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Rigorous approach to quantum integrable models at finite temperature

Approche rigoureuse aux modèles intégrable quantique à température finie

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Résumé

Cette thèse développe un cadre rigoureux qui permet de démontrer des représentations exactes associées à divers observables de la chaîne XXZ de Heisenberg de spin-1/2 à température finie. On commence avec une description de la chaîne XXZ dans le Chapitre 2 de la thèse. Nous introduisons l'énergie libre par site dans la limite du volume infinie. L'existence de cette limite à était établie par Ruelle. Nous la reproduisons pour une chaîne de spin de taille L. Afin de pouvoir décrire la matrice de transfert quantique et les maniements associés, il est utile de rappeler la construction de la matrice de transfert de la chaîne XXZ de spin-1/2 dans le cadre de l'Ansatz de Bethe algébrique. La description de la matrice de transfert quantique nous permet donc d'expliquer comment l'énergie libre par site peut-être exprimer en terme sa plus grande valeur propre. La possibilité d'en faire autant repose sur des hypothèses telles que: l'existence d'une valeur propre réelle, non-dégénérée de module maximale et de l'échangeabilitée de la limite du volume infinie et du nombre de Trotter à l'infinie. Suite à cela, nous introduisons le cadre nécéssaire nous permettant d'établir de manière rigoureuse ces hypothèses. Cela nous permet de construire des opérateurs issues du développement de la matrice de transfert quantique à haute température. Les propriétés analytiques de ces opérateurs sont rigoureusement établies et constituent la base des analyses qui s'en suivent. Cela nous permet de fournir des estimations rigoureuses sur la valeur propre dominante ainsi que sur les valeurs propres sous-dominante de la matrice de transfert quantique. Nous donnons finalement une preuve rigoureuse de l'échangeabilitée de la limite du volume infinie et du nombre de Trotter à l'infinie.

Dans le Chapitre 3, nous nous focalisons sur le spectre de la matrice de transfert quantique décrite *via* les équations intégrales non-linéaires. Nous rappelons l'Ansatz de Bethe algébrique pour la matrice de transfert quantique. Cela nous permet de representer les valeurs propres de la matrice de transfert quantiques en terms des racines de Bethe et nous permet d'introduire le formalisme décrivant la fonction auxiliaire. Nous rappelons ensuite la characterisation de la fonction auxiliaire en terme des équations intégrales non-linéaires. Ce formalisme nous permet de prendre la limite de Trotter vers l'infinie directement aux niveau de l'equation intégrale non-linéaire. Dans le reste de ce chapitre, nous développons la théorie de solvabilité de cette classe d'équation intégrales non-linéaires admettent des solutions et que ces dernières sont uniques. Nous établissons aussi que la limite infinie du nombre de Trotter peut être rigoureusement prise au niveau des solutions de telles équations intégrales non-linéaires.

Dans le Chapitre 4 nous nous basons sur les deux chapitres précédent afin de construire des representations intégrales pour les quantités physiques associées, telles que l'énergie libre et les longueurs de corrélation. En particulier, nous derivons de manière rigoureuse la représentation intégrale de la valeur propre dominante. Ceci nous permet d'écrire un représentation intégrale de l'énergie libre par site. Dans ce même cadre nous écrivons la représentation intégrale pour une certaine classe de valeurs propre sous-dominante. Cela nous permet donc donner une représentation intégrale ces longueurs de correlation. Pour la classe spécifique d'états "excités" de la matrice de transfert quantiques que nous considérons, nous démontrons de façon rigoureuse que les racines trous convergent vers zero dans le regime de haute température et que les racines particules satisfont les équations de Bethe pour la chaîne XXZ de spin-1. Nous exprimons donc les longueurs de corrélation en terme de contributions dominante de ces racine particules et trous à haute température.

Chapter 1

Introduction

1.1 The early civilisations

The comprehension of the laws of nature is a journey spanning through the millennia and is the result of a combination of intellectual leaps that has greatly impacted civilizations. This journey, albeit a rather treacherous one in human history, is nonetheless very interesting. Ever since the earlier times the identification of regular occurrences, such as the phases of the moon and the seasons, have led humans of that period to develop a certain sense for understanding and classifying such patterns, thus strongly improving their chances of survival. However, even though the association between a particular series of events and a system of communications in order to keep track of such events can be noted, such activities were still very far from any kind of abstract reasoning. Hence before going any deeper within the literature related to the subject studied in this thesis we provide an account on the development of the understanding and manipulation of abstract ideas throughout the centuries. It was not only about 4000 years B.C that the Sumerian civilisation in Mesopotamia would introduce a more orderly way of dealing with information. This was due to the growing administrative requirements coupled with the distribution of plots of lands¹ as the civilisation settled. As from 2700 years B. C, trades among the regions surrounding the Mediterranean Sea intensified with the rise of the Egyptian Empire. They had developed a base 10 numerical system as well as a notation for fractions as a result of developing their framework for multiplications and divisions. However the concept of place values was absent making dealing with large numbers difficult. The Egyptians also acquired a rather sophisticated understanding of dealing with geometrical problems concretely. A more efficient way of calculation would emerge from the Babylonian civilization who flourished from 2000 B.C to about 575 B.C. They would introduce description of large numbers and had a rather efficient counting system relying on a base 60. This efficiency is reflected in the fact that till today the sexagesimal base is implemented in our analogue clocks. Such developments arising from the settlements of the Mesopotamian and Egyptian civilisations constituted an *impetus* for the progress of mathematics. This knowledge of mathematics would soon be adopted by the Greeks who would begin to incorporate higher levels of abstract thinking to problems of geometry in particular. One of the first to do so was Thales who established the famous theorem, after whom it is named and much more. The works of geometers, that would follow, such as Pythagoras, immensely influenced the world of mathematics and, in part, contributed into forming the basis of Euclid's Elements. Aside to the advanced problems in geometry discussed by the Greeks, they also applied their mathematical studies to more concrete problems. These include, Archimedes' famous experiments on the measurement of the volume of irregular objects as well as his contributions to calculating the area or volume of an object by repeated computations, an early example of iterations. However, aside to the many foundational contributions to science, it is important to note that the Greeks were also the first to instil the notion of proofs. This reinforced the deductive approach allowing one to prove or disprove a given claim by relying on axioms.

¹The concept of a number multiplied by itself can also be traced to Sumerian and Babylonians civilisations as a result of measuring the plots of land needed for agriculture.

This axiomatic approach evolved throughout the centuries to become the guiding principle for rigorously establishing results in modern mathematics. From the 9th to the 15th centuries, the Middle Eastern school would gather and translate the earlier works of the Greeks, Indians and Chinese and build on those to develop powerful geometric techniques of resolution of algebraic equations of degree two, hence revolutionising the world of mathematics. This was the point where distinct fields of geometry and algebra, such as trigonometry and number theory, for example were being established. The Persian mathematician (or philosopher at the time), Al-Khwarizmi was the first to recognise the importance of implementing the Hindu numerical system, *viz.* use of numbers ranging from 1 to 9 and the 0, what greatly enhanced the efficiency of the counting system. Towards the end of the 15th century, the translations into Latin helped transferring the Greek-Islamic body of work in mathematics (and other fields of science such as medicine and optics for example) back to Europe. By the end of the 16th century, François Viète wrote the first manuscript [171] providing a consistent and coherent description of an algebraic equation in the modern sense. At this time, mathematics has been very much implemented in everyday life while the tools developed by the earlier civilisations have been largely revisited and refined.

Galileo's experiments, which build on such mathematical constructions, concerned the motion of moving bodies. His formulations and descriptions of the natural world via experiments would later become the basis for classical physics. Galileo's interests, just like his predecessors of the earlier centuries, were drawn to the intricacies of the night sky. Guided by Copernicus' heliocentric paradigm, he carried out a number of planetary observations and produced interesting observations. It was not long before his influence reached Kepler who was also studying the motion of planets. During the beginning of the 17th century, Tycho-Brahé and his assistant Kepler collected an important amount of information on the movement of planets. This allowed Kepler to formulate his three famous laws of planetary motion [79, 80, 81]. However, there was still no apparent theoretical explanation supporting Kepler's claims. It was not until towards the mid-17th century that light was shed on Kepler's observations through the *corpus* of Newton [136], the *Principia* -a body of work spanning three volumes-. The first two books of the *Principia* established the fundamental concepts of classical dynamics on the basis of first principle considerations. Newton was able to describe the motion of celestial bodies within his formalism and established the claims made by Kepler. Newton's approach to solve an associated system of equations of motion led to the development of the theory of infinitesimal changes which is referred today as differential calculus^{2,3}. This was an extremely effective way of dealing with the prevailing equations of motion in the *Principia*. Newton's achievements constituted an important foundation of the body of works emerging from Lagrange [116, 117] and shortly after, Hamilton [63], which contributed to the understanding of many-body systems.

1.2 Motivations from many-body systems

Towards the end of the eighteenth century, the equations governing the motion of two bodies interacting through a r^{-1} potential, a problem initially treated by Newton, were very well understood to admit an exact solution. Newton's equations for that problem actually correspond to the first system that one can identify as *explicitly solvable by integration*. However, it was soon realised [63, 116, 117] that it was not possible to obtain explicit solutions to the dynamics describing the motion of three or more bodies subject to r^{-1} two-body interactions. In his two important volumes of "*mécanique analytique*", Lagrange established the theory of static and dynamic systems and in doing so first provided a way to deal efficiently with differential equations governing the motion of many-body systems. In particular, his approach allowed one to find explicit solutions to certain instances of such equations. Lagrange's works⁴ were complemented, independently, by the contributions of Hamilton [63],

²It is important to point out that Leibniz [122] was also contributing, independently, around the same period, to the theory of infinitesimal changes.

³It is also important to note that in her translation of the *Principia* in French, Emilie du Châtelet derived Newton's results using differential calculus [25]. In the *Principia* Newton's approach is essentially geometrical.

⁴We point the interested reader to Note VI of "*mécanique analytique*, tome 1" of the eleventh volume of Lagrange collected works for a detailed exposition of the Hamilton-Jacobi equation and of the construction of the Poisson brackets. [116]

Liouville⁵ [131, 132] and Jacobi [73]. The works cited are important in the sense that they shaped an essential part of classical integrability by offering a way to solve complicated problems via the technique known as separation of variables as we will see in the later parts of this section and in the remaining of chapter. Now, for a brief moment we will focus our attention on the foundational work of Hamilton and Jacobi. For an extensive review we refer to a paper by Kozlov [104]. The problem of solving classical many-body systems by building on Newton's theory as established in the *Principia* had already been discussed by people like Bernouilli, d'Alembert, Euler and Lagrange. However, at the time, the understanding of solvability was not relying on the so-called *canonical variables* approach. This concept was introduced by Hamilton in 1834 [63] and independently by Jacobi three years later [73]. Their idea is to canonically reexpress the equations of classical mechanics for a given n-dimensional system, viz. the Euler-Lagrange equations issuing from a variational principle, into a system relative to a new set of variables in such a way that the latter could be directly integrated. Hamilton and Jacobi essentially found a way to effectively compute *n*-independent integrals of motions of a certain specific *n*-dimensional system. Shortly after Bour [19] and Liouville [132] managed to construct and show that the Poisson bracket of these *n*-independent integrals of motions are zero. All of this resulted in the setting up of a technique which -if applicable- allowed one to solve an *n*-dimensional problem by considering *n*-problems in one dimension which is the essence of the separation of variables. As a result of this, classical systems admitting independent integrals of motion which satisfy the conservation properties in the sense of Lagrange, Hamilton, Liouville and Jacobi are classified as *integrable systems*. Studying and solving classical systems belonging to this class would become a prime interest in the years that followed.

