$T(\hat{\rho}, \hat{\rho}') \equiv \frac{1}{2} \|\hat{\rho} - \hat{\rho}'\|_1 = \frac{1}{2} \text{Tr} \left[ \sqrt{(\hat{\rho} - \hat{\rho}')^\dagger (\hat{\rho} - \hat{\rho}')} \right].$$

**Lemma 3.2** (Contractive property) *Under the action of any CPTP-map  $\mathcal{E}$ , the trace distance between density operators  $\hat{\rho}$  and  $\hat{\rho}'$  does not increase,*

$$\|\mathcal{E}(\hat{\rho}) - \mathcal{E}(\hat{\rho}')\|_1 \leq \|\hat{\rho} - \hat{\rho}'\|_1 \quad \forall \hat{\rho}, \hat{\rho}'.$$

*Proof.* Let us first prove that for any states  $\hat{\rho}$  and  $\hat{\rho}'$ , we may perform the spectral decomposition  $\hat{\rho} - \hat{\rho}' = \hat{Q}_+ - \hat{Q}_-$ , with  $\hat{Q}_+$ ,  $\hat{Q}_-$  positive operators with support on orthogonal vector spaces.

<sup>23</sup>This statement might cause confusion at first, because it is easy to slip up and believe that  $\mathcal{L}$  itself is trace-preserving, in which case  $\text{Tr } \mathcal{L}(\cdot) \neq 0$  in general. But this is not true: the Lindbladian *generates* a trace-preserving map  $e^{\mathcal{L}t}$  and is not itself a trace-preserving map. At the infinitesimal level, we then need  $\text{Tr}[\mathcal{L}(\hat{\rho})] = 0 \quad \forall \hat{\rho}$  which is apparent from eq. (65) (the trace of a commutator is always zero and the trace of the dissipative part is also zero because of the cyclicity of the trace). A further subtlety is that we have then established  $\text{Tr}[\mathcal{L}(\hat{\rho})] = 0$  for all density matrices  $\hat{\rho}$ , while in eq. (66) we do not know a priori that  $\mathcal{E}_t(\hat{\rho})$  will be a density matrix. Nevertheless we can motivate this heuristically (mathematicians please look away) by arguing that density matrices form a complete subset of the linear operator space and the Lindbladian is linear, so  $\mathcal{L}(\hat{\rho})$  being zero on all density matrices extends by linearity to the entire space of linear operators.



For convenience, we make the case by going to a matrix representation for the operators. Since  $\hat{\rho} - \hat{\rho}'$  is Hermitian, there exists a unitary matrix  $\hat{U}$  and a real, diagonal matrix  $D = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_N)$  such that  $\hat{\rho} - \hat{\rho}' = \hat{U} \hat{D} \hat{U}^\dagger$ . Now define

$$\begin{aligned}\hat{D}^+ &= \text{diag}(\max(\lambda_1, 0), \max(\lambda_2, 0), \dots, \max(\lambda_N, 0)), \\ \hat{D}^- &= \text{diag}(-\min(\lambda_1, 0), -\min(\lambda_2, 0), \dots, -\min(\lambda_N, 0)),\end{aligned}$$

i.e. diagonal matrices containing the positive and negative eigenvalues of  $\hat{D}$ . Then  $\hat{\rho} - \hat{\rho}' = \hat{U} \hat{D}^+ \hat{U}^\dagger + \hat{U} \hat{D}^- \hat{U}^\dagger \equiv \hat{Q}_+ - \hat{Q}_-$ , with  $\hat{Q}_+$  and  $\hat{Q}_-$  positive operators with supports that are disjoint parts of the eigenbasis of  $\hat{\rho} - \hat{\rho}'$ , and therefore orthogonal. This justifies the spectral decomposition.

Now, let  $\hat{P}_+$  be the projection operator onto the positive spectral subspace of  $\mathcal{E}(\hat{Q}_+) - \mathcal{E}(\hat{Q}_-)$ . Observe that

$$\text{Tr}[\hat{Q}_+ - \hat{Q}_-] = \text{Tr}[\hat{\rho} - \hat{\rho}'] = \text{Tr}[\hat{\rho}] - \text{Tr}[\hat{\rho}'] = 0,$$

so  $\text{Tr}[\hat{Q}_+] = \text{Tr}[\hat{Q}_-]$ , which means that  $\text{Tr}[\mathcal{E}(\hat{Q}_+)] = \text{Tr}[\mathcal{E}(\hat{Q}_-)]$  (because the map is trace-preserving). Then

$$\begin{aligned}T(\hat{\rho}, \hat{\rho}') &= \frac{1}{2} \text{Tr}|\hat{\rho} - \hat{\rho}'| = \frac{1}{2} \text{Tr}|\hat{Q}_+ - \hat{Q}_-| = \frac{1}{2} \text{Tr}[\hat{Q}_+] + \frac{1}{2} \text{Tr}[\hat{Q}_-] = \frac{1}{2} \text{Tr}[\mathcal{E}(\hat{Q}_+)] + \frac{1}{2} \text{Tr}[\mathcal{E}(\hat{Q}_-)] \\ &= \text{Tr}[\mathcal{E}(\hat{Q}_+)] \geq \text{Tr}[\hat{P}_+ \mathcal{E}(\hat{Q}_+)] \geq \text{Tr}[\hat{P}_+ (\mathcal{E}(\hat{Q}_+) - \mathcal{E}(\hat{Q}_-))] = \text{Tr}[\hat{P}_+ (\mathcal{E}(\hat{\rho}) - \mathcal{E}(\hat{\rho}'))] = T(\mathcal{E}(\hat{\rho}), \mathcal{E}(\hat{\rho}')).\end{aligned}$$

The third equality follows from

$$\begin{aligned}|\hat{\rho} - \hat{\rho}'| &= |\hat{Q}_+ - \hat{Q}_-| = \sqrt{(\hat{Q}_+ - \hat{Q}_-)^\dagger (\hat{Q}_+ - \hat{Q}_-)} \\ &= \sqrt{\hat{Q}_+^2 - \hat{Q}_+ \hat{Q}_- - \hat{Q}_- \hat{Q}_+ + \hat{Q}_-^2} = \sqrt{(\hat{Q}_+ + \hat{Q}_-)^2} = \hat{Q}_+ + \hat{Q}_-, \end{aligned}$$

because the cross terms such as  $\hat{Q}_+ \hat{Q}_- = (\hat{U} \hat{D}^+ \hat{U}^\dagger)(\hat{U} \hat{D}^- \hat{U}^\dagger) = -\hat{U} \hat{D}^+ \hat{D}^- \hat{U}^\dagger$  vanish since  $\hat{D}^+ \hat{D}^- = 0$ . This completes the proof.  $\square$

We are now ready to prove the theorem that we are after:

**Theorem 3.5 (Non-positive real part)** *For a Markovian system with a finite-dimensional Hilbert space, the real part of the spectrum of  $\mathcal{L}$  is non-positive.*

*Proof.* The hard work has already been done in Lemma 3.1 and 3.2. It remains to conclude that, due to the contractive property, for finite-dimensional Hilbert spaces all eigenvalues  $\epsilon_n$  of  $\mathcal{E}_t$  lie within unit distance of the origin in the complex plane,

$$\mathcal{E}_t(\hat{R}) = \epsilon_n \hat{R} \quad \xRightarrow{\text{Lemma 3.2}} \quad |\epsilon_n| = \frac{\|\mathcal{E}_t(\hat{R})\|_1}{\|\hat{R}\|_1} \leq 1.$$

From  $\mathcal{E}_t = e^{\mathcal{L}t}$ , we see that the eigenvalues of the Liouvillian are  $\lambda_n = \frac{1}{t} \ln \epsilon_n$ , and since  $|\epsilon_n| \leq 1$ , we have  $\text{Re}\{\lambda_n\} \leq 0$ .  $\square$

### 3.3. Finding the spectrum of the non-Hermitian Lieb-Liniger model

We will now apply our knowledge of open quantum systems to find the spectrum of the Lindbladian for a Lieb-Liniger model with dissipation.

### 3.3.1. Discussion of work by Torres [118]

In the paper “Closed-form solution of Lindblad master equations without gain” by Torres [118], an approach is worked out for diagonalizing open quantum systems satisfying four assumptions. The **key insight** of this paper is that for open quantum systems satisfying these assumptions, the spectrum of the Liouvillian  $\mathcal{L}$  is completely determined by the spectrum of the part of the master equation that conserves excitations,  $\mathcal{K}$ . This means that if we know the eigenvalues of  $\mathcal{K}$ , we can find all eigenvalues of the Liouvillian.

**System** We are dealing with a system governed by a slight generalization of the master equation (65), because we now also include a damping rate  $\gamma_s$  paired to each of the jump operators  $A_s$  associated with a dissipative channel indexed by  $s$ . The damping rates allow us to ramp up or tone down the amount of dissipation. The dynamical evolution is given in terms of the Liouville superoperator as

$$\mathcal{L}\rho = \frac{1}{i\hbar}[H, \rho] + \sum_s \frac{\gamma_s}{2} (2L_s \rho L_s^\dagger - L_s^\dagger L_s \rho - \rho L_s^\dagger L_s), \quad (67)$$

where, as before, we can distinguish a coherent Hamiltonian part (the von Neumann equation), plus a dissipative part in Lindblad form.

Note: Physical interpretation of jump operators

Jump operators represent specific (irreversible) dissipative processes in open quantum systems that arise from the interaction between system and environment. They can for example represent spontaneous emission, absorption, stimulated emission, dephasing or damping of bosonic modes in a cavity.

**Assumptions** The following assumptions apply:

1. The Hamiltonian part has no source of driving;
2. An observable  $I$  exists that commutes with  $H$  (it is a constant of motion), which is a measure of the excitations in the system;
3. The system is defined on a Hilbert space  $\mathcal{H}$ , and there exists a complete basis set  $\{|n, j\rangle\}$  with  $\mathcal{N}$  elements, in which  $I$  is diagonal and there exist  $d_n$  states with the same integer eigenvalue of  $I$  ( $d_n$  is the algebraic multiplicity of the eigenvalues)

$$I |n, j\rangle = n |n, j\rangle, \quad n = 0, \dots, N,$$

and  $\mathcal{N} = \sum_{n=0}^N d_n$ . Another way to say this is that  $|n, j\rangle$  describes an eigenstate of  $I$  with  $n$  particles, where  $j$  labels eigenstates having the same particle number;

4. For the dissipative part, we consider only Lindblad operators  $A_s$  that represent either pure losses or pure gains in the system, formalized by the commutation relation<sup>24</sup>

$$[A_s, I] = \pm A_s.$$

**Consequences** We can immediately note two consequences of this construction:

1. Because  $H$  commutes with  $I$ ,  $H$  has a block-diagonal form in the basis where  $I$  is diagonal, with each block  $H^{(n)}$  of size  $d_n \times d_n$ ;
2. From the last assumption, it follows that each Hermitian operator  $A_s^\dagger A_s$  also commutes with  $I$ . To see this, note that

$$[A_s^\dagger A_s, I] = A_s^\dagger [A_s, I] + [A_s^\dagger, I] A_s = A_s^\dagger A_s - A_s^\dagger A_s = 0,$$

<sup>24</sup>For example, in the case of pure loss we have the relation  $[A_s, I] = +A_s$  such that  $I(A_s |n, j\rangle) = (A_s I - A_s) |n, j\rangle = (n-1)A_s |n, j\rangle$  i.e.  $A_s$  acts as a lowering operator on eigenstates of  $I$ .

where we used

$$[A_s^\dagger, I] = A_s^\dagger I - I A_s^\dagger = (I^\dagger A_s - A_s I^\dagger)^\dagger = -(A_s I - I A_s)^\dagger = -[A_s, I]^\dagger = -A_s^\dagger,$$

and  $I^\dagger = I$  since  $I$  is an observable. This again implies a block-diagonal form for  $A_s^\dagger A_s$  in the basis where  $I$  is diagonal.

This suggests splitting the master equation (67) in a part that conserves excitations,<sup>25</sup>  $\mathcal{K}\rho$ , and a part that describes de-excitation of the system,  $\mathcal{A}\rho$ :

$$\mathcal{L}\rho = \mathcal{K}\rho + \mathcal{A}\rho,$$

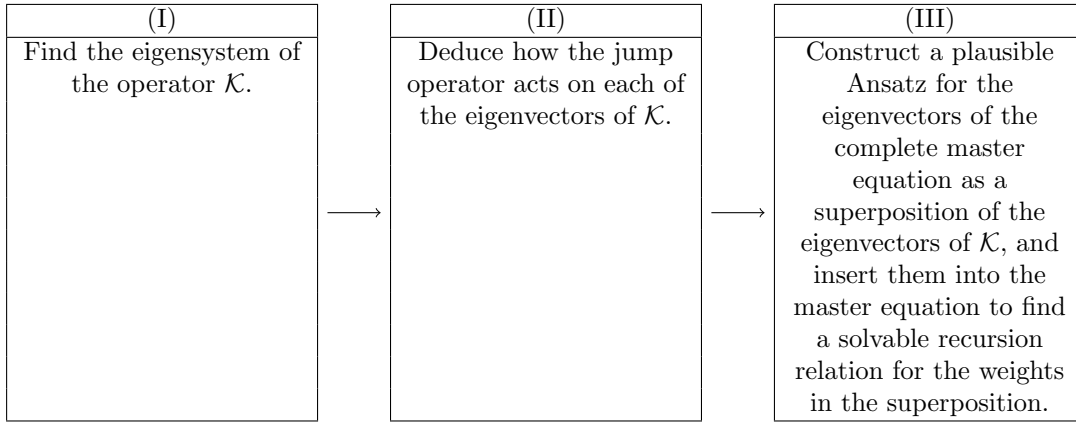
with

$$\mathcal{K}\rho = \frac{1}{i\hbar}(K\rho - \rho K^\dagger), \quad \mathcal{A}\rho = \sum_s \gamma_s A_s \rho A_s^\dagger, \quad (68)$$

and non-Hermitian Hamiltonian

$$K = H - i\hbar \sum_s \frac{\gamma_s}{2} A_s^\dagger A_s. \quad (69)$$

The flow of the paper, of which we will discuss only part (I), can be summarized in three steps:



The final achievement is the solution of the full master equation (67).

**Discussion of part (I)** The goal will be to find the eigensystem of  $\mathcal{K}$ . Note that  $[K, I] = 0$ , such that  $K$  is also block-diagonal in the basis  $\{|n, j\rangle\}$  that diagonalizes  $I$ :

$$K |n, k\rangle = \sum_{j=1}^{d_n} K_{j,k}^{(n)} |n, j\rangle.$$

This means that  $K$  does not mix/couple eigenvectors of  $I$  with different values of  $n$ . Assume that each block of  $K$  can be diagonalized by the transformation

$$\tilde{K}^{(n)} = Q^{\dagger(n)} K^{(n)} R^{(n)}, \quad \text{with } Q^{\dagger(n)} R^{(n)} = \mathbb{1}_{d_n},$$

where  $\tilde{K}^{(n)}$  is a diagonal matrix with the eigenvalues of the  $n$ -th block of  $K$  on its diagonal,  $\mathbb{1}_{d_n}$  the  $d_n \times d_n$  identity matrix and  $Q^{\dagger(n)}$  and  $R^{(n)}$  are the blocks of the operators  $Q^\dagger$  and  $R$  which diagonalize the  $n$ -th

---

<sup>25</sup>It conserves excitations since  $\frac{1}{i\hbar}[H, \rho]$  conserves excitations and the other two terms contain number operators  $A_s^\dagger A_s$ , which also do not change the total particle number.

block of  $K$ . We will use a tilde  $\sim$  to denote matrices expressed in the eigenbasis of  $K$ . The columns (rows) of  $R$  ( $Q^\dagger$ ) are the right (left) eigenvectors of  $K$  and in the original basis  $\{|n, j\rangle\}$  they can be expanded as

$$|r_j^n\rangle = \sum_{k=1}^{d_n} R_{k,j}^{(n)} |n, k\rangle, \quad |q_j^n\rangle = \sum_{k=1}^{d_n} Q_{k,j}^{(n)} |n, k\rangle.$$

These are linear combinations of the  $|n, j\rangle$  and hence also eigenstates of  $I$ . It follows that they are orthogonal and complete:<sup>26</sup>

$$\langle q_k^n | r_j^m \rangle = \delta_{k,j} \delta_{n,m}, \quad \sum_{n=0}^N \sum_{j=1}^{d_n} |r_j^n\rangle \langle q_j^n| = \mathbb{1}.$$

The eigenvalue equation for  $K$  is then

$$K |r_j^n\rangle = \epsilon_j^{(n)} |r_j^n\rangle, \quad K^\dagger |q_j^n\rangle = \epsilon_j^{*(n)} |q_j^n\rangle,$$

with complex eigenvalues  $\epsilon_j^{(n)}$ . The eigensystem of  $\mathcal{K}$  can be constructed from the eigensystem of  $K$ . From the expression for  $\mathcal{K}\rho$ , it can be seen (by inspection) that

$$\hat{\varrho}_{j,k}^{(l,n)} = |r_j^{n+l}\rangle \langle r_k^n|, \quad \check{\varrho}_{j,k}^{(l,n)} = |q_j^{n+l}\rangle \langle q_k^n|,$$

with  $j = 1, \dots, d_{n+l}$  and  $k = 1, \dots, d_n$ , are the right & left eigenvectors of  $\mathcal{K}$ : they solve the eigenvalue equation

$$\mathcal{K} \hat{\varrho}_{j,k}^{(l,n)} = \lambda_{j,k}^{(l,n)} \hat{\varrho}_{j,k}^{(l,n)}, \quad \mathcal{K}^\dagger \check{\varrho}_{j,k}^{(l,n)} = \lambda_{j,k}^{*(l,n)} \check{\varrho}_{j,k}^{(l,n)},$$

with eigenvalues

$$\lambda_{j,k}^{(l,n)} = \frac{1}{i\hbar} \left[ \epsilon_j^{(n+l)} - \epsilon_k^{*(n)} \right], \quad (70)$$

where the indices run over  $n+l, n = 0, \dots, N$ ,  $j = 1, \dots, d_{n+l}$  and  $k = 1, \dots, d_n$ . In the context of the Lieb-Liniger model:  $\epsilon_j^{(n)}$  is the energy of the  $n$ -particle eigenstate  $|n, j\rangle$ , i.e. an eigenstate with  $n$  particles with excitations labeled by  $j$ , where  $j = 1$  corresponds to the ground state and  $j = 2, 3, \dots$  correspond to excitations above the ground state – to be constructed by progressively shifting the Bethe numbers away from the ground state distribution,  $I_j \in \{-\frac{N}{2}+1, -\frac{N}{2}+2, \dots, \frac{N}{2}\}$  for  $N$  even and  $I_j \in \{-\frac{N-1}{2}, -\frac{N-1}{2}+1, \dots, \frac{N-1}{2}\}$  for  $N$  odd.

**Remarks** The fact that  $\mathcal{L}$  and  $\mathcal{K}$  share the same spectrum follows from the observation that  $\mathcal{L}$  has an upper triangular form in the basis where  $\mathcal{K}$  is diagonal; for the motivation of this statement (step II and III), we refer to the rest of the paper.

Application of these ideas can be found in for example Nakagawa, Kawakami, and Ueda [88] where the Liouvillian spectrum of a 1D dissipative Hubbard model is computed. Using the methods outlined here, the Liouvillian is diagonalized. After that, the steady state behaviour, Liouvillian gap, Hubbard gap and correlation length are investigated.

### 3.3.2. Numerical implementation

The Lieb-Liniger model with dissipation is described by the non-Hermitian Hamiltonian

$$\begin{aligned} \tilde{H}_{LL} &\equiv \int dx [\partial_x \Psi^\dagger(x) \partial_x \Psi(x) + (\gamma + i\omega) \Psi^\dagger(x) \Psi^\dagger(x) \Psi(x) \Psi(x)] \\ &= H_{LL} + i\omega \int dx \Psi^\dagger(x) \Psi^\dagger(x) \Psi(x) \Psi(x), \end{aligned} \quad (71)$$

---

<sup>26</sup>Complete because the  $\{|n, j\rangle\}$  is a complete basis.

Table 3: Identifications between the non-Hermitian Lieb-Liniger model discussed in this section and the paper by Torres [118].

	Torres [118]		Model	
	symbol	eq.	symbol	eq.
Lindbladian jump operators	$\mathcal{L}$	(67)	$\mathcal{L}_{LL}$	(72)
	$A$	generic	$L$	$\Psi(x)\Psi(x)$
Non-Hermitian Hamiltonian, eigenvalues	$K, \epsilon_n^l$	(69)	$\tilde{H}_{LL}, E_n^l$	(71)
Operator conserving excitations eigenvalues	$\mathcal{K}$	(68)	$\mathcal{K}_{LL}$	(73)
	$\lambda_{j,k}^{(l,n)}$	(70)	$\lambda_{j,k}^{(l,n)}$	(74)

with  $\gamma, \omega \in \mathbb{R}$  and  $H_{LL}$  given by eq. (24) (with  $c = \gamma$ ). We identify the jump operators as the double fields  $L = \Psi(x)\Psi(x)$ . The corresponding master equation is

$$\begin{aligned} \mathcal{L}_{LL}\rho = & \frac{1}{i\hbar}[H_{LL}, \rho] + \frac{i\omega}{2} \int dx [2\Psi(x)\Psi(x)\rho\Psi^\dagger(x)\Psi^\dagger(x) \\ & - \Psi^\dagger(x)\Psi^\dagger(x)\Psi(x)\Psi(x)\rho - \rho\Psi^\dagger(x)\Psi^\dagger(x)\Psi(x)\Psi(x)]. \end{aligned} \quad (72)$$

The operator  $\mathcal{K}_{LL}$ , that is responsible for the part of the dynamics that conserves excitations, is identified with

$$\mathcal{K}_{LL}\rho = \frac{1}{i\hbar}(\tilde{H}_{LL}\rho - \rho\tilde{H}_{LL}^\dagger). \quad (73)$$

The eigenvalues of  $\mathcal{K}_{LL}$  are, from eq. (70):

$$\lambda_{j,k}^{(l,n)} = \frac{1}{i\hbar} \left[ E^{(n+l)} - E^{*(n)} \right]. \quad (74)$$

Therefore, we propose the following three-step strategy for finding the spectrum of the Lindbladian  $\mathcal{L}$  for the complexified Lieb-Liniger Hamiltonian:

1. Numerically solve the Bethe equations eq. (32) for the non-Hermitian Hamiltonian  $\tilde{H}_{LL}$  to find the set of Bethe roots/rapidities  $\{k_j\}$ ,  $j = 1, \dots, N$ .
2. From the rapidities, build the energies  $E = \sum_i^N k_i^2$ , which are the eigenvalues of  $\tilde{H}_{LL}$ .
3. From the energies  $E$ , build the eigenvalues of the operator  $\mathcal{K}_{LL}$ , by considering eq. (70). By the arguments in Torres [118], we have then also found the spectrum of the Lindbladian  $\mathcal{L}$  ‘for free’.

To avoid confusion about the notation and make everything as explicit as possible, Table 3 lists the various identifications we make between our model and the objects in Torres [118].

**Step 1** After trying out various methods which all suffered from stability and scaling issues, we settled on an optimized Newton-Raphson solver with damping and LU-decomposition to solve the Bethe equations with imaginary coupling. We first rewrite the Bethe equations as

$$F_j(k_1, k_2, \dots, k_N) = k_j L - 2\pi I_j - \sum_{l=1}^N \theta(k_j - k_l) = 0, \quad j = 1, 2, \dots, N.$$

The Newton-Raphson method updates the values of the rapidities  $\{k_j\}$  according to the rule:

$$\vec{k}^{(n+1)} = \vec{k}^{(n)} - J^{-1} F(\vec{k}^{(n)}),$$

where  $F(\mathbf{k}^{(n+1)})$  is the vector of Bethe equations and  $J$  is the Jacobian matrix with elements

$$J_{jl} = \frac{\partial F_j}{\partial k_l} = L\delta_{jl} - \frac{d\theta(k_j - k_l)}{dk_j}.$$

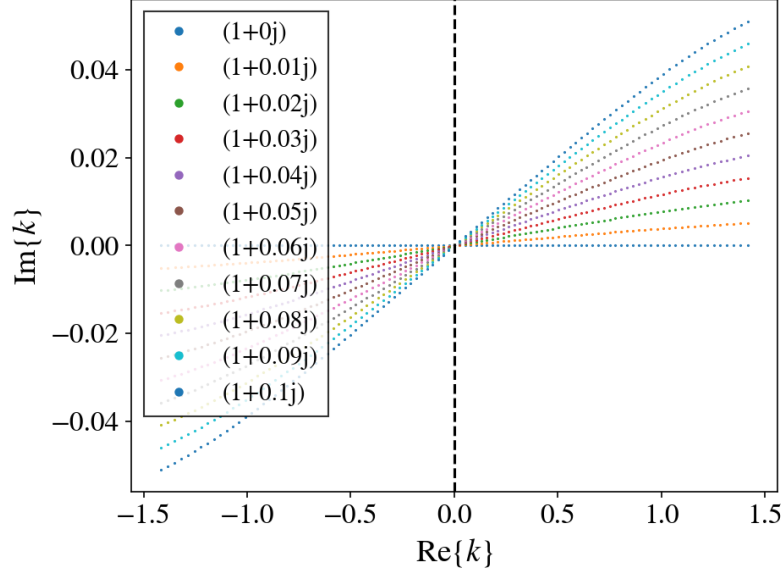


Figure 15: Real- and complex-valued parts of the Bethe roots  $\{k_j\}$  for couplings with small imaginary parts, at density  $\rho = 1$ . For  $c = 1 + 0j$ , the Bethe roots are completely real-valued, in accordance with Theorem 3.2.

The derivative is

$$\frac{d\theta(k)}{dk} = -\frac{2}{c} \frac{1}{1 + (k/c)^2}.$$

We use a damped update step: instead of  $\mathbf{k}^{(n+1)} = \mathbf{k}^{(n)} + \Delta\mathbf{k}^{(n)}$ , we use  $\mathbf{k}^{(n+1)} = \mathbf{k}^{(n)} + \alpha\Delta\mathbf{k}^{(n)}$ , with  $\alpha = 0.5$ . This prevents overshooting and improves stability, especially when far from the solution. Furthermore, instead of directly inverting the Jacobian matrix, we implement an LU-decomposition of  $J$  to attain the desired levels of stability and computational speed, and solve the system  $L_J U_J \Delta\mathbf{k}^{(n)} = -F(\mathbf{k}^{(n)})$ .<sup>27</sup> The initial conditions are chosen to mimic a free-particle approximation, where the initial rapidities are chosen as  $\frac{2\pi}{L}\{-\frac{N-1}{2}, -\frac{N-3}{2}, \dots, \frac{N-1}{2}\}$  for  $N$  odd and  $\{-\frac{N}{2} + 1, -\frac{N}{2} + 2, \dots, \frac{N}{2}\}$  for  $N$  even. The real- and complex-valued parts of the Bethe roots for couplings with small imaginary parts are shown in Figure 15.

For high densities, the current implementation of the Newton-Raphson solver does not converge, and non-sensical results are obtained. Notably, the method is found to break down for densities  $\rho \gtrsim 2-3$ , even if initial conditions are dynamically adapted to match the solution of the previous iteration. Interestingly, the LU-based solver with damping reproduces the results produced by Mathematica [56] to a high degree of precision, whereas previous methods suffered from a significant disparity away from  $\text{Im}\{c\} = 0$ .

**Step 2 and 3** We construct the spectrum of  $\mathcal{L}$ . Results are displayed in Figures 16, 17, 18 and 19, where we vary the imaginary part of the coupling, the number of excitations above the ground state, the number of particles  $N$  and the density  $\rho = N/L$ , respectively. Note that, in accordance with Theorem 3.5, the real parts of the roots are strictly non-positive.

<sup>27</sup>The cost of factorizing an  $N \times N$ -matrix into LU-form is  $\mathcal{O}(N^3)$ , and once the factorization is known, the cost of solving the system  $LU\mathbf{x} = \mathbf{b}$  is  $\mathcal{O}(N^2)$ : first solve  $L\mathbf{y} = \mathbf{b}$  and then  $U\mathbf{x} = \mathbf{y}$ . Hence, the total cost of solving  $LU\mathbf{x}_1 = \mathbf{b}_1, U\mathbf{x}_2 = \mathbf{b}_2, \dots, LU\mathbf{x}_r = \mathbf{b}_r$  for  $r$  right-hand side vectors scales as  $\mathcal{O}(N^3 + rN^2)$ , while the total cost of Gaussian elimination scales as  $\mathcal{O}(rN^3)$ , since each Gaussian elimination independently costs  $\mathcal{O}(N^3)$ .

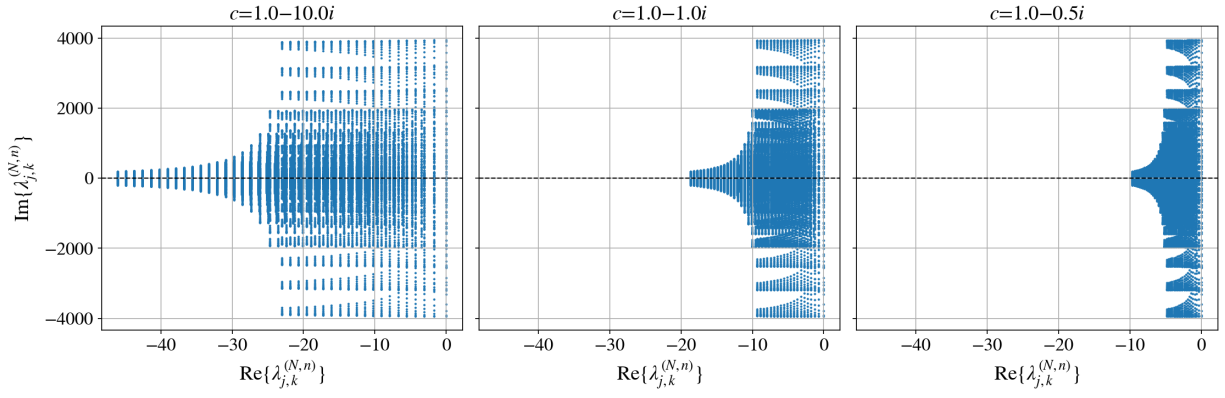


Figure 16: Lindbladian spectrum for  $\rho = 1$ , 10 excitations and varying imaginary contributions to the coupling.

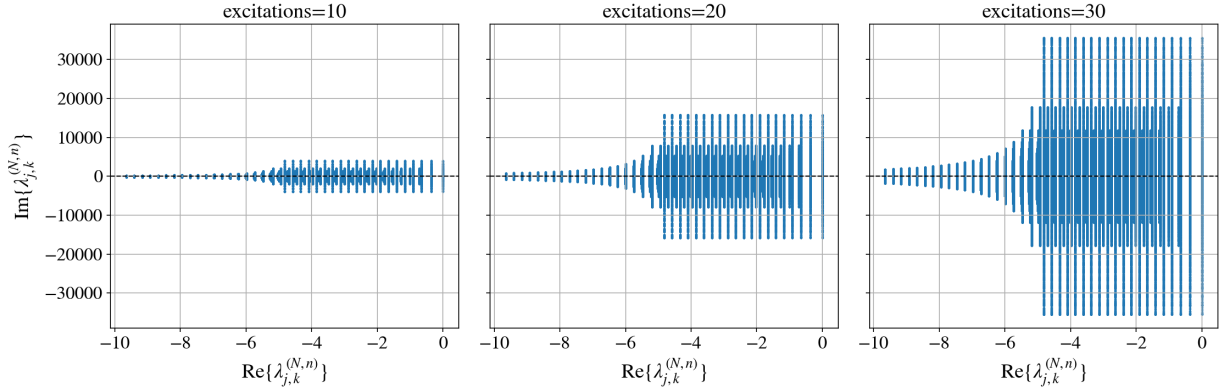


Figure 17: Lindbladian spectrum for  $\rho = 1$ ,  $c = 1 - 0.5i$  and varying number of excitations.