Following the approach developed by Hamilton and Jacobi, the separation of variables method was becoming more apparent in the analysis of Hamiltonian mechanics especially Delauney's *action-angle variable* method in 1860 [29]. This approach was found to be particularly suited for studying perturbations related to motion of celestial bodies. It was found to be also useful in the early instances of the development of quantum mechanics at the beginning of the twentieth century, namely for the Bohr-Sommerfeld quantisation. The separation of variables is a very effective approach to solve explicitly the dynamics of a system when the separate variables are known⁶. In the wake of discussing the integrals of motion in physical systems and for the sake of completeness, we extend the discussion to a continuous model of non-linear wave theory, namely the Korteweg and de Vries equation [103]. The early observations related to the model can be found in [20] and [143]. What is interesting with this model is that it admits solutions which signal the existence of an infinite number of conserved quantities. This would be formally studied in Gardner, Green, Kruskal and Miura [52] and independently by Lax [121] and later rigorously established in [54, 184, 185, 133]. The methods initially developed for solving partial differential equations describing many-body systems turn out to be extremely versatile and apply to many different fields of theoretical physics.

So far, we have only discussed classical systems. Yet, the early twentieth century, gave birth to a new paradigm in physics: *quantum mechanics*. Naturally, integrability also appeared in that setting. However, before discussing some of the aspects of integrability in quantum many-body systems, -in particular those at finite temperature-, it is interesting to recall the initial motivations for constructing such systems. These emerge from the early phenomenological approaches in classical statistical mechanics aiming at understanding magnetisation and phase transitions.

⁵Liouville was the first to produce a rigorous exposition on the integrals of motion of a system through an explicit example.

 $^{^{6}}$ It must be pointed out that the construction of such separate variables simply through the information about the complete set of independent conserved quantities in involution (with respect to the Poisson brackets) at the level of the Liouville-Arnold theorem [3] of classical integrability is not enough. Indeed, this needs to incorporate additional structures of algebraic nature, particularly a Lax matrix, its associated *r*-matrix and the Yang-Baxter algebra satisfied by the latter [5, 150].

1.2.1 Exact solvability in statistical mechanics

In the early 1900's, magnetism was one of the phenomena that could not be explained, in particular due to the lack of a clear mechanism that would lead to the emergence of the spontaneous magnetisation⁷ occurring at a low enough temperatures. It took almost two decades before the first realistic model of magnetism appeared, an achievement due to Lenz [123]. He was trying to explain the effect of ferromagnetism by proposing a lattice model consisting of atoms interacting *via* their discrete magnetic moments $\sigma_i = \{-1, +1\}$, where the interactions extends only to nearest neighbours. The Hamiltonian describing such interactions is

$$\mathbf{H} = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \tag{1.2.1}$$

where $\langle i, j \rangle$ indicates a summation over all nearest neighbour configurations. J is the nearest neighbour strength interaction. This model is the well-known Ising model [68]. Ising's name is attached to it after he managed to calculate the partition function associated to H in one dimension. His explicit solution of the model relied on the use of the so-called transfer matrices. In his setting, this brought down the problem to a diagonalisation of 2×2 matrices. Upon further studying his results, Ising understood that the one-dimensional model (1.2.1) does not exhibit a phase transition and falsely conjectured that classical statistical models even in dimensions two and higher, would also not exhibit phase transitions. Hence this motivated people to focus their attention on developing quantum models of magnetism as the belief was that only the recently invented quantum theory was able to grasp magnetism. In particular, Heisenberg derived his famous model of quantum magnetism, the Heisenberg magnet [65]. However in 1941, through an argument of duality, Kramers and Wannier [108] argued that the two-dimensional Ising model does exhibit a phase transition at a critical temperature $T_c > 0$. Three years later, Onsager managed to solve the two-dimensional Ising model [139]: he was able to compute explicitly the *per*-site free energy by evaluating the thermodynamical limit of the statistical sum defining the model's partition function. He was successful in characterising the magnetisation and the occurrence of an order-disorder transition by showing that the *per*-site free energy admits a singularity of order two and computed the associated critical exponents. However, while the transfer matrices of the one-dimensional model could be explicitly diagonalised through elementary means this turned out to be a non-trivial challenge in dimension two. Onsager achieved this by constructing a symmetric representation of an algebra of operators building up the transfer matrix and using it to diagonalise the transfer matrix by means of symmetries. Onsager's analysis was further extended and simplified by Kauffman [77]. Shortly after the publications of Onsager's and Kauffman's results, Yang was able to compute the spontaneous magnetisation of the model [177]. The works of Lenz, Ising, Onsager and Kauffman definitely constituted another milestone towards the understanding of more complicated exactly solvable models.

1.3 Towards quantum integrable models

On top of discussing the developments related to aforementioned incentives, we will see how these models and their quantum analogues are tightly related. And further, how this relation would set the grounds for the establishing deep algebraic structures in the search of exact solutions to the so-called *quantum integrable systems*. We will discuss the models and review the developments related to their solvability before entering the literature around the specific problems we contributed in resolving. In this way, we provide a framework for discussing the problematic in question but also try to instil a sense of appreciation for the difficulty of the problems around quantum spin chains in general. Since the introduction of the Heisenberg magnet [65] models, the search for characterising their spectrum and consequently associated physical quantities has only intensified with new and more powerful methods for doing so. This was (and still is) a formidable problem. As the calculations throughout the decades following the work of Ising, Onsager and Kauffmann evolved, the computation of physical quantities of interest such as the free energy, the correlation lengths or correlation functions, seemed to be within the realm of possibility. The algebraic approach, which appeared towards the end of the 1970's, to quantum integrable

⁷This is the apparent ordering of the spins of the system in the absence of a magnetic field at temperatures below the Curie temperature.

models would provide a plethora of powerful computational techniques⁸. We will review those ground-breaking developments in a later sub-section.

1.3.1 The coordinate Bethe Ansatz

In 1931, Hans Bethe [18] proposed an Ansatz allowing one to construct the Eigenfunctions of the Heisenberg XXX spin-1/2 chain in one-dimension. The latter corresponds to the isotropic limit $\Delta = 1$ of the XXZ spin-1/2 chain, whose Hamiltonian takes the form

$$H_{XXZ} = J \sum_{a=1}^{L} \left\{ \sigma_a^x \sigma_{a+1}^x + \sigma_a^y \sigma_{a+1}^y + \Delta (\sigma_a^z \sigma_{a+1}^z + 1) \right\} - \frac{h}{2} \sum_{a=1}^{L} \sigma_a^z$$
(1.3.1)

with periodic boundary conditions $\sigma_{L+1}^{\alpha} = \sigma_1^{\alpha}$ for $\alpha = \{x, y, z\}$. In the above, we noted σ_a^{α} as the operator acting non-trivially as the Pauli matrix σ^{α} on the a^{th} site of the quantum space of the chain. *J* is the coupling constant and *h* the magnetic field. Bethe provided a description of the coefficients of the Eigenvectors of the Heisenberg XXX spin-1/2 chain. He made the Ansatz that these coefficients are expressed as linear combinations of planewaves and has argued that their rapidities λ_a need to satisfy a set of algebraic equations in many variables and of degree going with *L* in order to obtain an Eigenvector. Orbach [140] generalised Bethe approach to the case of general anisotropy. The Bethe equations for the XXZ chain with $-1 < \Delta < 1$, *viz*. $\Delta = \cos(\zeta)$ and $\zeta \in]0; \pi[$ take the form

$$\left[\frac{\sinh(\lambda_a - \mathrm{i}\zeta/2)}{\sinh(\lambda_a + \mathrm{i}\zeta/2)}\right]^L \cdot \prod_{\substack{l=1\\l\neq k}}^M \left\{\frac{\sinh(\lambda_b - \lambda_a - \mathrm{i}\zeta)}{\sinh(\lambda_b - \lambda_a + \mathrm{i}\zeta)}\right\} = 1$$
(1.3.2)

where *M* corresponds to the number of Bethe roots. The associated Eigenvalues of H_{XXZ} are expressed as sums of functions evaluated at those rapidities. It is important to note here that Bethe himself was very much aware of the issue of completeness in his construction. In this setting, this essentially boils down to the question; does the number of distinct solutions to the Bethe ansatz equations, satisfied by *M* Bethe roots, M = 0, ..., L and the dimensionality of the Hilbert space of the model coincide? Bethe analysed all the structure of solutions for large *L* and argued that these solutions organise themselves into regular patterns called *strings*. These strings are essentially the complex solutions to the Bethe Ansatz equations. Bethe manage to count the number of all string solutions and showed that the latter reproduces the correct number of Eigenstates. While leading to the correct result [6, 24, 30, 40], one should stress that the whole approach to establishing completeness by counting string solutions is wrong since there do exist many non-string like solutions to the Bethe Ansatz equations while some of the claimed string solutions simply do not exist. However, we point out that there are works which discusses the issue of completeness without having to rely on the string solutions [33, 119, 120, 135, 137, 168].

The strings correspond to a particular form taken by a subset of Bethe roots [24, 163]. When $L \to \infty$, in the regime $-1 < \Delta < 1$, it is argued that solutions $\{\lambda_a\}_{a=1}^M$ should organise in groups of *j*-strings

$$\{\lambda_a\}_{a=1}^M \equiv \{\mu_{\alpha,k}^{(j)}\}$$
(1.3.3)

with

$$\mu_{\alpha,k}^{(j)} = \mu_{\alpha}^{(j)} + \frac{\mathrm{i}\zeta}{2}(j+1-2k) + \frac{\mathrm{i}\pi}{2}p_0 + d_{\alpha,k}^{(j)}$$
(1.3.4)

⁸Another reason, motivated by findings around the period, this time coming from conformal field theory [23, 17, 142], for studying quantum integral models, pertains to the *universality principle*. The latter provides a basis for studying such correlation functions. Namely if the critical exponent of a particular model is known then the critical exponents of models belonging to the same universality can be readily accessed. The Luttinger liquid [64] and two dimensional conformal field theories [17, 142] are examples of massless theories whose spectra and critical exponents can be explicitly characterised. The universality principle then allows one to argue the long distance behaviour of the correlation functions in a massless model belonging to one of such universality classes. Verifying the universality principle against an independent result obtained on the basis of first principle considerations has grown to become an important problem in mathematical physics. In fact, it turns out that one may carry out completely such a program in certain instances of one-dimensional quantum integrable models.

with $p_0 \in \{0, 1\}$ and fixed for k = 1, ..., j and

$$d_{\alpha,k}^{(j)} = \mathscr{O}(L^{-\infty}). \tag{1.3.5}$$

In (1.3.4), $\mu_{\alpha}^{(j)}$ is called the string center and $d_{\alpha,k}^{(j)}$, the string deviation. The interest in the solutions (real and complex) to Bethe equations was mostly due to the works related to the study of thermodynamics of quantum integrable systems which arised in the early 1970's. Since then there is now a large literature on the subject, see [6, 24, 30, 40, 42, 43, 49, 50, 51, 67, 82, 83, 84, 98, 99, 119, 120, 138, 149, 163, 168, 173, 176].

The work of Bethe opened the floodgates to the study of quantum many body integrable systems and this solicited the efforts of a large number of people. The technique devised by Bethe for computing the spectrum of the Heisenberg chain became known as the *coordinate Bethe Ansatz*. In 1938, Húlthen [66], albeit heuristically, identified the Eigenvector corresponding to the model's ground state in presence of a zero magnetic field. Further, he conjectured that, in the thermodynamic limit $L \rightarrow \infty$, the set of Bethe roots characterising the model's ground state at h = 0 condense on \mathbb{R} with a density $\rho_{H_{XXX}}$. He constructed the function $\rho_{H_{XXX}}$ by solving a linear integral equation which he derived for the latter. Shortly after, when studying his generalisation of Bethe's approach to the XXZ spin-1/2 chain (1.3.1), Orbach [140] adapted Húlthen's approach to the case of a generic anisotropy. He was able to derive an adequate linear integral equation describing the density of ground state Bethe roots for the XXZ chain at vanishing magnetic field but he could not offer an exact solution for the latter. The latter would appear in a paper by Walker [174] who considered a change of variable allowing him to transform the linear integral equation obtained by Orbach for $\Delta > 1$ into a π -periodic Wiener Hopf operator acting on $L^2([0;\pi])$. This allowed him to build on Fourier series expansions to solve the linear integral equation in question at $\Delta > 1$. These calculations were generalised by Griffiths [62] for the XXZ chain with $-1 < \Delta < 1$ and in a non-vanishing magnetic field, although the solution is not explicit anymore. These considerations allowed one to compute -in terms of the density- the thermodynamic limit of the ground state energy. The thermodynamic limit of the energies of the excited states for the Heisenberg XXX chain was considered by des Cloiseaux and Pearson [27]. In their work [27], they managed to derive the associated dispersion relation characterising the low-lying excitations. This analysis was then generalised to the XXZ case by des Cloiseaux and Gaudin [26]. However as pointed out by Faddeev and Takhtajan in 1981 [49], even with the correct dispersion law des Cloiseaux and Pearson gave a wrong interpretation for the spin content⁹ of the low-lying excitations.

In 1966, Yang and Yang [179, 180, 181] would bring in numerous elements of rigour related to the Bethe Ansatz approach to the spectrum of the XXZ spin chain. In particular they proved Húlthen's conjecture and were able to establish the existence of solutions to the Bethe equations describing the ground state. However they did not give a rigorous proof of the condensation of the Bethe roots on \mathbb{R} . The earlier methods discussed above, based on the densities, were developed only at a formal level and the possibility to take the large-*L* limit of sums over the Bethe roots by an integration *versus* the density of the Bethe roots was always assumed to be true. Recently, some light was shed on the matter through the work of Dorlas and Samsonov [35]. In their paper, they studied this problem for regimes of $\Delta > 1$ and $-1 < \Delta < 0$. In the sector $\Delta \in [-1,0)$, they followed the approach by Yang and Yang [179, 180, 181] and employed a convexity argument of a certain functional to establish the condensation property. They also managed to treat the case when Δ is much greater than 1 by perturbative techniques. Finally, in 2015, Kozlowski [105] gave a rigorous proof of the condensation property for all values of the anisotropy.

The complex solutions to the Bethe Ansatz equations were also investigated more thoroughly. In 1982 Destri and Lowenstein [30] managed to forge a way allowing them to study more precisely the solutions to the Bethe Ansatz equations of the chiral-invariant Gross-Neveu model in the large-L limit. In fact, these equation were structurally similar to the Bethe Ansatz equations of the Heisenberg XXX chain. Shortly after, Woynarovich

⁹des Cloiseaux and Pearson describe the low-lying excitations as triply degenerate spin-1 excitations. This was actually a one-particle excitation consisting of a doublet of spin-1/2 representations [49].

[176] and Babelon, de Vega and Viallet [6] built on the work of Destri and Lowenstein to analyse the excitation spectrum of the XXZ chain above the h = 0 ground state. These works have demonstrated that the string hypothesis does not hold in full generality and that there exist other structures of complex solutions to the Bethe equations in this magnetisation sector: *close* and *wide* pairs or quartets. These roots satisfy a set of coupled equations which are referred to as the *higher level Bethe Ansatz equations*. An analysis of the higher level Bethe Ansatz equation in the massive regime was then given by Virosztek and Woynarovich in 1984 [172] who corrected some of the statements made by Babelon, Viallet and de Vega [6]. In 1985, de Vega and Woynarovich [170] revisited the analysis of the massive regime of the XXZ chain and proposed a novel approach for dealing with the densities of the Bethe roots. The latter turned out to be much more effective to computing the finite-size corrections to the thermodynamics limit. A few years later, Klümper and Batchelor [93] developed an alternative approach based on non-linear integral equations for computing the finite-size corrections. In this way, they manage to avoid dealing explicitly with the root densities. This work was further extended in 1991 [94] and in 1993 [97]. One should mentioned that Destri and de Vega [31, 32] also developed a non-linear integral based framework for analysing finite-size corrections.

The XXZ chain is of course not the only instance of a quantum many-body exactly solvable model. One can cite as other examples of quantum integrable models, the non-linear Schrödinger model, the lattice sine-Gordon, or various other higher rank models, for example those defined by a $d^2 \times d^2$ fundamental R-matrix $R(\lambda,\mu) \in \mathscr{L}(\mathbb{C}^d \otimes \mathbb{C}^d)$, see for *e.g.* [74, 113] for reviews. For the case of the non-linear Schrödinger model, it is described by the Hamiltonian

$$\mathbb{H}_{\mathrm{NLS}} = \int_0^L dx \left\{ \partial_x \Phi^{\dagger}(x) \partial_x \Phi(x) + c \Phi^{\dagger}(x) \Phi^{\dagger}(x) \Phi(x) \Phi(x) \right\} - h \int_0^L dx \Phi^{\dagger}(x) \Phi(x).$$
(1.3.6)

It describes bosonic particles created/annihilated by the fields $\Phi^{\dagger}(x)/\Phi(x)$, and evolving on a circle of length *L*. *h* is to the chemical potential and c > 0 corresponds to the coupling constant. The Hamiltonian is subject to periodic boundary conditions. The above model was solved, within Bethe's approach, for all values of the coupling constant *c*. In 1960, Girardeau [55] considered the model with $c = +\infty$, which corresponds to the impenetrable Bose gas and produced the Eigenvalues and Eigenvectors of the model. Shortly after, in 1964, the model (1.3.6) was considered in its entire generality by Brézin, Pohil and Finkelberg [21]. They determined the spectrum of the latter *via* the coordinate Bethe Ansatz in the sector with three particles. The computation of the spectrum of the model (1.3.6) for *N* particles was done by Lieb and Lineger [129] simultaneously and independently to the work of Brézin, Pohil and Finkelberg. Towards the end of the 60's, Lieb [130] produced an extensive analysis of the excitation spectrum of the non-linear Schrödinger model characterising the low-lying excited states in the large-*L* limit: these were shown to consist of particles and holes. The particles are those excitations whose momenta lie away from the model's Fermi zone while the holes have their momenta inside this zone. The particle and holes form essentially the elementary excitations which Lieb differentiates from the quasi-particles which are defined as the isolated singularities of the Green's functions.

1.3.2 The algebraic Bethe Ansatz approach

The ground-breaking work of Onsager and Kauffman in being able to effectively study and diagonalise the transfer matrix of the two-dimensional Ising model would greatly influence research in the field in the years to come. The powerful results describing particular physical properties of the model would motivate people to consider more general models. Examples being the ice type [125] and antiferro/ferro-electric models [126, 128] studied by Lieb. He managed, *via* the transfer matrix method, to compute the entropies for the ice-type and antiferro/ferroelectric models and show the existence of phase transitions in those models. Lieb observed that the transfer matrix of the six-vertex model has the same Eigenfunctions as the XXZ spin-1/2 Hamiltonian. McCoy and Wu in 1968 [134] pushed these observations further by showing that the six-vertex transfer matrix and the XXZ spin-1/2 Hamiltonian explicitly commute. This result was later generalised to the Heisenberg XYZ model by Sutherland in 1970 [159]. The actual direct connection between the eight-vertex model and the Heisenberg XYZ Hamiltonian is due to Baxter [11]-[15] what also revealed the deep algebraic structure underlying the models. Baxter [12] constructed a one-parameter family of transfer matrices of the eight vertex model, $t_{8V}(\lambda)$, where λ is the spectral parameter. The transfer matrix constructed by Baxter is essentially the trace of a product of L-matrices. Such a product is now known as the monodromy matrix and the L matrix is the Lax matrix, in this case, of the eight vertex model. One of the many important results of Baxter is that he showed that these transfer matrices satisfy commutation relations which close for different values of the spectral parameter. Another foundational result by Baxter [11] is that he showed that the Heisenberg XYZ Hamiltonian is equal to $\partial_{\lambda} \ln t_{8V}(\lambda)|_{\lambda=0}$. This relation indicates the direct link between two-dimensional statistical models and one-dimensional quantum integrable models. It is important to note here that it is Baxter's work which first hinted the deep algebraic structure at the root of quantum integrable models. The Hamiltonian is explicitly embedded into of an abelian algebra of charges generated by a family of commuting transfer matrices. Many of the results obtained by Baxter established with the help of a set of equations satisfied by the weights of the eight vertex model. Baxter coined these as the star-triangle relation. This star-triangle relation can be recast as a relation of products of 4×4 matrices $R_{12}L_1L_2 = L_2L_1R_{12}$ where the indices 1,2 are the auxiliary spaces associated with the Lax matrices while R is a 4×4 matrix acting in the tensor product of the spaces 1 and 2. Independently upon studying an N-body problem with repulsive δ -interactions, Yang [178] obtained an equation of the same form. Nowadays the equation $R_{12}L_1L_2 = L_2L_1R_{12}$ is famously referred to as the Yang-Baxter equation.

In 1979, Faddeev, Sklyanin and Takhtajan [47] pushed further the use of the profound algebraic structure underlying quantum integrable models. Their main observations was that one may use the relations issuing from an RTT = TTR equation so as to provide a set of exchange relations between the entries of the monodromy matrix. These may then further be used so as to construct the Eigenvectors of the model in a simple algebraic way, by means of a repetitive action of some of the entries of the monodromy matrix on some reference state. Originally, Fadeev, Sklyanin and Takhtajan developed the methods for the lattice discretisation of the sine-Gordon model in (1 + 1)- dimension. However, soon the method was extended to many other models: the spin-s XXZ chain [7]-[9], the XYZ model [48], higher rank spin chains [109]-[114] so as to name a few. This algebraic approach, precisely due to its relative simplicity, opened the way towards the computation of the main object of interest: the *correlation functions*. This was developed, in particular, in the works [72], [86]-[90].

1.4 Quantum integrable models at finite temperature

So far, the mentioned results allow one to discuss quantum integrable models at zero temperature. Incorporating the elements related to the temperature in the studies pertaining to one-dimensional quantum integrable models was a completely different issue. This presented new sets of challenges and new techniques had to be invented in order to solve these new problems. It was not until 1969 that the first paper on the subject appeared. In their work [182], Yang and Yang formally argued an integral representation of the *per*-site free energy of the non-linear Schrödinger model in the infinite volume limit and at finite temperature as

$$f_{\rm NLS} = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \ln\left[1 + e^{-\frac{\varepsilon(k)}{T}}\right]. \tag{1.4.1}$$

There $\varepsilon(k)$ is the unique solution of the below non-linear integral equation called the Yang-Yang equation:

$$\varepsilon(k) = -h + k^2 - \frac{T}{\pi} \int_{-\infty}^{\infty} dq \, \frac{c}{c^2 + (k-q)^2} \ln\left[1 + e^{-\frac{\varepsilon(q)}{T}}\right], \qquad 0 < c \le \infty.$$
(1.4.2)

Here *h* and *c* are as appearing in (1.3.6). In fact, this non-linear integral equation can be seen as the prototypical form of the class non-linear integral equations that will be dealt with in this thesis. The approach of [182] is inspired from Landau and Lifschitz derivation of the non-equilibrium entropy density for a free quantum gas [118], what allowed Yang and Yang to characterise the entropy density of the non-linear Schrödinger model.

We point out that later on Yang and Yang's result was framed rigorously by Dorlas, Lewis and Pulé [34] upon characterising the thermodynamic limit of the free energy of that model within the context of large deviations and Varadhan's Lemma. The work of Dorlas, Lewis and Pulé relied on the completeness of the Bethe Ansatz Eigenfunctions. The latter was established by Dorlas in the following year [33].

Shortly after the work of Yang and Yang, Takahashi derived the thermodynamics of the Heisenberg XXX spin-1/2 chain [160]. Gaudin, simultaneously and independently, managed to obtain the thermodynamics of the XXZ spin chain [53] when $\Delta > 1$. By implementing the setting of Yang and Yang, Gaudin and Takahashi wrote down an integral representation for the *per*-site free energy of the model they studied. Gaudin also wrote down the entropy of the chain. The following year Takahashi generalised his approach to the XXZ chain for $-1 < \Delta < 1$ [161]. The results obtained in the mentioned works heavily built on the string hypothesis, namely assumed that "all" solutions to the Bethe equations organise themselves into concatenations of strings as shown in (1.3.4). They argued an infinite set of coupled non-linear integral equations governing the densities of the string centers supposed to grasp the "dominant" contribution to $\ln \operatorname{tr}_{\mathfrak{h}_{XXZ}}\left[e^{-\frac{H_{XXZ}}{T}}\right]$ when $L \to \infty$. Such handlings based on strings turned out -independently of the lack of validity of the string hypothesis- to be quite tricky and needed to be improved due to "wrong" counting of the string contributions, as pointed out in 1972 by Johnson, McCoy and Lai [76]. This was due to the fact that for the XXZ chain, for $-1 < \Delta < 1$, only strings of a certain length are allowed. While, in the overall, the results stemming from that approach are believed ¹⁰ to be correct, there seems to be little chance of making the approach rigorous, in the spirit of Dorlas, Lewis and Pulé's approach. Furthermore, the cumbersomeness and technical complications related to the use of infinitely many non-linear integral equations were calling for a different approach which would allow for string hypothesis free reasonings.