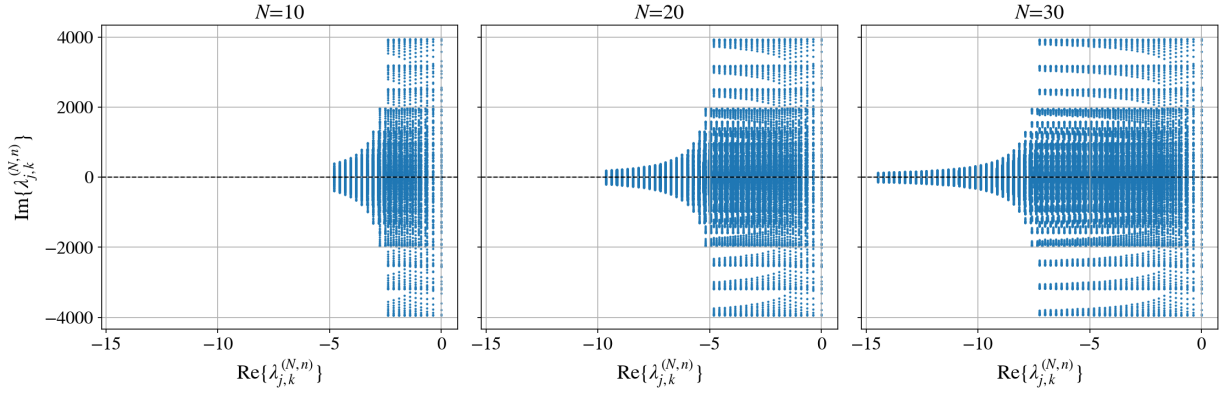


Figure 18: Lindbladian spectrum for  $\rho = 1$ ,  $c = 1 - 0.5i$ , 10 excitations and varying  $N$ .

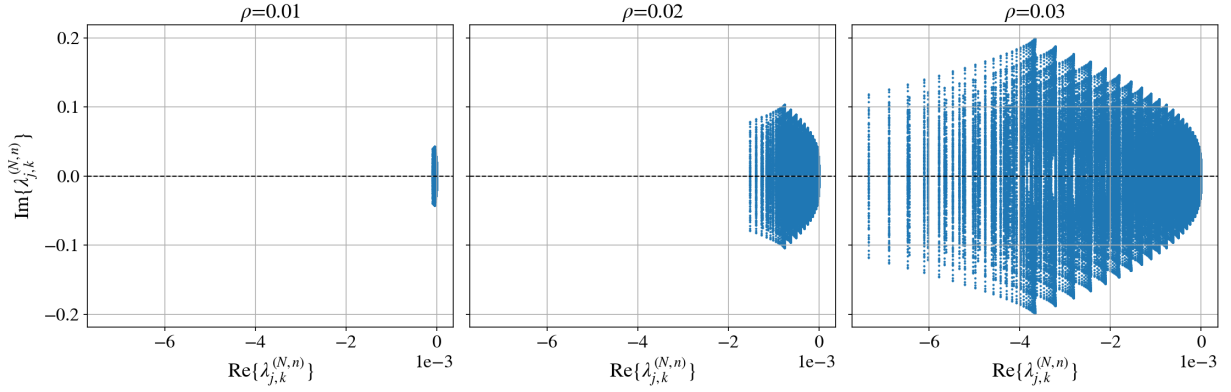


Figure 19: Lindbladian spectrum for  $c = 1 - 0.5i$ , 10 excitations and varying  $\rho$ .



## 4. Algebraic Bethe Ansatz and Richardson-Gaudin models

In this section, we introduce algebraic Bethe Ansatz (ABA) and Richardson-Gaudin (RG) models, drawing mainly on [20], [87], [26] and [113]. The algebraic Bethe Ansatz can be seen as an Ansatz for the underlying *operator algebra*<sup>28</sup> of a model, in contrast to coordinate Bethe Ansatz, which is an Ansatz for the wavefunction. ABA was developed by a group of Soviet mathematical physicists in the 1970s, now known as the Leningrad school, with a leading role for Ludvig Faddeev. They generalized earlier work by Rodney Baxter in the early 1970s, who managed to solve the classical 8-vertex model and the XXZ- and XYZ-models using a transfer matrix approach [8, 9, 10]. The *quantum inverse scattering method* (QISM, see for example Sklyanin [107]), which is a quantum mechanical adaptation of the classical inverse scattering method that is used to solve nonlinear classical wave equations with solitonic solutions, is practically synonymous to solution by algebraic Bethe Ansatz.

If you read this thesis chronologically, you will at this point have encountered the coordinate, thermodynamic and – now – the algebraic Bethe Ansatz. But the story does not end here. In literature, you will in fact find even more exotic flavours of the Bethe Ansatz: nested Bethe Ansatz [109] for a hierarchical application of the algebraic Ansatz in models with multiple species or spin components, analytic/functional Bethe Ansatz [106] based on functional relations like Baxter’s TQ-equation, off-diagonal Bethe Ansatz [125] for systems with non-diagonal boundaries (e.g. open Hubbard chains) and extended Bethe Ansatz [59] adapted to long-range or elliptic systems or systems with integrable dissipative dynamics. In addition, a class of systems known as Richardson-Gaudin models is solvable by an approach that is in many ways a rewriting of the algebraic Bethe Ansatz, producing the same output (the Bethe equations) – see Section 4.3. *The unifying principle underlying all these variations is the assumption that the many-body wavefunction or transfer matrix eigenstates can be constructed from two-body scattering events that factorize consistently across the entire system.* To elaborate, it is assumed that the system’s dynamics are completely elastic and non-diffractive, such that multi-particle scattering events can be reduced to a sequence of two-particle scattering events. Furthermore, the many-particle S-matrix is assumed to factorize into two-body S-matrices, and the two-body scattering events must satisfy the Yang Baxter equation, which we will see shortly. The system’s solvability then reduces to finding quantization conditions (Bethe equations) that consistently describe these interactions. I gave my best to organize known models solvable by Bethe Ansatz and Richardson-Gaudin methods in Table 4, which I do not believe to be exhaustive, but which should go a long way in listing some of the more well-known models to which the BA/RG-approach is applied.

The ABA, which I present schematically in Figure 20, is in some sense a ‘reverse’ method, in that one first specifies the Yang-Baxter algebra and its representation and that a physical model is then a consequence, rather than the starting point. Another perspective is that one views ABA as somewhat of a black box containing a vast amount of models and that one tries to extract the physics by (systematically) feeding it different representations of the Yang-Baxter algebra. This is sometimes called the *constructive approach*.

Despite its overall success in providing a framework for the systematic study of quantum integrable models, ABA has two major weaknesses. Firstly, ABA is not universally applicable to all quantum integrable systems. For example, the XYZ-model fails to be solvable by ‘traditional’ ABA due to the lack of a unique pseudovacuum state, although modified versions of Bethe Ansatz exist that are able to overcome this impediment. Secondly, the ABA suffers from a *completeness problem* in the sense that it does not necessarily yield all eigenstates of the system; this problem can sometimes be circumvented by introducing new parameters to the Yang-Baxter algebra.

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<sup>28</sup>Because the notion of an algebra occurs so frequently throughout this thesis, let us be complete and recall that an algebra (over a field) is essentially a vector field with an additional operation that gives it a multiplicative structure. Informally and in the way we are interested, an algebra is just a bunch of operators and their commutation relations.

<sup>29</sup>Extension of the Lieb-Liniger model from bosons to spin-1/2 fermions with Dirac delta interactions.

Table 4: Table of models solvable by Bethe Ansatz and the related Richardson-Gaudin approach. C: coordinate, A: algebraic, N: nested, F: functional, O: off-diagonal, E: extended. Rational, trigonometric and elliptic pertain to the RG-class, see eq. (104) and accompanying text. For many of the models listed here, thermodynamic Bethe Ansatz methods were developed to describe the system at finite temperature. The table is based on my limited literature review and the sources I have consulted to compose this chapter, and I do not claim that it is by any means exhaustive. Furthermore, the distinction between BA/RG-solvable models is not as rigid as the table suggests; the class I assign to a model merely reflects the context in which I have seen their solution presented. In fact, from Section 4.3 it will hopefully be clear that the RG-approach can be seen as a rewriting of the ABA.

	Model	Type	refs.
BA	Lieb-Liniger	C/A	Section 3 & 4.2.2
	Gaudin-Yang <sup>29</sup>	C/N	[48, 127]
	6- and 8-vertex	A/F	[72, 11]
	Thirring	C	[12]
	Kondo	C	[3]
	(Generalized) 1D Hubbard-type	C/A/N/O	[77, 97, 125]
	Bose-Hubbard dimer	A	[78]
	Anderson impurity	C	[103]
	Inozemtsev chain	E	[59, 58, 57]
	1D $\delta$ -function anyons	C	[7]
BA/RG	Heisenberg XXX <sub>1/2</sub>	C rational	[13]
	Heisenberg XXZ <sub>1/2</sub> /XYZ <sub>1/2</sub>	C/A trigonometric	Section 4.2 & [72]
	Higher-spin XXX <sub>s</sub> /XXZ <sub>s</sub>	N elliptic	[72]
RG	Central spin	rational	[47]
	(Generalized) Dicke	rational	[113]
	BCS pairing	rational	[39]

#### 4.1. The machinery of ABA

Our goal is to construct integrable models from scratch. We will do this through a generative function approach, where we construct a generative function for the charges, which we will name the **transfer matrix**:

$$\tau(\lambda) = \exp \left[ \sum_{n=0}^{\infty} \frac{i_n}{n!} Q_n (\lambda - \xi)^n \right] \quad (75)$$

(the  $i_n$ 's are arbitrary numerical constants). The charges are constructed by taking derivatives of the transfer matrix:

$$Q_n = i_n^{-1} \frac{d^n}{d\lambda^n} \ln \tau(\lambda) \Big|_{\lambda=\xi}. \quad (76)$$

At this point, we have not attached any physical meaning to the  $Q_n$ 's, but they will correspond to conserved quantities such as the Hamiltonian. Note that while the transfer matrix is a highly non-local object (it is a nontrivial product over an infinite chain), the charges generated via the logarithm are additive and local. Sometimes, the transfer matrix is written instead as an expansion in  $\lambda$  around the complex number  $\xi$ , with operator-valued coefficients given by the conserved charges centered at  $\xi$ :

$$\tau(\lambda) = \sum_{n=-\infty}^{\infty} Q_n^{(\xi)} (\lambda - \xi)^n.$$

Since the  $\tau(\lambda)$  commute, the  $Q_n^{(\xi)}$  will commute as well, and, in addition, they will share eigenstates with  $\tau(\lambda)$ . This way of writing the transfer matrix makes it convenient to extract the eigenvalues of the charges

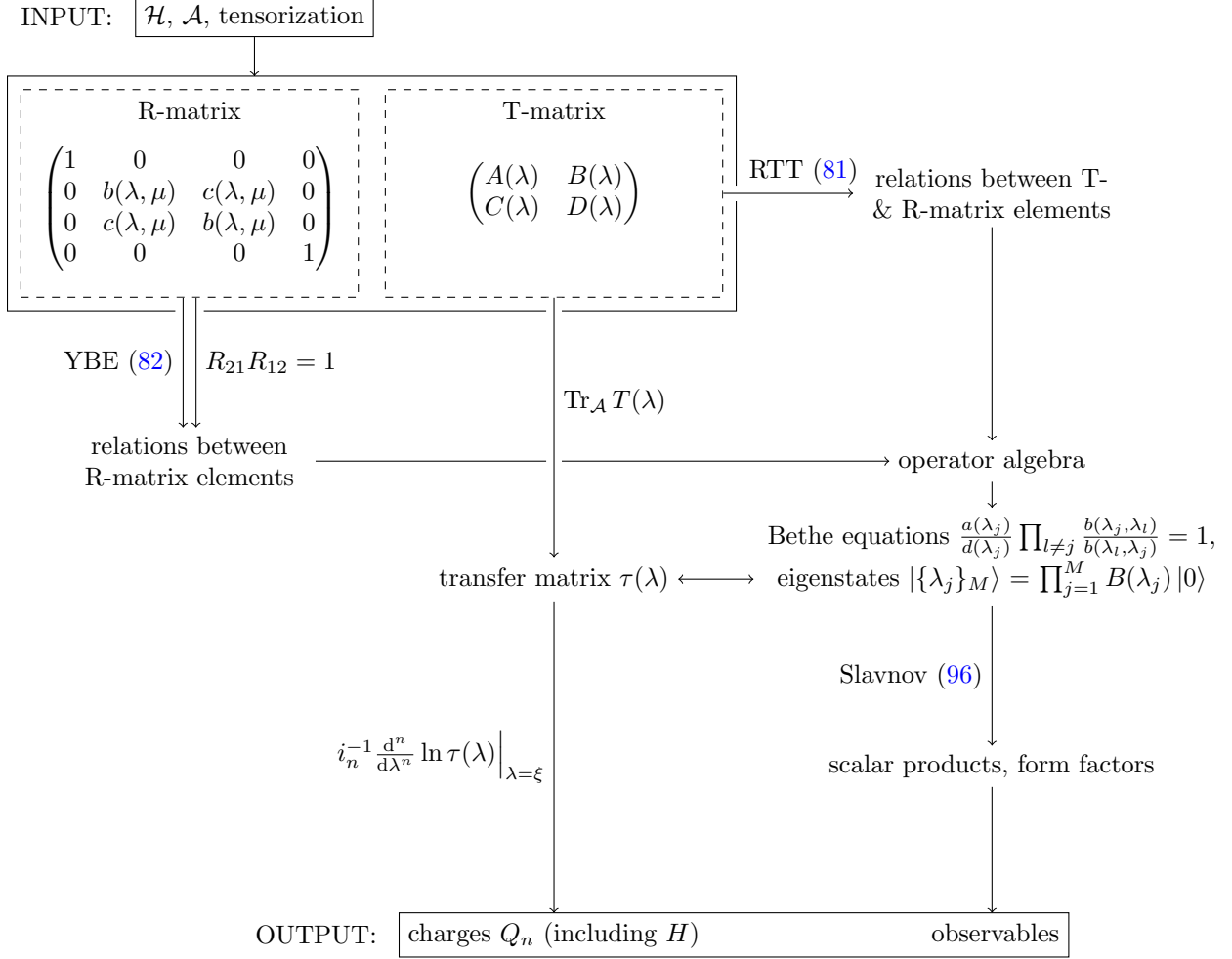


Figure 20: Schematic overview of algebraic Bethe ansatz (ABA). Input consists of a choice for the local Hilbert space  $\mathcal{H}$  and the auxiliary space  $\mathcal{A}$ , and, once these are decided upon, a choice for the entries of the  $R$ -matrix (for concreteness, we show a particular choice of an  $R$ -matrix with two off-diagonal elements). The output comprises conserved charges and eigenstates, which can be used to construct scalar products and form factors through Slavnov's formula.

by contour integration, since, for a generic eigenstate  $|\psi\rangle$  of  $\tau(\lambda)$  with eigenvalue  $\Lambda(\lambda)$ , the eigenvalue of  $Q_n^{(\xi)}$  will be given by evaluating  $\frac{1}{2\pi i} \oint_{\mathcal{C}} (\lambda - \xi)^{-1-n} \Lambda(\lambda) d\lambda$  around  $\xi$ , where  $\mathcal{C}$  is a contour encircling  $\xi$ .

The statement that all conserved charges are in involution is equivalent to stating that the transfer matrix commutes for all values of the spectral parameter:

$$[\tau(\lambda), \tau(\mu)] = 0 \quad \forall \lambda, \mu. \quad (77)$$

This can be easily seen by realizing that if the charges (76) should commute, then  $[\frac{1}{\tau(\lambda)} \frac{d}{d\lambda} \tau(\lambda), \frac{1}{\tau(\mu)} \frac{d}{d\mu} \tau(\mu)] = \frac{1}{\tau(\lambda)\tau(\mu)} \frac{d}{d\lambda} \frac{d}{d\mu} \tau(\lambda)\tau(\mu) - \frac{1}{\tau(\mu)\tau(\lambda)} \frac{d}{d\mu} \frac{d}{d\lambda} \tau(\mu)\tau(\lambda) = 0$  and this trivially holds if (77) holds (and similarly for higher order derivatives).

The big idea behind the algebraic Bethe ansatz (ABA) approach is to provide a formalism for finding such commuting transfer matrices. In order to do this, we need to find representations of (77), which we attempt by first phrasing the problem in a different way, using a somewhat formal mathematical construction.

- We introduce an auxiliary space  $\mathcal{A}$  and let  $\tau(\lambda)$  be the trace over  $\mathcal{A}$  of some new object  $T(\lambda)$  called

the **monodromy matrix**:

$$\tau(\lambda) = \text{Tr}_{\mathcal{A}} T(\lambda).$$

Note: Monodromy

In differential geometry, monodromy refers to the change to an object after parallel transport along a closed path. To understand the connection between this concept and  $T(\lambda)$ , we will express the monodromy matrix as a product of so-called Lax operators,  $L_j(\lambda)$ , that relate the auxiliary space with the (physical) lattice sites (see section C.4):

$$T(\lambda) = L_N(\lambda)L_{N-1}(\lambda) \cdots L_1(\lambda).$$

This construction is reminiscent of the parallel transport of a solution in a fiber bundle, if we interpret the  $L$ -operators as representing a discrete evolution (akin to the notion of parallel transport induced by a connection); a sequence of these operators then tells us how the solution changes after ‘moving’ through the system. If we think about the trajectory as a closed path,  $T(\lambda)$  tells us the total transformation after traversing one loop – just like monodromy in differential geometry.

Note that the monodromy matrix acts in the space  $\mathcal{A} \otimes \mathcal{H}$ . For concreteness, we take  $\mathcal{A} \simeq \mathbb{C}^2$ , i.e. a two-dimensional vector space isomorphic to  $\mathbb{C}^2$ , but in general, the choice of  $\mathcal{A}$  depends on the details of the problem. The requirement (77) now becomes

$$[\text{Tr}_{\mathcal{A}} T(\lambda), \text{Tr}_{\mathcal{A}}(\mu)] = 0. \quad (78)$$

Since the product of traces is the trace in the tensor product space, i.e.  $\text{Tr}(A \otimes B) = \text{Tr}(A) \text{Tr}(B)$ , the condition (78) can be written as

$$[\tau(\lambda), \tau(\mu)] = \text{Tr}_{\mathcal{A}} T(\lambda) \text{Tr}_{\mathcal{A}} T(\mu) - \text{Tr}_{\mathcal{A}} T(\mu) \text{Tr}_{\mathcal{A}} T(\lambda) = \text{Tr}_{\mathcal{A} \otimes \mathcal{A}} (T(\lambda) \otimes T(\mu) - T(\mu) \otimes T(\lambda)) = 0. \quad (79)$$

- We consider the tensor product of two separate auxiliary spaces  $\mathcal{A}_{1,2}$  and define the operators  $T_i(\lambda)$ ,  $i \in \{1, 2\}$  acting in  $\mathcal{A}_1 \otimes \mathcal{A}_2 \otimes \mathcal{H}$  as

$$T_1(\lambda) = T(\lambda) \otimes \mathbb{1}_2, \quad T_2(\lambda) = \mathbb{1}_1 \otimes T(\lambda),$$

where the subscript on  $\mathbb{1}$  denotes that it acts as the identity in this space. In terms of the auxiliary spaces, eq. (79) becomes

$$\begin{aligned} & \text{Tr}_{\mathcal{A}_1 \otimes \mathcal{A}_2} (T(\lambda) \otimes T(\mu) - T(\mu) \otimes T(\lambda)) \\ &= \text{Tr}_{\mathcal{A}_1 \otimes \mathcal{A}_2} (T_1(\lambda)T_2(\mu) - T_2(\mu)T_1(\lambda)) = \text{Tr}_{\mathcal{A}_1 \otimes \mathcal{A}_2} [T_1(\lambda), T_2(\mu)] = 0. \end{aligned} \quad (80)$$

In the first equality, we used  $T(\lambda) \otimes T(\mu) = (T(\lambda) \otimes \mathbb{1}_2)(\mathbb{1}_1 \otimes T(\mu)) = T_1(\lambda)T_2(\mu)$ . This is really a relation in  $\mathcal{H}$ , since we are tracing out  $\mathcal{A}_1$  and  $\mathcal{A}_2$ .

- We conclude that  $\text{Tr}_{\mathcal{A}_1 \otimes \mathcal{A}_2} (T_1(\lambda)T_2(\mu)) = \text{Tr}_{\mathcal{A}_1 \otimes \mathcal{A}_2} (T_2(\mu)T_1(\lambda))$ ,<sup>30</sup> and since the trace is invariant under a similarity transform, we argue that the products  $T_1T_2$  and  $T_2T_1$  are related by a similarity transformation  $R_{12}(\lambda, \mu) \in \mathcal{A}_1 \otimes \mathcal{A}_2$ , where the indices specify in which spaces this so-called **R-matrix** acts. We can therefore solve eq. (80) by requiring that  $T_1$  and  $T_2$  be *intertwined* by an invertible  $R$ -matrix,

$$R_{12}(\lambda, \mu)T_1(\lambda)T_2(\mu)R_{12}^{-1}(\lambda, \mu) = T_2(\mu)T_1(\lambda),$$

and hence we obtain the so-called **RTT-relation**:

$$R_{12}(\lambda, \mu)T_1(\lambda)T_2(\mu) = T_2(\mu)T_1(\lambda)R_{12}(\lambda, \mu). \quad (81)$$

<sup>30</sup>Naively, this would seem trivial because of the cyclic property of the trace. Note however that this is a partial trace over  $\mathcal{A}_1 \otimes \mathcal{A}_2$  (the resulting object is not a scalar but a matrix in  $\mathcal{H}$ ), and hence we cannot hope that it is generally true.

Table 5: Objects of ABA.  $\mathcal{H}$  represents the Hilbert space and  $\mathcal{A}$  stands for auxiliary space.

Object	Notation	Notes	Space
transfer matrix	$\tau(\lambda)$	$\tau(\lambda) = \text{Tr}_{\mathcal{A}} T(\lambda)$	$\mathcal{H}$
monodromy matrix	$T(\lambda)$ $T_i(\lambda), i \in \{1, 2\}$	$T_1(\lambda) = T(\lambda) \otimes \mathbb{1}_2$	$\mathcal{A} \otimes \mathcal{H}$ $\mathcal{A}_1 \otimes \mathcal{A}_2 \otimes \mathcal{H}$
R-matrix	$R_{12}$	in the presence of a Hilbert space, it is understood that $R_{12} = R_{12} \otimes \mathbb{1}_{\mathcal{H}}$	$\mathcal{A}_1 \otimes \mathcal{A}_2 \otimes \mathcal{H}$

Note: Intertwining [53]

In quantum mechanics, an intertwining operator  $D$  is a linear operator that satisfies the intertwining relation

$$H_1 D = D H_2,$$

where  $H_1$  and  $H_2$  are two different Hamiltonians. From this relation, it can be deduced that for an eigenfunction  $\psi_{2,n}$  of  $H_2$  obeying  $H_2 \Psi_{2,n} = E_{2,n} \Psi_{2,n}$ ,

$$H_1(D\Psi_{2,n}) = D(H_2\Psi_{2,n}) = E_{2,n}(D\Psi_{2,n}),$$

which shows that  $D\Psi_{2,n}$  is an eigenfunction of  $H_1$ . Thus the intertwining operator  $D$  maps eigenfunctions for  $H_2$  into eigenfunctions of  $H_1$ .

**Constraining the  $R$ -matrix** Finding a representation of the relation (81) (finding an  $R$ -matrix and a monodromy matrix that satisfies it) lies at the heart of defining a set of commuting quantum operators and hence a class of quantum integrable models. What obvious restrictions on the  $R$ -matrix can we think of at this point?

1.  $R$  has to be non-singular, i.e.  $\det R_{12}(\lambda, \mu) \neq 0$  (except possibly for isolated points  $\lambda$  and  $\mu$ ), which guarantees the existence of an inverse;
2. Since we may want to rescale  $R$  by an arbitrary scalar function, we can impose without loss of generality that  $R_{12}(\lambda, \mu)R_{21}(\mu, \lambda) = 1$ ;
3. The RTT-relation (81) relating different auxiliary spaces is not constraining enough, in the sense that it does not specify completely how tensor products of monodromy matrices are related under permutation. To see what is going on and what additional consistency relation on the  $R$ -matrix we need, consider a tensor product of three monodromy matrices  $T(\lambda) \otimes T(\mu) \otimes T(\nu)$ . We use the notation

$$T(\lambda) \otimes T(\mu) \otimes T(\nu) = T_1 T_2 T_3,$$

$$T_1 = T(\lambda) \otimes \mathbb{1}_2 \otimes \mathbb{1}_3, \quad T_2 = \mathbb{1}_1 \otimes T(\mu) \otimes \mathbb{1}_3, \quad T_3 = \mathbb{1}_1 \otimes \mathbb{1}_2 \otimes T(\nu).$$

We can permute  $T_1 T_2 T_3 \rightarrow T_3 T_2 T_1$  in two different ways, using eq. (81) and  $[R_{ij}, T_k] = 0$  for  $i \neq j \neq k$  (they act in different spaces):

$$T_1 T_2 T_3 = R_{12}^{-1} T_2 T_1 T_3 R_{12} = R_{12}^{-1} R_{13}^{-1} T_2 T_3 T_1 R_{13} R_{12} = R_{12}^{-1} R_{13}^{-1} R_{23}^{-1} T_3 T_2 T_1 R_{23} R_{13} R_{12},$$

$$T_1 T_2 T_3 = R_{23}^{-1} T_1 T_3 T_2 R_{23} = R_{23}^{-1} R_{13}^{-1} T_3 T_1 T_2 R_{13} R_{23} = R_{23}^{-1} R_{13}^{-1} R_{12}^{-1} T_3 T_2 T_1 R_{12} R_{13} R_{23}.$$

Demanding that these permutations yield the same outcome, we see that a sufficient (but not necessary) condition for the result to be identical is for the  $R$ -matrix to obey the **Yang-Baxter equation** (YBE):

$$\boxed{R_{12}(\mu, \lambda) R_{13}(\lambda, \nu) R_{23}(\mu, \nu) = R_{23}(\mu, \nu) R_{13}(\lambda, \nu) R_{12}(\lambda, \mu)}, \quad (82)$$

where we reinserted spectral parameters. In fact, we can play the same game for a product of  $n$  monodromy matrices and find, after reordering all  $R$ -matrices using  $[R_{ij}, R_{kl}] = 0$  for  $i \neq j \neq k \neq l$

$l$ , a product of Yang-Baxter equations; put differently, we can break any such relation between  $n$  monodromy matrices down into relations involving three  $R$ -matrices. This is a direct manifestation of the factorizability of scattering events in integrable systems. The Yang-Baxter equation for its own sake has been well-studied by physicists and mathematicians alike because it has an interesting structure and because of its connection to braid groups and their representations. For a primer on some of the interesting aspects of the YBE, see Appendix C.

Note: The mysterious  $R$ -matrix

What *is* the  $R$ -matrix? The Yang-Baxter equation has spiked its own field of research, which means that the name  $R$ -matrix has proliferated greatly in the literature. We can, of course, define the  $R$ -matrix in the abstract sense:

*The  $R$ -matrix is an invertible matrix intertwining the monodromy matrices of two auxiliary Hilbert spaces.*

But is there, maybe, another, more physical (and more elucidating) interpretation? I have thought about it for quite some time, and have yet to come across one.

We may now attempt to construct the  $R$ -matrix explicitly, subject to the constraints imposed by requirement 2 and 3.

We stress again that we have settled on  $\mathcal{A} \simeq \mathbb{C}^2$ , such that the smallest  $R$ -matrices of interest are  $4 \times 4$  matrices, which we may parametrize as

$$R(\lambda, \mu) = \begin{pmatrix} r_{11}(\lambda, \mu) & r_{12}(\lambda, \mu) & r_{13}(\lambda, \mu) & r_{14}(\lambda, \mu) \\ r_{21}(\lambda, \mu) & r_{22}(\lambda, \mu) & r_{23}(\lambda, \mu) & r_{24}(\lambda, \mu) \\ r_{31}(\lambda, \mu) & r_{32}(\lambda, \mu) & r_{33}(\lambda, \mu) & r_{34}(\lambda, \mu) \\ r_{41}(\lambda, \mu) & r_{42}(\lambda, \mu) & r_{43}(\lambda, \mu) & r_{44}(\lambda, \mu) \end{pmatrix}.$$

For the monodromy matrix, we choose the representation

$$T(\lambda) \equiv \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}, \quad (83)$$

where the entries are operators in the (yet unspecified!) Hilbert space. Then

$$T_1(\lambda) = \begin{pmatrix} A(\lambda) & 0 & B(\lambda) & 0 \\ 0 & A(\lambda) & 0 & B(\lambda) \\ C(\lambda) & 0 & D(\lambda) & 0 \\ 0 & C(\lambda) & 0 & D(\lambda) \end{pmatrix}, \quad T_2(\lambda) = \begin{pmatrix} A(\mu) & B(\mu) & 0 & 0 \\ C(\mu) & D(\mu) & 0 & 0 \\ 0 & 0 & A(\mu) & B(\mu) \\ 0 & 0 & C(\mu) & D(\mu) \end{pmatrix},$$

and

$$T_1(\lambda)T_2(\mu) = \begin{pmatrix} A(\lambda)A(\mu) & A(\lambda)B(\mu) & B(\lambda)A(\mu) & B(\lambda)B(\mu) \\ A(\lambda)C(\mu) & A(\lambda)D(\mu) & B(\lambda)C(\mu) & B(\lambda)D(\mu) \\ C(\lambda)A(\mu) & C(\lambda)B(\mu) & D(\lambda)A(\mu) & D(\lambda)B(\mu) \\ C(\lambda)C(\mu) & C(\lambda)D(\mu) & D(\lambda)C(\mu) & D(\lambda)D(\mu) \end{pmatrix},$$

$$T_2(\mu)T_1(\lambda) = \begin{pmatrix} A(\mu)A(\lambda) & B(\mu)A(\lambda) & A(\mu)B(\lambda) & B(\mu)B(\lambda) \\ C(\mu)A(\lambda) & D(\mu)A(\lambda) & C(\mu)B(\lambda) & D(\mu)B(\lambda) \\ A(\mu)C(\lambda) & B(\mu)C(\lambda) & A(\mu)D(\lambda) & B(\mu)D(\lambda) \\ C(\mu)C(\lambda) & D(\mu)C(\lambda) & C(\mu)D(\lambda) & D(\mu)D(\lambda) \end{pmatrix}.$$

Choosing a form of the  $R$ -matrix thus fixes the commutation relations between the  $A$ ,  $B$ ,  $C$  and  $D$  operators. Let us gain intuition by studying two, simple forms:

- **the diagonal  $R$ -matrix:** Let

$$R(\lambda, \mu) = \begin{pmatrix} r_{11}(\lambda, \mu) & & & \\ & r_{22}(\lambda, \mu) & & \\ & & r_{33}(\lambda, \mu) & \\ & & & r_{44}(\lambda, \mu) \end{pmatrix}.$$

This form of  $R$ -matrix satisfies the YBE trivially; for any  $r_{ij}$ , requirement 3 holds. Invariance under rescaling by an arbitrary function (see Lemma C.1) furthermore allows us to set  $r_{11}(\lambda, \mu) = 1$ . Requirement 2 imposes the constraints  $r_{22}(\lambda, \mu)r_{33}(\mu, \lambda) = 1$  and  $r_{44}(\lambda, \mu)r_{44}(\mu, \lambda) = 1$ . So we write

$$r_{22}(\lambda, \mu) = e^{s(\lambda, \mu)}, \quad r_{33}(\lambda, \mu) = e^{-s(\lambda, \mu)}, \quad r_{44}(\lambda, \mu) = (-1)^\theta e^{t(\lambda, \mu)},$$

with  $s(\lambda, \mu)$  an arbitrary function,  $t(\lambda, \mu) = -t(\mu, \lambda)$  and  $\theta \in \{0, 1\}$ .

- **the simplest non-diagonal  $R$ -matrix:** Let

$$R(\lambda, \mu) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & b(\lambda, \mu) & c(\lambda, \mu) & 0 \\ 0 & c(\lambda, \mu) & b(\lambda, \mu) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

$R$  must satisfy (2) and (3).