This change of perspective was achieved by Koma [100, 101]. Koma built on the ideas of Suzuki [155] and Suzuki and Inoue [156] which consisted in discretising the Boltzmann statistical operator in an appropriate way. In his analysis, Koma introduced this Trotter-Suzuki approximant of the finite volume partition function of the Heisenberg chain [100] and the Heisenberg-Ising chain [101] what allowed him to express the trace of the Boltzmann weight as

$$\frac{1}{L}\ln \operatorname{tr}_{\mathfrak{h}_{XXZ}}\left[\mathrm{e}^{-\frac{1}{T}\mathrm{H}_{XXZ}}\right] = \lim_{N \to \infty} \frac{1}{L}\ln \operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}}\left[\mathscr{T}_{N,T}^{L}\right].$$
(1.4.3)

Thus, the initial partition function in finite volume is isolated by taking the infinite Trotter limit $N \to \infty$ of the trace of the L^{th} -power of an operator $\mathscr{T}_{N,T}$ acting on an auxiliary Hilbert space $\mathfrak{h}_{\mathfrak{q}}$. The operator $\mathscr{T}_{N,T}$ hence constructed by Koma corresponds to the transfer matrix of a vertex model related to the product of two Ising models. Representations of the type (1.4.3) become particularly efficient in the thermodynamic limit, at least if one is able to prove the exchangeability of the thermodynamic limit of (1.4.3) with the Trotter limit appearing in the right hand side of this formula. By implementing the setting of Suzuki [155] and Suzuki and Inoue [156] Koma was able to prove the exchangeability of the $L \to \infty$ and $N \to \infty$ for his transfer matrix $\mathscr{T}_{N,T}$. He also established that $\mathscr{T}_{N,T}$ admits a non-degenerate, real and maximal in modulus Eigenvalue $\Lambda_{\max}(\mathscr{T}_{N,T})$. This allowed him to express the *per*-site free energy as

$$f = -T \lim_{N \to \infty} \left\{ \ln \left[\Lambda_{\max}(\mathscr{T}_{N,T}) \right] \right\}.$$
(1.4.4)

Koma was thus able to produce a simple formula for the *per*-site free energy of the Heisenberg-Ising chain in terms of the dominant Eigenvalue of the transfer matrix where it still remained to characterise the Trotter limit. He managed to rigorously treat the calculation of the Trotter limit when $\Delta = 0$ case which was already treated in [156] in another approach. Away from the free fermion, Koma could only perform numerical analysis for the case $\Delta = 1$ [101].

¹⁰In fact it was demonstrated in [96] that the quantum transfer matrix and the Gaudin/Takahashi approach are equivalent.

Koma's approach represented a huge step forward in understanding rigorously one dimensional quantum spin systems at finite temperature since it did not rely on string based approaches. Albeit, Koma's approach did not produce a characterisation of the Trotter limit, it certainly formed the basis of the works that would follow. In 1991 Takahashi treated the infinite Trotter limit of the dominant Eigenvalue of Koma's transfer matrix formally at the level of the Bethe Ansatz equations [162]. In his setting, he expressed this limit via an infinite sequence of Bethe roots. This way of calculating the infinite Trotter limit of the dominant Eigenvalue made Takahashi's approach difficult to implement in practice even on numerical grounds because Takahashi's approach involved an infinite number of variables satisfying an infinite number of constraints. In fact, from today's point of view, one may also see that Koma's transfer matrix does not exhibit enough algebraic structure so as to allow one to study more problems such as the evaluation of thermal correlations function. Later on, Suzuki, Akutsu and Wadati [158] introduced another Transfer matrix $t_{\mathfrak{q}}(0)$, related to a staggered six-vertex model, which enjoyed the property (1.4.3). The construction was generalised to the presence of a spectral parameter by Klümper [91, 92] and Destri- de Vega [31, 32]. Later on, it turned out, starting from the work of Göhmann, Klümper and Seel [59, 60] that this transfer matrix is very well suited for computing the thermal correlators. This was confirmed by the large amount of works, on the subject, that followed [36, 39, 57, 59, 60]. More importantly, however, the case of the quantum transfer matrix $t_{\mathfrak{q}}(\lambda)$ allows one to take the Trotter limit quite effectively. The possibility to do so goes back to the seminal works of Klümper [91, 92] and Destri-de Vega [31, 32]. Their idea consists, first, in introducing a certain auxiliary function a which is shown to satisfy a non-linear integral equation in which the dependence on the Trotter number only appears in the driving term. Then, one writes an integral representation for the dominant Eigenvalue, in which $\mathfrak{a}(\lambda)$ appears in the integrand. Such handlings greatly reduce, at least on formal grounds, the taking of the Trotter limit in that it is enough to take it on the level of the driving term in the non-linear integral equation. In fact Klümper was also able to characterise, within this setting, the correlation lengths of the model [41, 59, 92, 95, 107, 106, 162].

Albeit, the above works produced powerful results and pioneered extremely interesting techniques for studying quantum integrable systems at finite temperature, they were introduced and treated only on a formal level. The various assumptions on which the construction of a non-linear integral equations based description of the *per*-site free energy rested were not rigorously established. The goal of this thesis is to fill this gap and rigorously prove these assumptions. Namely to prove the existence of a dominant non-degenerate, real Eigenvalue of $t_q(0)$, to establish the exchangeability of the Trotter and the thermodynamic limits. While these were proven for Koma's transfer matrix $\mathscr{T}_{N,L}$, they were not for $t_q(0)$. It turns out that the techniques to do so are drastically different. Also, we lay the whole theory of the non-linear integral equations, for temperatures large enough, on rigorous grounds and provide a rigorous identification of the dominant Eigenvalue of $t_q(0)$.

1.5 Outline of the thesis

This thesis is organised as follows. The second chapter of the thesis opens with some description of the XXZ spin-1/2 chain which is the model used in our analysis in this thesis. We then introduce our quantity of interest, namely the *per*-site free energy. In order to describe the quantum transfer matrix t_q and the handlings based on the latter, we feel necessary to remind of the construction of the transfer matrix of the XXZ spin-1/2 chain within the setting of the algebraic Bethe Ansatz. After describing the quantum transfer matrix, we explain how it is used to express the *per*-site free energy in terms of its largest Eigenvalue. The possibility to do so is based on assumptions, namely: the existence of a real, non-degenerate maximal in modulus Eigenvalue of t_q and the validity of the exchangeability of the $L \rightarrow \infty$ and $N \rightarrow \infty$ limits. After this, we introduce the setting allowing us to rigorously establish the aforementioned assumptions. This allows us to construct operators issued from the high temperature expansion of t_q . The analytical properties of these operators are then rigorously characterised as they form the basis for the analysis which follows. We hence provide rigorous estimates on the dominant as well as the sub-leading Eigenvalues of the quantum transfer matrix. We conclude this chapter with the rigorous proof of the exchangeability of the infinite volume and the infinite Trotter limits.

Chapter 3 focuses on the non-linear integral equation based approach to the spectrum of the quantum transfer matrix. We first recall the algebraic Bethe Ansatz framework for the quantum transfer matrix. This yields a representation for the Eigenvalues of the quantum transfer matrix in terms of the Bethe roots and allows us to introduce the auxiliary function formalism. Then, we recall the alternative characterisation of the auxiliary function in terms of the non-linear integral equations. Such a setting allows one to take formally the infinite Trotter number limit on the level of the non-linear integral equation and show that, in the high temperature limit these do admit solutions and that these are unique. We also establish that the infinite Trotter number limit may be taken rigorously on the level of the solution to such non-linear integral equation. This constitutes the final result of the chapter.

In Chapter 4 we build on the last two chapters to construct integral representations for associated physical quantities, namely the free energy and the correlation lengths. In particular, we rigorously derive the integral representation of the dominant Eigenvalue. Consequently this allows us to write down an integral representation of the *per*-site free energy. Within the same setting we write down the integral representation for a certain class of the sub-leading Eigenvalues. This allows us to write down some of the correlation lengths in integral form. For the specific class of "excited" states of the quantum transfer matrix we consider, we rigorously show that the hole roots converge to zero in the large temperature limit and that the particle roots satisfy the XXZ spin-1 Bethe Ansatz equations. We conclude by writing down the high temperature behaviour of correlation lengths in terms of these dominant particle and hole roots contributions.

Chapter 2

Combinatorial based approach to the spectrum of quantum transfer matrix

In this chapter we rigorously prove a number of conjectures pertaining to the analysis of quantum integrable models at finite temperature. This is achieved by establishing various properties of the high temperature expansion of the quantum transfer matrix. While we shall focus our attention on the XXZ chain case, the methodology developed in this chapter is applicable to a large class of quantum integrable models whose finite temperature behaviour can be grasped with the quantum transfer matrix approach.

In Section 2.1, we provide a concise introduction to the algebraic Bethe Ansatz for the transfer and quantum transfer matrices associated with the XXZ chain. The quantum transfer matrix allows one to express pertinent observables such as the free energy in a very simple form which only involves maximum Eigenvalue and the associated Eigenvectors and/or a few sub-leading ones. However the validity of such formulae relies on a certain number of assumptions related to the spectrum of the quantum transfer matrix. In Section 2.2 we present the first original results of the thesis which consist in a rigorous proof of these assumptions. We obtain a new expansion of the quantum transfer matrix which is well adapted for studying various properties of its spectrum in the high temperature regime. These results allow us to demonstrate that the quantum transfer matrix does admit a non-degenerate, maximal in modulus and real Eigenvalue. Building further on these techniques we produce a rigorous proof of the exchangeability of the Trotter and infinite volume limits in Section 2.3.

2.1 The XXZ spin-1/2 chain at finite temperature

This section recalls several known facts about the XXZ spin-1/2 chain. In particular, we review the quantum inverse scattering method based approach to the diagonalisation of the model and then describe the construction of the quantum transfer matrix.

2.1.1 The model

As an archetypal example of a quantum integrable model, the XXZ chain represents an extraordinary laboratory for studying quantum integrable models. The XXZ spin-1/2 chain refers to the Hamiltonian operator

$$H_{XXZ} = J \sum_{a=1}^{L} \left\{ \sigma_a^x \sigma_{a+1}^x + \sigma_a^y \sigma_{a+1}^y + \Delta (\sigma_a^z \sigma_{a+1}^z + id) \right\} - \frac{h}{2} \sum_{a=1}^{L} \sigma_a^z.$$
(2.1.1)

 \mathfrak{H}_{XXZ} acts on the Hilbert $\mathfrak{h}_{XXZ} = \bigotimes_{a=1}^{L} \mathfrak{h}_a$ assembled from a tensor product of the local quantum spaces \mathfrak{h}_a with $\mathfrak{h}_a \simeq \mathbb{C}^2$. The operator σ_a^{α} where $\alpha \in \{x, y, z\}$ acts as the Pauli matrix σ^{α} on the space \mathfrak{h}_a and as the identity

matrix on all the other spaces

$$\sigma_a^{\alpha} = \underbrace{\operatorname{id} \otimes \ldots \otimes \operatorname{id}}_{a-1} \otimes \sigma^{\alpha} \otimes \underbrace{\operatorname{id} \otimes \ldots \otimes \operatorname{id}}_{L-a}.$$
(2.1.2)

In the above, J > 0 is an overall coupling constant characterising the strength of the exchange interaction and $L \in 2\mathbb{N}$ corresponds to the number of sites ¹. The model is subject to periodic boundary conditions $\sigma_{L+1}^{\alpha} = \sigma_1^{\alpha}$. $\Delta \in \mathbb{R}$ is the anisotropy and *h* is an overall magnetic field oriented along the same direction as the anisotropy. When $\Delta = 1, h = 0$ the model (2.1.1) reduces to the XXX Heisenberg anti-ferromagnet. When $\Delta < -1$, the model is in the ferromagnetic regime for any magnetic field *h*. The same holds true for $\Delta \ge -1$ if $|h| \ge 4J(1+\Delta)$. However, if $|h| < 4J(1+\Delta)$ and $\Delta \ge -1$, the model is in its antiferromagnetic regime. The latter splits into the distinct phases

- $\Delta > 1$ for magnetic field $0 \le |h| < 4J(1 \Delta)$ corresponds to the massive antiferromagnetic regime;
- $\Delta > 1$ for magnetic field $h_{\ell} \le |h| < 4J(1 + \Delta)$ corresponds to the massless antiferromagnetic model.
- $-1 < \Delta \le 1$ for magnetic field $0 \le |h| < 4J(1 + \Delta)$ corresponds to the massless antiferromagnetic model.