□ From (2), we find the conditions

$$b(\lambda, \mu)b(\mu, \lambda) + c(\lambda, \mu)c(\mu, \lambda) = 1, \quad (84a)$$

$$b(\lambda, \mu)c(\mu, \lambda) + c(\lambda, \mu)b(\mu, \lambda) = 0. \quad (84b)$$

□ From (3), we find

$$(b(\lambda, \mu) - b(\lambda, \nu))c(\mu, \nu) + c(\lambda, \mu)c(\lambda, \nu)b(\mu, \nu) = 0, \quad (85a)$$

$$c(\lambda, \mu)(b(\lambda, \nu) - b(\mu, \nu)) - b(\lambda, \mu)c(\lambda, \nu)c(\mu, \nu) = 0, \quad (85b)$$

$$(1 - b(\lambda, \mu)b(\mu, \nu))c(\lambda, \nu) - c(\lambda, \mu)c(\mu, \nu) = 0. \quad (85c)$$

Writing out both sides of the intertwining relation (81) in matrix form gives rise to a whole bunch of commutation/product relations between the operators in the monodromy matrix, involving the entries of  $R(\lambda, \mu)$ . Two of those – which we will need shortly – are

$$A(\lambda)B(\mu) = f(\lambda, \mu)B(\mu)A(\lambda) + g(\mu, \lambda)B(\lambda)A(\mu), \quad (86a)$$

$$[B(\lambda), B(\mu)] = 0, \quad (86b)$$

where we defined

$$f(\mu, \lambda) \equiv \frac{1}{b(\lambda, \mu)}, \quad g(\mu, \lambda) \equiv \frac{c(\lambda, \mu)}{b(\lambda, \mu)}. \quad (87)$$

Note that the second condition in (84) implies that  $g(\mu, \lambda) = -g(\lambda, \mu)$ . The complete set of commutation/product relations is the *operator algebra* generated by the monodromy matrix for this particular choice of  $R$ -matrix, called the **Yang-Baxter algebra**, see Appendix C.

**Transfer matrix: Eigenstates** In our representation of the monodromy matrix (83), the generating function for conserved charges, the transfer matrix  $\tau$  (recall that this is the trace of the monodromy matrix over the auxiliary space  $\mathcal{A}$ ) takes the form

$$\tau(\lambda) = \text{Tr}_{\mathcal{A}} T(\lambda) = A(\lambda) + D(\lambda). \quad (88)$$

States simultaneously diagonalizing all conserved charges are obtained by finding the eigenstates of the transfer matrix itself, so our objective will be to look for eigenstates of  $A(\lambda) + D(\lambda)$ . The form of the monodromy matrix suggest to interpret  $B$  as a raising operator and  $C$  as a lowering operator in the Hilbert space.<sup>31</sup>

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<sup>31</sup>This interpretation is very natural when the underlying algebra is  $\mathfrak{su}(2)$ , for example in a spin-1/2 chain.

To build the eigenstates, we will assume the existence of a pseudovacuum  $|0\rangle$  which has the interpretation of the highest weight state of the monodromy operator algebra<sup>32</sup> We also assume that it simultaneously diagonalizes  $A$  and  $D$ , and that  $C$  (the ‘lowering operator’) annihilates it:

$$A(\lambda)|0\rangle = a(\lambda)|0\rangle, \quad D(\lambda)|0\rangle = d(\lambda)|0\rangle, \quad C(\lambda)|0\rangle = 0, \quad (89)$$

with arbitrary functions  $a(\lambda)$ ,  $d(\lambda)$ . Hence, by construction, the pseudovacuum is an eigenstate of the transfer matrix:

$$\tau(\lambda)|0\rangle = \tau(\lambda|\emptyset)|0\rangle, \quad \tau(\lambda|\emptyset) = a(\lambda) + d(\lambda). \quad (90)$$

To construct further eigenstates of the transfer matrix, we repeatedly apply the ‘raising operator’  $B(\lambda)$  on the pseudovacuum. We consider the **algebraic Bethe Ansatz**<sup>33</sup>

$$|\psi\rangle \equiv |\{\lambda_j\}_M\rangle \equiv \prod_{j=1}^M B(\lambda_j)|0\rangle, \quad (91)$$

for generic  $M$  and  $\{\lambda_j\}_M$ . These states are also called *Bethe vectors*. Note that, because of  $[B(\lambda), B(\mu)] = 0$ , the order in the product does not matter. To study how the transfer matrix acts on the state (91), we work out the action of  $A$  and  $D$  on  $|\psi\rangle$ .

- For  $A$ , we find:

$$A(\lambda) \prod_{j=1}^M B(\lambda_j)|0\rangle = \Lambda^A \prod_{j=1}^M B(\lambda_j)|0\rangle + \sum_{l=1}^M \Lambda_l^A B(\lambda) \prod_{j \neq l}^M B(\lambda_j)|0\rangle, \quad (92)$$

with

$$\Lambda^A = a(\lambda) \prod_{j=1}^M b^{-1}(\lambda_j, \lambda), \quad \Lambda_l^A = -a(\lambda_l) \frac{c(\lambda_l, \lambda)}{b(\lambda_l, \lambda)} \prod_{j \neq l}^M b^{-1}(\lambda_j, \lambda_l).$$

Note: derivation for  $M = 3$

We will make use of the parametrizations (87) and the commutation/product relations in (86). We want to compute

$$A(\lambda) \prod_{j=1}^3 B(\lambda_j)|0\rangle.$$

We will do this by commuting  $A(\lambda)$  all the way to the right to let it act on  $|0\rangle$ . Everytime we commute  $A(\lambda)$  past a  $B(\lambda_j)$ , we generate additional terms, while we can exchange the order of the  $B(\lambda_j)$ ’s at no cost.

$$\begin{aligned} A(\lambda) \prod_{j=1}^3 B(\lambda_j)|0\rangle &= A(\lambda)B(\lambda_1)B(\lambda_2)B(\lambda_3)|0\rangle \\ &= [f(\lambda, \lambda_1)B(\lambda_1)A(\lambda) + g(\lambda_1, \lambda)B(\lambda)A(\lambda_1)]B(\lambda_2)B(\lambda_3)|0\rangle \\ &= f(\lambda, \lambda_1)B(\lambda_1)[f(\lambda, \lambda_2)B(\lambda_2)A(\lambda) + g(\lambda_2, \lambda)B(\lambda)A(\lambda_2)]B(\lambda_3)|0\rangle \\ &\quad + g(\lambda_1, \lambda)B(\lambda)[f(\lambda_1, \lambda_2)B(\lambda_2)A(\lambda_1) + g(\lambda_2, \lambda_1)B(\lambda_1)A(\lambda_2)]B(\lambda_3)|0\rangle \\ &= f(\lambda, \lambda_1)f(\lambda, \lambda_2)B(\lambda_1)B(\lambda_2)[f(\lambda, \lambda_3)B(\lambda_3)A(\lambda) + g(\lambda_3, \lambda)B(\lambda)A(\lambda_3)]|0\rangle \\ &\quad + f(\lambda, \lambda_1)g(\lambda_2, \lambda)B(\lambda_1)B(\lambda)[f(\lambda_2, \lambda_3)B(\lambda_3)A(\lambda_2) + g(\lambda_3, \lambda_2)B(\lambda_2)A(\lambda_3)]|0\rangle \\ &\quad + g(\lambda_1, \lambda)f(\lambda_1, \lambda_2)B(\lambda)B(\lambda_2)[f(\lambda_1, \lambda_3)B(\lambda_3)A(\lambda_1) + g(\lambda_3, \lambda_1)B(\lambda_1)A(\lambda_3)]|0\rangle \\ &\quad + g(\lambda_1, \lambda)g(\lambda_2, \lambda_1)B(\lambda)B(\lambda_1)[f(\lambda_2, \lambda_3)B(\lambda_3)A(\lambda_2) + g(\lambda_3, \lambda_2)B(\lambda_2)A(\lambda_3)]|0\rangle \end{aligned}$$

<sup>32</sup>Note that depending on the field of study, this can also be called the *lowest* weight state!

<sup>33</sup>Yes, there it is, finally.



$$\begin{aligned}
&= f(\lambda, \lambda_1) f(\lambda, \lambda_2) f(\lambda, \lambda_3) a(\lambda) B(\lambda_1) B(\lambda_2) B(\lambda_3) |0\rangle \\
&\quad + f(\lambda, \lambda_1) f(\lambda, \lambda_2) g(\lambda_3, \lambda) a(\lambda_3) B(\lambda) B(\lambda_1) B(\lambda_2) |0\rangle \\
&\quad + f(\lambda, \lambda_1) g(\lambda_2, \lambda) f(\lambda_2, \lambda_3) a(\lambda_2) B(\lambda) B(\lambda_1) B(\lambda_3) |0\rangle \\
&\quad + f(\lambda, \lambda_1) g(\lambda_2, \lambda) g(\lambda_3, \lambda_2) a(\lambda_3) B(\lambda) B(\lambda_1) B(\lambda_2) |0\rangle \\
&\quad + g(\lambda_1, \lambda) f(\lambda_1, \lambda_2) f(\lambda_1, \lambda_3) a(\lambda_1) B(\lambda) B(\lambda_2) B(\lambda_3) |0\rangle \\
&\quad + g(\lambda_1, \lambda) f(\lambda_1, \lambda_2) g(\lambda_3, \lambda_1) a(\lambda_3) B(\lambda) B(\lambda_1) B(\lambda_2) |0\rangle \\
&\quad + g(\lambda_1, \lambda) g(\lambda_2, \lambda_1) f(\lambda_2, \lambda_3) a(\lambda_2) B(\lambda) B(\lambda_1) B(\lambda_3) |0\rangle \\
&\quad + g(\lambda_1, \lambda) g(\lambda_2, \lambda_1) g(\lambda_3, \lambda_2) a(\lambda_3) B(\lambda) B(\lambda_1) B(\lambda_2) |0\rangle .
\end{aligned}$$

It is immediately clear that the first line in the final result represents the first term in (92):

$$a(\lambda) \prod_{j=1}^3 b^{-1}(\lambda_j, \lambda) \prod_{j=1}^3 B(\lambda_j) |0\rangle = \Lambda^A \prod_{j=1}^3 B(\lambda_j) |0\rangle .$$

Furthermore, using  $g(\mu, \lambda) = -g(\lambda, \mu)$ , the **purple** line can be rewritten as

$$\begin{aligned}
& - \frac{c(\lambda_1, \lambda)}{b(\lambda_1, \lambda)} b^{-1}(\lambda_2, \lambda_1) b^{-1}(\lambda_3, \lambda_1) a(\lambda_1) B(\lambda) B(\lambda_2) B(\lambda_3) |0\rangle \\
&= \underbrace{\left[ -a(\lambda_1) \frac{c(\lambda_1, \lambda)}{b(\lambda_1, \lambda)} \prod_{j \neq 1}^3 b^{-1}(\lambda_j, \lambda_1) \right]}_{\Lambda_1^A} B(\lambda) \prod_{j \neq 1}^3 B(\lambda_j) |0\rangle .
\end{aligned}$$

Using the identities in eq. (84) and (85), the **magenta** lines can be massaged into the  $\Lambda_2^A B(\lambda) \prod_{j \neq 2}^3 B(\lambda_j) |0\rangle$  term. Similarly, the **blue** lines make up the  $\Lambda_3^A B(\lambda) \prod_{j \neq 3}^3 B(\lambda_j) |0\rangle$  term.

The sum of **purple**, **magenta** and **blue** lines now gives us the second term in (92):

$$\text{purple} + \text{magenta} + \text{blue} = \sum_{l=1}^3 \Lambda_l^A B(\lambda) \prod_{j \neq l}^3 B(\lambda_j) |0\rangle ,$$

which completes the ‘proof’.

- For  $D$ , we find:

$$D(\lambda) \prod_{j=1}^M B(\lambda_j) |0\rangle = \Lambda^D \prod_{j=1}^M B(\lambda_j) |0\rangle + \sum_{l=1}^M \Lambda_l^D B(\lambda) \prod_{j \neq l}^M B(\lambda_j) |0\rangle ,$$

with

$$\Lambda^D = d(\lambda) \prod_{j=1}^M b^{-1}(\lambda, \lambda_j) , \quad \Lambda_l^D = -d(\lambda_l) \frac{c(\lambda, \lambda_l)}{b(\lambda, \lambda_l)} \prod_{j \neq l}^M b^{-1}(\lambda_l, \lambda_j) .$$

Hence, the action of the transfer matrix on the Bethe state can be expressed as

$$\begin{aligned}
\tau(\lambda) \prod_{j=1}^M B(\lambda_j) |0\rangle &= (A(\lambda) + D(\lambda)) \prod_{j=1}^M B(\lambda_j) |0\rangle \\
&= \underbrace{\Lambda^A \prod_{j=1}^M B(\lambda_j) |0\rangle}_{\text{diagonal}} + \underbrace{\sum_{l=1}^M \Lambda_l^A B(\lambda) \prod_{j \neq l}^M B(\lambda_j) |0\rangle}_{\text{off-diagonal}} + \underbrace{\Lambda^D \prod_{j=1}^M B(\lambda_j) |0\rangle}_{\text{diagonal}} + \underbrace{\sum_{l=1}^M \Lambda_l^D B(\lambda) \prod_{j \neq l}^M B(\lambda_j) |0\rangle}_{\text{off-diagonal}} . \quad (93)
\end{aligned}$$

To make the Bethe state an eigenstate of the transfer matrix, we need to get rid of the off-diagonal terms:

$$\sum_{j=1}^M (\Lambda_j^A + \Lambda_j^D) B(\lambda) \prod_{l \neq j}^M B(\lambda_l) |0\rangle = 0,$$

and hence

$$\Lambda_j^A + \Lambda_j^D = 0, \quad \forall j,$$

which translates to

$$\frac{a(\lambda_j)}{d(\lambda_j)} \frac{c(\lambda_j, \lambda) b(\lambda, \lambda_j)}{b(\lambda_j, \lambda) c(\lambda, \lambda_j)} \prod_{l \neq j}^M \frac{b(\lambda_j, \lambda_l)}{b(\lambda_l, \lambda_j)} = -1.$$

Finally, using eq. (84b) to simplify the fraction involving  $b$  and  $c$ , we find:

$$\boxed{\frac{a(\lambda_j)}{d(\lambda_j)} \prod_{l \neq j} \frac{b(\lambda_j, \lambda_l)}{b(\lambda_l, \lambda_j)} = 1, \quad \forall j = 1, \dots, N.} \quad (94)$$

These are the **Bethe equations** (constraints on the rapidities), guaranteeing that  $|\{\lambda_j\}_M\rangle$  are eigenstates of the transfer matrix  $\tau(\lambda)$ :

$$\tau(\lambda) |\{\lambda_j\}_M\rangle = \tau(\lambda) |\{\lambda_j\}_M\rangle |\{\lambda_j\}_M\rangle, \quad \tau(\lambda) |\{\lambda_j\}_M\rangle = a(\lambda) \prod_{j=1}^M b^{-1}(\lambda_j, \lambda) + d(\lambda) \prod_{j=1}^M b^{-1}(\lambda, \lambda_j). \quad (95)$$

We may now formalize the statement as a theorem:

**Theorem 4.1**  $|\{\lambda_j\}_M\rangle \equiv \prod_{j=1}^M B(\lambda_j) |0\rangle$  is an eigenstate of the transfer matrix  $\tau(\lambda)$  iff the rapidities  $\lambda_j$  satisfy the Bethe equations.

We also wish to define a measure in the Hilbert space, and so we introduce the dual pseudovacuum  $\langle 0| = |0\rangle^\dagger$ , with the properties

$$\langle 0|0\rangle = 1, \quad \langle 0|A(\lambda) = a(\lambda) \langle 0|, \quad \langle 0|D(\lambda) = d(\lambda) \langle 0|, \quad \langle 0|B(\lambda) = 0.$$

Note how the roles of  $B$  and  $C$  have flipped. The *dual states*

$$\langle \{\lambda_j\}_M| \equiv \langle 0| \prod_{j=1}^M C(\lambda_j)$$

are eigenstates of the transfer matrix  $\tau(\lambda)$  with eigenvalue  $\tau(\lambda) |\{\lambda_j\}_M\rangle$  given in eq. (95) if the  $\{\lambda_j\}_M$  satisfy the Bethe equations (94). We can also obtain an orthogonality condition by noting  $\tau(\lambda) |\{\lambda_j^C\}_M\rangle \neq \tau(\lambda) |\{\lambda_k^B\}_M\rangle$  for  $\{\lambda_j^C\}_M \neq \{\lambda_k^B\}_M$ , such that

$$\langle \{\lambda_j^C\}_M| \tau(\lambda) |\{\lambda_k^B\}_M\rangle = \tau(\lambda) |\{\lambda_j^C\}_M\rangle \langle \{\lambda_j^C\}_M| \{\lambda_k^B\}_M\rangle = \tau(\lambda) |\{\lambda_k^B\}_M\rangle \langle \{\lambda_j^C\}_M| \{\lambda_k^B\}_M\rangle,$$

and hence

$$\langle \{\lambda_j^C\}_M| \{\lambda_k^B\}_M\rangle = \langle 0| \prod_{j=1}^M C(\lambda_j^C) \prod_{k=1}^M B(\lambda_k^B) |0\rangle = 0, \quad \{\lambda_j^C\}_M \neq \{\lambda_k^B\}_M.$$

Take a moment here to contemplate what we have accomplished thus far:

- We have not made any assumptions on the Hilbert space, except that it contains a highest-weight state (pseudovacuum).
- We have not yet defined the transfer matrix  $\tau$ , besides assuming its existence.
- Our  $R$ -matrix still contains unspecified functions.

Defining an integrable model thus amounts to finding a specific representation of the algebraic structure we have defined, which makes it extremely flexible and generalizable.

### Slavnov's determinant formula

N. Slavnov found a convenient way to compute scalar products of states constructed by acting with  $B(\lambda)$  and  $C(\lambda)$  on the vacuum. The object we seek to compute is

$$S_M(\{\mu\}, \{\lambda\}) = \langle 0 | \prod_{j=1}^M C(\mu_j) \prod_{k=1}^M B(\lambda_k) | 0 \rangle .$$

**Slavnov's theorem** says that for  $\{\lambda\}$  a set of solutions to the Bethe equations and for  $\{\mu\}$  an arbitrary set of parameters, the scalar product  $S_M$  can be represented as the following determinant:

$$S_M(\{\mu\}, \{\lambda\}) = S_M(\{\lambda\}, \{\mu\}) = \frac{\prod_{j=1}^M \prod_{k=1}^M \varphi(\mu_j - \lambda_k)}{\prod_{j < k} \varphi(\mu_j - \mu_k) \prod_{j > k} \varphi(\lambda_j - \lambda_k)} \det T(\{\mu\}, \{\lambda\}) , \quad (96)$$

where

$$T_{ab} = \frac{\partial}{\partial \lambda_a} \tau(\mu_b | \{\lambda\}) , \quad \varphi(\lambda) \equiv \begin{cases} \lambda , & \Delta = 1 , \\ \sinh \lambda , & |\Delta| < 1 . \end{cases}$$

and  $\Delta$  is the anisotropy.

### Quantum inverse problem

Up to this point, we have constructed our eigenstates and managed to normalize them properly. Eventually, we want to land back onto local operators with clear, physical relevance. In other words, we want to make contact between the ‘abstract’  $A, B, C, D$  operators from ABA and the physical operators, which are e.g. the local spins in a Heisenberg spin chain. The relation between the operator entries of the monodromy matrix and local (spin) operators of the system is known as the **quantum inverse problem**. Once we have a representation for the local operators in terms of  $A, B, C, D$ , we can throw in Slavnov's formula and obtain an explicit expression for the matrix element of an operator between eigenstates, which means we are in a position to answer any question about expectation values of products of spin operators, at different spacetime points, in a spin chain. We will illustrate the quantum inverse problem by example, see Section 4.2.1.

#### ABA: Summary

Starting from the (naive) definition of quantum integrability (the existence of a complete set of conserved charges in involution), the **goal** is to construct integrable models from scratch. Instead of finding charges one-by-one, we use a generating function from which we peel off charges by taking derivatives. We call the generating function the transfer matrix  $\tau(\lambda)$ , with  $\lambda$  the spectral parameter. Via a simple argument, we deduce that involution of all charges is equivalent to commutativity of the transfer matrix for all values of  $\lambda$ . The **main idea** of the algebraic Bethe Ansatz is to provide a formalism for generating such commuting transfer matrices.

- We start the process by introducing an auxiliary space  $\mathcal{A}$  that extends the Hilbert space  $\mathcal{H}$ , and we demand that  $\tau(\lambda)$  be the trace of some new object  $T(\lambda)$  in  $\mathcal{A}$ : the monodromy matrix.
- Following simple steps, we are able to show that the involution condition can be phrased as a matrix equation of monodromy matrices (in a tensored auxiliary space  $\mathcal{A}_1 \otimes \mathcal{A}_2$ ), and a similarity transform matrix, the  $R$ -matrix. This is the RTT-relation eq. (81).

The ‘updated’ problem is therefore to find a representation of the  $R$ -matrix and the associated monodromy matrix.

- We figure out two important restrictions on  $R$ : an inversion requirement, ‘ $R_{21}R_{12} = 1$ ’, and compatibility with the Yang-Baxter equation, eq. (82). The restrictions on  $R$  induced by these relations translate into a bunch of product/commutation relations between the operators in the monodromy matrix (operator algebra), which we worked out schematically for diagonal  $R$  and

then for the simplest non-diagonal  $R$ . We did this for  $\mathcal{A} \simeq \mathbb{C}^2$ , s.t.  $R$  and  $T$  are  $4 \times 4$ -matrices.

- The equivalence between involution of charges and commutativity of the transfer matrices for different  $\lambda$  means that by diagonalizing the transfer matrix, we solve the problem. So we aim to find the eigenstates of the transfer matrix. In the process, we find the Bethe equations eq. (94) as the consistency equations that the elements of  $R$  need to fulfill.

We are done: we found the charges  $Q_n$  and the eigenstates of the transfer matrix  $|\{\lambda_j\}_M\rangle$ . From here, we can use Slavnov's formula eq. (96) to compute scalar products and form factors. In the process, we never specified  $\mathcal{H}$ , or the precise form of  $R$  or  $T$ .

## 4.2. Examples

In the previous section, we have gone through the procedure of picking a simple  $R$ -matrix and assigning it a model. Let's now turn things around in another example: we start with the known  $R$ -matrix of a model, and see what nice things we can do.

**A simple  $R$ -matrix** What can we say about the  $b$  and  $c$  functions in the  $R$ -matrix? Let's list some requirements and assumptions:

- We want rapidity-dependent operators (constant-valued functions would yield a trivial model).
- To simplify matters, we choose our two-parameter functions to depend only on the difference of the parameters, i.e.  $b(\lambda, \mu) \equiv b(\lambda - \mu)$  and  $c(\lambda, \mu) \equiv c(\lambda - \mu)$ .<sup>34</sup>
- We suppose that  $b(\lambda)$  and  $c(\lambda)$  are analytic, and are bounded at  $|\lambda| \rightarrow \infty$ .

The simplest non-constant form of  $c$  is then a one-pole form<sup>35</sup>

$$c(\lambda, \mu) \equiv \frac{c_0}{\lambda - \mu + i\eta},$$

where  $c_0, \eta$  are generic (complex-valued) constants. The inversion condition (84) dictates that  $b(\lambda, \mu)$  must have a single pole at  $\lambda = -\eta$ , and that it has asymptotic value  $\lim_{\lambda \rightarrow \infty} b(\lambda, \mu) = 1$ .

$$b(\lambda, \mu) \equiv 1 + \frac{b_0}{\lambda - \mu + i\eta}.$$

Plugging  $b(\lambda, \mu)$  and  $c(\lambda, \mu)$  into eq. (84b), it is easy to see that the equation is satisfied if  $b_0 = -i\eta$  and  $c_0 = i\eta$ . Thus, we obtain:

$$b(\lambda, \mu) = \frac{\lambda - \mu}{\lambda - \mu + i\eta}, \quad c(\lambda, \mu) = \frac{i\eta}{\lambda - \mu + i\eta}.$$

This 'simplest' form of the  $R$ -matrix with  $\eta = 1$  turns out to describe the XXX-chain. If we take a slightly more general form for  $b(\lambda, \mu)$  and  $c(\lambda, \mu)$ , we can in fact also describe the XXX-chain. If we allow this modification, we find, in conclusion:

$$R(\lambda, \mu) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & b(\lambda, \mu) & c(\lambda, \mu) & 0 \\ 0 & c(\lambda, \mu) & b(\lambda, \mu) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

<sup>34</sup>Choosing the  $R$ -matrix to depend only on the difference of spectral parameters is very common in literature. Besides simplifying the structure of the  $R$ -matrix and the YBE and the ensuing algebra, physically you should be comfortable with this simplification from the viewpoint of relativistic field theories, to maintain Lorentz invariance.

<sup>35</sup>A physical motivation for this choice of  $R$ -matrix element is the following: we know intuitively that if two plane waves with similar momenta collide, there will be some kind of resonance, whereas if they have vastly different momenta, they tend to pass through each other without scattering. Formally, we then want to have something that has a big effect on the ordering/commutation relations (which are defined in terms of the  $R$ -matrix elements) when the momenta (almost) coincide, and less of an effect when the momenta differ substantially, and zero when they are infinitely different. So we want an off-diagonal entry that looks like a single pole.

$$b(\lambda, \mu) = \frac{\varphi(\lambda - \mu)}{\varphi(\lambda - \mu + i\eta)}, \quad c(\lambda, \mu) = \frac{\varphi(i\eta)}{\varphi(\lambda - \mu + i\eta)},$$

$$\varphi(\lambda) = \begin{cases} \lambda, & \text{XXX: } \eta = 1, \\ \sinh(\lambda), & \text{XXZ: } |\Delta = \cos \eta| < 1, \\ \sin(\lambda), & \text{XXZ: } \Delta = \cosh \eta > 1. \end{cases} \quad (97)$$

Note that for the  $XXX$ -model, we have the relation  $b(\mu, \lambda) + c(\mu, \lambda) = 1$ . In the next section, we will show explicitly that the  $R$ -matrix (97) with  $\varphi(\lambda) = \sin(\lambda)$  is indeed the  $R$ -matrix for the  $XXZ$ -model. Concretely, our objective will be to show that with this choice of elements, we find the conserved charges for the  $XXZ$ -chain, including the Hamiltonian  $H_{XXZ}$ . Such relations are called *trace identities*, because they express the conserved charges as derivatives of the transfer matrix, which is the trace of the monodromy matrix. We will also treat the Lieb Liniger model in the context of ABA.

Note: Some notational convention

In literature, the  $R$ -matrix for the  $XXX$ -model is often written in the form

$$R_{ru}(\lambda, \mu) = \begin{pmatrix} f(\mu, \lambda) & 0 & 0 & 0 \\ 0 & g(\mu, \lambda) & 1 & 0 \\ 0 & 1 & g(\mu, \lambda) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad f(\mu, \lambda) = 1 + \frac{ic}{\mu - \lambda}, \quad g(\mu, \lambda) = \frac{ic}{\mu - \lambda}, \quad (98)$$

(98) is related to (97) by

$$R(\lambda - \mu) = f^{-1}(\mu, \lambda) P R_{ru}(\lambda, \mu)|_{c=i\eta}.$$

#### 4.2.1. ABA for the $XXZ$ -model [87]

**Setup** We will show that, under certain assumptions, the simplest form of  $R$ -matrix as defined in eq. (97) with the choice  $\varphi(\lambda) = \sin(\lambda)$  returns the conserved charges of the  $XXZ$ -chain. The Hilbert space  $\mathcal{H}$  of an  $N$ -site spin-1/2 is constructed by tensoring  $N$  elemental Hilbert spaces  $\mathcal{H}_i$ :

$$\mathcal{H} = \bigotimes_{i=1}^N \mathcal{H}_i.$$

We express the monodromy matrix as a product of  $N$  so-called  $L$ -operators living in  $\mathcal{A} \otimes \mathcal{H}_j$

$$T(\lambda) = L_N(\lambda, \xi_N) L_{N-1}(\lambda, \xi_{N-1}) \cdots L_1(\lambda, \xi_1),$$

where the  $\xi_i$  represent inhomogeneity parameters (all of them are equal for a homogeneous chain). Recall that the  $R$ -matrix we have defined lives in  $\mathcal{A} \otimes \mathcal{A}$ , and we chose  $\mathcal{A} \simeq \mathbb{C}^2$ . This suggests to start from basic two-dimensional Hilbert spaces isomorphic to auxiliary space,  $\mathcal{H}_j \sim \mathcal{A}$ . We now define

$$L_j(\lambda, \xi_j) = R_{aj}(\lambda, \xi_j),$$

where the subscript means the matrix acts on  $\mathcal{A} \otimes \mathcal{H}_j$ . Employing the YBE (82), it is straightforward to demonstrate the following intertwining relation, where we use  $j$  and  $a_i$  as indices for the Hilbert and auxiliary spaces, respectively:

$$R_{a_1 a_2}(\lambda, \mu) T_{a_1}(\lambda) T_{a_2}(\mu) = R_{a_1 a_2}(\lambda, \mu) [R_{a_1 N}(\lambda, \mu) \cdots R_{a_1 1}(\lambda, \xi)] [R_{a_2 N}(\mu, \xi_N) \cdots R_{a_2 1}(\mu, \xi_1)]$$

$$\stackrel{(82)}{=} [R_{a_2 N}(\mu, \xi_N) \cdots R_{a_2 1}(\mu, \xi_1)] [R_{a_1 N}(\lambda, \xi_N) \cdots R_{a_1 1}(\lambda, \xi_1)] R_{a_1 a_2}(\lambda, \mu).$$

From now on, we consider a homogenous chain with all  $\xi_j = i\eta/2$ , such that the  $L$ -operator takes the form

$$L_j(\lambda, i\eta/2) = R_{aj}(\lambda, -i\eta/2) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{\sin(\lambda - i\eta/2)}{\sin(\lambda + i\eta/2)} & \frac{\sin(i\eta)}{\sin(\lambda + i\eta/2)} & 0 \\ 0 & \frac{\sin(i\eta)}{\sin(\lambda + i\eta/2)} & \frac{\sin(\lambda - i\eta/2)}{\sin(\lambda + i\eta/2)} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

The  $L$ -operator can be written in terms of the permutation matrix  $\mathbb{P}_{aj}$  that interchanges the auxiliary space with the  $j$ -th site Hilbert space as follows:

$$L_j(\lambda, i\eta/2) = \frac{1}{\sin(\lambda + i\eta/2)} [c_1 \mathbb{1}_{aj} + c_P \mathbb{P}_{aj} + c_z \sigma_0^z \otimes \sigma_j^z],$$

where  $\sigma_j^z$  represents the Pauli- $z$  matrix on site  $j$ , and where we introduced the coefficients:

$$\begin{aligned} c_1 &= \frac{1}{2} (\sin(\lambda + i\eta/2) + \sin(\lambda - i\eta/2) - \sin(i\eta)), \\ c_P &= \sin(i\eta), \\ c_z &= \frac{1}{2} (\sin(\lambda + i\eta/2) - \sin(\lambda - i\eta/2) - \sin(i\eta)). \end{aligned}$$

Note: The permutation operator

In general, the permutation operator  $\mathbb{P}_{jk}$  exchanges the  $j$ -th and  $k$ -th space:  $\mathbb{P}_{jk}(V_j \otimes V_k) = V_k \otimes V_j$ . It satisfies the relations

$$\mathbb{P}_{0j} \mathbb{P}_{0k} \mathbb{P}_{0j} = \mathbb{P}_{jk}, \quad (99a)$$

$$\mathbb{P}_{0j}^2 = \mathbb{1}_{0j}. \quad (99b)$$

Note that for  $\lambda = i\eta/2$ , we find  $c_1 = c_z = 0$ , and hence  $L_j(i\eta/2, i\eta/2) = P_{aj}$ . This means that

$$T(i\eta/2) = \sin(\lambda + i\eta/2)^{-N} [c_1 \mathbb{1} + c_P \mathbb{P} + c_z \sigma^z \otimes \sigma^z]_{aN} \cdots [c_1 \mathbb{1} + c_P \mathbb{P} + c_z \sigma^z \otimes \sigma^z]_{a1} \Big|_{\lambda=i\eta/2} = \mathbb{P}_{aN} \cdots \mathbb{P}_{a1}.$$

If we now evaluate the transfer matrix (also at  $\lambda = i\eta/2$ ) and use the property (99), we can shift  $\mathbb{P}_{01}$  all the way to the left in such a way that what remains in the auxiliary trace is a single operator:

$$\begin{aligned} \tau(i\eta/2) &= \text{Tr}_a T(i\eta/2) = \text{Tr}_a [\mathbb{P}_{aN} \cdots \mathbb{P}_{a1}] = \text{Tr} [\mathbb{P}_{aN} \cdots \mathbb{P}_{a3} \mathbb{P}_{a1} \mathbb{P}_{a1} \mathbb{P}_{a2} \mathbb{P}_{a1}] \\ &= \text{Tr}_a [\mathbb{P}_{aN} \cdots \mathbb{P}_{a3} \mathbb{P}_{a1} \mathbb{P}_{12}] = \text{Tr}_a [\mathbb{P}_{a1}] \mathbb{P}_{1N} \cdots \mathbb{P}_{13} \mathbb{P}_{12} = \mathbb{P}_{1N} \cdots \mathbb{P}_{13} \mathbb{P}_{12} \equiv U, \end{aligned} \quad (100)$$

where we used  $\text{Tr}_a \mathbb{P}_{aj} = \mathbb{1}_j$ . Note that we could take the  $\mathbb{P}_{1N} \cdots \mathbb{P}_{12}$  outside of the trace, because the trace is taken over a different space. The operator  $U$  is called the *cyclic shift operator*. Its repeated action on an operator  $A_{j,k}$  defined in the  $j$ -th and  $k$ -th space is

$$A_{j,k} U^n = U^n A_{j-n, k-n}. \quad (101)$$

**Charges** Having obtained the transfer matrix, we can now construct the integrals of motion using eq. (76). We will construct  $\mathcal{Q}_0$  and  $\mathcal{Q}_1$  explicitly, and state  $\mathcal{Q}_2$ .<sup>36</sup>

- $\hat{\mathcal{Q}}_0$  is simply given by

$$\mathcal{Q}_0 = \ln \tau(i\eta/2) = \ln U \equiv i\hat{P}.$$

Note that  $U = e^{i\hat{P}}$  and hence  $\hat{P}$  carries the interpretation of momentum operator for systems with periodic boundary conditions.<sup>37</sup>

- The derivative with respect to  $\lambda$  of an  $L$ -operator is

$$\left. \frac{d}{d\lambda} L_j(\lambda, i\eta/2) \right|_{\lambda=i\eta/2} = \frac{1}{\sin i\eta} [c'_1 \mathbb{1} + c'_P \mathbb{P} + c'_z (\sigma^z \otimes \sigma^z)]_{aj},$$

with

$$c'_1 = \cos^2(i\eta/2), \quad c'_P = -\cos(i\eta), \quad c'_z = -\sin^2(i\eta/2).$$

<sup>36</sup>We place a hat on the operator  $\hat{P}$  to distinguish it from its eigenvalue  $P$ .

<sup>37</sup>Since  $U^N = 1$  and therefore we can interpret  $\hat{P}$  as the generator of translations.

We then find:

$$\begin{aligned}
\left. \sin(i\eta) \frac{d}{d\lambda} \tau(\lambda) \right|_{\lambda=i\eta/2} &= \left. \sin(i\eta) \operatorname{Tr}_a T(\lambda) \right|_{\lambda=i\eta/2} \\
&= \operatorname{Tr}_a \left[ [c'_1 \mathbb{1} + c'_P \mathbb{P} + c_z(\sigma^z \otimes \sigma^z)]_{aN} L_{N-1}(i\eta/2, i\eta/2) \cdots L_1(i\eta/2, i\eta/2) \right. \\
&\quad \left. + L_N(i\eta/2, i\eta/2) [c'_1 \mathbb{1} + c'_P \mathbb{P} + c_z(\sigma^z \otimes \sigma^z)]_{a(N-1)} L_{N-2}(i\eta/2, i\eta/2) \cdots \right. \\
&\quad \left. + \dots \right] \\
&= \operatorname{Tr}_a \left[ [c'_1 \mathbb{1} + c'_P \mathbb{P} + c_z(\sigma^z \otimes \sigma^z)]_{aN} \mathbb{P}_{a(N-1)} \cdots \mathbb{P}_{a1} \right] \\
&\quad + \mathbb{P}_{aN} [c'_1 \mathbb{1} + c'_P \mathbb{P} + c_z(\sigma^z \otimes \sigma^z)]_{a(N-1)} \mathbb{P}_{a(N-2)} \cdots \\
&\quad + \dots \left] \\
&= [c'_1 \mathbb{1} + c'_P \mathbb{P} + c_z(\sigma^z \otimes \sigma^z)]_{1N} \mathbb{P}_{1(N-1)} \mathbb{P}_{1(N-2)} \cdots \mathbb{P}_{12} \\
&\quad + \mathbb{P}_{1N} [c'_1 \mathbb{1} + c'_P \mathbb{P} + c_z(\sigma^z \otimes \sigma^z)]_{1(N-1)} \mathbb{P}_{1(N-2)} \cdots \mathbb{P}_{12} \\
&\quad + \dots,
\end{aligned}$$

where in the last line we used eq. (100), and where the dots represent the remaining cyclic permutations. Now take the logarithm:

$$\begin{aligned}
\left. \sin(i\eta) \frac{d}{d\lambda} \ln \tau(\lambda) \right|_{\lambda=i\eta/2} &= \sin(i\eta) \frac{1}{\tau(\lambda)} \left. \frac{d}{d\lambda} \tau(\lambda) \right|_{\lambda=i\eta/2} \\
&= \sum_{j=1}^N [c'_1 \mathbb{P} + c'_P \mathbb{1} + c_2(\sigma^z \otimes \sigma^z) \mathbb{P}]_{j(j+1)} \\
&= \sum_{j=1}^N \frac{1}{2} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \cos(i\eta) \sigma_j^z \sigma_{j+1}^z - \cos(i\eta) \mathbb{1}).
\end{aligned}$$

For the last equality we used the identity  $\sum_a \sigma_j^a \otimes \sigma_l^a = 2\mathbb{P}_{jl} - \mathbb{1}_{jl}$ , relating the Pauli matrices and the permutation operator. But this is the Hamiltonian for the XXZ-model, if we identify  $\cos(i\eta) \equiv \Delta$ :

$$\mathcal{Q}_1 = H_{XXZ} = \sum_{j=1}^N S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta(S_j^z S_{j+1}^z - \frac{1}{4}) = \frac{1}{2} \sin(i\eta) \left. \frac{d}{d\lambda} \ln \tau(\lambda) \right|_{\lambda=i\eta/2}.$$

- Without computation, we state the first non-trivial higher conserved charge, which is  $\mathcal{Q}_3$ :

$$\mathcal{Q}_2 = \frac{1}{\varphi(i\eta)^2} \left( 4 \sum_{j=1}^N [S_j^z (S_{j-1}^+ S_{j+1}^- + S_{j+1}^+ S_{j-1}^-) - \Delta(S_{j-1}^z + S_{j+1}^z)(S_j^+ S_{j+1}^- - S_{j+1}^+ S_j^-)] - N \right).$$

Using eq. (95), noting that, since  $a(i\eta/2) = 1$  and  $d(i\eta/2) = 0$ , the eigenvalues of the transfer matrix are

$$\tau\left(\frac{i\eta}{2}, \{\lambda_j\}\right) = \prod_{j=1}^M b^{-1}(\lambda_j, \frac{i\eta}{2}),$$

we can also compute the associated eigenvalues of  $\mathcal{Q}_0$  and  $\mathcal{Q}_1$ , which we will call  $P$  and  $E$ , respectively:

$$\begin{aligned}
P &= -i \ln \tau\left(\frac{i\eta}{2}, \{\lambda_j\}\right) = -i \sum_{j=1}^M \ln \left( b^{-1}(\lambda_j, \frac{i\eta}{2}) \right), \\
E &= \frac{1}{2} \sin(i\eta) \left. \frac{d}{d\lambda} \ln \tau(\mu, \{\lambda_j\}) \right|_{\mu=i\eta/2} = \frac{1}{2} \sin(i\eta) \sum_{j=1}^M \left. \frac{d}{d\lambda} \ln b^{-1}(\lambda_j, \mu) \right|_{\mu=i\eta/2}.
\end{aligned}$$

**Quantum inverse problem** We have reformulated the XXZ-model in an algebraic way in terms of the non-local operators  $A(\lambda)$ ,  $B(\lambda)$ ,  $C(\lambda)$  and  $D(\lambda)$ . However, we would now like to relate these operators back to local operators, such as the spin-flip operator  $S_j^+$ . In other words, we would like to express  $S_j^+$  in terms of  $A(\lambda)$ ,  $B(\lambda)$ ,  $C(\lambda)$  and  $D(\lambda)$ . We will present the quantum inverse problem for the homogeneous case ( $\xi_i = \xi$ ). The first step is to consider the monodromy matrix at  $\lambda = \xi$ :

$$T(\xi) = \mathbb{P}_{aN} \mathbb{P}_{a(N-1)} \cdots \mathbb{P}_{a1} = \mathbb{P}_{a1} \mathbb{P}_{1N} \mathbb{P}_{1(N-1)} \cdots \mathbb{P}_{12} = \mathbb{P}_{a1} U.$$

where in the second equation we used eq. (100) without the trace. In auxiliary space, we find

$$T(\xi) = \begin{pmatrix} A(\xi) & B(\xi) \\ C(\xi) & D(\xi) \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} U = \begin{pmatrix} \frac{1+\sigma_1^z}{2} & \sigma_1^- \\ \sigma_1^+ & \frac{1-\sigma_1^z}{2} \end{pmatrix} U,$$

where  $\sigma_1^z$  and  $\sigma_1^\pm = (\sigma_1^x \pm i\sigma_1^y)/2$  are the Pauli matrices on site 1. This system can be solved in a straightforward manner:

$$A(\xi) + D(\xi) = U, \quad A(\xi) - D(\xi) = \sigma_1^z U, \quad B(\xi) = \sigma_1^- U, \quad C(\xi) = \sigma_1^+ U.$$

Similar expressions for local operators acting on the other sites can be obtained with the translation operator from eq. (101):  $\sigma_j^a = U^{j-1} \sigma_1^a U^{1-j}$  together with the condition  $U^N = 1$  for periodic boundaries. For example:

$$\begin{aligned} \sigma_j^z &= U^{j-1} ((A(\xi) - D(\xi)) U^{-1}) U^{1-j} = U^{j-1} (A(\xi) - D(\xi)) U^{-j} \\ &= U^{j-1} (A(\xi) - D(\xi)) U^{N-j} = [A(\xi) + D(\xi)]^{j-1} (A(\xi) - D(\xi)) [A(\xi) + D(\xi)]^{N-j}. \end{aligned}$$

We find:

$$\begin{aligned} \sigma_j^z &= [A(\xi) + D(\xi)]^{j-1} (A(\xi) - D(\xi)) [A(\xi) + D(\xi)]^{N-j}, \\ \sigma_j^- &= [A(\xi) + D(\xi)]^{j-1} B(\xi) [A(\xi) + D(\xi)]^{N-j}, \\ \sigma_j^+ &= [A(\xi) + D(\xi)]^{j-1} C(\xi) [A(\xi) + D(\xi)]^{N-j}. \end{aligned}$$

The mapping for the inhomogeneous case is more challenging, but has been solved by working in the basis of so-called  $F$ -matrices [69].

#### 4.2.2. ABA for the Lieb-Liniger model

We will briefly apply the ABA to the Lieb-Liniger model, and state the main results. The  $R$ -matrix for the Lieb-Liniger model is

$$R_{LL}(\lambda, \mu) = \begin{pmatrix} f(\lambda, \mu) & 0 & 0 & 0 \\ 0 & g(\lambda, \mu) & 1 & 0 \\ 0 & 1 & g(\lambda, \mu) & 0 \\ 0 & 0 & 0 & f(\lambda, \mu) \end{pmatrix}.$$

It is closely related to the  $R$ -matrix of the XXX-chain:  $R_{XXX}(\lambda, \mu) = \mathbb{P} R_{LL}(\lambda, \mu) / f(\lambda, \mu) \big|_{c \rightarrow 1}$ . Unlike the XXX-chain, however, the Lieb-Liniger model is a continuum model. To work the magic of ABA on the Lieb-Liniger model, we effectively regularize it by putting it on a lattice with lattice constant  $a$  and  $M = L/a$  sites. The  $L$ -operator, to leading order, is

$$L_n(\lambda) = \begin{pmatrix} 1 - i\frac{\lambda a}{2} & -i\sqrt{c}\Psi_n^\dagger a \\ i\sqrt{c}\Psi_n^\dagger a & 1 + i\frac{\lambda a}{2} \end{pmatrix} + \mathcal{O}(a^2), \quad n \in \{1, \dots, M\}.$$

The fields are subject to the commutation relation  $[\Psi_m, \Psi_n^\dagger] = \frac{1}{a} \delta_{m,n}$ . We construct the monodromy matrix in the usual way:

$$T(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix} = L_M(\lambda) \cdots L_1(\lambda),$$



where the  $A(\lambda)$ ,  $B(\lambda)$ ,  $C(\lambda)$  and  $D(\lambda)$  operators satisfy the commutation relations in eq. (86) (the full set) if we replace  $1/b(\lambda, \mu) \rightarrow f(\lambda, \mu)$  and  $c(\lambda, \mu)/b(\lambda, \mu) \rightarrow g(\lambda, \mu)$ . The conserved charges are constructed from the transfer matrix. The first few of them are stated below:

$$\begin{aligned}\mathcal{Q}_0 &= N = \int_0^L \Psi^\dagger \Psi dx, \\ \mathcal{Q}_1 &= \hat{P} = -\frac{i}{2} \int_0^L (\Psi^\dagger \Psi_x - \Psi_x^\dagger \Psi) dx, \\ \mathcal{Q}_2 &= H = \int_0^L (\Psi_x^\dagger \Psi_x + c \Psi^\dagger \Psi^\dagger \Psi \Psi) dx, \\ \mathcal{Q}_3 &= i \int_0^L (\Psi^\dagger \Psi_{xxx} - 3c \Psi^\dagger \Psi^\dagger \Psi \Psi_x) dx, \\ \mathcal{Q}_4 &= \int_0^L [\Psi_{xx}^\dagger \Psi_{xx} + 2c((\Psi^\dagger)^2)_x (\Psi^2)_x + c(\Psi_x^\dagger)^2 \Psi^2 \\ &\quad + c(\Psi^\dagger)^2 (\Psi_x)^2 + c^2 (\Psi^\dagger)^3 \Psi^3 + c^2 (\Psi^\dagger)^2 \Psi \Psi^\dagger \Psi^2] dx.\end{aligned}$$

See Mossel [87] for a more elaborate treatment.

### 4.3. Richardson-Gaudin models

In the previous sections, we introduced the algebraic Bethe ansatz as a framework for constructing integrable systems through an algebraic approach. We have seen that the Bethe equations emerge as a necessary condition for Bethe states to be eigenvectors of the transfer matrix, and that Bethe equations pertaining to specific models are the result of choosing specific representations of the Yang-Baxter algebra.

In this section, we will build out the approach one step further by shifting our attention from ABA to Richardson-Gaudin models, which will occupy a pivotal position in the numerical methods of Section 5. As we will see, these represent in many ways a reformulation of the ABA, and the object of interest that they produce is the same: the Bethe equations of the system. We will mainly follow Claeys [26], with additions inspired by Sträter [113] and the seminal paper on Gaudin models by Gaudin (in French) [47].

#### 4.3.1. The Gaudin equations

Consider a spin-1/2 chain of  $L$  sites, labeled by  $i = 1, \dots, L$ . Each separate spin corresponds to a realization of the  $\mathfrak{su}(2)$  algebra, generated by the  $\hat{S}^+$ ,  $\hat{S}^-$  and  $\hat{S}^z$  operators with commutation relations

$$[\hat{S}_i^z, \hat{S}_j^\pm] = \delta_{ij} \hat{S}_i^\pm, \quad [\hat{S}_i^z, \hat{S}_j^\mp] = -\delta_{ij} \hat{S}_i^\mp, \quad [\hat{S}_i^+, \hat{S}_j^-] = 2\delta_{ij} \hat{S}_i^z.$$

The simplest non-interacting Hamiltonian that can be constructed out of these operators is

$$\hat{H} = \sum_{i=1}^L \hat{H}_i = \sum_{i=1}^L \frac{\omega_i}{2} \hat{S}_i^z, \quad (102)$$

where the  $\omega_i$  represent a magnetic field applied along the  $z$ -axis at site  $i$ . The conserved charges for this Hamiltonian are  $\hat{Q}_i = \hat{S}_i^z$  (since  $[\hat{H}, \hat{Q}_i] = 0$ ). In terms of the conserved charges, the Hamiltonian can be expressed as

$$\hat{H} = \sum_{i=1}^L \frac{\omega_i}{2} \hat{Q}_i.$$

We now propose a set of interacting conserved charges, characterized by an interaction strength  $g$ , such that in the non-interacting limit ( $g \rightarrow 0$ ) we recover eq. (102):

$$\hat{Q}_i = \hat{S}_i^z + g \sum_{j \neq i}^L [X_{ij}(\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+) + Z_{ij} \hat{S}_i^z \hat{S}_j^z], \quad i = 1, \dots, L. \quad (103)$$

These are parametrized by a set of  $X$  and  $Z$ -variables. In the limit  $g \rightarrow \infty$ , they define the class of  $XXZ$  *Gaudin magnets*. We require  $[\hat{Q}_i, \hat{Q}_j] = 0$  for these operators, to enforce the standard integrability conditions. By explicit computation, this is seen to hold if

$$X_{ij} + X_{ji} = 0, \quad Z_{ij} + Z_{ji} = 0, \quad \forall i \neq j, \quad (104a)$$

$$X_{ij}X_{jk} - X_{ik}(Z_{ij} + Z_{jk}) = 0, \quad \forall i \neq j \neq k, \quad (104b)$$

which are known as **Gaudin equations**. Obtaining a class of conserved charges amounts to solving the Gaudin equations simultaneously. Three well-known classes of solutions (up to normalization) are the following:

1. *XXX rational model*:

$$X_{ij} = Z_{ij} = \frac{g}{\epsilon_i - \epsilon_j}.$$

2. *XXZ trigonometric model*:

$$X_{ij} = \frac{g}{\sin(\epsilon_i - \epsilon_j)}, \quad Z_{ij} = g \cot(\epsilon_i - \epsilon_j).$$

3. *XXZ hyperbolic model*:

$$X_{ij} = \frac{g}{\sinh(\epsilon_i - \epsilon_j)}, \quad Z_{ij} = g \coth(\epsilon_i - \epsilon_j),$$

with  $g$  a real parameter. These are functional relations which are odd in some arbitrary parameter  $\epsilon_i - \epsilon_j$ . Any linear combination of the conserved charges (103) gives rise to a *Richardson-Gaudin integrable Hamiltonian*  $H = \sum_{i=1}^L \omega_i \hat{Q}_i / 2$ . Note as well that rational models follow from trigonometric models in the limit ( $\epsilon_i \rightarrow \epsilon_j$ ) and similarly that hyperbolic models follow from trigonometric models by the substitution  $\epsilon_i \rightarrow i\epsilon_j$ ,  $\epsilon_j \rightarrow i\epsilon_i$  and  $g \rightarrow -ig$ .

In keeping with the treatment of Claeys [26], we compromised on the fact that the conserved charges eq. (103) are not quite of the form presupposed by Gaudin [47]:

$$\hat{Q}_i = \sum_{j \neq i}^L [\Gamma_{ij}^x \hat{S}_i^x \hat{S}_j^x + \Gamma_{ij}^y \hat{S}_i^y \hat{S}_j^y + \Gamma_{ij}^z \hat{S}_i^z \hat{S}_j^z], \quad i = 1, \dots, L. \quad (105)$$

Note that the Gaudin's charges eq. (105), although lacking an external magnetic field, are fully anisotropic, and the resulting Gaudin equations take the form

$$\Gamma_{ij}^\alpha = -\Gamma_{ij}^\alpha, \quad \forall i \neq j, \\ \Gamma_{ij}^\alpha \Gamma_{jk}^\beta + \Gamma_{ki}^\beta \Gamma_{ij}^\gamma + \Gamma_{jk}^\gamma \Gamma_{ki}^\alpha = 0, \quad \forall i \neq j \neq k,$$

for any permutation  $(\alpha, \beta, \gamma)$  of  $(x, y, z)$ . In addition to the previously found classes of solutions, these Gaudin equations also admit the *XYZ elliptic model*, defined in terms of Jacobi elliptic functions  $\text{sn}(\cdot, \cdot)$ ,  $\text{cn}(\cdot, \cdot)$  and  $\text{dn}(\cdot, \cdot)$  with arbitrary elliptic modulus  $k$ :

$$\Gamma_{ij}^x = \frac{1 + k \text{sn}^2(\epsilon_i - \epsilon_j, k)}{\text{sn}(\epsilon_i - \epsilon_j, k)}, \quad \Gamma_{ij}^y = \frac{1 - k \text{sn}^2(\epsilon_i - \epsilon_j, k)}{\text{sn}(\epsilon_i - \epsilon_j, k)}, \quad \Gamma_{ij}^z = \frac{\text{cn}(\epsilon_i - \epsilon_j, k) \text{dn}(\epsilon_i - \epsilon_j, k)}{\text{sn}(\epsilon_i - \epsilon_j, k)}.$$

Finally, it is worth mentioning that Claeys et al. [27] work out the fully anisotropic case including a magnetic field for spin-1/2 systems,<sup>38</sup> with charges of the form

$$\hat{Q}_i = B_i^x \hat{S}_i^x + B_i^y \hat{S}_i^y + B_i^z \hat{S}_i^z + \sum_{j \neq i}^L [\Gamma_{ij}^x \hat{S}_i^x \hat{S}_j^x + \Gamma_{ij}^y \hat{S}_i^y \hat{S}_j^y + \Gamma_{ij}^z \hat{S}_i^z \hat{S}_j^z],$$

<sup>38</sup>While the previous relations hold for arbitrary spin- $s$  representations, restricting to spin-1/2 allows one to use the additional relation  $\hat{S}_i^\alpha \hat{S}_i^\beta = \frac{i}{2} \sum_\gamma \epsilon_{\alpha\beta\gamma} \hat{S}_i^\gamma + \frac{1}{4} \delta_{\alpha\beta} \mathbb{1}$ , which makes these results possible. Here,  $\epsilon_{\alpha\beta\gamma}$  represents the Levi-Civita symbol.

where now the  $\hat{S}_i^\alpha$ ,  $i = 1, \dots, L$  are distinct realizations of the spin-1/2 algebra  $\mathfrak{su}(2)$ . The Gaudin equations are seen to incorporate the external magnetic field, and take the form:

$$\begin{aligned}\Gamma_{ij}^\alpha B_j^\alpha + \Gamma_{ji}^\gamma B_i^\alpha &= 0, \quad \forall i \neq j, \\ \Gamma_{ik}^\alpha \Gamma_{jk}^\beta - \Gamma_{ij}^\alpha \Gamma_{jk}^\gamma - \Gamma_{ji}^\beta \Gamma_{ik}^\gamma &= 0, \quad \forall i \neq j \neq k.\end{aligned}$$

Note that the anti-symmetry condition on the  $\Gamma_{ij}^\alpha$  is not present any longer. The exact solution to these integrability constraints can be parametrized in terms of 7 free variables  $\{\alpha_x, \beta_x, \alpha_y, \beta_y, \gamma, \lambda, g\}$ :

$$\begin{aligned}B_i^x &= \frac{\gamma}{\sqrt{\alpha_x \epsilon_i + \beta_x}}, & \Gamma_{ij}^x &= g \frac{\sqrt{(\alpha_x \epsilon_i + \beta_x)(\alpha_y \epsilon_j + \beta_y)}}{\epsilon_i - \epsilon_j}, \\ B_i^y &= \frac{\lambda}{\sqrt{\alpha_y \epsilon_i + \beta_y}}, & \Gamma_{ij}^y &= g \frac{\sqrt{(\alpha_y \epsilon_i + \beta_y)(\alpha_x \epsilon_j + \beta_x)}}{\epsilon_i - \epsilon_j}, \\ B_i^z &= 1, & \Gamma_{ij}^z &= g \frac{\sqrt{(\alpha_x \epsilon_j + \beta_x)(\alpha_y \epsilon_j + \beta_y)}}{\epsilon_i - \epsilon_j},\end{aligned}$$

and the conserved charges are given by

$$\begin{aligned}\hat{Q}_i &= \left( \hat{S}_i^z + \frac{1}{2} \right) + \frac{\gamma}{\sqrt{\alpha_x \epsilon_i + \beta_x}} \hat{S}_i^x + \frac{\lambda}{\sqrt{\alpha_y \epsilon_i + \beta_y}} \hat{S}_i^y \\ &+ g \sum_{j \neq i}^L \frac{1}{\epsilon_i - \epsilon_j} \left[ \sqrt{\alpha_x \epsilon_i + \beta_x} \sqrt{\alpha_y \epsilon_j + \beta_y} \hat{S}_i^x \hat{S}_j^x + \sqrt{\alpha_y \epsilon_i + \beta_y} \sqrt{\alpha_x \epsilon_j + \beta_x} \hat{S}_i^y \hat{S}_j^y \right] \\ &+ g \sum_{j \neq i}^L \frac{\sqrt{\alpha_x \epsilon_j + \beta_x} \sqrt{\alpha_y \epsilon_j + \beta_y}}{\epsilon_i - \epsilon_j} \left( \hat{S}_i^z \hat{S}_j^z - \frac{1}{4} \right).\end{aligned}$$

Their eigenvalues can be found from a set of quadratic equations (Dimo and Faribault [35]), a property that may be exploited if one wishes to build efficient ways of extracting eigenvalues and Bethe roots from such models; we will gratefully use it in Section 5.

#### 4.3.2. Generalized Gaudin algebra

The original idea behind the Gaudin algebra was to take a special parameter limit of the ABA, the *quasi-classical limit*, in which the  $R$ -matrix reduces to the identity operator  $\mathbb{1}$  plus higher order corrections. Concretely, a Gaudin algebra emerges in models that have a parameter limit  $\eta \rightarrow 0$  in which the  $R$ -matrix reduces to the identity operator (to first order); this allows for the expansions:

$$\begin{aligned}R(u, v) &= \mathbb{1} + \eta \mathcal{R}(u, v) + \mathcal{O}(\eta^2), \\ T(u, v) &= \mathbb{1} + \eta \mathcal{T}(u, v) + \mathcal{O}(\eta^2), \\ A(u) &= \mathbb{1} + \eta \mathcal{A}(u) + \mathcal{O}(\eta^2), \\ B(u) &= \eta \mathcal{B}(u) + \mathcal{O}(\eta^2), \\ C(u) &= \eta \mathcal{C}(u) + \mathcal{O}(\eta^2), \\ D(u) &= \mathbb{1} + \eta \mathcal{D}(u) + \mathcal{O}(\eta^2).\end{aligned}$$

The **Gaudin algebra**  $\mathcal{Y}$  is formed by the operators  $\mathcal{A}(u)$ ,  $\mathcal{B}(u)$ ,  $\mathcal{C}(u)$ ,  $\mathcal{D}(u)$  and their commutation relations.

The procedure was initiated in a seminal paper by Gaudin [47] in 1976, and the framework was later systemized by Sklyanin and Takebe [108], and further worked out into a closed algebraic treatment, without the need for a quasi-classical limit,<sup>39</sup> by Ortiz et al. [91] in a 2005 paper – this is what became known as the

<sup>39</sup>The need for a quasi-classical limit is cumbersome because non-trivial results emerge only at quadratic order in  $\eta$ , due to the fact that the transfer matrix  $\hat{t}(u) = \mathcal{A}(u) + \mathcal{D}(u)$  is (to linear order) a Casimir of the Gaudin algebra and hence (by Schur's lemma) proportional to  $\mathbb{1}$ .

generalized Gaudin algebra. The fact that the Gaudin algebra emerges as a parameter limit of ABA has the merit of firmly emphasizing the connection between the two approaches.

As stated, the **generalized Gaudin algebra** (GGA) provides a more or less closed, algebraic framework for Richardson-Gaudin integrable models. In many ways, it can be seen as a rewriting of the ABA.

A GGA is defined by operators  $\hat{S}^x(u)$ ,  $\hat{S}^y(u)$  and  $\hat{S}^z(u)$ , satisfying the commutation relations

$$[\hat{S}^x(u), \hat{S}^y(v)] = i(Y(u, v)\hat{S}^z(u) - X(u, v)\hat{S}^z(v)), \quad (106a)$$

$$[\hat{S}^y(u), \hat{S}^z(v)] = i(Z(u, v)\hat{S}^x(u) - Y(u, v)\hat{S}^x(v)), \quad (106b)$$

$$[\hat{S}^z(u), \hat{S}^x(v)] = i(X(u, v)\hat{S}^y(u) - Z(u, v)\hat{S}^y(v)), \quad (106c)$$

$$[\hat{S}^\kappa(u), \hat{S}^\kappa(v)] = 0, \quad \kappa = x, y, z, \quad u, v \in \mathbb{C}, \quad u \neq v, \quad (106d)$$

with three functions  $X(u, v)$ ,  $Y(u, v)$  and  $Z(u, v)$  depending on (possibly complex-valued) *spectral parameters*  $u$ ,  $v$  and  $w$ . These functions are demanded to be anti-symmetric under exchange of  $u$  and  $v$ , and are meromorphic with a simple pole at  $u = v$ . The limiting behaviour at this point is

$$\lim_{\epsilon \rightarrow 0} \epsilon X(u, u + \epsilon) = \lim_{\epsilon \rightarrow 0} \epsilon Y(u, u + \epsilon) = \lim_{\epsilon \rightarrow 0} \epsilon Z(u, u + \epsilon) = f(u).$$

At coinciding points  $u = v$ , we therefore find

$$\begin{aligned} [\hat{S}^x(u), \hat{S}^y(u)] &= \lim_{\epsilon \rightarrow 0} [\hat{S}^x(u), \hat{S}^y(u + \epsilon)] = \lim_{\epsilon \rightarrow 0} i[Y(u, u + \epsilon)\hat{S}^z(u) - X(u, u + \epsilon)\hat{S}^z(u + \epsilon)] \\ &= \lim_{\epsilon \rightarrow 0} i \left[ \epsilon Y(u, u + \epsilon) \frac{\hat{S}^z(u) - \hat{S}^z(u + \epsilon)}{\epsilon} \right] = -if(u) \frac{\partial \hat{S}^z(u)}{\partial u}, \\ [\hat{S}^y(u), \hat{S}^z(u)] &= -if(u) \frac{\partial \hat{S}^x(u)}{\partial u}, \\ [\hat{S}^z(u), \hat{S}^x(u)] &= -if(u) \frac{\partial \hat{S}^y(u)}{\partial u}, \\ [\hat{S}^\kappa(u), \hat{S}^\kappa(u)] &= 0. \end{aligned}$$

Because of this, we recognize the structure of an infinite dimensional Lie algebra. Note also from eq. (106) the strong resemblance to the  $\mathfrak{su}(2)$  algebra, which may come as no surprise because of the connection to non-interacting models in the  $g \rightarrow 0$  limit, which is described by  $\mathfrak{su}(2)$ . In fact, eq. (106) describes an  $\mathfrak{sl}(2)$  algebra (the complexified version of  $\mathfrak{su}(2)$ ).

Let us now exploit the Lie algebraic structure to construct two equations relating the functions  $X$ ,  $Y$  and  $Z$ .