Above, h_{ℓ} [181] can be explicitly expressed in terms of theta functions, see [38]. The last case corresponds to the range of values of Δ within which we restrict ourselves in this thesis. Accordingly, we choose the parametrisation

$$\Delta = \cos(\zeta) \quad \text{with} \quad \zeta \in]0; \pi[. \tag{2.1.3})$$

We do however stress that the techniques described below do hold for any value of the anisotropy Δ and magnetic field *h*.

2.1.2 The free energy of the XXZ chain at finite temperature

We shall focus mainly on the simplest most pertinent quantity associated to the XXZ spin chain (2.1.1), namely the *per*-site free energy. The latter is defined as

$$f_{\rm XXZ} = -T \cdot \lim_{L \to \infty} \frac{1}{L} \ln \operatorname{tr}_{\mathfrak{h}_{\rm XXZ}} \left[e^{-\frac{1}{T} \operatorname{H}_{\rm XXZ}} \right].$$
(2.1.4)

The well-definedness of the thermodynamic limit above has been rigorously established provided that $L \rightarrow \infty$ in an adequate sense which follows from Ruelle's rigorous treatment [145]. For the reader's convenience we reproduce the proof below.

Theorem 2.1.1. [145] Let f_L be the per-site free energy of a chain of L-sites defined as

$$f_L = -\frac{T}{L} \ln \operatorname{tr}_{\mathfrak{h}_{XXZ}} \left[e^{-\frac{\mathfrak{H}^{(k;L)}}{T}} \right].$$
(2.1.5)

The limit $L \rightarrow \infty$ *of the finite* L *per-site free energy exists*

$$\lim_{L \to \infty} f_L = f_{\text{XXZ}}.$$
 (2.1.6)

Proof. For the purpose of the proof, we need to introduce the XXZ chain Hamiltonian acting on a segment (k;L)

$$\mathbf{H}^{(k;L)} = \sum_{a=k}^{L-1} \mathbf{h}_{aa+1} - \frac{h}{2} \sum_{a=1}^{L} \sigma_a^z + \mathbf{h}_{L;k}$$
(2.1.7)

where

$$\mathbf{h}_{aa+1} = J \big\{ \sigma_a^x \sigma_{a+1}^x + \sigma_a^y \sigma_{a+1}^y + \Delta (\sigma_a^z \sigma_{a+1}^z + \mathrm{id}) \big\}.$$
(2.1.8)

¹While the case $L \in \mathbb{N}$ may be treated without problems, assuming an even *L* allows for some simplifications.

The above XXZ Hamiltonian acts on $\mathfrak{h}^{(k;L)} = \bigotimes_{a=k}^{L} \mathfrak{h}_{a}$. We then have that

$$\mathbf{H}^{(1:2L)} = \mathbf{H}^{(1:L)} + \mathbf{H}^{(L+1:2L)} + \overbrace{\mathbf{h}_{L;L+1} - \mathbf{h}_{L;1} - \mathbf{h}_{2L;L+1} + \mathbf{h}_{1;2L}}^{\delta \mathbf{h}_{L}}.$$
(2.1.9)

Upon using that, for two Hermitian matrices A and B,

$$\left|\ln \operatorname{tr}(\mathbf{e}^{A+B}) - \ln \operatorname{tr}(\mathbf{e}^{A})\right| \le ||B||$$
(2.1.10)

where $\|\cdot\|$ is the operator norm, we have

$$\left| \ln \operatorname{tr}_{\mathfrak{h}^{(1;2L)}} \left[e^{-\frac{1}{T} (\mathfrak{H}^{(1;L)} + \mathfrak{H}^{(L+1;2L)} + \delta \mathfrak{h}_{L})} \right] - \ln \operatorname{tr}_{\mathfrak{h}^{(1;2L)}} \left[e^{-\frac{1}{T} (\mathfrak{H}^{(1;L)} + \mathfrak{H}^{(L+1;2L)})} \right] \right| \leq \frac{1}{T} \| \delta \mathfrak{h}_{L} \|.$$

$$(2.1.11)$$

Since it also holds

$$\mathrm{tr}_{\mathfrak{h}^{(1;2L)}}\left[\mathrm{e}^{-\frac{1}{T}(\mathrm{H}^{(1;L)}+\mathrm{H}^{(L+1;2L)})}\right] = \left(\mathrm{tr}_{\mathfrak{h}^{(1;L)}}\left[\mathrm{e}^{-\frac{1}{T}\mathrm{H}^{(1;L)}}\right]\right)^{2},\tag{2.1.12}$$

we infer that

$$\left| f_{2L} - f_L \right| = \frac{T}{2L} \left| \ln \operatorname{tr}_{\mathfrak{h}^{(1;2L)}} \left[e^{-\frac{1}{T} \mathbf{H}^{(1;2L)}} \right] - 2 \ln \operatorname{tr}_{\mathfrak{h}^{(1;L)}} \left[e^{-\frac{1}{T} \mathbf{H}^{(1;L)}} \right] \right| \le \frac{\| \delta \mathbf{h}_L \|}{2L} \le \frac{C}{2L}$$
(2.1.13)

for some constant C > 0 and where we used that $\parallel \sigma_a^{\alpha} \parallel = 1$. Hence for the particular choice $L = 2^{n-1}$ with $n \in \mathbb{Z}$

$$\left|f_{2^{n}} - f_{2^{n-1}}\right| \le \frac{C}{2^{n}} \tag{2.1.14}$$

and thus more generally,

$$\left|f_{2^{n+m}} - f_{2^n}\right| \le \sum_{k=1}^m \left|f_{2^{n+k}} - f_{2^{n+k-1}}\right| \le C \sum_{k=1}^m \frac{1}{2^{n+k}} \le \frac{C}{2^n}.$$
(2.1.15)

Hence f_{2^n} is a Cauchy sequence on \mathbb{R} as such it converges towards a limit, *viz*.

$$f_{\text{XXZ}} = \lim_{n \to \infty} f_{2^n}.$$
 (2.1.16)

It remains to show that f_L also converges to f_{XXZ} . First of all, one has the bound

$$\left|f_{2^{n}L} - f_{L}\right| \le \sum_{k=1}^{n} \left|f_{2^{k}L} - f_{2^{k-1}L}\right| \le \frac{C}{2^{k}L} \le \frac{C}{L}.$$
 (2.1.17)

On the other hand we can understand f_{2^nL} as built up from L chains of length 2^n .

$$\mathbf{H}^{(1;2^{n}L)} = \sum_{k=0}^{L-1} \left\{ \mathbf{H}^{(k2^{n}+1;(k+1)2^{n})} - \mathbf{h}_{(k+1)2^{n};k2^{n}+1} + \mathbf{h}_{(k+1)2^{n};(k+1)2^{n}+1} \right\}$$
(2.1.18)

and hence, upon following the same strategy, we get, for some constant C' > 0,

$$|f_{2^{n}L} - f_{2^{n}}| \le \frac{(L+1)C'}{2^{n}L} \xrightarrow[n \to \infty]{} 0.$$
 (2.1.19)

One then has $\lim_{n\to\infty} f_{2^nL} = f_{XXZ}$ and upon taking the $n \to \infty$ limit in (2.1.17), we have that

$$\left| f_{\rm XXZ} - f_L \right| \le \frac{C}{L} \tag{2.1.20}$$

for some C > 0. This entails the claim.

2.1.3 The algebraic Bethe Ansatz solution of the XXZ chain

The spectrum and Eigenvectors of the Hamiltonian (2.1.1) can be accessed by means of the coordinate Bethe Ansatz developed by Bethe [18] and Orbach [140] and through its refinement due to Faddeev, Sklyanin and Takhtadjan [47] in the form of the algebraic Bethe Ansatz. The quantum inverse scattering method approach to the diagonalisation of the Hamiltonian (2.1.1) relies on the R-matrix

$$R(\lambda) = \frac{1}{\sinh(-i\zeta)} \begin{pmatrix} \sinh(-i\zeta + \lambda) & 0 & 0 & 0\\ 0 & \sinh(\lambda) & \sinh(-i\zeta) & 0\\ 0 & \sinh(-i\zeta) & \sinh(\lambda) & 0\\ 0 & 0 & 0 & \sinh(-i\zeta + \lambda) \end{pmatrix}, \quad \zeta \in [0;\pi[$$
 (2.1.21)

where $\lambda \in \mathbb{C}$ is the spectral parameter. $R(\lambda)$ corresponds to the trigonometric or six-vertex solution [16] of the Yang-Baxter equation

$$R_{12}(\lambda)R_{13}(\lambda-\mu)R_{23}(\mu) = R_{23}(\mu)R_{13}(\lambda-\mu)R_{12}(\lambda)$$
(2.1.22)

defined on $\mathscr{L}(\mathfrak{h}_1 \otimes \mathfrak{h}_2 \otimes \mathfrak{h}_3)$. In the above \mathbb{R}_{ab} corresponds to the embedding of \mathbb{R} on $\mathscr{L}(\mathbb{C}^2 \otimes \mathbb{C}^2)$ into an operator on $\mathscr{L}(\mathfrak{h}_1 \otimes \mathfrak{h}_2 \otimes \mathfrak{h}_3)$ which acts as the identity operator on the space $\mathfrak{h}_m, m \neq a, b$ and as $\mathbb{R}(\lambda)$ on $\mathfrak{h}_a \otimes \mathfrak{h}_b$. This solution of the Yang-Baxter equation not only allows one to diagonalize the Hamiltonian (2.1.1) through the algebraic Bethe Ansatz but also allows one to introduce the quantum transfer matrix at finite temperatures as we will discuss later on.

Upon considering an ordered product of R matrices acting on the tensor-product of local quantum spaces and one auxiliary space, one obtains the monodromy matrix $T_k(\lambda)$ of the XXZ chain:

$$\mathbf{T}_{k}(\boldsymbol{\lambda}) = \mathbf{R}_{kL}(\boldsymbol{\lambda}) \dots \mathbf{R}_{k1}(\boldsymbol{\lambda}), \qquad (2.1.23)$$

where the index *k* refers to the auxiliary space. The entries of the monodromy matrix are operators acting in the XXZ chain's Hilbert space \mathfrak{h}_{XXZ} . Thus, it is convenient to express $T_k(\lambda)$ as a 2 × 2 operator valued matrix on the auxiliary space \mathfrak{h}_k

$$\mathbf{T}_{k}(\boldsymbol{\lambda}) = \begin{pmatrix} \mathbf{A}(\boldsymbol{\lambda}) & \mathbf{B}(\boldsymbol{\lambda}) \\ \mathbf{C}(\boldsymbol{\lambda}) & \mathbf{D}(\boldsymbol{\lambda}) \end{pmatrix}_{[k]}.$$
 (2.1.24)

Since for $k \neq k'$ and $a \neq b$ it holds

$$[\mathbf{R}_{ka}(\lambda),\mathbf{R}_{k'b}(\mu)] = 0, \qquad (2.1.25)$$

it follows from L application of the Yang-Baxter equation (2.1.22) that

$$\mathbf{R}_{kk'}(\lambda - \mu)\mathbf{T}_k(\lambda)\mathbf{T}_{k'}(\mu) = \mathbf{T}_{k'}(\mu)\mathbf{T}_k(\lambda)\mathbf{R}_{kk'}(\lambda - \mu)$$
(2.1.26)

where $T_k(\lambda)$, $T_{k'}(\mu)$ act on two distinct auxiliary spaces h_k and $h_{k'}$ respectively. The relation (2.1.26) contains all the commutation relations satisfied by the elements of the monodromy matrix [44, 45, 47].