- We know that for the generators to define a Lie algebra, they need to satisfy the Jacobi identity, for example:

$$[\hat{S}^x(u), [\hat{S}^x(v), \hat{S}^y(w)]] + [\hat{S}^y(w), [\hat{S}^x(u), \hat{S}^x(v)]] + [\hat{S}^x(v), [\hat{S}^y(w), \hat{S}^x(u)]] = 0,$$

The Jacobi identities can be evaluated using eq. (106), and the first four (out of seven) non-trivial identities are listed below:

$$[\hat{S}^x(u), [\hat{S}^x(v), \hat{S}^y(w)]] + [\hat{S}^y(w), [\hat{S}^x(u), \hat{S}^x(v)]] + [\hat{S}^x(v), [\hat{S}^y(w), \hat{S}^x(u)]] = 0, \quad (107a)$$

$$\begin{aligned} \implies & Y(v, w)(X(v, u)\hat{S}^y(u) - Z(u, v)\hat{S}^y(v)) - X(v, w)(X(w, u)\hat{S}^y(w) - Z(w, u)\hat{S}^y(u)) \\ & - Y(u, w)(X(u, v)\hat{S}^y(u) - Z(u, v)\hat{S}^y(v)) + X(u, w)(X(w, v)\hat{S}^y(w) - Z(w, v)\hat{S}^y(v)) = 0, \end{aligned}$$

$$[\hat{S}^x(u), [\hat{S}^x(v), \hat{S}^z(w)]] + [\hat{S}^z(w), [\hat{S}^x(u), \hat{S}^x(v)]] + [\hat{S}^x(v), [\hat{S}^z(w), \hat{S}^x(u)]] = 0, \quad (107b)$$

$$\begin{aligned} \implies & X(w, v)(Y(u, w)\hat{S}^z(u) - X(u, w)\hat{S}^z(w)) - Z(w, v)(Y(u, v)\hat{S}^z(u) - X(u, v)\hat{S}^z(v)) \\ & - X(w, u)(Y(v, w)\hat{S}^z(v) - X(v, w)\hat{S}^z(w)) + Z(w, u)(Y(v, u)\hat{S}^z(v) - X(v, u)\hat{S}^z(u)) = 0, \end{aligned}$$

$$[\hat{S}^y(u), [\hat{S}^y(v), \hat{S}^x(w)]] + [\hat{S}^x(w), [\hat{S}^y(u), \hat{S}^y(v)]] + [\hat{S}^y(v), [\hat{S}^x(w), \hat{S}^y(u)]] = 0, \quad (107c)$$

$$\begin{aligned} \implies & Y(w, v)(Z(u, w)\hat{S}^x(u) - Y(u, w)\hat{S}^x(w)) - X(w, v)(Z(u, v)\hat{S}^x(u) - Y(u, v)\hat{S}^x(v)) \\ & - Y(w, u)(Z(v, w)\hat{S}^x(v) - Y(v, w)\hat{S}^x(w)) + X(w, u)(Z(v, u)\hat{S}^x(v) - Y(v, u)\hat{S}^x(u)) = 0, \end{aligned}$$

$$[\hat{S}^y(u), [\hat{S}^y(v), \hat{S}^z(w)]] + [\hat{S}^z(w), [\hat{S}^y(u), \hat{S}^y(v)]] + [\hat{S}^y(v), [\hat{S}^z(w), \hat{S}^y(u)]] = 0, \quad (107d)$$

$$\begin{aligned} \implies & Z(v, w)(Y(v, u)\hat{S}^z(v) - X(v, u)\hat{S}^z(u)) - Y(v, w)(Y(w, u)\hat{S}^z(w) - X(w, u)\hat{S}^z(u)) \\ & - Z(u, w)(Y(u, v)\hat{S}^z(u) - X(u, v)\hat{S}^z(v)) + Y(u, w)(Y(w, v)\hat{S}^z(w) - X(w, v)\hat{S}^z(v)) = 0, \end{aligned}$$

...

Taking for example eq. (107b) and using the anti-symmetry property of the functions  $X$ ,  $Y$  and  $Z$ , it is easy to see that

$$[X(v, w)Y(w, u) + Y(u, v)Z(v, w) + Z(w, u)X(u, v)]\hat{S}^z(u) - [u \Leftrightarrow v]\hat{S}^z(v) = 0,$$

and similarly for the other identities. Thus, we find that combining the various Jacobi identities yields the following consistency equations for the  $X$ -,  $Y$ - and  $Z$ -functions:

$$X(u, v)Y(v, w) + Y(w, u)Z(u, v) + Z(v, w)X(w, u) = 0. \quad (108)$$

This is a continuous equivalent of the Gaudin equations and serves as an incarnation of the Yang Baxter equation in the framework of GGA.

- From the non-trivial Jacobi identities (107), it is also possible to derive the relations

$$X(u, v)^2 - Z(u, v)^2 = \Gamma_1, \quad X(u, v)^2 - Y(u, v)^2 = \Gamma_2, \quad \forall u, v \in \mathbb{C}, \quad (109)$$

with  $\Gamma_1$  and  $\Gamma_2$  constants.

Finally, we define a continuous family of mutually commuting operators

$$\hat{S}^2(u) = \hat{S}^x(u)^2 + \hat{S}^y(u)^2 + \hat{S}^z(u)^2.$$

It follows from eq. (106) that

$$[\hat{S}^2(u), \hat{S}^2(v)] = 0, \quad \forall u, v \in \mathbb{C},$$

and hence the  $\hat{S}^2(u)$  define a continuous set of conserved charges (which lands us back onto integrability).

#### 4.3.3. The XXZ-parametrization

We now make the connection with the  $\mathfrak{su}(2)$  algebra by going to the so-called *XXZ-parametrization*. For the XXZ-model, setting  $X_{ij} = Y_{ij} = X(\epsilon_i, \epsilon_j)$ ,  $Z_{ij} = Z(\epsilon_i, \epsilon_j)$  and exploiting the anti-symmetry under exchange of  $u$  and  $v$  makes the similarity between equations (104b) and (108) manifest:

$$\begin{aligned} X(\epsilon_i, \epsilon_j)Y(\epsilon_j, \epsilon_k) - Y(\epsilon_i, \epsilon_k)Z(\epsilon_i, \epsilon_j) - X(\epsilon_i, \epsilon_k)Z(\epsilon_j, \epsilon_k) &= 0, \\ X(\epsilon_i, \epsilon_j)Y(\epsilon_j, \epsilon_k) + Y(\epsilon_k, \epsilon_i)Z(\epsilon_i, \epsilon_j) + Z(\epsilon_j, \epsilon_k)X(\epsilon_k, \epsilon_i) &= 0, \end{aligned}$$

where, in the second line, we were free to exchange the  $X$ - and the  $Z$ -term, since these are just (scalar) functions. Furthermore, using (109), equation (108) can be written exclusively in terms of  $Z$  as

$$Z(u, v)Z(v, w) + Z(w, u)Z(u, v) + Z(v, w)Z(w, u) = \Gamma.$$

which is the XXZ-parametrization. In terms of the raising and lowering operators

$$\hat{S}^+(u) = \hat{S}^x(u) + i\hat{S}^y(u), \quad \hat{S}^-(u) = \hat{S}^x(u) - i\hat{S}^y(u),$$

the commutation relations (106) simplify to

$$[\hat{S}^z(u), \hat{S}^\pm(v)] = \pm(X(u, v)\hat{S}^\pm(u) - Z(u, v)\hat{S}^\pm(v)), \quad (110a)$$

$$[\hat{S}^-(u), \hat{S}^+(v)] = -2X(u, v)(\hat{S}^z(u) - \hat{S}^z(v)), \quad (110b)$$

$$[\hat{S}^\pm(u), \hat{S}^\pm(v)] = 0. \quad (110c)$$

#### 4.3.4. Bethe equations from GGA

Finally, we go through the process of obtaining the Bethe equations to reveal the structural parallels with the ABA-approach. We define a pseudovacuum  $|0\rangle$ , defined as the lowest-weight representation with the usual property

$$\hat{S}^-(u) |0\rangle = 0.$$

It then follows from eq. (110a) that  $\hat{S}^- \hat{S}^z |0\rangle = 0$ , and hence

$$\hat{S}^z(u) |0\rangle = F_z |0\rangle$$

(similarly, it is straightforward to show that  $\hat{S}^2(u) |0\rangle = F_2(u) |0\rangle$ ).

We also define a Bethe-Ansatz wavefunction depending on a set of (possibly complex-valued) rapidities/Bethe roots  $\{v_1, \dots, v_N\}$ , acting on  $|0\rangle$ :

$$|v_1, \dots, v_N\rangle = \hat{S}^+(v_1) \hat{S}^+(v_2) \cdots \hat{S}^+(v_N) |0\rangle = \prod_{a=1}^N \hat{S}^+(v_a) |0\rangle.$$

Recall that  $\hat{S}(u)$  commutes at different values of the spectral parameter  $u$ , which implies that the conserved charges possess a common set of eigenstates and simultaneous diagonalization is achieved by finding the eigenstates of a single  $\hat{S}^2(u)$ . The action of  $\hat{S}^2(u)$  on a Bethe state can be obtained by explicit computation (by commuting it through all the raising operators, in the same way as for the ABA, but with the commutation relations from the GGA):

$$\begin{aligned} \hat{S}^2(u) \left( \prod_{a=1}^N \hat{S}^+(v_a) \right) |0\rangle &= \sum_{a=1}^N \sum_{b=a+1}^N \left( \prod_{c \neq a, b}^N \hat{S}^+(v_c) \right) [[\hat{S}^2(u), \hat{S}^+(v_a)], \hat{S}^+(v_b)] |0\rangle \\ &\quad + \sum_{a=1}^N \left( \prod_{b \neq a}^N \hat{S}^+(v_b) \right) [\hat{S}^2(u), \hat{S}^+(v_a)] |0\rangle + \underbrace{\left( \prod_{a=1}^N \hat{S}^+(v_a) \right) \hat{S}^2(u) |0\rangle}_{F_2(u) |v_1 \cdots v_N\rangle}, \\ [\hat{S}^2(u) - F_2(u)] |v_1 \cdots v_N\rangle &= \sum_{a=1}^N \sum_{b=a+1}^N \left( \prod_{c \neq a, b}^N \hat{S}^+(v_c) \right) [[\hat{S}^2(u), \hat{S}^+(v_a)], \hat{S}^+(v_b)] |0\rangle \\ &\quad + \sum_{a=1}^N \left( \prod_{b \neq a}^N \hat{S}^+(v_b) \right) [\hat{S}^2(u), \hat{S}^+(v_a)] |0\rangle. \end{aligned}$$

Note that higher commutators of the form  $[[[\hat{S}^2(u), \hat{S}^+(v_a)], \hat{S}^+(v_b)], \hat{S}^+(v_c)]$  vanish<sup>40</sup> and therefore do not appear in the above expression. Using the commutation relations in eq. (110), the previous equation reduces to the sum of a diagonal and an off-diagonal part:

$$[\hat{S}^2(u) - F_2(u)] |v_1 \cdots v_N\rangle = - \underbrace{\sum_{a=1}^N [\Gamma + Z(u, v_a)(2F_z(u) - \sum_{b \neq a}^N Z(u, v_b))]}_{\text{diagonal}} |v_1 \cdots v_N\rangle$$

<sup>40</sup>The innermost commutator  $[\hat{S}^2(u), \hat{S}^+(v_a)] = [\hat{S}^x(u)^2 + \hat{S}^y(u)^2 + \hat{S}^z(u), \hat{S}^x(v_a) + i\hat{S}^y(v_a)]$  can be expanded with the commutator identity  $[AB, C] = A[B, C]C + [A, C]B$  and yields

$$X(u, v_a)(\hat{S}^+(u)\hat{S}^z(v_a) + \hat{S}^z(v_a)\hat{S}^+(u)) - Z(u, v_a)(\hat{S}^z(u)\hat{S}^+(v_a) + \hat{S}^+(v_a)\hat{S}^z(u)).$$

The next commutation relation gives

$$\begin{aligned} [[\hat{S}^2(u), \hat{S}^+(v_a)], \hat{S}^+(v_b)] &= X(u, v_a)(\hat{S}^+(u)[\hat{S}^z(v_a), \hat{S}^+(v_b)] + [\hat{S}^z(v_a), \hat{S}^+(v_b)]\hat{S}^+(u)) \\ &\quad - Z(u, v_a)([\hat{S}^z(u), \hat{S}^+(v_b)]\hat{S}^+(v_a) + \hat{S}^+(v_a)[\hat{S}^z(u), \hat{S}^+(v_b)]). \end{aligned}$$

Since all the commutators in this expression are proportional to  $\hat{S}^+$  and  $[\hat{S}^+(u), \hat{S}^+(v)] = 0$ , the final, outermost commutator in  $[[[\hat{S}^2(u), \hat{S}^+(v_a)], \hat{S}^+(v_b)], \hat{S}^+(v_c)]$  will vanish.

$$+ 2 \underbrace{\sum_{a=1}^N X(u, v_a) [F_z(v_a) + \sum_{b \neq a}^N Z(v_b, v_a)]}_{\text{off-diagonal}} |v_1 \cdots v_a \rightarrow u \cdots v_N\rangle,$$

where  $v_a \rightarrow u$  means that one rapidity has been replaced by the spectral parameter  $u$ . **This is the counterpart of eq. (93) in the ABA framework.** For the off-diagonal part to vanish and an exact eigenstate to be obtained, we need the rapidities to satisfy the Bethe equations (Richardson-Gaudin equations):

$$F_z(v_a) + \sum_{b \neq a}^N Z(v_b, v_a) = 0, \quad \forall a = 1, \dots, N.$$

These do not depend on the spectral parameter  $u$ . This makes sense, because the Bethe states are eigenstates at each value of the spectral parameter (recall that we found  $[\hat{S}^2(u), \hat{S}^2(v)] = 0$ ).

#### RG-models: Summary

We have defined the generalized Gaudin algebra. Demanding commutation of the operator  $\hat{S}^2(u)$  for different values of the spectral parameter  $u$ , we can deduce the Bethe equations by demanding that the action of  $\hat{S}^2(u)$  on a Bethe-Ansatz wavefunction  $|v_1, \dots, v_N\rangle$  yields an eigenstate, in strong correspondence with the procedure of finding the Bethe equations in the ABA-framework.

**Spin models from a GGA** To construct specific spin models, we will choose a specific spin representation and construct the GGA-generators in terms of interacting spins. Recall that a spin- $s$  particle can be realized by an irrep  $|s, m_s\rangle$  with  $m_s = -s, -s+1, \dots, s$ . A specific representation in terms of  $\otimes_{i=1}^L \mathfrak{su}(2)$  generators can be introduced as

$$\hat{S}^\pm(u) = \sum_{i=1}^L X(u, \epsilon_i) \hat{S}_i^\pm, \quad \hat{S}^z(u) = -\frac{1}{g} - \sum_{i=1}^L Z(u, \epsilon_i) \hat{S}_i^z,$$

with  $g, \epsilon_1, \dots, \epsilon_L \in \mathbb{R}$ . Writing out

$$\hat{S}^2(u) = \frac{1}{2}(\hat{S}^+(u)\hat{S}^-(u) + \hat{S}^-(u)\hat{S}^+(u)) + \hat{S}^z(u)^2,$$

it can be shown that

$$\hat{S}^2(u) = \frac{2}{g} \sum_{i=1}^L Z(u, \epsilon_i) \hat{Q}_i - \Gamma \left( \sum_{i=1}^L \hat{S}_i^z \right)^2 + \text{cst},$$

with

$$\hat{Q}_i = \hat{S}_i^z + g \sum_{j \neq i}^L \left[ \frac{1}{2} X(\epsilon_i, \epsilon_j) (\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+) + Z(\epsilon_i, \epsilon_j) \hat{S}_i^z \hat{S}_j^z \right].$$

It can also be checked that the lowest weight state  $|0\rangle = \otimes_{i=1}^L |s_i, -s_i\rangle$  satisfies the properties of a vacuum state, and the following Bethe wavefunction leads to the eigenvalue equation:

$$\hat{Q}_i |v_1 \cdots v_N\rangle = -s_i \left[ 1 + g \sum_{a=1}^N Z(\epsilon_i, v_a) - g \sum_{j \neq i}^L Z(\epsilon_i, \epsilon_j) s_j \right] |v_1 \cdots v_N\rangle,$$

provided that the rapidities satisfy the Bethe equations

$$\frac{1}{g} + \sum_{i=1}^L Z(\epsilon_i, v_a) s_i - \sum_{b \neq a}^L Z(v_b, v_a) = 0, \quad a = 1, \dots, N.$$

#### 4.4. ABA and RG-models: final remarks

Let us (re)state some of the main take-aways of this section.

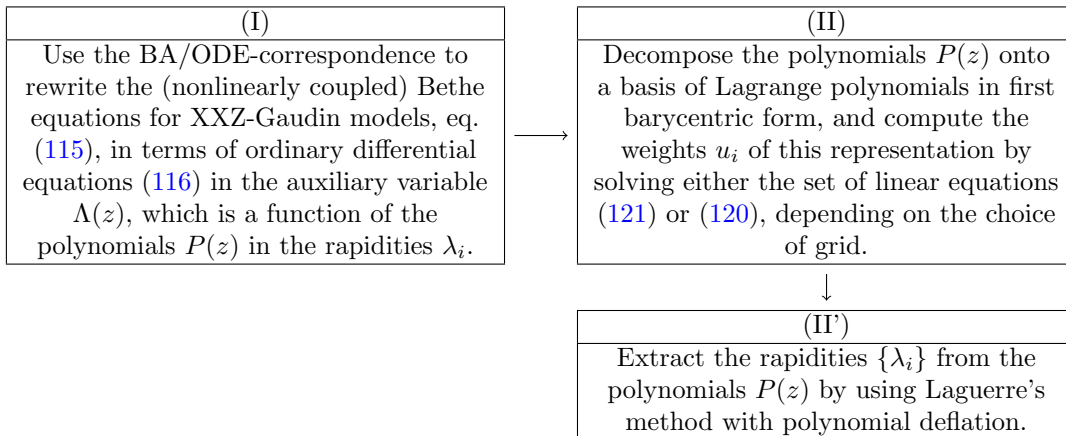
- The ABA contains an enormous variety of models due to its high degree of flexibility. The inputs of ABA are extensive: the local Hilbert space, the conventions for tensorization, the dimensionality of the auxiliary space, the form of the  $R$ -matrix, the form of the functions inside the  $R$ -matrix, and the choice for monodromy – to illucidate the last piont, there are many other monodromy matrices than the ones we defined that will obey the RTT-relation eq. (81) for the same  $R$ -matrix. Once all choices have been made, a model comes out, in line with what we called the ‘constructive’ (or black box) approach. The algebraic Bethe Ansatz is able to solve a huge variety of models, and once the framework is understood the rest is essentially representation theory.
- In this regard, one can promote the Heisenberg spin chain as the simplest, non-trivial quantum model that one can write down, since it derives from all the simplest (non-trivial) choices in the process.
- Slavnov’s formula, eq. (96), is what makes ABA truly *practical*, since it bridges the gap between (abstract) objects from ABA (two states, one of which is on-shell/an eigenstate, i.e. satisfies the Bethe equations and hence diagonalizes the transfer matrix) with observables (correlation functions). It is what gives us a numerical value that can be used in experiment, after doing all the abstract juggling with states and operators.
- As mentioned in the introduction, ABA suffers from a completeness problem. It is often difficult to prove that the set of eigenstates we find by solving the Bethe equations, is indeed a complete set of states.
- In the framework of ABA, the operator algebra we find is not an ordinary Lie algebra (in which bilinears map onto linears), but a quadratic algebra, meaning that products of two operators commute into products of two operators.



## 5. Efficient computation of rapidities for BA-solvable models

Let us now remind ourselves why, in this thesis, we choose to tread the elegant, but somewhat tedious, path of Bethe Ansatz and Gaudin models. After all, at the end of the day, all we are really looking to do is to find the spectrum and the charges of a class of fairly common physical models. Even if we choose to add imaginary parts to the coupling constants, we could still in principle brute-force the diagonalization and be done with it. *The key point here is that we could do this, but that it would be disastrously inefficient for large system sizes.* This is where we revert back to our information-theoretic viewpoint on integrability: in a regular  $N$ -particle quantum system – that is, in an  $N$ -particle quantum system without any special structure – the Hilbert space scales as  $\exp(N)$ . On the other hand, systems that admit an ABA-integrable structure are completely specified by the  $M$  rapidities  $\{\lambda_\alpha\}$  which are solutions to the Bethe equations, and of which there are typically of the order of  $N$  (exactly  $N$  if there is no degeneracy). This seemingly innocent property has far-reaching implications in the thermodynamic limit and is the reason why we can look at large system sizes!

In this chapter, we give a detailed review (with intermediate steps) of Faribault et al. [44] and El Araby, Gritsev, and Faribault [41], who present numerical methods for finding the rapidities of a particular class of rational Gaudin models by writing the quadratic Bethe equations as a system of ordinary differential equations in a different variable (the ‘BA/ODE-correspondence’; see Dorey and Tateo [37] for the seminal paper and Dorey, Dunning, and Tateo [36] for a more comprehensive overview). Subsequently, a new set of quadratic equations in the new variable is obtained, and then a polynomial inversion method (such as Laguerre’s method with deflation on a basis of barycentric polynomials) is used to extract the rapidities:



The reason for using the BA/ODE correspondence is that the rapidities  $\lambda_k$  are either real or come in pairs of complex conjugates, and in the latter case numerical instabilities can occur when working directly with the  $\lambda_k$ . By focusing on a different set of quantities, we can circumvent the canceling divergence which can occur for certain values of the coupling strength.

Once the review is complete and all methods are in place, we discuss some technicalities involved with upgrading the method to handle complex-valued couplings. We propose to implement a modification of the grid definition and apply the methods to the central spin model.

A logical step in the direction of open quantum systems would be to apply the BA/ODE-method to the generalized Dicke model with complex-valued coupling, aided by the work of Sträter [113] who considered the non-complex case, and to efficiently extract the rapidities of this model. The feature of the (generalized) Dicke model that makes it well-suited for our purposes is the fact that once complexified, it has the correct form of jump operators for a direct application of the methods developed by Torres [118] (see Section 3.3.1). In other words, once we find the rapidities of the generalized Dicke model, we could find the spectrum of its Lindbladian in the exact same fashion as we worked out for the Lieb-Liniger model in Section 3.3.2, by simply reusing the code with different equations and parameters.

### 5.1. The BA/ODE correspondence

The Bethe equations for a generic systems can be written in the form

$$F(\lambda_i) = \sum_{j \neq i} \frac{1}{\lambda_i - \lambda_j}, \quad (111)$$

where the left-hand side  $F$  is model-dependent. In this formulation, it is immediately obvious that for coinciding rapidities the right-hand side will diverge. While similar terms on the left-hand side will formally cancel out the divergences, numerical stability and computation time are negatively affected. What we can do, however, is to introduce a new function  $\Lambda(z)$  (Sträter [113] calls this ‘a clever substitution’), defined in terms of the polynomials  $P(z)$  as

$$\Lambda(z) = \sum_{k=1}^M \frac{1}{z - \lambda_k} = \frac{P(z)}{P'(z)}, \quad P(z) = \prod_{k=1}^M (z - \lambda_k). \quad (112)$$

The **BA/ODE correspondence** now consists of rewriting the (nonlinearly coupled) Bethe equations, eq. (111), in terms of ordinary differential equations. The first step in this direction is to realize that the  $\Lambda(z)$  satisfy the following Riccati-type differential equation:

$$\frac{\partial \Lambda(z)}{\partial z} + \Lambda^2(z) = - \sum_{\alpha} \frac{1}{(z - \lambda_{\alpha})^2} + \sum_{\alpha, \beta} \frac{1}{(z - \lambda_{\alpha})(z - \lambda_{\beta})} = \sum_{\alpha < \beta} \frac{2}{(z - \lambda_{\alpha})(z - \lambda_{\beta})},$$

where (implicitly)  $\alpha, \beta = 1, \dots, M$ . If the set  $\{\lambda_i\}$  is a solution to the Bethe equations, we can write

$$\boxed{\Lambda'(z) + \Lambda^2(z) - \sum_{\alpha} \frac{2F(\lambda_{\alpha})}{z - \lambda_{\alpha}} = 0}, \quad (113)$$

and by repeatedly taking derivatives, we generate the set of equalities:

$$\begin{cases} \Lambda'(z) + \Lambda^2(z) - \sum_{\alpha} \frac{2F(\lambda_{\alpha})}{z - \lambda_{\alpha}} & = 0, & (114a) \\ \Lambda''(z) + 2\Lambda(z)\Lambda'(z) + \sum_{\alpha} \frac{2F(\lambda_{\alpha})}{(z - \lambda_{\alpha})^2} & = 0, & (114b) \\ \Lambda'''(z) + 2\Lambda(z)\Lambda''(z) + 2\Lambda'(z)^2 - \sum_{\alpha} \frac{4F(\lambda_{\alpha})}{(z - \lambda_{\alpha})^3} & = 0, & (114c) \\ \dots & & \end{cases}$$

From now on, we restrict to XXZ Gaudin models, which possess the following, particular form of the  $F$ -function:

$$\boxed{F(\lambda_{\alpha}) = - \sum_{i=1}^N \frac{A_i}{(\epsilon_i - \lambda_{\alpha})} + \frac{B}{2g} \lambda_{\alpha} + \frac{C}{2g}}, \quad (115)$$

with  $g$  (‘coupling constant’) and  $\epsilon_i$  (‘energy levels’) model-dependent parameters. In (pseudo)spin models,  $A_i = |s_i|\Omega$  with  $|s_i|$  the norm of the spin degree of freedom and  $\Omega$  integer related to the degeneracy (the number of elements of the set  $\{\epsilon_j\}$  equal to  $\epsilon_i$ ), such that  $A_i$  can take on any integer or half-integer values.

Using this form of  $F(\lambda_\alpha)$  and taking the limit  $z \rightarrow \epsilon_j$ , the system can be written as

$$\left\{ \begin{aligned} (1 - 2A_j)\Lambda'(\epsilon_j) + \Lambda^2(\epsilon_j) + \frac{B}{g}M - \frac{B\epsilon_j + C}{g}\Lambda(\epsilon_j) + \sum_{i \neq j} 2A_i \frac{\Lambda(\epsilon_j) - \Lambda(\epsilon_i)}{\epsilon_i - \epsilon_j} &= 0, \quad (116a) \\ (1 - A_j)\Lambda''(\epsilon_j) + 2\Lambda(\epsilon_j)\Lambda'(\epsilon_j) - \frac{B}{g}\Lambda(\epsilon_j) - \frac{B\epsilon_j + C}{g}\Lambda'(\epsilon_j) \\ + \sum_{i \neq j} 2A_i \frac{\Lambda(\epsilon_j) - \Lambda(\epsilon_i)}{(\epsilon_i - \epsilon_j)^2} + \Lambda'(\epsilon_j) \sum_{i \neq j} \frac{2A_j}{\epsilon_i - \epsilon_j} &= 0, \quad (116b) \\ (1 - \frac{2}{3}A_j)\Lambda'''(\epsilon_j) + 2\Lambda(\epsilon_j)\Lambda''(\epsilon_j) + 2\Lambda'(\epsilon_j)^2 - 2\frac{B}{g}\Lambda'(\epsilon_j) - \frac{B\epsilon_j + C}{g}\Lambda''(\epsilon_j) \\ + \sum_{i \neq j} 4A_i \frac{\Lambda(\epsilon_j) - \Lambda(\epsilon_i)}{(\epsilon_i - \epsilon_j)^3} + \sum_{i \neq j} \frac{4A_i\Lambda'(\epsilon_j)}{(\epsilon_i - \epsilon_j)^2} + 2\sum_{i \neq j} \frac{2A_i\Lambda''(\epsilon_j)}{\epsilon_i - \epsilon_j} &= 0, \quad (116c) \\ \dots & \end{aligned} \right.$$

Let us show this explicitly for the second equation, eq. (116b). For convenience, we list the first two derivatives of  $\Lambda(z)$ :

$$\Lambda(z) = \sum_{k=1}^M \frac{1}{z - \lambda_k}, \quad \Lambda'(z) = -\sum_{k=1}^M \frac{1}{(z - \lambda_k)^2}, \quad \Lambda''(z) = 2\sum_{k=1}^M \frac{1}{(z - \lambda_k)^3}.$$

Eq. (114b) can be written as

$$\begin{aligned} \Lambda''(z) + 2\Lambda(z)\Lambda'(z) + \sum_{\alpha} \frac{2F(\lambda_{\alpha})}{(z - \lambda_{\alpha})^2} &= 0, \\ \Lambda''(z) + 2\Lambda(z)\Lambda'(z) + 2\sum_{\alpha} \frac{1}{(z - \lambda_{\alpha})^2} \left[ -\sum_{i=1}^N \frac{A_i}{\epsilon_i - \lambda_{\alpha}} + \frac{B}{2g}\lambda_{\alpha} + \frac{C}{2g} \right] &= 0, \\ \Lambda''(\epsilon_j) + 2\Lambda(\epsilon_j)\Lambda'(\epsilon_j) - 2\underbrace{\sum_{\alpha} \sum_{i=1}^N \frac{A_i}{(\epsilon_j - \lambda_{\alpha})^2(\epsilon_i - \lambda_{\alpha})}}_{\text{I}} + \underbrace{\frac{B}{g} \sum_{\alpha} \frac{\lambda_{\alpha}}{(\epsilon_j - \lambda_{\alpha})^2}}_{\text{II}} + \underbrace{\frac{C}{g} \sum_{\alpha} \frac{1}{(\epsilon_j - \lambda_{\alpha})^2}}_{\text{III}} &= 0, \end{aligned}$$

where in the third line, we took the limit  $z \rightarrow \epsilon_j$ .

- For term I, we write:

$$\begin{aligned} \sum_{\alpha} \sum_{i=1}^N \frac{A_i}{(\epsilon_j - \lambda_{\alpha})^2(\epsilon_i - \lambda_{\alpha})} &= \sum_{\alpha} \frac{A_j}{(\epsilon_j - \lambda_{\alpha})^3} + \sum_{\alpha} \sum_{i \neq j} \frac{A_i}{(\epsilon_j - \lambda_{\alpha})^2(\epsilon_i - \lambda_{\alpha})} \\ &= \frac{1}{2}A_j\Lambda''(\epsilon_j) + \sum_{\alpha} \sum_{i \neq j} \frac{A_i(\epsilon_i - \epsilon_j)^2}{(\epsilon_i - \epsilon_j)^2(\epsilon_j - \lambda_{\alpha})^2(\epsilon_i - \lambda_{\alpha})} \\ &= \frac{1}{2}A_j\Lambda''(\epsilon_j) + \sum_{\alpha} \sum_{i \neq j} \frac{A_i(\epsilon_i^2 - 2\epsilon_i\epsilon_j + \epsilon_j^2)}{(\epsilon_i - \epsilon_j)^2(\epsilon_j - \lambda_{\alpha})^2(\epsilon_i - \lambda_{\alpha})} \\ &= \frac{1}{2}A_j\Lambda''(\epsilon_j) + \sum_{\alpha} \sum_{i \neq j} \frac{A_i[(\epsilon_i - \epsilon_j)(\epsilon_i - \lambda_{\alpha}) - (\epsilon_j - \lambda_{\alpha})(\epsilon_i - \epsilon_j)]}{(\epsilon_i - \epsilon_j)^2(\epsilon_j - \lambda_{\alpha})^2(\epsilon_i - \lambda_{\alpha})} \\ &= \frac{1}{2}A_j\Lambda''(\epsilon_j) + \sum_{\alpha} \sum_{i \neq j} A_i \left[ \frac{\epsilon_i - \epsilon_j}{(\epsilon_i - \epsilon_j)^2} \left( \frac{1}{(\epsilon_j - \lambda_{\alpha})^2} \right) - \frac{1}{(\epsilon_i - \epsilon_j)^2} \left( \frac{\epsilon_i - \lambda_{\alpha} - (\epsilon_j - \lambda_{\alpha})}{(\epsilon_j - \lambda_{\alpha})(\epsilon_i - \lambda_{\alpha})} \right) \right] \\ &= \frac{1}{2}A_j\Lambda''(\epsilon_j) + \sum_{\alpha} \sum_{i \neq j} A_i \left[ \frac{1}{\epsilon_i - \epsilon_j} \left( \frac{1}{(\epsilon_j - \lambda_{\alpha})^2} \right) - \frac{1}{(\epsilon_i - \epsilon_j)^2} \left( \frac{1}{\epsilon_j - \lambda_{\alpha}} - \frac{1}{\epsilon_i - \lambda_{\alpha}} \right) \right] \end{aligned}$$

$$= \frac{1}{2} A_j \Lambda''(\epsilon_j) + \sum_{i \neq j} A_i \left[ -\frac{\Lambda'(\epsilon_j)}{\epsilon_i - \epsilon_j} - \frac{\Lambda(\epsilon_j) - \Lambda(\epsilon_i)}{(\epsilon_i - \epsilon_j)^2} \right].$$

- For term II:

$$\begin{aligned} \sum_{\alpha} \frac{\lambda_{\alpha}}{(\epsilon_j - \lambda_{\alpha})^2} &= \sum_{\alpha} \left[ -\frac{\epsilon_j - \lambda_{\alpha}}{(\epsilon_j - \lambda_{\alpha})^2} + \frac{\epsilon_j}{(\epsilon_j - \lambda_{\alpha})^2} \right] \\ &= -\sum_{\alpha} \frac{1}{\epsilon_j - \lambda_{\alpha}} + \sum_{\alpha} \frac{\epsilon_j}{(\epsilon_j - \lambda_{\alpha})^2} \\ &= -\Lambda(\epsilon_j) - \epsilon_j \Lambda'(\epsilon_j). \end{aligned}$$

- For term III:

$$\sum_{\alpha} \frac{1}{(\epsilon_j - \lambda_{\alpha})^2} = -\Lambda(\epsilon_j).$$

Putting the results together, we recover eq. (116b).

The relevant question now is how many of the equalities presented in eq. (116) we actually require. Inspection of the equations reveals that the answer boils down to the value of  $A_j$ :

- for  $A_j = 1/2$  (a non-degenerate spin-1/2), the coefficient  $(1 - 2A_j)$  in the first equation vanishes and we obtain a quadratic equation which we can solve for the set of variables  $\{\Lambda(\epsilon_j)\}$ ;
- for  $A_j = 1$  (a spin-1 or a twofold degenerate spin-1/2), the first two equations form a quadratic systems of equations for  $\{\Lambda(\epsilon_j)\}$  and  $\{\Lambda'(\epsilon_j)\}$ ;
- For  $A_j = 3/2$ , we need  $\{\Lambda(\epsilon_j)\}$ ,  $\{\Lambda'(\epsilon_j)\}$  and  $\{\Lambda''(\epsilon_j)\}$ ;
- Etc.

Note: The  $n$ -th derivative for arbitrary  $A_j$

To whom it may concern, I want to remark that in appendix A of El Araby, Gritsev, and Faribault [41], it is proven that the  $n$ -th derivative  $\mathcal{E}_j^{(n)}$  of eq. (113) at the point  $g$  with  $F$ -function of the form eq. (115) reads

$$\mathcal{E}_j^{(n)}(g) = \kappa_j^{(n)}(g) + \sum_{k=0}^n \binom{n}{k} \Lambda_j^{(k)} \Lambda_j^{(n-k)} - \left( \frac{Bn\epsilon_j}{g} \Lambda_j^{(n-1)} + C \Lambda_j^{(n)} \right) + \left( 1 - \frac{d_j}{n+1} \right) \Lambda_j^{(n+1)} = 0,$$

where

$$\begin{aligned} \Lambda_j^{(n)} &= g^{n+1} \Lambda(\epsilon_j)^{(n)} \equiv g^{n+1} \frac{d^n \Lambda(z)}{dz^n} \Big|_{z=\epsilon_j}, \\ \kappa_j^{(n)}(g) &\equiv - \sum_{i \neq j}^N d_i n! \left( g^{n+1} \frac{\Lambda_i - \Lambda_j}{(\epsilon_i - \epsilon_j)^{n+1}} - \sum_{k=1}^n \frac{1}{(n+1-k)!} \frac{\Lambda_j^{(n+1-k)}}{(\epsilon_i - \epsilon_j)^k} \right). \end{aligned}$$

As prescribed, for  $A_j = 1/2$  ( $d_j = 1$  for spin 1/2), we solve  $\mathcal{E}^{(0)}$  in terms of  $\Lambda_j^{(0)}$ , for  $A_j = 1$  we solve  $(\mathcal{E}^{(0)}, \mathcal{E}^{(1)})$  in terms of  $(\Lambda_j^{(0)}, \Lambda_j^{(1)})$ , etc.

## 5.2. Root extraction

What remains to be done is to extract the rapidities from the ‘auxiliary’ variables  $\{\Lambda_i\}$ :

$$\{\Lambda_i\} \rightarrow \{\lambda_i\}.$$

This comes down to finding the roots of  $P(z)$ , since  $P(z) = \prod_{k=1}^M (z - \lambda_k)$ . We can do this in different ways: Faribault et al. [44] use an elementary method based on simple monomial expansion  $P(z) = \sum_{n=0}^M P_n(\{\lambda_i\})z^n$ , while the follow-up paper by El Araby, Gritsev, and Faribault [41] employ a more efficient approach; we will opt for the second method, because the first method was shown to suffer from problems in the numerical implementation.

The ODE eq. (113) with the specific form of Bethe equations eq. (115) with  $A_i = \frac{1}{2}d_i$  becomes

$$\Lambda'(z) + \Lambda^2(z) - \sum_{\alpha=1}^N \left[ \left( \sum_{i=1}^N \frac{d_i}{\lambda_\alpha - \epsilon_i} + \frac{B}{g} \lambda_\alpha + \frac{C}{g} \right) \frac{1}{z - \lambda_\alpha} \right] = 0.$$

We note from eq. (112) that  $\Lambda'(z) = (P(z)P''(z) - P'(z)^2)/P(z)^2$ , and hence

$$P''(z) - P(z) \left[ \sum_{\alpha=1}^N \sum_{i=1}^N \frac{d_i}{\lambda_\alpha - \epsilon_i} \frac{1}{z - \lambda_\alpha} + \sum_{\alpha=1}^N \frac{B}{g} \frac{\lambda_\alpha}{z - \lambda_\alpha} + \sum_{\alpha=1}^N \frac{C}{g} \frac{1}{z - \lambda_\alpha} \right] = 0.$$

The first term between square brackets can be simplified using partial fraction decomposition. This yields

$$\sum_{\alpha=1}^N \sum_{i=1}^N \frac{d_i}{\lambda_\alpha - \epsilon_i} \frac{1}{z - \lambda_\alpha} = \sum_{\alpha=1}^N \sum_{i=1}^N \left( \frac{d_i}{(z - \epsilon_i)(\lambda_\alpha - \epsilon_i)} + \frac{d_i}{(z - \epsilon_i)(z - \lambda_\alpha)} \right) = \sum_{i=1}^N \left( \frac{-d_i \Lambda(\epsilon_i)}{z - \epsilon_i} + \frac{d_i \Lambda(z)}{z - \epsilon_i} \right).$$

The second term can be simplified as follows:

$$\frac{B}{g} \sum_{\alpha=1}^N \frac{\lambda_\alpha}{z - \lambda_\alpha} = \frac{B}{g} \sum_{\alpha=1}^N \left( \frac{\lambda_\alpha - z}{z - \lambda_\alpha} + \frac{z}{z - \lambda_\alpha} \right) = \frac{B}{g} (-M + z\Lambda(z)).$$

The third term is instantly seen to be  $C\Lambda(z)/g$ . Thus, after writing  $P'(z) = \Lambda(z)P(z)$ , we find the equation

$$\boxed{P''(z) - F(z)P'(z) + G(z)P(z) = 0}, \quad (117)$$

with

$$F(z) = \frac{C}{g} + \frac{Bz}{g} + \sum_{j=1}^N \frac{d_j}{z - \epsilon_j},$$

$$G(z) = \frac{MB}{g} + \sum_{j=1}^N \frac{d_j \Lambda(\epsilon_j)}{z - \epsilon_j}.$$

**Barycentric representation** We decompose the polynomials  $P(z)$  onto the basis of Lagrange polynomials in first barycentric form (see Appendix B.2):

$$P(z) = \ell(z) \sum_{i=1}^{M+1} \frac{w_i}{z - z_i} P(z_i) \equiv \ell(z) \sum_{i=1}^{M+1} \frac{u_i}{z - z_i}, \quad (118)$$

with  $\ell(z) \equiv \prod_{i=1}^{M+1} (z - z_i)$ ,  $w_i = \prod_{j=1, j \neq i}^{M+1} (z_i - z_j)^{-1}$ ,  $u_i = w_i P(z_i)$ .

This gives rise to the equations

$$\begin{cases} \frac{P(z)}{\ell(z)} &= \sum_{i=1}^{M+1} \frac{u_i}{z - z_i}, \\ \frac{P'(z)}{\ell(z)} &= \sum_{i \neq j(=1)}^{M+1} \frac{u_i}{(z - z_i)(z - z_j)}, \\ \frac{P''(z)}{\ell(z)} &= \sum_{i \neq j \neq k(=1)}^{M+1} \frac{u_i}{(z - z_i)(z - z_j)(z - z_k)}. \end{cases} \quad (119)$$

In the barycentric representation (119), the equation (117) can take on a general or a simplified form, depending on whether the grid points are chosen (not to) coincide with the  $\epsilon_i$ :

- for general  $z = z_i$  (provided  $z_i$  differs from every  $\epsilon_j$ , such that  $F(z_i)$  and  $G(z_i)$  do not blow up):

$$\sum_{j \neq k(\neq i)}^{M+1} \frac{u_i}{(z_i - z_j)(z_i - z_k)} + 2 \sum_{j \neq k(\neq i)}^{M+1} \frac{u_j}{(z_i - z_j)(z_i - z_k)} - F(z_i) \left( \sum_{j \neq i}^{M+1} \frac{u_i}{z_i - z_j} + \sum_{j \neq i}^{M+1} \frac{u_j}{z_i - z_j} \right) + G(z_i)u_i = 0; \quad (120)$$

- for a grid point  $z_i = \epsilon_i$  (using  $P'(\epsilon_i) = \Lambda(\epsilon_i)P(\epsilon_i)$ ):

$$\sum_{j(\neq i)}^{M+1} \frac{u_i}{\epsilon_i - z_j} + \sum_{j(\neq i)}^{M+1} \frac{u_j}{\epsilon_i - z_j} = \Lambda(\epsilon_i)u_i. \quad (121)$$

Note: Derivation of eq. (120)

Substituting the expressions for  $P''(z)$ ,  $P'(z)$  and  $P(z)$  into eq. (117) gives the equations

$$\underbrace{\sum_{i \neq j \neq k(=1)}^{M+1} \frac{u_i}{(z - z_i)(z - z_j)(z - z_k)}}_{\text{I}} - \underbrace{F(z) \sum_{i \neq j(=1)}^{M+1} \frac{u_i}{(z - z_i)(z - z_j)}}_{\text{II}} + \underbrace{G(z) \sum_{i=1}^{M+1} \frac{u_i}{z - z_i}}_{\text{III}} = 0.$$

The form (120) can be derived by computing the residues of I, II and III as  $z \rightarrow z_l$  (we renamed the fixed grid point  $z_l$  here to avoid confusion with the summation index) and demanding that they sum to zero.

- The sum in the third term can be split as

$$G(z) \left( \frac{u_l}{z - z_l} + \sum_{i \neq l}^{M+1} \frac{u_i}{z - z_i} \right).$$

To find the residue, multiply by  $(z - z_l)$  and take the limit as  $z \rightarrow z_l$ :

$$\lim_{z \rightarrow z_l} (z - z_l) G(z) \left( \frac{u_l}{z - z_l} + \sum_{i \neq l}^{M+1} \frac{u_i}{z - z_i} \right) = \lim_{z \rightarrow z_l} G(z) u_l = G(z_l) u_l.$$

- The second term can be decomposed into two contributions for either  $i = l$  or  $j = l$ :

$$-F(z) \left[ \sum_{j \neq l}^{M+1} \frac{u_l}{(z - z_l)(z - z_j)} + \sum_{i \neq l}^{M+1} \frac{u_i}{(z - z_i)(z - z_l)} \right],$$

and the residue is given by

$$\begin{aligned} \lim_{z \rightarrow z_l} (z - z_l) \left( -F(z) \left[ \sum_{j \neq l}^{M+1} \frac{u_l}{(z - z_l)(z - z_j)} + \sum_{i \neq l}^{M+1} \frac{u_i}{(z - z_i)(z - z_l)} \right] \right) \\ = -F(z_l) \left( \sum_{j \neq l}^{M+1} \frac{u_l}{z_l - z_j} + \sum_{i \neq l}^{M+1} \frac{u_i}{z_l - z_i} \right). \end{aligned}$$

Relabeling the dummy index in the second sum, we get

$$-F(z_l) \left( \sum_{j \neq l}^{M+1} \frac{u_l}{z_l - z_j} + \sum_{i \neq l}^{M+1} \frac{u_j}{z_l - z_j} \right).$$

- The first term can similarly be decomposed into three contributions for either  $i = l$ ,  $j = l$  or  $k = l$ :

$$\sum_{j,k \neq l, j \neq k}^{M+1} \frac{u_l}{(z - z_l)(z - z_j)(z - z_k)} + \sum_{i,k \neq l, i \neq k}^{M+1} \frac{u_i}{(z - z_i)(z - z_l)(z - z_k)} + \sum_{i,j \neq l, i \neq j}^{M+1} \frac{u_i}{(z - z_i)(z - z_j)(z - z_l)},$$

with residues

$$\begin{aligned} & \lim_{z \rightarrow z_l} (z - z_l) \left( \sum_{j,k \neq l, j \neq k}^{M+1} \frac{u_l}{(z - z_l)(z - z_j)(z - z_k)} + \sum_{i,k \neq l, i \neq k}^{M+1} \frac{u_i}{(z - z_i)(z - z_l)(z - z_k)} \right. \\ & \quad \left. + \sum_{i,j \neq l, i \neq j}^{M+1} \frac{u_i}{(z - z_i)(z - z_j)(z - z_l)} \right) \\ &= \sum_{j,k \neq l, j \neq k}^{M+1} \frac{u_l}{(z - z_j)(z - z_k)} + \sum_{i,k \neq l, i \neq k}^{M+1} \frac{u_i}{(z - z_i)(z - z_k)} + \sum_{i,j \neq l, i \neq j}^{M+1} \frac{u_i}{(z - z_i)(z - z_j)}. \end{aligned}$$

After relabeling the second and third sums, we get

$$\sum_{j,k \neq l, j \neq k}^{M+1} \frac{u_l}{(z_l - z_j)(z_l - z_k)} + 2 \sum_{j,k \neq l, j \neq k}^{M+1} \frac{u_j}{(z_l - z_j)(z_l - z_k)}.$$

Adding the contributions I, II and III lands us on eq. (120).

In the examples considered by Faribault et al. [44] and El Araby, Gritsev, and Faribault [41], the grid is chosen to coincide with the  $\epsilon_i$ , which warrants the use of the equations (121). For models with complex-valued coupling, we found better stability using a grid that changes dynamically: we assume that the rapidities change more or less smoothly with the coupling and choose the grid at coupling strength  $c$  to coincide with the rapidities at coupling strength  $c - \Delta c$ , which should then guarantee that the grid is close enough to the actual roots. In this case, it is necessary to find the coefficients of the Lagrange basis representation by solving for the  $\{u_i\}$  in the linear equations (120).

Regardless of whether the  $\{z_i\}$  are chosen to coincide with the grid points  $\{\epsilon_i\}$ , the core of the argument is that for any given grid  $\{z_i\}$ , the coefficients  $\{u_i\}$  of the Lagrange basis representation can be obtained by solving a set of linear equations (linear in the coefficients  $u_i$ ), namely eq. (120) or (121). Once we have the coefficients, we have a representation of the polynomial, and we can use a standard root-finding algorithm such as Laguerre's method with polynomial deflation to find the roots  $\{\lambda_i\}$ .

### 5.3. Implementation

In the previous section, we described a method to efficiently compute Bethe roots through the BA/ODE-correspondence. The starting point of this method are the Bethe equations (111). In late February, Alexandre Faribault and his PhD student Raphael Burgun (Université de Lorraine) graciously agreed to share a Python script of Raphael's making – one that computes conserved charges and Bethe roots of the central spin model as a function of the coupling strength. The purpose of this ‘mini project’ was to let me tinker with the script and adapt it in a way that would make it suitable for handling complex-valued couplings.

Although major parts of the script are direct implementations of or have clearly been influenced by [44, 41], it circumvents the BA/ODE-correspondence and instead hinges on (1) a particular form of the conserved charges that lets us express squares of eigenvalues of charges as a linear combination of the other eigenvalues,

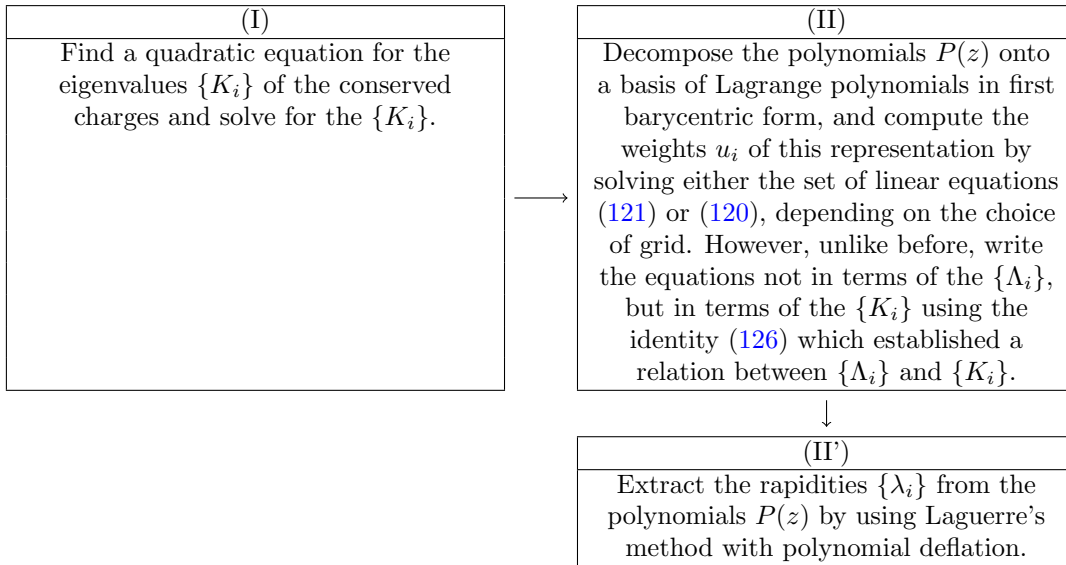
based on Dimo and Faribault [35], and (2) a non-trivial identity that directly relates the eigenvalues of conserved charges  $\{K_i\}$  with the auxiliary variables  $\{\Lambda_i\}$ , see eq. (126) based on Faribault and Schuricht [43]. Put differently, in Sections 5.1 and 5.2 we used the BA/ODE-correspondence to find a set of auxiliary variables  $\{\Lambda_i\}$  which we massaged into a set of linear equations for the coefficients  $\{u_i\}$  of the Lagrange basis representation, and then the Bethe roots  $\{\lambda_i\}$  were to be extracted with a root-finding algorithm:

$$(\text{BA/ODE-correspondence} \rightarrow) \{\Lambda_i\} \rightarrow \{u_i\} \rightarrow \{\lambda_i\}.$$

In the numerical implementation of Raphael's script, however, we use a nontrivial identity between the eigenvalues of the conserved charges  $\{K_i\}$  and the auxiliary variables  $\{\Lambda_i\}$  to circumvent the BA/ODE-correspondence, and go from charge eigenvalues to the coefficients of the basis representation before extracting the roots:

$$\{K_i\} \rightarrow \{u_i\} \rightarrow \{\lambda_i\}.$$

To reflect the different approach, we may modify the schematic that was featured in the introduction of this chapter:



The method put forth in this section has been found to work well (based on my own assessment) for a broad range of system sizes and accepts a variable number of excitations. An obvious disadvantage of going about things the way we do here, relying on a particular form of the conserved charges and on a relation between the  $\{K_i\}$  and the  $\{\Lambda_i\}$  that holds only for Gaudin models realized in terms of finite magnitude (pseudo-)spins<sup>41</sup> to provide the necessary relations between variables, is that the method is less generally applicable, whereas an BA/ODE-based solver is applicable to any system that admits Bethe equations.

In the following, we illustrate the method directly in the context of the central spin model, described by the Hamiltonian:

$$H = \hat{S}_j^z + g \sum_{k=1 \neq j}^N \frac{1}{\epsilon_j - \epsilon_k} \vec{S}_j \cdot \vec{S}_k,$$

with  $g = 1/B_z$ ,  $\vec{S} = (\hat{S}^x, \hat{S}^y, \hat{S}^z)$  and  $\vec{S}_j$  the ‘central spin’. Clearly, the quantity  $\hat{Q}_j = \hat{S}_j^z + g \sum_{k=1 \neq j}^N \frac{1}{\epsilon_j - \epsilon_k} \vec{S}_j \cdot \vec{S}_k$  is itself a conserved charge.

<sup>41</sup>For example, any model containing bosonic degrees of freedom such as Jaynes-Cummings-Dicke like models will not satisfy the identity.



**Quadratic equation for the charges** Dimo and Faribault [35] prove that any RG-model with charges of the form

$$\hat{Q}_i = \vec{B}_i \cdot \vec{\sigma}_i + \sum_{k \neq i}^N \sum_{\alpha=x,y,z} \Gamma_{i,k}^\alpha \hat{\sigma}_i^\alpha \hat{\sigma}_k^\alpha$$

(with Greek subscripts denoting orientations  $\{x, y, z\}$ , Latin subscripts labeling spins  $\{1, 2, \dots, N\}$  and  $\vec{\sigma}$  the Pauli matrices), the square of charges can be expressed as the following linear combination of the other charges:

$$\hat{Q}_i^2 = -2 \sum_{j \neq i} \frac{\Gamma_{ij}^\alpha \Gamma_{ij}^\gamma}{\Gamma_{ji}^\beta} \hat{Q}_j + \sum_{\alpha} (B_i^\alpha)^2 + \sum_{\alpha} \sum_{k \neq i} (\Gamma_{ik}^\alpha)^2. \quad (122)$$

The equality then also trivially holds for the eigenvalues  $K_j$ :

$$K_i^2 = -2 \sum_{j \neq i} \frac{\Gamma_{ij}^\alpha \Gamma_{ij}^\gamma}{\Gamma_{ji}^\beta} K_j + \sum_{\alpha} (B_i^\alpha)^2 + \sum_{\alpha} \sum_{k \neq i} (\Gamma_{ik}^\alpha)^2. \quad (123)$$

To apply the result, we write our  $\hat{Q}_j$  as

$$\begin{aligned} \hat{Q}_j &= \hat{S}_j^z + g \sum_{k=1 \neq j}^N \frac{1}{\epsilon_j - \epsilon_k} \vec{S}_j \cdot \vec{S}_k \\ &= \frac{1}{2} \hat{\sigma}_j^z + \frac{g}{4} \sum_{k=1 \neq j}^{N-1} \sum_{\alpha=x,y,z} \frac{1}{\epsilon_j - \epsilon_k} \hat{\sigma}_j^\alpha \hat{\sigma}_k^\alpha \\ &= \frac{1}{2} \hat{\sigma}_j^z + \sum_{k=1 \neq j}^{N-1} \sum_{\alpha=x,y,z} \Gamma_{jk}^\alpha \hat{\sigma}_j^\alpha \hat{\sigma}_k^\alpha. \end{aligned}$$

Note that we have switched to Pauli operators in the second line (they are of course simply related by a factor  $\hbar/2$ , and we set  $\hbar = 1$ ). We then identify

$$\Gamma_{ik}^\alpha = \frac{1}{4} \frac{g}{\epsilon_i - \epsilon_k}, \quad \text{and} \quad \vec{B}_i = \begin{pmatrix} 0 \\ 0 \\ 1/2 \end{pmatrix}.$$

Substituting the identifications into eq. (123) gets us

$$F_j(K_1, K_2, \dots, K_N; g) \equiv K_j^2 - \frac{g}{2} \sum_{i \neq j}^N \frac{K_j}{\epsilon_j - \epsilon_i} - \frac{3}{16} g^2 \sum_{i \neq j}^N \frac{1}{(\epsilon_j - \epsilon_i)^2} - \frac{1}{4} = 0, \quad j = 1, 2, \dots, N.$$

We have thus obtained a quadratic equation for the eigenvalues of the charges. This is extremely useful, since we can now numerically solve for these eigenvalues, for example using a Newton-Raphson algorithm. The Newton-Raphson method updates the values of the vector  $\vec{K} = (K_1, K_2, \dots, K_N)$  according to the rule

$$\vec{K}^{(n+1)} = \vec{K}^{(n)} - J^{-1} F(\vec{K}^{(n)}),$$

where  $F(\vec{K})$  is the vector of equations for the charges and  $J$  is the Jacobian matrix with elements

$$J_{jl} = \frac{\partial F_j}{\partial K_l} = 2K_j \delta_{jl} - \frac{g}{2} \sum_{i \neq j}^N \frac{1}{\epsilon_j - \epsilon_i} \delta_{il}.$$

Because our solver will evolve the eigenvalues of the conserved charges with the coupling strength  $g$ , we also want to know  $\vec{K}'$ , the derivative of  $\vec{K}$  with respect to  $g$ . Following Sträter [113], in particular Section 3.5, it

follows that we can compute  $\vec{K}'$  by solving the linear system

$$J\vec{K}' = -\frac{\partial \vec{F}}{\partial g} \equiv \vec{B}_1, \quad (124)$$

$$\text{with } B_{1,j} = \frac{1}{g} \left( K_j^2 + \frac{3}{16} g^2 \sum_{i \neq j}^{N-1} \frac{1}{(\epsilon_i - \epsilon_j)^2} - \frac{1}{4} \right),$$

which is easy to solve numerically for  $\vec{K}'$  using a standard linear algebra solver.

**Bethe root extraction from polynomials** As explained in Section 5.2 on root extraction, we first want to find the  $\{u_i\}$ , which represent the displacements in the barycentric representation of  $P(z)$ . To do this, we solve eq. (121) if we choose our gridpoints  $z_i$  to coincide with the  $\epsilon_i$ , or we use eq. (120) if this is not the case.

Let us illustrate how one would set up the system of linear equations for the ‘on-grid’ central spin model. We write eq. (121) as

$$\left[ \sum_{j \neq i}^{M+1} \frac{1}{\epsilon_i - \epsilon_j} - \Lambda(\epsilon_i) \right] u_i + \sum_{j \neq i}^{M+1} \frac{1}{\epsilon_i - \epsilon_j} u_j = 0,$$

and now we rewrite this as a matrix equation of the following form:<sup>42</sup>

$$\text{Mat} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_M \\ u_{M+1} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}, \quad (125)$$

where Mat has **diagonal** terms

$$\text{Mat}_{ii} = \left[ \sum_{j \neq i}^{M+1} \frac{1}{\epsilon_i - \epsilon_j} - \Lambda(\epsilon_i) \right] = \frac{2}{g} \left[ K_i - \frac{g}{4} \sum_{j \neq i}^N \frac{1}{\epsilon_i - \epsilon_j} + \frac{1}{2} \right] + \sum_{k \neq i}^{M+1} \frac{1}{\epsilon_i - \epsilon_k}.$$

The rewriting in the second equality follows Faribault and Schuricht [43], in particular eq. (12), which (in our notation) is the identity

$$\Lambda(\epsilon_i) = \frac{2}{g} \left[ K_i - \frac{g}{4} \sum_{j \neq i}^N \frac{1}{\epsilon_i - \epsilon_j} + \frac{1}{2} \right]. \quad (126)$$

The **off-diagonal** terms are simply

$$\text{Mat}_{ij} = \frac{1}{\epsilon_i - \epsilon_j} \quad (i \neq j)$$

The assembled matrix (filling the last row with all 1’s) is:

$$\text{Mat} = \begin{pmatrix} \frac{2}{g} \left[ K_1 - \frac{g}{4} \sum_{k \neq 1}^N \frac{1}{\epsilon_1 - \epsilon_k} + \frac{1}{2} \right] + \sum_{k \neq 1}^{M+1} \frac{1}{\epsilon_1 - \epsilon_k} & \frac{1}{\epsilon_1 - \epsilon_2} & \cdots & \frac{1}{\epsilon_1 - \epsilon_{M+1}} \\ \frac{1}{\epsilon_2 - \epsilon_1} & \frac{2}{g} \left[ K_2 - \frac{g}{4} \sum_{k \neq 2}^N \frac{1}{\epsilon_2 - \epsilon_k} + \frac{1}{2} \right] + \sum_{k \neq 2}^{M+1} \frac{1}{\epsilon_2 - \epsilon_k} & \cdots & \frac{1}{\epsilon_2 - \epsilon_{M+1}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{\epsilon_M - \epsilon_1} & \frac{1}{\epsilon_M - \epsilon_2} & \cdots & \frac{2}{g} \left[ K_M - \frac{g}{4} \sum_{k \neq M}^N \frac{1}{\epsilon_M - \epsilon_k} + \frac{1}{2} \right] + \sum_{k \neq M}^{M+1} \frac{1}{\epsilon_M - \epsilon_k} \\ 1 & 1 & 1 & 1 \end{pmatrix}.$$

<sup>42</sup>Note that we have a 1 in the last position of the vector on the rhs. We will also fill the last row of the matrix Mat with 1’s. This is not a typo. Since the polynomial  $P(z)$  is the product  $(z - \lambda_1)(z - \lambda_2) \cdots (z - \lambda_M) = z^M + \mathcal{O}(z^{M-1})$ , it has coefficient 1 for the  $z^M$  term. As a consequence, in the limit  $z \rightarrow \infty$ , we have  $P(z) \rightarrow z^M$  and for the basis polynomials  $\ell(z) \rightarrow z^{M+1}$ . Therefore, the barycentric representation of  $P(z)$ , eq. (118), becomes  $z^M = z^{M+1} \sum_{i=1}^{M+1} \frac{u_i}{z}$ , i.e.  $\frac{1}{z} = \sum_{i=1}^{M+1} \frac{u_i}{z}$ . This gives us an additional equation to complete the set of linear equations:  $\sum_i^{M+1} u_i = 1$ .

The  $\{u_i\}$  are obtained by solving the linear system (125) with this form of Mat. After we have the  $\{u_i\}$ , we can construct the polynomials  $P(z)$  using eq. (119). It is computationally more efficient to express  $P(z)/\ell(z)$ ,  $P'(z)/\ell(z)$  and  $P''(z)/\ell(z)$  in terms of one another, using again the identity (126):

$$\begin{cases} \frac{P(z)}{\ell(z)} &= \sum_i^N \frac{u_i}{z-z_i}, \\ \frac{P'(z)}{\ell(z)} &= \sum_i^N \left\{ -\frac{2}{g} \left[ K_i - \frac{g}{4} \sum_{j \neq i}^N \frac{1}{\epsilon_i - \epsilon_j} + \frac{1}{2} \right] \frac{u_i}{z-z_i} \right\}, \\ \frac{P''(z)}{\ell(z)} &= \sum_i^N \left\{ \frac{1}{z-z_i} \left[ \frac{P'(z)}{\ell(z)} + \frac{2}{g} \left[ K_i - \frac{g}{4} \sum_{j \neq i}^N \frac{1}{\epsilon_i - \epsilon_j} + \frac{1}{2} \right] \frac{u_i}{z-z_i} \right] \right\}. \end{cases}$$

Finally, we implement Laguerre's method to extract the rapidities  $\{\lambda_\alpha\}$  from the eigenvalues  $\{K_i\}$ :

1. Compute  $G \equiv \frac{P'(\lambda_k)}{P(\lambda_k)}$ .
2. Compute  $H \equiv G^2 - \frac{P''(\lambda_k)}{P(\lambda_k)}$ .
3. Compute  $a \equiv \frac{n}{G \pm \sqrt{(n-1)(nH-G^2)}}$ , where  $n$  is the degree of the polynomial and we choose the sign such that the denominator has the largest value.
4. Set  $\lambda_{k+1} = \lambda_k - a$ .