Note that the monodromy matrix (2.1.23) constitutes a representation of the RTT relation given in (2.1.26). By choosing a different representation on the quantum spaces, one would end up with a different integrable model (see *e.g.* [7]-[9], [22, 69, 85, 93, 111]). By taking the trace with respect to the auxiliary space, one constructs the transfer matrix

$$\mathbf{t}(\boldsymbol{\lambda}) = \operatorname{tr}_{\mathfrak{h}_{k}}[\mathbf{T}_{k}(\boldsymbol{\lambda})] = \mathbf{A}(\boldsymbol{\lambda}) + \mathbf{D}(\boldsymbol{\lambda}). \tag{2.1.27}$$

An important consequence of the relation (2.1.26) is the commutation relation for the transfer matrices

$$[t(\lambda), t(\mu)] = 0, \ \forall \lambda, \mu \in \mathbb{C},$$
(2.1.28)

so that $t(\lambda)$ forms a one parameter λ commutative family of operators. The coefficients of the expansion of $t(\lambda)$, for example around $\lambda = 0$, provide the quantum integrals of motion. The main point is that the XXZ Hamiltonian

can be retrieved from the transfer matrix $t(\lambda)$. When the spectral parameter λ is set to 0, the R-matrix reduces to the permutation operator P:

$$R(0) = P, \text{ where } P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$
 (2.1.29)

Therefore by (2.1.27),

$$t(0) = tr_k \{ R_{kL}(0) \dots R_{k1}(0) \} = P_{12} \dots P_{N-1N}$$
(2.1.30)

where we used the fact that $P_{kN}P_{kM} = P_{NM}P_{kN}$ and $tr_k \{P_{kN}\} = id_N$. The product $P_{12} \dots P_{N-1N}$ is the shift operator U. After some elementary manipulation one has that

$$t'(0) = \mathbf{U} \cdot \sum_{i=1}^{L} \mathbf{R}'_{ii+1}(0) \mathbf{P}_{ii+1}, \qquad (2.1.31)$$

Multiplying by $t^{-1}(0)$ on both sides leads to

$$\frac{d}{d\lambda} \ln t(\lambda) \big|_{\lambda=0} = t^{-1}(0) \cdot t'(0) = \sum_{i=1}^{L} \mathbf{R}'_{ii+1}(0) \mathbf{P}_{ii+1}.$$
(2.1.32)

From the definition of the R-matrix (2.1.21) one computes $R'_{ii+1}(0)$ and upon multiplication with the permutation operator P_{ii+1} this leads to

$$\sum_{i=1}^{L} \mathsf{R}'_{ii+1}(0) \cdot \mathsf{P}_{ii+1} = \frac{1}{2\sinh(-i\zeta)} \sum_{i=1}^{L} \left\{ \sigma_i^x \otimes \sigma_{i+1}^x + \sigma_i^y \otimes \sigma_{i+1}^y + \cosh(-i\zeta) \cdot \left[\mathrm{id}_i \otimes \mathrm{id}_{i+1} + \sigma_i^z \otimes \sigma_{i+1}^z \right] \right\}.$$
(2.1.33)

Hence

$$H_{XXZ}|_{h=0} = 2J\sinh(-i\zeta)\frac{d}{d\lambda}\ln t(\lambda)|_{\lambda=0}$$
(2.1.34)

upon using the parametrisation $\Delta = \cos(\zeta)$ introduced in (2.1.3). It is clear that H_{XXZ} commutes with the transfer matrix $t(\lambda)$ for all λ which is a hallmark of integrability of the model. Hence H_{XXZ} and $t(\lambda)$ share the same Eigenvalues whose construction we explain below.

We first introduce the pseudo-vacuum or reference state $|0\rangle$. It is built out of a tensor product of the vectors e_1 where $\{e_1, e_2\}$ is the canonical basis of \mathbb{C}^2 :

$$\boldsymbol{e}_1 = \begin{pmatrix} 1\\ 0 \end{pmatrix}, \quad \boldsymbol{e}_2 = \begin{pmatrix} 0\\ 1 \end{pmatrix}.$$
 (2.1.35)

Namely,

$$|0\rangle = \underbrace{\boldsymbol{e}_1 \otimes \ldots \otimes \boldsymbol{e}_1}_{L-\text{times}}.$$
(2.1.36)

 $|0\rangle$ is an Eigenstate of the operators $A(\lambda)$ and $D(\lambda)$

$$A(\lambda)|0\rangle = a(\lambda)|0\rangle$$
 and $D(\lambda)|0\rangle = d(\lambda)|0\rangle$ (2.1.37)

where $a(\lambda) = \sinh^L(\lambda - i\zeta/2)$ and $d(\lambda) = \sinh^L(\lambda + i\zeta/2)$. $|0\rangle$ is also annihilated by the operator $C(\lambda)$, viz.

$$C(\lambda)|0\rangle = 0 \quad \forall \lambda \in \mathbb{C}.$$
(2.1.38)

Owing to $[H_{XXZ}, \sum_{a=1}^{L} \sigma_a^z] = 0$ one can look for Eigenvectors in sectors of fixed spin $S^z = \frac{1}{2} \sum_{a=1}^{L} \sigma_a^z$ since

$$S^{z}|\Psi(\{\lambda_{a}\}_{a=1}^{M})\rangle = \left(\frac{L}{2} - M\right)|\Psi(\{\lambda_{a}\}_{a=1}^{M})\rangle.$$

$$(2.1.39)$$

The other Eigenstates of the transfer matrix are obtained by acting on $|0\rangle$ with a string of B operators

$$|\Psi(\{\lambda_a\}_{a=1}^M)\rangle = \prod_{a=1}^M \mathsf{B}(\lambda_a)|0\rangle \text{ for } M \in \{1,\dots,L\},$$
(2.1.40)

where *M* is the number of rapidities λ_a . For $|\Psi(\{\lambda_a\}_{a=1}^M)\rangle$ to give rise to an Eigenstate of $t(\lambda)$, one needs to impose constraints on the set $\{\lambda_a\}_{a=1}^M$. By using the various commutation relations between the operators $A(\lambda), D(\lambda)$ and $B(\lambda)$ which follow from (2.1.26), one may write down the result of the action of the transfer matrix on the state $|\Psi(\{\lambda_a\}_{a=1}^M)\rangle$.

Theorem 2.1.2. [47] The action of the operators $A(\lambda)$ and $D(\lambda)$ on the state $|\Psi(\{\lambda_a\}_{a=1}^M)\rangle$ takes the form

$$\begin{aligned} \{\mathbf{A}(\lambda) + \mathbf{D}(\lambda)\} |\Psi(\{\lambda_a\}_{a=1}^M)\rangle \\ &= \Lambda(\lambda|\{\lambda_a\}_{a=1}^M) |\Psi(\{\lambda_a\}_{a=1}^M)\rangle + \sum_{a=1}^M \left\{ \mathbf{a}(\lambda_a) \cdot \frac{\sinh(-i\zeta)}{\sinh(\lambda_a - \lambda)} \cdot \prod_{\substack{b=1\\b\neq a}}^M \frac{\sinh(\lambda_a - \lambda_b - i\zeta)}{\sinh(\lambda_a - \lambda_b)} \right. \end{aligned} \tag{2.1.41} \\ &+ \mathbf{d}(\lambda_a) \cdot \frac{\sinh(-i\zeta)}{\sinh(\lambda - \lambda_a)} \cdot \prod_{\substack{b=1\\b\neq a}}^M \frac{\sinh(\lambda_b - \lambda_a - i\zeta)}{\sinh(\lambda_b - \lambda_a)} \left. \right\} |\Psi(\{\lambda_a\}_{a=1}^M)\rangle \end{aligned}$$

where

$$\Lambda(\lambda|\{\lambda_a\}_{a=1}^M) = a(\lambda) \cdot \prod_{a=1}^M \frac{\sinh(\lambda - \lambda_a + i\zeta)}{\sinh(\lambda - \lambda_a)} + d(\lambda) \cdot \prod_{a=1}^M \frac{\sinh(\lambda - \lambda_a - i\zeta)}{\sinh(\lambda - \lambda_a)}.$$
 (2.1.42)

 $|\Psi(\{\lambda_a\}_{a=1}^M)\rangle \neq 0$ is an Eigenstate of the transfer matrix $t(\lambda)$ and $\Lambda(\lambda|\{\lambda_a\}_{a=1}^M)$ the Eigenvalue of the transfer matrix $t(\lambda)$ if the second term on the right hand side of (2.1.41) vanishes. For pairwise distinct λ'_a s such that $\lambda_a \neq \pm i\zeta$ for all a and $\lambda_a - \lambda_b \neq \pm i\zeta$, this implies that it holds

$$\frac{\mathbf{a}(\lambda_a)}{\mathbf{d}(\lambda_a)} \cdot \prod_{\substack{b=1\\b\neq a}}^{M} \frac{\sinh(\lambda_a - \lambda_b + \mathrm{i}\zeta)}{\sinh(\lambda_a - \lambda_b - \mathrm{i}\zeta)} = 1, \ a = 1, \dots, M.$$
(2.1.43)

Equations (2.1.43) correspond to the Bethe equations of the XXZ chain. $\{\lambda_a\}_{a=1}^M$ are called the Bethe roots. The Eigenstates of the transfer matrix can also be constructed by using the covector

$$\langle \Psi\{\lambda_a\}_{a=1}^M | = \langle 0| \prod_{a=1}^M C(\lambda_a).$$
(2.1.44)

The above result does not ensure that the algebraic Bethe Ansatz provides one with a complete set of Eigenvectors of the XXZ spin-1/2 chain. The issue of completeness in the case of the inhomogeneous model was settled in a generic setting in the works [119, 120, 168]. In [137], completeness is shown for the case of the anti-periodic XXX chain for arbitrary spin again, in the generic inhomogeneous model setting. And finally, one is directed to the paper of Mukhin, Tarasov and Varchenko [135] where completeness of the Bethe vectors, in an appropriate sense, was established for the *per se* XXX chain.

Aside to the completeness issues, there are other problems associated to the description of the solutions to the Bethe Ansatz equation (2.1.43). In 1938, Húlthen identified the Bethe roots characterising the ground state

of the XXX spin chain. A satisfactory proof of the identification of Bethe roots for the ground state of the XXZ chain was given in 1966 by Yang and Yang [179]. They prove that the ground state of the XXZ chain is unique by applying the Perron-Frobenius theorem. This problem is most conveniently studied by presenting the Bethe equations in their logarithmic form:

$$\frac{\mathrm{i}}{2\pi} \ln\left[\frac{\sinh(\lambda_a + \mathrm{i}\zeta/2)}{\sinh(\lambda_a - \mathrm{i}\zeta/2)}\right] - \frac{1}{2\pi L} \sum_{a=1}^M \theta(\lambda_a - \lambda_b) + \frac{M}{2L} = \frac{n_a}{L}$$
(2.1.45)

where the function θ is defined as

$$\theta(\lambda) = \begin{cases} \operatorname{iln}\left[\frac{\sinh(i\zeta+\lambda)}{\sinh(i\zeta-\lambda)}\right], & \text{for } |\mathfrak{I}(\lambda)| < \zeta_{\mathrm{m}} = \min(\zeta, \pi - \zeta), \\ -\pi \operatorname{sgn}(\pi - 2\zeta) + \operatorname{iln}\left[\frac{\sinh(i\zeta+\lambda)}{\sinh(\lambda-i\zeta)}\right], & \text{for } \zeta_{\mathrm{m}} < |\mathfrak{I}(\lambda)| < \pi/2 \end{cases}$$
(2.1.46)

with ln corresponding to the principle branch of the logarithm. The function $\lambda \mapsto \theta(\lambda)$ is an $i\pi$ -periodic analytic function on $\mathbb{C} \setminus \{\mathbb{R}^+ \pm i\zeta_m + i\pi\mathbb{Z}\}$ with cuts on $\mathbb{R}^+ \pm i\zeta_m + i\pi\mathbb{Z}$. We will denote by $\theta_{\pm}(z)$ the \pm boundary value of θ , *viz*. the limit $\theta_{\pm}(z) = \lim_{\epsilon \to 0^+} \theta(z \pm i\epsilon)$. Note that the \pm boundary values differ only if $z \in \{\mathbb{R}^+ \pm i\zeta_m + i\pi\mathbb{Z}\}$.