In Algorithm 1, we describe the steps of the Python implementation for real-valued coupling in pseudocode.

---

**Algorithm 1** Pseudocode.

---

```

1: dim ← comb(N, M)                                ▷ Calculate dim( $\mathcal{H}$ ) with N spins and M excitations
2: for j = 0 to dim - 1 do                             ▷ Loop over configurations in  $\mathcal{H}$ 
3:   Kj ← config(j, N, M)                             ▷ Initiate Kj with a configuration
4:   for ng = 0 to nbpts do                               ▷ Loop over coupling values
5:      $\delta \leftarrow 0.025$ 
6:     g ← ng ·  $\delta$                                          ▷ Coupling strength
7:     Kj ← Kj + Kj'(g -  $\delta$ , Kj) ·  $\delta$                  ▷ Compute estimate of new Kj by adding gradient term (124)
8:     Kj ← NewtonRaphson(Kj, g,  $\varepsilon$ )                 ▷ Use estimate as initial guess for N-R;  $\varepsilon$  is the tolerance
9:      $\vec{K}[ng, :, j] \leftarrow K_j$ 
10:    if ng mod 2 = 0 and ng ≠ 0 then                     ▷ Compute roots for every 2nd step
11:      new_ng ← round(ng/2)
12:       $\lambda_k \leftarrow \frac{e_0 + e_1}{2} + e_1$                      ▷ Initial guess for the root
13:      newu ← u_grid(res, g)                             ▷ Find ui from (121)
14:      newM ← M
15:      newK ← Kj
16:      for k = 0 to M - 1 do                               ▷ Loop over excitations
17:         $\lambda_k \leftarrow \text{Laguerre}(\lambda_k, \text{newu}, \varepsilon, \text{grid}, \text{newM}, g, \text{newK})$ 
18:        roots[new_ng - 1, k, j] ←  $\lambda_k$                  ▷ Laguerre's method
19:        newM ← newM - 1
20:        newu[i] ← newu[i] ·  $\frac{\text{grid}[i] - \text{grid}[\text{newM} + 1]}{\text{grid}[i] - \lambda_k}$    ▷ Deflate: shift displacements
21:        for i = 0 to newM
22:          newK[i] ← newK[i] +  $\frac{g}{2} \cdot \frac{1}{e[i] - \lambda_k}$ 
23:        for i = 0 to N - 1
24:           $\lambda_k \leftarrow \text{conjugate}(\lambda_k)$                  ▷ If g real, roots come in pairs
25:        end for
26:      end if
27:    end for
28:  end for

```

---

To achieve better stability for complex-valued couplings, we switch from *u\_grid* to *u\_offgrid* in line 13: we solve eq. (120) instead of eq. (121).

#### 5.4. Example computation with complex-valued coupling

We plot the Bethe roots of a central spin model featuring 8 sites and 4 excitations, and contrast their distributions for real-valued and complex-valued couplings.

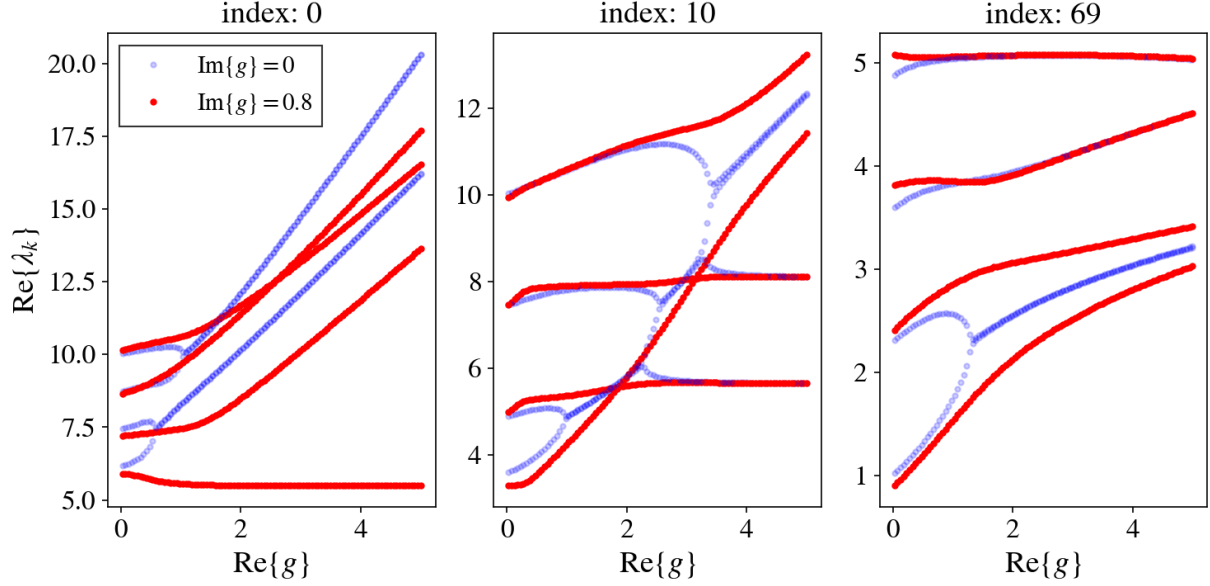


Figure 21: Central spin model: real part of the Bethe roots as a function of the real part of the coupling  $g$ , with  $N = 8$  spins and  $M = 4$  excitations. ‘index’ labels the configurations in the  $\dim(\mathcal{H}) = N!/(M!(N-M)!) = 70$  dimensional Hilbert space.

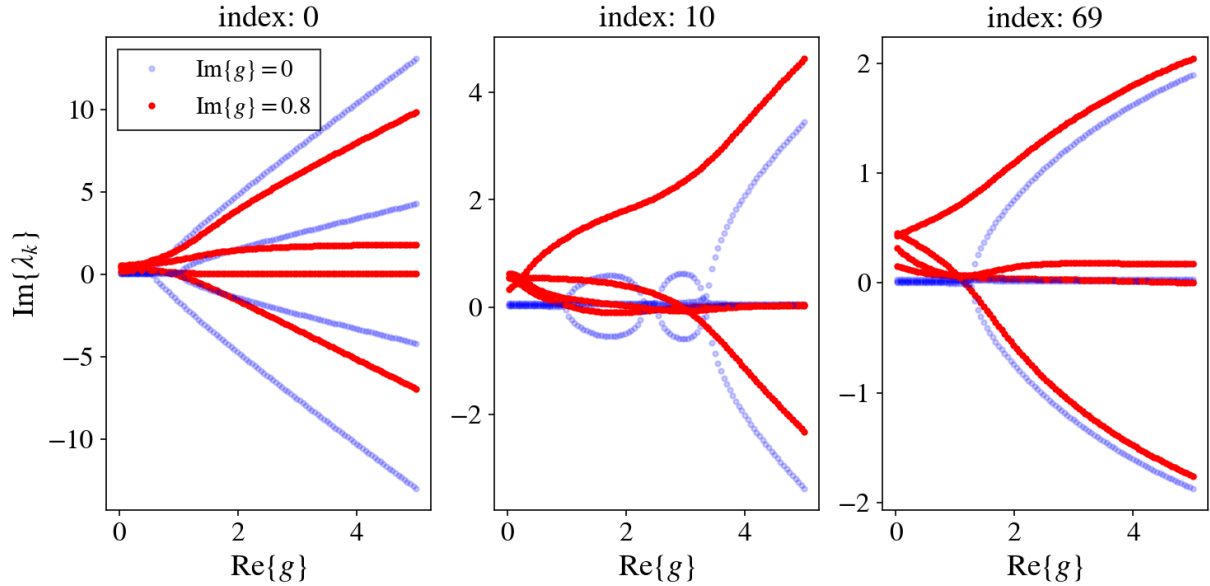


Figure 22: Central spin model: imaginary part of the Bethe roots as a function of the real part of the coupling  $g$ , with  $N = 8$  spins and  $M = 4$  excitations. ‘index’ labels the configurations in the  $\dim(\mathcal{H}) = N!/(M!(N-M)!) = 70$  dimensional Hilbert space.

### 5.5. Relation to work by Bakker [5]

In Chapter 4 of his PhD thesis (in preparation), Bakker [5] reformulates the task of finding the  $N$ -point correlation functions for a system of noisy, driven, dissipative spins, into solving a time-evolution equation governed by an  $N$ -site non-Hermitian RG-Hamiltonian.

Concretely, he shows that in the system governed by the Lindblad equation

$$\partial_t \rho = \mathcal{L} \rho \equiv -i[H, \rho] + \sum_{\alpha} D_{\alpha}[\rho],$$

$$\text{with } H = \sum_j^{N_s} (2\epsilon_j) s_j^z, \quad D_{\alpha}[\rho] = L_{\alpha} \rho L_{\alpha}^{\dagger} - \frac{1}{2} \{L_{\alpha}^{\dagger} L_{\alpha}, \rho\}, \quad L_{\alpha} = \sqrt{g_{\alpha}} \sum_j^{N_s} s_j^{\alpha}, \quad \text{and } \alpha = \{z, +, -\},$$

the time evolution of the vector  $\tilde{\mathcal{C}}$  containing the correlation functions of the spins,

$$c_{a_1, \dots, a_N} = \text{Tr} \left[ \rho^{(N)} \sigma_1^{a_1} \otimes \dots \otimes \sigma_N^{a_N} \right], \quad \text{with } a_j = \{0, x, y, z\},$$

is governed by the non-Hermitian spin-1 Hamiltonian

$$H_{RG} = - \sum_j^N 2i\epsilon_j S_j^z - g_+ \sum_{j,k}^N (S_j^x S_k^x + S_j^y S_k^y),$$

namely,

$$\frac{d}{dt} \tilde{\mathcal{C}} = H_{RG} \tilde{\mathcal{C}}. \tag{127}$$

Reversing the argument, we could in principle (practical challenges aside) start with an  $N$ -site non-Hermitian RG-Hamiltonian such as the complexified central spin Hamiltonian, and map it to a system of noisy, driven, dissipative spins via its correlation functions, which are the solution to the dynamical equation (127) (knowledge of all the correlation functions fully specifies the theory).

The Bethe root solver presented in Section 5.3 can aid in this process by providing the rapidities needed to build correlation functions, following Slavnov's formula eq. (96). In other words, having an efficient solver for the Bethe roots of a class of non-Hermitian RG-Hamiltonians, we may solve for their rapidities, build the full set of correlation functions using Slavnov's formula, and – given the appropriate mapping – we would then also have solved for a system of noisy, driven, dissipative spins.

## 6. Conclusion

In this thesis, we spent most of our efforts investigating quantum systems that are both *integrable* and *open*: integrable, in the sense of admitting a Bethe Ansatz formulation, and open, in the sense of being non-Hermitian, with imaginary couplings that give the system a dissipative character. To understand how these concepts work together to produce interesting behaviour, we dedicated Section 2 to a fairly heuristic discussion on the notion of classical integrability, and the proper way to extend integrability to quantum-mechanical systems. Starting from Hamiltonian mechanics and the Liouville-Arnold theorem, we painted integrability in the context of chaos and ergodicity, before framing the integrability of quantum mechanical systems in terms of their ergodic properties and the density character of their conserved charges.

In Section 3, we explored the first example of a Bethe-Ansatz solvable, quantum integrable system: the Lieb-Liniger model for bosons with Dirac delta interactions in one dimension. We discussed the solution of the model by coordinate Bethe Ansatz and the various regimes of qualitatively different behaviour that the model can exhibit, depending on the sign of the interaction term. In the second half of the section, we introduced open quantum systems. Building on recent advancements, we performed a numerical study of the spectrum of a Lindbladian for an open Lieb-Liniger model, starting from its Bethe roots.

Section 4 served to present two faces of solution by Bethe Ansatz: the framework of *algebraic Bethe Ansatz* and the framework of *Richardson-Gaudin models*. Both methods produce the same object of interest, namely the Bethe equations of the system, but their construction builds up from different starting positions. We studied the origin of the lauded Yang-Baxter equation, and derived a general expression for the Bethe equations as a set of consistency equations restraining the rapidities. The main objective of this section was to outline the methods in a way that is tractable for physicists without a deep understanding of the mathematical aspects of Lie algebras, representation theory and quantum groups, and to lay the groundwork for the numerical methods presented in Section 5.

The last section, Section 5, started with an in-depth review of two papers on numerical procedures for solving Bethe equations, based on the BA/ODE-correspondence. We then modified and optimized a Bethe root solver to deal with non-Hermitian Richardson-Gaudin models realized in terms of finite magnitude (pseudo-)spins, and with a particular form of conserved charges. This solver was applied the solver to the complexified central spin model, and the distribution of rapidities was presented.

Naturally, a one-year thesis is usually finished with more questions than there are answers. If any future master's student has a particular interest in continuing this branch of research, I would suggest to look for other identities that can make the Bethe solver more generally applicable to systems not limited by their form of conserved charges, or with bosonic degrees of freedom. Alternatively, one may try to implement the solver using the full machinery of the BA/ODE-correspondence without any 'shortcuts', but this has undoubtedly already been done. Nevertheless, it could still be interesting to investigate stability of a BA/ODE-based solution method in the context of dissipative systems, since the introduction of imaginary numbers in the couplings has been seen to degrade numerical performance if no adequate countermeasures are taken.

## A. Proof of the Liouville-Arnold theorem

We prove Theorem 2.2. The proof is basically identical to the combination of the two proofs in Section 1.2 and Appendix A of Dunajski [40], but some aspects have been written down more explicitly and with additional comments. I do not claim originality, and will note that the proof is insightful but not fully rigorous in all places.

*Proof.* Motion takes place on the surface

$$f_1(p, q) = c_1, \quad f_2(p, q) = c_2, \quad \dots, \quad f_n(p, q) = c_n$$

of dimension  $2n - n = n$ . This surface is a torus.

*Subproof.* We prove that this surface is indeed a torus. The gradients  $\nabla f_k$  are independent, thus the set

$$M_f \equiv \{(p, q) \in M : f_k(p, q) = c_k\}$$

defines a manifold of dimension  $n$ . Introduce local coordinates  $\xi^a = (p, q)$  on  $M$  with Poisson bracket

$$\{f, g\} = \omega^{ab} \frac{\partial f}{\partial \xi^a} \frac{\partial g}{\partial \xi^b}, \quad a, b = 1, 2, \dots, 2n,$$

and  $\omega$  the constant anti-symmetric matrix

$$\omega = \begin{pmatrix} 0 & \mathbb{1}_n \\ -\mathbb{1}_n & 0 \end{pmatrix}.$$

Since the Poisson brackets  $\{f_j, f_k\}$  vanish, the Hamiltonian vector field

$$X_{f_k} = \omega^{ab} \frac{\partial f_k}{\partial \xi^b} \frac{\partial}{\partial \xi^a}$$

is orthogonal to any of the gradients  $\partial_a f_j$  with  $a = 1, \dots, 2n$  and  $k = 1, \dots, n$ . Furthermore, the gradients are perpendicular to  $M_f$ , so the Hamiltonian vectors fields are tangent to  $M_f$ . They also commute, since

$$[X_{f_j}, X_{f_k}] = -X_{\{f_j, f_k\}} = 0.$$

We see that the vectors generate an action of the Abelian group  $\mathbb{R}^n$  on  $M$ , which restricts to an  $\mathbb{R}^n$  action on  $M_f$ . Let  $p_0 \in M_f$  and let  $\Gamma$  be a lattice of all vectors in  $\mathbb{R}^n$  which fix  $p_0$  under the group action, i.e. vectors in  $\text{Stab}(p_0)$  by  $\mathbb{R}^n$ . Evidently,  $\Gamma$  is a finite subgroup of  $\mathbb{R}^n$ . We can invoke the orbit-stabilizer theorem (see below) to conclude that

$$M_f = \mathbb{R}^n / \Gamma.$$

Assuming  $M_f$  is compact, this quotient space is diffeomorphic to  $T^n$ , the  $n$ -torus. ■

Note: Orbit-Stabilizer theorem

Let  $G$  be a group and  $\Omega$  a finite set, and let  $x \in \Omega$ . The **group orbit** of  $x$  is the subset of all images of  $x$  under the action of elements in  $G$ , i.e.  $G(x) = \{g(x) : g \in G\}$ . The **stabilizer** subgroup (isotropy group, little group) of  $x$  by  $G$  is given by  $\{g \in G : g(x) = x\}$ , i.e. the elements in  $G$  that produce group fixed points in  $x$ . The **orbit stabilizer theorem** states that there exists a bijection between  $G/\text{Stab}(x)$ , the set of cosets for the stabilizer subgroup, and  $\text{Orb}(x)$ . Invoking Lagrange's theorem, it then follows immediately that,  $\forall x \in \Omega$ ,

$$|G| = |\text{Orb}(x)| \cdot |\text{Stab}(x)|.$$

### Example

The orbit of 1 under the permutation group  $\{(1)(2)(3)(4), (12)(3)(4), (1)(2)(34), (12)(34)\}$  is  $\{1, 2\}$ . The stabilizer of 1 (and also 2) is  $\{(1)(2)(3)(4), (1)(2)(34)\}$ . So indeed, we find that  $4 = 2 \cdot 2$ .

For each point in  $M$ , there exists precisely one torus  $T^n$  that passes through that point. As a consequence,  $M$  admits a foliation by  $n$ -dimensional leaves,<sup>43</sup> the leaves being tori (labeled by the constants  $c_1, \dots, c_n$ ).

We assume that

$$\det \left( \frac{\partial f_j}{\partial p_k} \right) \neq 0,$$

which amounts to assuming the first integrals are functionally independent. Doing this, we can solve the system  $f_k(p, q) = c_k$  for the momenta  $p_i : p_i = p_i(q, c)$ , and the relations  $f_i(q, p(q, c)) = c_i$  hold identically.<sup>44</sup> We differentiate the relations with respect to  $q_j$ , and then multiply by  $\sum_j \frac{\partial f_m}{\partial p_j}$  to obtain

$$\begin{aligned} \frac{\partial f_i}{\partial q_j} + \sum_k \frac{\partial f_i}{\partial p_k} \frac{\partial p_k}{\partial q_j} &= 0, \\ \sum_j \frac{\partial f_m}{\partial p_j} \frac{\partial f_i}{\partial q_j} + \sum_{j,k} \frac{\partial f_m}{\partial p_j} \frac{\partial f_i}{\partial p_k} \frac{\partial p_k}{\partial q_j} &= 0. \end{aligned}$$

Next, subtract the same expression with  $m \leftrightarrow i$ :

$$\begin{aligned} \{f_i, f_m\} + \sum_{j,k} \left( \frac{\partial f_m}{\partial p_j} \frac{\partial f_i}{\partial p_k} \frac{\partial p_k}{\partial q_j} - \frac{\partial f_i}{\partial p_j} \frac{\partial f_m}{\partial p_k} \frac{\partial p_k}{\partial q_j} \right) &= 0, \\ \sum_{j,k} \frac{\partial f_i}{\partial p_k} \frac{\partial f_m}{\partial p_j} \left( \frac{\partial p_k}{\partial q_j} - \frac{\partial p_j}{\partial q_k} \right) &= 0, \end{aligned}$$

where  $\{f_i, f_m\}$  vanishes because  $f_i$  and  $f_m$  are in involution. Note that from the last line we conclude that

$$\frac{\partial p_k}{\partial q_j} - \frac{\partial p_j}{\partial q_k} = 0, \tag{A.1}$$

because the matrices  $\partial f_i / \partial p_k$  are invertible (by assumption). Now recall Stokes' theorem (for  $n = 3$ ): for a surface  $D$  with boundary  $\partial D$ , it states that

$$\oint_{\partial D} \vec{p} \cdot d\vec{q} = \int_D (\vec{\nabla} \times \vec{p}) \cdot d\vec{q}, \quad (\vec{\nabla} \times \vec{p})_m = \frac{1}{2} \epsilon_{jkm} \left( \frac{\partial p_k}{\partial q_j} - \frac{\partial p_j}{\partial q_k} \right),$$

with  $\epsilon$  the totally anti-symmetric symbol. The condition (A.1) can be written as

$$\begin{aligned} \frac{1}{2} \left( \frac{\partial p_k}{\partial q_j} - \frac{\partial p_j}{\partial q_k} \right) \epsilon_{jkm} &= 0, \\ \frac{1}{2} \epsilon_{jkm} \left( \frac{\partial p_k}{\partial q_j} - \frac{\partial p_j}{\partial q_k} \right) dq_m &= 0, \end{aligned}$$

<sup>43</sup>Recall that, informally, a foliation means a decomposition into submanifolds. If the submanifolds all have the same dimension, the foliation is called *regular*.

<sup>44</sup>The non-zero determinant means that the Jacobian is invertible; by virtue of the implicit function theorem, we can untangle the variables and write the momenta  $p$  in terms of  $q$  and the constants  $c$ .



$$\int_D (\vec{\nabla} \times \vec{p}) \cdot d\vec{q} \stackrel{\text{Stokes'}}{=} \oint_{\partial D} p_m dq_m = 0,$$

where in going from the second to the third line, we have recognized the expression for the curl of  $\vec{p}$  and we integrated over  $D$ . Here,  $\partial D$  is any closed contractible curve on  $T^n$  and summation over  $m$  is implied.

In the next part of the proof, we construct the action coordinates. We first note that there are  $n$  closed curves that cannot be contracted down to a point, and therefore their corresponding integrals will not vanish. Hence, the integrals can be used to build coordinates, which we will name the action coordinates:

$$I_k \equiv \frac{1}{2\pi} \oint_{\Gamma_k} \sum_j p_j dq_j. \quad (\text{A.2})$$

Here, the closed curve  $\Gamma_k$  is the  $k$ -th basic cycle (submanifold without boundary) of the torus  $T^n$ :

$$\Gamma_k = \{(\tilde{\phi}_1, \dots, \tilde{\phi}_n) \in T^n : 0 \leq \tilde{\phi}_k \leq 2\pi, \tilde{\phi}_j = \text{const}, \text{ for } j \neq k\},$$

where  $\tilde{\phi}$  are some (yet unspecified) coordinates on  $T^n$ .

By Stokes' theorem, the action coordinates are independent of the choice of  $\Gamma_k$ . This is because

$$\oint_{\Gamma_k} \sum_j p_j dq_j + \oint_{\hat{\Gamma}_k} \sum_j p_j dq_j = \int \left( \frac{\partial p_i}{\partial q_j} - \frac{\partial p_j}{\partial q_i} \right) dq_j \wedge dq_i = 0,$$

where we take  $\hat{\Gamma}_k$  to have the opposite orientation with respect to  $\Gamma_k$ .<sup>45</sup>

The action variables (A.2) are also first integrals, since  $\oint p(q, c) dq$  only depends on  $c_k = f_k$  and the  $f_k$  are themselves first integrals. To convince ourselves, we show that they are in involution:

$$\begin{aligned} \{I_i, I_j\} &= \sum_{r,s,k} \left( \frac{\partial I_i}{\partial f_r} \frac{\partial f_r}{\partial q_k} \frac{\partial I_j}{\partial f_s} \frac{\partial f_s}{\partial p_k} - \frac{\partial I_i}{\partial f_r} \frac{\partial f_r}{\partial p_k} \frac{\partial I_j}{\partial f_s} \frac{\partial f_s}{\partial q_k} \right) \\ &= \sum_{r,s} \frac{\partial I_i}{\partial f_r} \frac{\partial I_j}{\partial f_s} \{f_r, f_s\} \\ &= 0, \end{aligned}$$

and in particular  $\{I_k, H\} = 0$ . The torus  $M_f$  may also be represented in terms of the action variables, as

$$I_1 = \tilde{c}_1, \quad \dots, \quad I_n = \tilde{c}_n,$$

for some new constants  $\tilde{c}_1, \dots, \tilde{c}_n$ .

Now, we can begin to construct the angle coordinates  $\phi_k$ , which we take canonically conjugate to the action coordinates. We do this by means of a generating function:

$$\begin{aligned} \phi_i &= \frac{\partial S(I, q)}{\partial I_i}, \quad p_i = \frac{\partial S(I, q)}{\partial q_i}, \\ S(I, q) &= \int_{q_0}^q \sum_j p_j dq_j. \end{aligned} \quad (\text{A.3})$$

Note that this definition is path-independent because of (A.1) and Stokes' theorem. The angle coordinates are periodic with period  $2\pi$  – considering two paths  $C$  and  $C_k$  (the  $k$ -th cycle), it follows that

$$S(q, I) = \int_{C \cup C_k} \sum_j p_j dq_j = \int_C \sum_j p_j dq_j + \int_{C_k} \sum_j p_j dq_j = S(q, I) + 2\pi I_k,$$

---

<sup>45</sup>For general deformations of  $\Gamma_k$ , the invariance follows from the Poincaré-Cartain theorem.

implying

$$\phi_k = \frac{\partial S}{\partial I_k} = \phi_k + 2\pi.$$

The transformations  $q = q(\phi, I)$ ,  $p = p(\phi, I)$  and  $\phi = \phi(q, p)$ ,  $I = I(q, p)$ , being defined by a generating function, are canonical, and they are also invertible. Thus,

$$\{I_j, I_k\} = 0, \quad \{\phi_j, \phi_k\} = 0, \quad \{\phi_j, I_k\} = \delta_{jk},$$

and the dynamics evolve according to

$$\dot{\phi}_k = \{\phi_k, \tilde{H}\}, \quad \dot{I}_k = \{I_k, \tilde{H}\},$$

where  $\tilde{H}(\phi, I) = H(q(\phi, I), p(\phi, I))$ . Since the  $I_k$ 's are first integrals,  $\dot{I}_k = -\partial\tilde{H}/\partial\phi_k = 0$ , so  $\tilde{H} = \tilde{H}(I)$  and therefore  $\dot{\phi}_k = \partial\tilde{H}/\partial I_k = \omega_k(I)$ . Integrating these canonical equations of motion yields

$$\phi_k(t) = \omega_k(I)t + \phi_k(0), \quad I_k(t) = I_k(0). \quad (\text{A.4})$$

Clearly, the solutions eq. (A.4) describes motion on the  $n$ -torus: the angle coordinate  $\phi_k$  grows linearly with time (modulo  $2\pi$ ) while the action coordinate  $I_k$  (the radius of the torus) remains constant. So we have motion that wraps around a toroidal circle at constant angular velocity  $\omega_k$ .  $\square$

If the  $\omega_k$  are incommensurate, the flow never returns to the same point: the trajectory is quasi-periodic (densely filling the torus).

Actually finding action-angle variables for a given integrable system proceeds by means of the **Hamilton-Jacobi equation**:

$$H\left(\frac{\partial S(I, q)}{\partial q}, q\right) = \bar{H}(I). \quad (\text{A.5})$$

An insightful example where the action-angle coordinates for a one-degree-of-freedom Hamiltonian are constructed explicitly can be found in Section 7.1.4 of Ott [92].

## B. Mathematical background

We give some very basic background on the Lebesgue measure and Lagrange polynomials.

### B.1. The Lebesgue measure and measure space

We introduce the notion of a  $\sigma$ -algebra, a measure(able) space and the Lebesgue measure.

Let  $X$  be a set and  $P(X)$  its power set (the set of all subsets of  $X$ , including  $X$  and  $\emptyset$ ). A subset  $\Sigma \subseteq P(X)$  is called a  **$\sigma$ -algebra** on  $X$  if and only if

1.  $X \in \Sigma$ ;
2.  $\Sigma$  is *closed under complementation*: if some set  $A$  is in  $\Sigma$ , then so is its complement  $X \setminus A$ ;
3.  $\Sigma$  is *closed under countable unions*: if  $A_1, A_2, \dots$  are in  $\Sigma$ , then so is  $A = A_1 \cup A_2 \cup \dots$ .

Elements of the  $\sigma$ -algebra are called *measurable sets*, and an ordered pair  $(X, \Sigma)$ , where  $X$  is a set and  $\Sigma$  is a  $\sigma$ -algebra over  $X$ , is called a *measurable space*.

Let  $X$  be a set and  $\Sigma$  a  $\sigma$ -algebra over  $X$ . A set function  $\mu$  from  $\Sigma$  to the extended real number line ( $\mathbb{R}$  together with  $\pm\infty$ ) is called a **measure** on  $(X, \Sigma)$  if the following conditions hold:

1. *non-negativity*: for all  $E \in \Sigma$ ,  $\mu(E) \geq 0$ ;
2.  $\mu(\emptyset) = 0$ ;
3. *countable additivity ( $\sigma$ -additivity)*: for all countable collections  $\{E_k\}_{k=1}^\infty$  of pairwise disjoint sets in  $\Sigma$ ,  
$$\mu\left(\bigcup_{k=1}^\infty E_k\right) = \sum_{k=1}^\infty \mu(E_k).$$

Condition 1 and 2 are rather intuitive. The third condition ties into the idea of monotonicity: the measure of a set is the sum of the measures of its subsets. A *measure space* is defined as the triple  $(X, \Sigma, \mu)$ , i.e. a measure space is a measurable space together with a measure on it.

The **Lebesgue measure** is the standard way of assigning a measure to subsets of  $\mathbb{R}^n$ . For simple geometric objects like intervals ( $\subset \mathbb{R}$ ), rectangles ( $\subset \mathbb{R}^2$ ) or boxes ( $\subset \mathbb{R}^3$ ), it coincides with the usual notion of length, area or volume. For a general set  $S \subset \mathbb{R}^n$ , the Lebesgue measure is defined as the infimum of the sum of boxes that cover  $S$ . More formally, let  $\text{Vol}(C) = \ell(I_1) \times \dots \times \ell(I_n)$  denote the volume of any rectangular cuboid  $C = I_1 \times \dots \times I_n$ , where  $I_i = (a_i, b_i)$ ,  $i = 1, \dots, n$  are open intervals and  $\ell(I_i) = b_i - a_i$  are their lengths. For any subset  $E \subseteq \mathbb{R}^n$ , the Lebesgue (outer) measure is given by

$$\lambda^*(E) = \inf \left\{ \sum_{k=1}^\infty \text{Vol}(C_k) : (C_k)_{k \in \mathbb{N}} \text{ is a sequence of products of open intervals with } E \subset \bigcup_{k=1}^\infty C_k \right\}.$$

### B.2. Lagrange polynomials

A **Lagrange (interpolating) polynomial**  $L(x)$  is the unique polynomial of lowest degree that interpolates a given set of data consisting of *nodes*  $x_j$  and *values*  $y_j$ , denoted as coordinate pairs  $(x_j, y_j)$ , with  $0 \leq j \leq k$ . The Lagrange polynomial  $L(x)$  has degree  $\leq k$ , and takes on each value at the corresponding node:  $L(x_j) = y_j$ .

A Lagrange polynomial for a set of  $k + 1$  nodes  $\{x_0, x_1, \dots, x_k\}$  (all distinct,  $x_j \neq x_m$  for  $j \neq m$ ) through the corresponding values  $\{y_0, y_1, \dots, y_k\}$  is the linear combination

$$L(x) = \sum_{j=0}^k y_j \ell_j(x),$$

expressed in terms of the *Lagrange basis* for polynomials of degree  $\leq k$ ,  $\{\ell_0(x), \ell_1(x), \dots, \ell_k(x)\}$ . Each basis polynomial are defined by the product

$$\ell_j(x) = \prod_{0 \leq m \leq k, m \neq j} \frac{x - x_m}{x_j - x_m}.$$

Note that  $\ell_j(x_m) = \delta_{jm}$ . Some properties:

- Each basis polynomial has degree  $k$ , so the linear combination  $L(x)$  has degree  $\leq k$ .
- $L(x)$  interpolates the data, since  $L(x_m) = \sum_{j=0}^k y_j \ell_j(x_m) = \sum_{j=0}^k y_j \delta_{mj} = y_m$ .
- The interpolating polynomial is unique. This is readily proved if we assume the existence of another polynomial of degree  $\leq k$ , say  $M(x)$ , which also interpolates the data. Then  $M(x) - L(x)$  is zero at the  $k+1$  distinct nodes  $\{x_0, x_1, \dots, x_k\}$ . But since the only polynomial with more than  $k$  roots is the constant zero function, this must mean that  $M(x) - L(x) = 0$ , or  $M(x) = L(x)$ .

Note: The barycentric form

We can always decompose the  $\ell_j(x)$  in the following manner:

$$\ell_j(x) = \ell(x) \frac{w_j}{x - x_j},$$

where  $\ell(x) = \prod_m (x - x_m)$  is shared by every basis polynomial,  $w_j = \prod_{m \neq j} (x_j - x_m)^{-1}$  is a node-specific constant (the *barycentric weight*) and the remaining factor represents the displacement from  $x_j$  to  $x$ . The Lagrange polynomial can then be written in so-called *first barycentric form*<sup>a</sup> as

$$L(x) = \ell(x) \sum_{j=0}^k \frac{w_j}{x - x_j} y_j.$$

If the weights  $w_j$  are pre-computed, finding  $L(x)$  in this way requires  $\mathcal{O}(k)$  operations instead of the  $\mathcal{O}(k^2)$  operations that have to be performed to evaluate each Lagrange basis polynomial  $\ell_j(x)$  individually.

---

<sup>a</sup>'barycenter' means center of mass.

## C. The Yang-Baxter equation

We state some properties of the Yang-Baxter equation and briefly discuss its connection to factorized scattering, the Lieb-Liniger model and braid groups. The introduction to properties of the YBE is based on Chapter 3 of Chowdhury and Choudhury [25]. The effort to explain the connection between the YBE, factorized scattering and the braid group were inspired by the online blog post [52]. The connection between factorized scattering and the Lieb-Liniger model on the level of the  $S$ -matrix follows Zamolodchikov [128] and [25]. We finish with some comments on the algebra generated by the Yang-Baxter equation, with Sträter [113] as the main source.

### C.1. Basic properties

Recall that the YBE is a matrix equation defined in  $V_1 \otimes V_2 \otimes V_3$  (the tensor product of three complex vector spaces). Keeping with notation from [25], we write the YBE in additive form as follows:

$$\boxed{R^{V_1 V_2}(u-v)R^{V_1 V_3}(u)R^{V_2 V_3}(v) = R^{V_2 V_3}(v)R^{V_1 V_3}(u)R^{V_1 V_2}(u-v)}, \quad (\text{C.1})$$

where the superscripts denote the two spaces of the direct product on which  $R$  acts, while in the remaining space it acts as  $\mathbb{1}$ . The additive formulation of the YBE differs from the multiplicative formulation eq. (82) in terms of the placement of the spectral parameters. The multiplicative form is more general, while the additive form implies a form of translational symmetry in the spectral parameters, but this will not matter for the properties we state below.

A convenient basis is the *Chevalley basis*  $e_{ij}$ : matrices with 1 on the intersection of row  $i$  and column  $j$ , and 0 everywhere else,

$$e_{ij}e_{kl} = \delta_{jk}e_{il}.$$

In this basis, the  $R$ -matrices are expressed as follows:

$$\begin{aligned} R^{V_1 V_2}(u) &= [R^{V_1 V_2}(u)]_{kl}^{ij} e_{ij}^{V_1} \otimes e_{kl}^{V_2} \otimes \mathbb{1}, \\ R^{V_1 V_3}(v) &= [R^{V_1 V_3}(v)]_{rs}^{pq} e_{pq}^{V_1} \otimes \mathbb{1} \otimes e_{rs}^{V_3}, \\ R^{V_2 V_3}(w) &= [R^{V_2 V_3}(w)]_{cd}^{ab} \mathbb{1} \otimes e_{ab}^{V_2} \otimes e_{cd}^{V_3}. \end{aligned}$$

Then the YBE, in terms of elements, is

$$\sum_{\alpha, \beta, \gamma} [R^{V_1 V_2}(u-v)]_{c\beta}^{a\alpha} [R^{V_1 V_3}(u)]_{e\gamma}^{\alpha b} [R^{V_2 V_3}(v)]_{\gamma f}^{\beta d} = \sum_{\alpha, \beta, \gamma} [R^{V_2 V_3}(v)]_{e\beta}^{c\alpha} [R^{V_1 V_3}(u)]_{\beta f}^{\alpha \gamma} [R^{V_1 V_2}(u-v)]_{\alpha d}^{\gamma b}.$$

Let us assume that the  $V_i$ 's ( $i = 1, 2, 3$ ) are identical vector spaces of dimension  $N$ .

A solution of the YBE is called a *Yang-Baxter sheaf*; it may depend on additional parameters (besides the spectral parameter), which we call *connection constants*. Here (for simplicity), we will consider  $R$  to be a function of a single connection constant  $\eta$ .

We proceed to state some basic definitions in the literature.

**Definition C.1** A *YB-sheaf*  $R(u, \eta)$  is

1. regular if  $R(u=0, \eta) = \mathcal{P}$ , the permutation operator ( $\mathcal{P}_{kl}^{ij} = \delta_{il}\delta_{jk}$ ).
2. quasi-classical if  $\exists \eta = \eta_c$  such that  $R(u, \eta_c) = \mathbb{1}$ , the identity operator in  $V \otimes V$ .

Furthermore, if in  $V$  the representation  $T(g)$  of some group  $G$  acts, then one says that the sheaf  $R(u)$  is invariant with respect to  $T(g)$ , if for any  $g \in G$  it holds that  $R(u)(T(g) \otimes T(g)) = (T(g) \otimes T(g))R(u)$ .

Without proof, we also state the following symmetry transformations:

**Lemma C.1** *The following symmetry transformations for the YBE exist:*

1. *If  $R(u)$  is a solution, then so is  $R'(u) = f(u)R(u)$ , with  $f(u)$  an arbitrary scalar function. It is said that the sheafs  $R(u), R'(u)$  are homothetic.*
2. *If  $T$  is some nondegenerate operator in  $V$ , then the sheaf  $R'(u) = (T \otimes T)R(u)(T \otimes T)^{-1}$  is a solution as well. One says that  $R'(u), R(u)$  are equivalent.*

Finally, we define two operations:

**Definition C.2** *Let  $R^{(1)}(u), R^{(2)}(u)$  be two solutions of the YBE of dimension  $N_1, N_2$  respectively. The tensor product of sheaves is the sheaf  $(R^{(1)} \otimes R^{(2)})(u) = R^{(1)}(u) \otimes R^{(2)}(u)$  of dimension  $N_1 \times N_2$ , defined by*

$$(R^{(1)} \otimes R^{(2)})(u) = R^{(1)}(u) \otimes R^{(2)}(u).$$

**Definition C.3** *The direct sum of sheaves is the sheaf  $(R^{(1)} \oplus R^{(2)})(u)$  of dimension  $N_1 + N_2$ , which is defined by its action on the basis vectors  $e_\alpha \otimes e_\beta$ . Let  $e_\alpha \otimes e_\beta$  denote basis vectors such that*

$$R(u)(e_\gamma \otimes e_\delta) = (e_\alpha \otimes e_\beta) R_{\gamma\delta}^{\alpha\beta}(u).$$

*The operator  $(R^{(1)}(u) \oplus R^{(2)}(u))$  acts on basis vectors of the form*

$$e_{\alpha_i}^{(i)} \otimes e_{\alpha_k}^{(k)} \quad (i, k = 1, 2; \alpha_i = 1, 2, \dots, N_i; e_{\alpha_i}^{(i)} \in V_i)$$

*of the space  $(V_1 + V_2) \otimes (V_1 + V_2)$  by*

$$\begin{aligned} (R^{(1)}(u) \oplus R^{(2)}(u) + R^{(2)}(u))(e_{\alpha_1}^{(1)} \otimes e_{\beta_1}^{(1)}) &= R^{(1)}(u)(e_{\alpha_1}^{(1)} \otimes e_{\beta_1}^{(1)}), \\ (R^{(1)}(u) \oplus R^{(2)}(u) + R^{(2)}(u))(e_{\alpha_1}^{(1)} \otimes e_{\beta_2}^{(2)}) &= (e_{\alpha_1}^{(1)} \otimes e_{\beta_2}^{(2)}), \\ (R^{(1)}(u) \oplus R^{(2)}(u) + R^{(2)}(u))(e_{\alpha_2}^{(2)} \otimes e_{\beta_1}^{(1)}) &= (e_{\alpha_2}^{(2)} \otimes e_{\beta_1}^{(1)}), \\ (R^{(1)}(u) \oplus R^{(2)}(u) + R^{(2)}(u))(e_{\alpha_2}^{(2)} \otimes e_{\beta_2}^{(2)}) &= R^{(2)}(u)(e_{\alpha_2}^{(2)} \otimes e_{\beta_2}^{(2)}). \end{aligned}$$

Both the tensor product and the direct sum of sheaves can be shown to satisfy the Yang-Baxter eq. (C.1). The tensor product of sheaves preserves regularity, while the direct sum preserves only quasi-classicalism. Note also that the direct sum of two sheaves is never a regular sheaf.

## C.2. YBE, factorized scattering and the braid group

The arguments presented here take a good deal of inspiration from the blog post [52] which I found very enlightening, and are informal on purpose. For a rigorous treatment, please refer to one of many available lecture notes or textbooks on the topic, such as Poulain d'Andecy [96].

In integrable systems where a scattering interpretation applies, a key characteristic is the ability to factorize scattering processes in terms of two-particle scattering events. The YBE makes this property palpable by breaking down a three-particle scattering event in terms of two-particle scattering events (the factorization of an  $N$ -particle scattering event follows from repeated application of three-particle factorization). It is a consistency equation for the factorized scattering of three particles.

There are exactly three ways in which three particles can scatter, see Figure 23. If we denote by  $(ijk)$  a scattering event between particles  $i, j$  and  $k$ , the three ways are:

$$(12) \rightarrow (13) \rightarrow (23), \quad (123), \quad (23) \rightarrow (13) \rightarrow (12), \quad (\text{C.2})$$

i.e. one scenario in which all three particles scatter simultaneously and two scenarios in which the three-particle scattering is decomposed into a sequence of two-particle scattering events, see Figure 23. The YBE imposes that the two decompositions be equal.

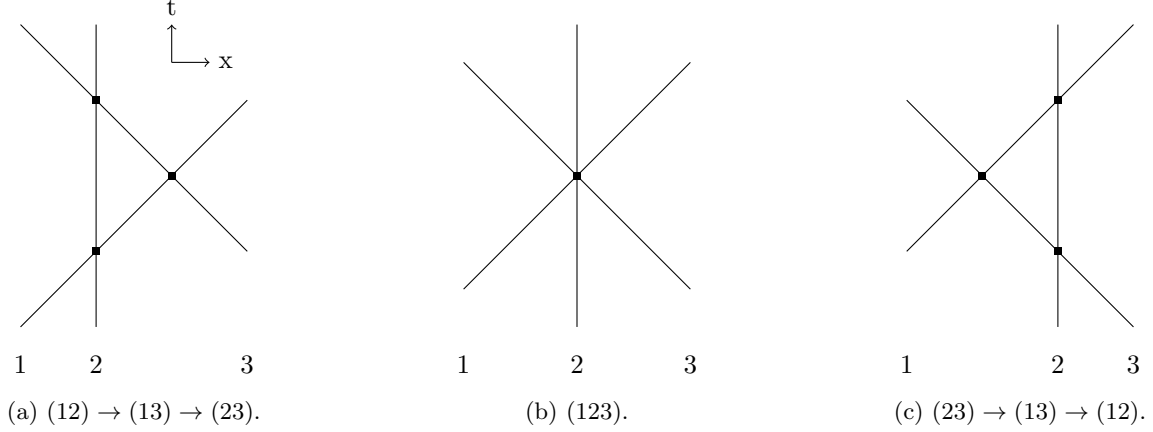


Figure 23: Possible three-particle scattering scenarios. Either all three particles scatter in one vertex, as in (b), or the three-particle scattering can be factorized into a sequence of two-particle scattering events, as in (a) and (c). The YBE imposes equivalency between the scattering scenarios  $(12) \rightarrow (13) \rightarrow (23)$  (left-hand side) and  $(23) \rightarrow (13) \rightarrow (12)$  (right-hand side).

Let us make this a little bit more formal. Imagine a bunch of particles on a line, each with a state that can be any element of a set  $X$ . We set out the following rules:

1. The only way particles can change their state is by interacting with each other.
2. An interaction occurs when two particles pass by each other,
3. Particles can interact only two at a time, and when they do, they swap positions and their state changes according to a function  $F : X \times X \rightarrow X \times X$ . Specifically, if two particles 1 and 2 (the labels) are in state  $x$  and  $y$  respectively, then their states after interacting will be

$$\begin{aligned} F(x, y) &= (F_a(x, y), F_b(x, y)) \\ &= (\text{new state of particle 1, new state of particle 2}), \end{aligned}$$

where  $F_a, F_b : X \times X \rightarrow X$ .

Now, imagine that we have three particles on our line. To keep an account of the whole system, we need an element of  $X \times X \times X$  to keep track of the states and a permutation  $\sigma \in S_3$  (the symmetric group of three elements) to keep track of the positions. For example, the configuration

$$\begin{array}{ccc} 1 & 3 & 2 \\ \bullet & \bullet & \bullet \\ x & z & y \end{array}$$

can be described by the states  $(x, y, z) \in X^3$  and the permutation  $132 \in S_3$  for the positions. To register how the states of the particles change over time we introduce three functions from  $X \times X \times X \rightarrow X \times X \times X$ , which we call  $F_{12}$ ,  $F_{13}$  and  $F_{23}$ . The function  $F_{ij}$  describes how the states of the particles changes when particle  $i$  and  $j$  interact, and is given by applying  $F$  to the  $i, j$  coordinates of  $(x, y, z)$  and acting as the identity on the remaining coordinates:

$$\begin{aligned} F_{12}(x, y, z) &= (F(x, y), z) = (F_a(x, y), F_b(x, y), z), \\ F_{13}(x, y, z) &= (F_a(x, z), y, F_b(x, z)), \\ F_{23}(x, y, z) &= (x, F(y, z)) = (x, F_a(y, z), F_b(y, z)). \end{aligned}$$

Now suppose that the particles begin in position 123 and states  $(x, y, z)$ . By the rules of our own making (rule #2), we cannot directly interact particles 1 and 3, since they are separated by particle 2. However,

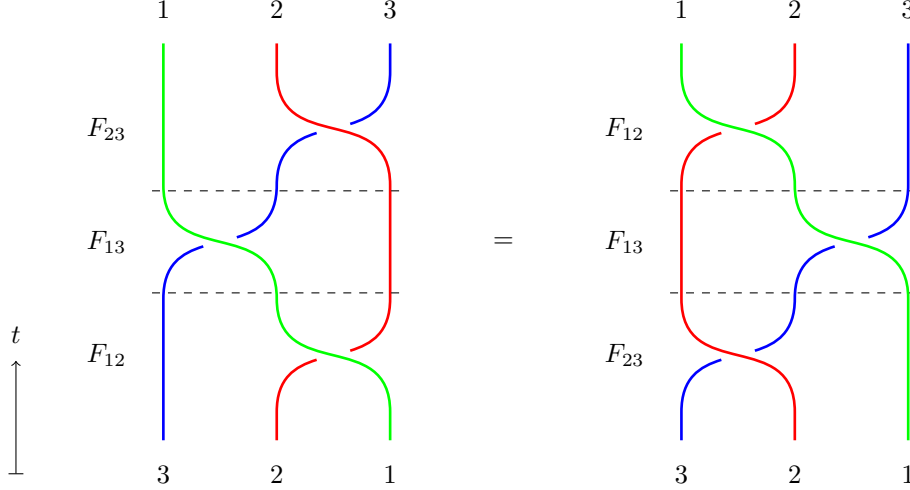


Figure 24: The YBE as a braiding relation. Graphic generated with elements of the [braids](#) package.

there are two ways in which we can pass through particle 2 to make particles 1 and 3 interact:

$$\begin{aligned}
 \text{first way : } & (x, y, z) \mapsto F_{23}^{123}(x, y, z) \mapsto F_{23}^{312}(F_{13}^{132}(x, y, z)) \mapsto F_{12}^{321}(F_{13}^{321}(F_{23}^{123}(x, y, z))), \\
 \text{second way : } & (x, y, z) \mapsto F_{12}^{123}(x, y, z) \mapsto F_{13}^{213}(F_{12}^{213}(x, y, z)) \mapsto F_{23}^{312}(F_{13}^{321}(F_{12}^{123}(x, y, z))),
 \end{aligned} \tag{C.3}$$

where the superscripts denote the positions of the particles.

But of course, at the end of the day (no matter if we used the first or the second way to move the particles around), we can demand that the final outcome is the same! The YBE is the formal way of implementing this: we define a solution to the YBE as a function  $F : X \times X \times X \rightarrow X \times X$  that satisfies

$$F_{12} \circ F_{13} \circ F_{23} = F_{23} \circ F_{13} \circ F_{12}.$$

Some example solutions to the YBE are:

- The identity map  $\mathbf{1} : X \times X \rightarrow X \times X$ .
- The swap map  $P : X \times X \rightarrow X \times X$ , given by  $P(x, y) = (y, x)$ .
- Let  $\rho$  be a permutation of  $X$ , then the map  $F(x, y) = (\rho(x), \rho^{-1}(y))$  is a solution and both sides are equal to the function  $(x, y, z) \mapsto (\rho^2(x), y, \rho^{-2}(z))$ .

Graphically, what we described in eq. (C.3) and what is the essence of the YBE is captured in Figure 24. In the depiction, we have given the scattering process the interpretation of a braiding relation: the particles are represented by braids (strings) that cross each other at various instants (the crossings represent interactions).

The *braid group*  $B_n$  on  $n$  strands has elements  $\{\sigma_1, \sigma_2, \dots, \sigma_{n-1}\}$  which represent elementary braid crossings between adjacent strands. They satisfy the relations:

- braid relation:  $\sigma_i \sigma_{i+1} \sigma_i = \sigma_{i+1} \sigma_i \sigma_{i+1}$ ;
- far commutativity:  $\sigma_i \sigma_j = \sigma_j \sigma_i$ , for  $|i - j| > 1$ .

The Yang-Baxter equation eq. (C.1) is equivalent to the braid relation if the R-matrix is interpreted as a braiding operator. In particular, if  $R : V \otimes V \rightarrow V \otimes V$  is a solution to the YBE, then it is possible to define a representation of the braid group  $B_n$  by assigning to each generator  $\sigma_i$  the R-matrix  $R$  acting on the  $i$ -th and  $(i + 1)$ -th spaces:

$$\sigma_i \mapsto R_{i, i+1}.$$



This gives a representation

$$B_n \rightarrow \text{End}(V^{\otimes n}).$$

### C.3. Lieb-Liniger as a limit of the factorizable, nonrelativistic $S$ -matrix with $Z_4$ -symmetry

It is insightful to see how factorized scattering plays out at the level of the  $S$ -matrix. Furthermore, using heuristic arguments, we can show that by imposing  $Z_4$ -symmetry on the  $S$ -matrix in the non-relativistic limit, the  $S$ -matrix of the Lieb-Liniger model is recovered with a suitable choice of parameters.

We study particles that have an internal state  $|A\rangle$  or  $|\bar{A}\rangle$  (particle-antiparticle pair or spin up-spin down), connected by an operator  $\hat{C}$  in the following way:

$$\hat{C}|A\rangle = \bar{A}, \quad \hat{C}|\bar{A}\rangle = |A\rangle.$$

A general  $\hat{Z}_N$  operator acts on these states as

$$\hat{Z}_N|A\rangle = e^{i\phi}|A\rangle, \quad \hat{Z}_N|\bar{A}\rangle = e^{-i\phi}|\bar{A}\rangle,$$

with  $\phi = 2\pi/N$ . For two-particle states, we choose the following basis:  $\{|AA\rangle, |\bar{A}\bar{A}\rangle, |A\bar{A}\rangle, |\bar{A}A\rangle\}$ . Now, the following constraints arise from invariance demands:

- Invariance under  $\hat{C}$ - and  $Z_N$ -symmetry:  $[\hat{C}, \hat{S}] = 0$  and  $[\hat{Z}_N, \hat{S}] = 0$ ;
- $\hat{C}$ -invariance:  $S_{ij} = S_{ji}$ ,  $i, j = 1, 2, 3, 4$ ;
- $Z_N$ -invariance:  $\langle A\bar{A}|\hat{S}|AA\rangle \sin \phi = 0$ ,  $\langle \bar{A}A|\hat{S}|AA\rangle \sin \phi = 0$ ,  $\langle \bar{A}\bar{A}|\hat{S}|AA\rangle \sin 2\phi = 0$ .

From these restrictions, the 2-body  $S$ -matrix with  $Z_4$ -symmetry is restricted to the form:

$$\hat{S}^{(2)}(\theta) = \begin{pmatrix} S & S_a & 0 & 0 \\ S_a & S & 0 & 0 \\ 0 & 0 & S_r & S_t \\ 0 & 0 & S_t & S_r \end{pmatrix}$$

Unitarity  $\hat{S}^{(2)}(\theta)\hat{S}^{(2)}(-\theta) = \mathbb{1}$  gives rise to the following equations:

$$S(\theta)S(-\theta) + S_a(\theta)S_a(-\theta) = 1, \quad (\text{C.4a})$$

$$S(\theta)S_a(-\theta) + S_a(\theta)S(-\theta) = 0, \quad (\text{C.4b})$$

$$S_r(\theta)S_r(-\theta) + S_t(\theta)S_t(-\theta) = 1, \quad (\text{C.4c})$$

$$S_r(\theta)S_t(-\theta) + S_t(\theta)S_r(-\theta) = 0. \quad (\text{C.4d})$$

For systems with an infinite number of integrals of motion, we furthermore have the factorization equation

$$\hat{S}^{(3)}((1)23, \theta_{23})\hat{S}^{(3)}(13(2), \theta_{13})\hat{S}^{(3)}((3)12, \theta_{12}) = \hat{S}^{(3)}(12(3), \theta_{12})\hat{S}^{(3)}((2)13, \theta_{13})\hat{S}^{(3)}(23(1), \theta_{23}), \quad (\text{C.5})$$

with  $\theta_{ij} = \theta_i - \theta_j$  and

$$\hat{S}^{(3)}(ij(k), \theta) = \begin{pmatrix} \tilde{S}^{(3)}(ij(k), \theta) & 0 \\ 0 & \tilde{S}^{(3)}(ij(k), \theta) \end{pmatrix}, \quad \hat{S}^{(3)}(k(ij), \theta) = \begin{pmatrix} \tilde{S}^{(3)}((k)ij, \theta) & 0 \\ 0 & \tilde{S}^{(3)}((k)ij, \theta) \end{pmatrix},$$

$$\tilde{S}^{(3)}(ij(k); \theta) = \begin{pmatrix} S & 0 & 0 & S_a \\ 0 & S_r & S_t & 0 \\ 0 & S_t & S_r & 0 \\ S_a & 0 & 0 & S \end{pmatrix}, \quad \tilde{S}^{(3)}((k)ij; \theta) = \begin{pmatrix} S & S_a & 0 & 0 \\ S_a & S & 0 & 0 \\ 0 & 0 & S_r & S_t \\ 0 & 0 & S_t & S_r \end{pmatrix}.$$

The interpretation of  $\hat{S}^{(3)}(ij(k); \theta)$  is that of particles  $ij$  colliding, while  $k$  remains to the right of the collision, and vice versa for  $\hat{S}^{(3)}(k(ij); \theta)$ . Writing out the cubic identity eq. (C.5) yields another set of relations:

$$SS_aS_r + S_aS_tS_t = S_aSS + SS_rS_a, \quad (\text{C.6a})$$

$$SS_aS_t + S_aS_tS_r = S_rS_tS_a + S_tS_aS, \quad (\text{C.6b})$$

$$S_rSS_r + S_tS_rS_t = S_aSS_a + SS_rS, \quad (\text{C.6c})$$

$$S_rSS_t + S_tS_rS_r = S_rS_tS + S_tS_aS_a, \quad (\text{C.6d})$$

with arguments  $\theta_{12}$ ,  $\theta_{13}$  and  $\theta_{23}$  for the  $S$ -elements (in that order) left implicit. We can solve eq. (C.6) to get

$$S(\theta) = \frac{\text{sn}(\mu\theta + 2\xi, l)}{\text{sn}(2\xi, l)} S_r(\theta), \quad (\text{C.7a})$$

$$S_t(\theta) = -\frac{\text{sn}(\mu\theta, l)}{\text{sn}(2\xi, l)} S_r(\theta), \quad (\text{C.7b})$$

$$S_a(\theta) = -l\text{sn}(\mu\theta, l)\text{sn}(\mu\theta + 2\xi, l) S_r(\theta), \quad (\text{C.7c})$$

with  $l$  the modulus of Jacobi's elliptic function  $\text{sl}(x, l)$  and  $\mu, \xi$  arbitrary constants. We can use this result to solve for  $S_r$  from the unitarity relations (C.4), and find

$$S_r(\theta) = \exp \left[ 4 \sum_{n=1}^{\infty} \frac{\sin^2 \left[ \frac{\pi n(2\xi + ik')}{2k} \right] \sin \left[ \frac{\pi n\mu\theta}{2k} \right] \sin \left[ \frac{\pi n(2\xi + \mu\theta)}{2k} \right]}{n \sinh \left[ \frac{\pi nk'}{k} \right] \cos \left[ \frac{\pi n\xi}{k} \right]} \right],$$

which can then be used to compute the remaining  $S$ -matrix elements –  $S$ ,  $S_t$  and  $S_a$  – from eq. (C.7).

In the limit  $\mu \rightarrow 0$  and  $2\xi \rightarrow -\pi$  with  $(\mu + 2\xi)/\mu \equiv -2i\kappa/\hbar$  fixed, it can be shown that the  $S$ -matrix reduces to:

$$S(p) = \frac{\frac{p}{2m} - \frac{i\kappa}{\hbar}}{\frac{p}{2m} + \frac{i\kappa}{\hbar}},$$

where we have replaced the rapidity variable  $\theta$  by the velocity  $p/m$  because we are taking the non-relativistic limit. This is the result found by Lieb and Liniger [76]. Thus, we have motivated that the imposition of  $Z_4$ -symmetry on a non-relativistic theory of factorizable  $S$ -matrices leads to the  $\delta$ -function Bose gas in a certain limit.

For a more complete account and intermediate steps, see [128] and Section 3.3 of [25].

## C.4. Some facts about the Yang-Baxter algebra

On a physical Hilbert space, the Yang-Baxter algebra  $Y$  is represented by the operators  $A(u)$ ,  $B(u)$ ,  $C(u)$  and  $D(u)$  and their commutation relations. The relation of these operators to (local) physical operators is the concern of the so-called *quantum inverse problem*.

An important characteristic of the Yang-Baxter algebra is that it admits a coproduct  $\Delta : Y \rightarrow Y \otimes Y$  which turns it into a bialgebra (and a Hopf algebra). The coproduct is defined by

$$\Delta \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} (u) = \begin{pmatrix} T_{11} \otimes T_{11} + T_{12} \otimes T_{21} & T_{11} \otimes T_{12} + T_{12} \otimes T_{22} \\ T_{21} \otimes T_{11} + T_{22} \otimes T_{21} & T_{21} \otimes T_{12} + T_{22} \otimes T_{22} \end{pmatrix} (u).$$

The coproduct structure allows us to ‘glue’ together single-particle representations to obtain the Yang-Baxter algebra for a multiparticle system. Concretely, let  $\pi : Y \rightarrow \mathcal{H}^a$  be a representation of the Yang-Baxter algebra on a Hilbert space  $\mathcal{H}^a$  corresponding to a single particle (e.g. a single spin). The representation of the monodromy matrix at each site is usually denoted as a *Lax operator*  $L(u) = \pi(T(u))$  acting on  $\mathcal{A} \otimes \mathcal{H}^a$ . Now, let  $\pi_a$  and  $\pi_b$  be representations of  $Y$  on the Hilbert spaces  $\mathcal{H}^a$  and  $\mathcal{H}^b$ . Then we use the coproduct construction to build a representation  $\pi_{ab}$  of  $Y$  on  $\mathcal{H}^a \otimes \mathcal{H}^b$  as follows:

$$\pi_{ab}(T(u)) = (\pi_a \otimes \pi_b)(\Delta(T(u))) = L_a(u)L_b(u),$$

where the notation is understood to mean that  $L_a(u)$  and  $L_b(u)$  are multiplied in the usual matrix sense on  $\mathcal{A}$  while the components are tensor-multiplied, such that  $L_a(u)L_b(u)$  acts on  $\mathcal{A} \otimes \mathcal{H}^a \otimes \mathcal{H}^b$ . For an  $N$ -particle

system, the same construction yields

$$T(u) \equiv \pi_{a_1 a_2 \dots a_N}(T(u)) = \begin{pmatrix} A(u) & B(u) \\ C(u) & D(u) \end{pmatrix} = \prod_{i=1}^N L_i(u).$$

Note that we assigned the same symbol to the monodromy matrix and its representation, which is the common practice. The elements  $A(u)$ ,  $B(u)$ ,  $C(u)$  and  $D(u)$  act on the  $N$ -particle tensor space.

For a mathematical treatment of the Yang-Baxter algebra and its connection to so-called ‘quantum groups’, please consult Kassel [\[64\]](#).

## D. Further reading

I include a list of helpful sources to get started with the main topics of this thesis.

### Section 2: Further reading

- An introductory treatment of dynamical systems and chaos:  
S. H. Strogatz. *Nonlinear dynamics and chaos: with applications to physics, biology, chemistry, and engineering*. CRC press, 2018. DOI: <https://doi.org/10.1201/9780429492563>.
- A nice article commenting on the relation between chaos and integrability:  
A. D. Stone. “Einstein’s unknown insight and the problem of quantizing chaos”. In: *Physics Today* 58.8 (2005), pp. 37–43. DOI: <https://doi.org/10.1063/1.2062917>.
- Lecture notes on classical integrability theory:  
M. Dunajski. “Integrable systems”. In: *University of Cambridge Lecture Notes* (2012). URL: [https://www.damtp.cam.ac.uk/user/md327/ISlecture\\_notes\\_2012.pdf](https://www.damtp.cam.ac.uk/user/md327/ISlecture_notes_2012.pdf).
- Full paper on the improved definition of quantum integrability:  
J.-S. Caux and J. Mossel. “Remarks on the notion of quantum integrability”. In: *Journal of Statistical Mechanics: Theory and Experiment* 2011.02 (2011), P02023. DOI: [10.1088/1742-5468/2011/02/P02023](https://doi.org/10.1088/1742-5468/2011/02/P02023). URL: <https://iopscience.iop.org/article/10.1088/1742-5468/2011/02/P02023>.

### Section 3: Further reading

- A fairly rigorous (but slightly antiquated) introduction to the basics of the Lieb-Liniger model, at both zero and finite temperature:  
V. E. Korepin, N. M. Bogoliubov, and A. G. Izergin. *Quantum Inverse Scattering Method and Correlation Functions*. Cambridge Monographs on Mathematical Physics. Cambridge University Press, 1993. ISBN: 9780511628832. DOI: [10.1017/CB09780511628832](https://doi.org/10.1017/CB09780511628832).
- A more readable introduction:  
F. Franchini. *An Introduction to Integrable Techniques for One-Dimensional Quantum Systems*. Springer International Publishing, 2017. ISBN: 9783319484877. DOI: [10.1007/978-3-319-48487-7](https://doi.org/10.1007/978-3-319-48487-7). URL: <http://dx.doi.org/10.1007/978-3-319-48487-7>.
- A first introduction to the Lindblad master equation:  
D. Manzano. “A short introduction to the Lindblad master equation”. In: *AIP Advances* 10.2 (Feb. 2020), p. 025106. ISSN: 2158-3226. DOI: [10.1063/1.5115323](https://doi.org/10.1063/1.5115323). eprint: [https://pubs.aip.org/aip/adv/article-pdf/doi/10.1063/1.5115323/12881278/025106\\_1\\_online.pdf](https://pubs.aip.org/aip/adv/article-pdf/doi/10.1063/1.5115323/12881278/025106_1_online.pdf). URL: <https://doi.org/10.1063/1.5115323>.

### Section 4: Further reading

- An accessible first reading on ABA including historical context:  
Chapter 2 of C. Sträter. *Quantum Integrability and its Application to the Dicke Model*. Geschwister-Scholl-Platz 1, Munich, Germany, 2011.
- A detailed step-by-step introductory treatment of ABA:  
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