In equation (2.1.45), n_a are certain integers whose choice allows one, in principle, to differentiate between different solutions. These integers can be chosen inside a certain subset of \mathbb{Z} which depends on L, M and ζ . For instance, Yang and Yang [179] have shown that the Bethe roots describing the ground state in the sector with fixed magnetisation $\frac{1}{2}L - M$ are given by the real valued solution to the equations (2.1.43) with $n_a = a - (M+1)/2$.

The computation of the spectrum of the transfer matrix of the XXZ spin-1/2 chain by the algebraic Bethe Ansatz represents an important achivement. However, despite the fact that the Eigenvalues (2.1.42) are accessible in an explicit way, the calculation of any thermal average, even $tr_{b_{XXZ}} \left[e^{-\frac{H_{XXZ}}{T}} \right]$, remains a rather difficult task. Consequently understanding the thermodynamics of the model also becomes a very complicated one. A great deal of effort [31, 32, 53, 59, 91, 92, 93, 100, 101, 155, 156, 158, 160, 175]-[166] was necessary in order to overcome this issue which culminated in the definition of an adequate *quantum transfer matrix* thus leading to more efficient computations of the physical quantities at finite temperature.

2.1.4 The quantum transfer matrix

The strategy behind the construction of the quantum transfer matrix relies on a simple yet very important ingredient which is the Trotter-Suzuki formula [155, 154]. Consider a sequence of bounded operators \mathfrak{A}_N , $N \in \mathbb{N}$, which converges in norm to a bounded operator \mathfrak{A} . Then we have the Trotter formula

$$\lim_{N \to \infty} \left(1 + \frac{\mathfrak{A}_N}{N} \right)^N = e^{\mathfrak{A}}.$$
(2.1.47)

The use of this formula to the description of the thermodynamics of quantum spin systems was pioneered by Suzuki [155, 154]. We now explain how (2.1.47) may be used for the description of the XXZ chain at finite temperature.

The R-matrix (2.1.21) allows one to introduce two types of monodromy matrices $T_k(\lambda)$ and $T_k(\lambda)$

$$\mathbf{T}_{k}(\lambda) = \mathbf{R}_{kL}(\lambda) \dots \mathbf{R}_{k1}(\lambda) \quad \text{and} \quad \mathbf{T}_{k}(\lambda) = \mathbf{R}_{1k}^{\mathbf{t}_{k}}(-\lambda) \dots \mathbf{R}_{Lk}^{\mathbf{t}_{k}}(-\lambda), \quad (2.1.48)$$

The superscript \mathfrak{t}_k corresponds to the partial transposition with respect to the space \mathfrak{h}_k . One can then write down the transfer matrices $\mathfrak{t}(\lambda)$ and $\tilde{\mathfrak{t}}(\lambda)$ defined as the traces with respect to the auxiliary spaces \mathfrak{h}_k of the monodromy matrices $\mathfrak{T}_k(\lambda)$ and $\tilde{\mathfrak{T}}_k(\lambda)$ respectively:

$$t(\lambda) = tr_{\mathfrak{h}_k}[T_k(\lambda)] \quad \text{and} \quad \widetilde{t}(\lambda) = tr_{\mathfrak{h}_k}[\widetilde{T}_k(\lambda)]. \quad (2.1.49)$$

For small λ these transfer matrices admit the expansion

$$t(\lambda) = U \cdot \left[id + \lambda \cdot \frac{H_{XXZ}|_{h=0}}{2J\sinh(-i\zeta)} + \mathcal{O}(\lambda^2) \right] \text{ and } \widetilde{t}(\lambda) = \left[id - \lambda \cdot \frac{H_{XXZ}|_{h=0}}{2J\sinh(-i\zeta)} + \mathcal{O}(\lambda^2) \right] \cdot U^{-1} \quad (2.1.50)$$

where U is the shift operator introduced in (2.1.30) and $H_{XXZ}|_{h=0}$ is the XXZ spin-1/2 Hamiltonian at zero magnetic field.

Then, as observed in [59, 98, 99, 158]

$$\lim_{N \to \infty} \left\{ \mathsf{t} \left(-\frac{\beta}{N} \right) \cdot \tilde{\mathsf{t}} \left(\frac{\beta}{N} \right) \right\}^{N} \times \prod_{a=1}^{L} e^{\frac{h}{2T} \sigma_{a}^{z}} \\
= \lim_{N \to \infty} \left\{ \mathsf{U} \cdot \left[1 - \frac{1}{N} \beta \frac{\mathsf{H}_{\mathsf{XXZ}}|_{h=0}}{2J \sinh(-\mathsf{i}\zeta)} + \mathscr{O} \left(\frac{1}{N^{2}} \right) \right] \cdot \left[1 - \frac{1}{N} \beta \frac{\mathsf{H}_{\mathsf{XXZ}}|_{h=0}}{2J \sinh(-\mathsf{i}\zeta)} + \mathscr{O} \left(\frac{1}{N^{2}} \right) \right] \cdot \mathsf{U}^{-1} \right\}^{N} \\
= \lim_{N \to \infty} \mathsf{U} \cdot \left[1 - \frac{1}{N} \beta \frac{\mathsf{H}_{\mathsf{XXZ}}|_{h=0}}{J \sinh(-\mathsf{i}\zeta)} + \mathscr{O} \left(\frac{1}{N^{2}} \right) \right]^{N} \cdot \mathsf{U}^{-1} = e^{-\frac{1}{T}\mathsf{H}_{\mathsf{XXZ}}} \tag{2.1.51}$$

since H_{XXZ} is translation invariant and where we introduced

$$\beta = \frac{J \cdot \sinh(-i\zeta)}{T}.$$
(2.1.52)

This Trotter discretisation of the Boltzmann operator introduces a new auxiliary space $\mathfrak{h}_{\mathfrak{q}} = \bigotimes_{k=0}^{2N} \mathfrak{h}_{a_k}$, realised as a tensor product of the 2*N* auxiliary spaces, that will appear in the construction of the transfer matrix. Indeed from (2.1.51) one has that

$$\mathbf{e}^{-\frac{1}{T}\mathbf{H}_{XXZ}} = \lim_{N \to \infty} \left\{ \mathrm{tr}_{a_{1} \dots a_{2N}} \left[\left\{ \mathbf{R}_{a_{2N}1}^{\mathbf{t}_{a_{2N}}} \left(-\frac{\beta}{N} \right) \mathbf{R}_{1a_{2N-1}} \left(\frac{\beta}{N} \right) \cdots \mathbf{R}_{a_{2}1}^{\mathbf{t}_{a_{2}}} \left(-\frac{\beta}{N} \right) \mathbf{R}_{1a_{1}} \left(\frac{\beta}{N} \right) \cdot \mathbf{e}^{\frac{h}{2T}\sigma_{1}^{z}} \right\} \right] \right\}$$
$$\cdots \left\{ \mathbf{R}_{a_{2N}L}^{\mathbf{t}_{a_{2N}L}} \left(-\frac{\beta}{N} \right) \mathbf{R}_{La_{2N-1}} \left(\frac{\beta}{N} \right) \cdots \mathbf{R}_{a_{2}L}^{\mathbf{t}_{a_{2}}} \left(-\frac{\beta}{N} \right) \mathbf{R}_{La_{1}} \left(\frac{\beta}{N} \right) \cdot \mathbf{e}^{\frac{h}{2T}\sigma_{L}^{z}} \right\} \right] \right\}$$
$$= \lim_{N \to \infty} \left\{ \mathrm{tr}_{a_{1} \dots a_{2N}} \left[\mathbf{T}_{\mathfrak{q};1}(0) \cdots \mathbf{T}_{\mathfrak{q};L}(0) \right] \right\}$$
$$(2.1.53)$$

where $T_{q;a}(\xi)$ is the quantum monodromy matrix

$$\mathbf{T}_{\mathfrak{q};a}(\xi) = \mathbf{R}_{a_{2N}a}^{\mathbf{t}_{a_{2N}a}} \left(\xi - \frac{\beta}{N}\right) \mathbf{R}_{aa_{2N-1}} \left(\xi + \frac{\beta}{N}\right) \cdots \mathbf{R}_{a_{2}a}^{\mathbf{t}_{a_{2}}} \left(\xi - \frac{\beta}{N}\right) \mathbf{R}_{aa_{1}} \left(\xi + \frac{\beta}{N}\right) \cdot \mathbf{e}^{\frac{h}{2T}\sigma_{a}^{z}}$$
(2.1.54)

which has \mathfrak{h}_a as its auxiliary space.

The quantum transfer matrix is defined as the trace with respect to this auxiliary space h_a of the quantum monodromy matrix

$$\mathbf{t}_{\mathfrak{q}}(\boldsymbol{\xi}) = \mathrm{tr}_{\mathfrak{h}_{a}} \big[\mathbf{T}_{\mathfrak{q};a}(\boldsymbol{\xi}) \big]. \tag{2.1.55}$$

The principal advantage of the quantum transfer matrix is that it provides an easier access to the information related to the thermodynamics of the system being studied. As we discussed earlier on, the computation of thermodynamically relevant quantities within the framework of the ordinary transfer matrix requires the knowledge of an infinite number of Eigenvalues of the Hamiltonian describing the system. Within the quantum transfer matrix approach numerous physical observables can be accessed from the knowledge of just a few Eigenvalues of the quantum transfer matrix "close" to the largest one. Recall the definition of the *per*-site free energy (2.1.4),

$$f_{\rm XXZ} = -T \cdot \lim_{L \to \infty} \frac{1}{L} \ln \operatorname{tr}_{\mathfrak{h}_{\rm XXZ}} \left[e^{-\frac{1}{T} \operatorname{H}_{\rm XXZ}} \right].$$
(2.1.56)

Upon employing (2.1.53) one gets

$$f_{XXZ} = -\lim_{L \to \infty} \lim_{N \to \infty} \frac{T}{L} \ln \left[\operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}}(\mathfrak{t}_{\mathfrak{q}}(0)^{L}) \right].$$
(2.1.57)

• If one can exchange the limits then it follows that

$$f_{\rm XXZ} = -\lim_{N \to \infty} \lim_{L \to \infty} \frac{T}{L} \ln \left[\operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}}(\mathfrak{t}_{\mathfrak{q}}(0)^{L}) \right].$$
(2.1.58)

• If $t_q(0)$ admits a maximal in modulus, non-degenerate Eigenvalue² $\widehat{\Lambda}_{max}$ then, since

$$\operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}}\left[\operatorname{t}^{L}_{\mathfrak{q}}(0)\right] = \widehat{\Lambda}^{L}_{\max} + \sum_{a=1}^{2^{N}-1} \widehat{\Lambda}^{L}_{a}, \qquad (2.1.59)$$

where $\widehat{\Lambda}_a$ are the other Eigenvalues of the quantum transfer matrix repeated according to their multiplicity, we then have that

$$f_{\rm XXZ} = -\lim_{N \to \infty} T \ln \widehat{\Lambda}_{\rm max} \tag{2.1.60}$$

where the hat above is used to indicate the *N*-dependence of the quantities on the Trotter number. In the remainder of the chapter, we shall establish these two properties rigorously.

2.2 Large temperature expansion of the quantum transfer matrix

2.2.1 A preliminary expansion

In this section we develop a setting which allows one to establish the existence of a spectral gap in the spectrum of the quantum transfer matrix and to rigorously characterise the latter. We, however, start by introducing some notations and definitions.

We recall that given an elementary matrix E^{ik} acting on $\mathscr{L}(\mathbb{C}^2)$, E_a^{ik} stands for its canonical embedding into an operator on $\mathfrak{h}_0 \otimes \mathfrak{h}_{\mathfrak{q}}$ acting non-trivially on the a^{th} tensor product

$$\mathbf{E}_{a}^{ik} = \underbrace{\mathrm{id} \otimes \ldots \otimes \mathrm{id}}_{a-1} \otimes \mathbf{E}^{ik} \otimes \underbrace{\mathrm{id} \otimes \ldots \otimes \mathrm{id}}_{2N-a}.$$
(2.2.1)

For instance, the permutation operator or its partial transpose on the a^{th} space $P_{ab}^{t_a}$ can be expressed as

$$P_{ab} = \sum_{i,k=1}^{2} E_a^{ik} E_b^{ki}, \qquad P_{ab}^{t_a} = \sum_{i,k=1}^{2} E_a^{ik} E_b^{ik}.$$
(2.2.2)

As *per* the explicit expression for the R - matrix (2.1.21) one writes that

$$\mathbf{R}_{ab}\left(-\frac{\beta}{N}\right) = \mathbf{P}_{ab} + \mathbf{N}_{ab},\tag{2.2.3}$$

$$\operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}}(\mathfrak{t}_{\mathfrak{q}}(0)^{L}) = \widehat{\Lambda}_{\max}^{L} \left(\mathrm{e}^{i\widehat{\phi}_{1}L} + \dots + \mathrm{e}^{i\widehat{\phi}_{l}L} \right) + \mathscr{O}(\widehat{\Lambda}_{\max}^{L} \cdot L^{-\infty}),$$

²One would obtain a similar result in case $\widehat{\Lambda}_{max}$ would be degenerate (even 2^N-fold) or if there would be several Eigenvalues of maximal modulus $\widehat{\Lambda}_{max}$ appearing with phases $e^{i\widehat{\phi}_1}, \ldots, e^{i\widehat{\phi}_l}$ as then

where the remainder corresponds to the lower in modulus Eigenvalues and where $e^{i\hat{\phi}_1L} + \cdots + e^{i\hat{\phi}_lL}$ is real. Since the Eigenvalue of the quantum transfer matrix appear in complex conjugate pairs. However, since this is not the case here, we will not dwell any longer on this note.

where

$$N_{ab} = \sum_{i,k=1}^{2} n_{ik} \cdot E_a^{ii} E_b^{kk} \quad \text{with} \quad \begin{cases} n_{11} = n_{22} = \cosh\left(\frac{\beta}{N}\right) - 1 - \coth(-i\zeta) \sinh\left(\frac{\beta}{N}\right) \\ n_{12} = n_{21} = -\frac{\sinh\left(\frac{\beta}{N}\right)}{\sinh(-i\zeta)} \end{cases} \quad . \tag{2.2.4}$$

Define the operators

$$\Pi_l = \mathsf{P}_{2l0}^{\mathfrak{t}_{2l}} \mathsf{P}_{02l-1} \tag{2.2.5}$$

and

$$W_l = \mathbb{R}_{2l0}^{\mathfrak{t}_{2l}} \left(-\frac{\beta}{N}\right) \mathbb{R}_{02l-1} \left(-\frac{\beta}{N}\right) - \Pi_l.$$
(2.2.6)

Further, given $l \ge m$, define

$$\mathbf{\Omega}_{l;m} = \begin{cases} \Pi_{l} \dots \Pi_{m+1} \cdot e^{\frac{h}{2T} \sigma_{0}^{z} \delta_{m0}}, \text{ if } l \ge m+1, \\ e^{\frac{h}{2T} \sigma_{0}^{z} \delta_{m0}}, \text{ if } l = m \end{cases}$$
(2.2.7)

Here and in the following δ_{ab} stands for the Kronecker symbol. We have now introduced enough notations to write down an expansion of the quantum transfer matrix that one may expect to be well structured relatively to the analysis of the high temperature properties of $t_q(0)$.

The expansion of the quantum monodromy matrix (2.1.54) is obtained upon expressing each factor associated to a pair of spaces $\mathfrak{h}_{2l} \otimes \mathfrak{h}_{2l+1}$ in (2.1.54) as $W_l + \Pi_l$ so that one obtains

$$\mathbf{T}_{\mathfrak{q};0}(0) = \mathbf{\Omega}_{N;0} + \sum_{n=1}^{N} \sum_{\boldsymbol{l} \in \mathscr{L}_{N}^{(n)}} \mathscr{O}_{\boldsymbol{l}} \quad \text{with} \quad \mathscr{O}_{\boldsymbol{l}} = \mathbf{\Omega}_{N;l_{n}} \cdot \mathbf{W}_{l_{n}} \cdot \mathbf{\Omega}_{l_{n-1};l_{n-1}} \cdots \mathbf{W}_{l_{1}} \cdot \mathbf{\Omega}_{l_{1}-1;0}, \quad (2.2.8)$$

with $T_{q;0}(\xi)$ given by (2.1.54) and where the summation runs through

$$\mathscr{L}_{N}^{(n)} = \{ \boldsymbol{l} = (l_{1}, \dots, l_{n}) : 1 \le l_{1} < \dots < l_{n} \le N \}.$$
(2.2.9)

The decomposition (2.2.8) entails a similar expansion for the quantum transfer matrix (2.1.55)

$$\mathbf{t}_{\mathfrak{q}}(0) = \boldsymbol{\omega}_{N;0} + \delta \mathbf{t}_{q}, \qquad (2.2.10)$$

where

$$\boldsymbol{\omega}_{N;0} = \operatorname{tr}_{\mathfrak{h}_0} \left[\boldsymbol{\Omega}_{N;0} \right] \quad \text{and} \quad \delta \mathsf{t}_q = \sum_{n=1}^N \sum_{\boldsymbol{l} \in \mathscr{L}_N^{(n)}} \mathsf{O}_{\boldsymbol{l}}, \quad \text{with} \quad \mathsf{O}_{\boldsymbol{l}} = \operatorname{tr}_{\mathfrak{h}_0} [\mathscr{O}_{\boldsymbol{l}}]. \tag{2.2.11}$$

The decomposition (2.2.10) of the quantum transfer matrix allows one to study its high temperature expansion. The strategy consists in expressing the operators $\boldsymbol{\omega}_{N;0}$ and $O_{\boldsymbol{l}}$ as sums of rank one operators what then allows to easily compute any power of $t_q(0)$ explicitly. We describe how this unfolds in the next subsection devoted to the analysis of the properties of $\boldsymbol{\omega}_{N;0}$. Then we characterise the sub-leading terms by repeating the, now more involved, procedure for the operator $O_{\boldsymbol{l}}$.

2.2.2 Analysis of the leading term of the quantum transfer matrix expansion at high temperature

We introduce the following convention for writing vectors in $\mathfrak{h}_{\mathfrak{q}} = \bigotimes_{a=1}^{2N} \mathfrak{h}_a$. Given vectors $\mathbf{v}_1, \ldots, \mathbf{v}_{2N}$ in $\mathfrak{h}_1, \ldots, \mathfrak{h}_{2N}$, we agree to denote their 2*N*-fold tensor product as

$$\boldsymbol{\nu}_1 \otimes \ldots \otimes \boldsymbol{\nu}_{2N} = \prod_{a=1}^{2N} \boldsymbol{\nu}_a^{(a)}. \tag{2.2.12}$$

In this notation $v_a^{(a)}$ thus stands for the *a*th vector appearing in the full tensor product. We remind that, as introduced in (2.1.35), $e_a, a = 1, 2$ is the canonical basis of \mathbb{C}^2 . We now establish several properties of the first term $\boldsymbol{\omega}_{N;0}$ of the expansion (2.2.10). These properties will be useful, later on, when characterising the leading Eigenvalue of the quantum transfer matrix.

Lemma 2.2.1. The operator $\boldsymbol{\omega}_{N;0}$ introduced in (2.2.11) has rank 1 and takes the form

$$\boldsymbol{\omega}_{N;0} = \boldsymbol{v} \cdot \boldsymbol{w}^{t} \quad with \quad \begin{cases} \boldsymbol{v} = \sum_{\boldsymbol{i} \in \{1,2\}^{N}} e^{\frac{h}{2T} \varepsilon_{i_{N}}} \prod_{s=1}^{N} \left\{ \boldsymbol{e}_{i_{s}}^{(2s)} \boldsymbol{e}_{i_{s-1}}^{(2s-1)} \right\}, \\ \boldsymbol{w} = \sum_{\boldsymbol{j} \in \{1,2\}^{N}} \prod_{s=1}^{N} \left\{ \boldsymbol{e}_{j_{s}}^{(2s)} \boldsymbol{e}_{j_{s}}^{(2s-1)} \right\} \end{cases}$$
(2.2.13)

where $\varepsilon_i = (-1)^{i-1}$, $\mathbf{i} = (i_1, \dots, i_N)$ and respectively $\mathbf{j} = (j_1, \dots, j_N)$. \mathfrak{t} represents the global transposition with respect to full tensor product space. Also we made use of periodic boundary conditions $i_0 \equiv i_N$.

Furthermore, it holds that

$$(\boldsymbol{w},\boldsymbol{v}) = 2\cosh\left(\frac{h}{2T}\right), \quad \|\boldsymbol{v}\|^2 = 2^N \cosh\left(\frac{h}{T}\right) \quad and \quad \|\boldsymbol{w}\|^2 = 2^N.$$
 (2.2.14)

Proof. The operator given by (2.2.7) can be recast as

$$\begin{aligned} \mathbf{\Omega}_{l;m} &= \mathbf{P}_{2l0}^{t_{2l}} \mathbf{P}_{02l-1} \cdots \mathbf{P}_{2m+2}^{t_{2m+2}} \mathbf{P}_{02m+1} \cdot \mathbf{e}_{2T}^{\frac{h}{2T}} \sigma_0^z \delta_{m0} \\ &= \left(\sum_{i,k=\{1,2\}} \mathbf{E}_{2l}^{ik} \mathbf{E}_{0}^{ik}\right) \left(\sum_{i,k=\{1,2\}} \mathbf{E}_{0}^{ik} \mathbf{E}_{2l-1}^{ki}\right) \cdots \left(\sum_{i,k=\{1,2\}} \mathbf{E}_{0}^{ik} \mathbf{E}_{2m+1}^{ki}\right) \cdot \mathbf{e}_{2T}^{\frac{h}{2T}} \sigma_0^z \delta_{m0}. \end{aligned}$$

Upon expanding the products, one gets

$$\mathbf{\Omega}_{l;m} = \sum_{\substack{i_s,k_s \in \{1,2\}\\s=2m+1,\dots,2l}} \prod_{s=2m+1}^{2l} \left\{ \mathsf{E}_s^{i_sk_s} \right\} \cdot \mathsf{E}_0^{i_{2l}k_{2l}} \mathsf{E}_0^{k_{2l-1}i_{2l-1}} \cdots \mathsf{E}_0^{k_{2m+1}i_{2m+1}} \cdot \mathsf{e}^{\frac{h}{2T}\varepsilon_{i_{2m+1}}\delta_{m0}}.$$
(2.2.15)

The algebra of elementary matrices $E^{ab}E^{cd} = \delta_{bc}E^{ad}$ then allows one to compute the product of matrices acting on the auxiliary space

$$\mathbf{E}_{0}^{i_{2l}k_{2l}}\mathbf{E}_{0}^{k_{2l-1}i_{2l-1}}\dots\mathbf{E}_{0}^{k_{2m+1}i_{2m+1}} = \mathbf{E}_{0}^{i_{2l}i_{2m+1}}\cdot\prod_{s=m+1}^{l}\left\{\delta_{k_{2s}k_{2s-1}}\right\}\cdot\prod_{s=m+2}^{l}\left\{\delta_{i_{2s-1}i_{2s-2}}\right\}.$$
(2.2.16)

The Kronecker symbols allow one to get rid of the summations over the odd labelled variables

 i_{2s-1} with $s = m+2, \dots, l$ and k_{2s-1} with $s = m+1, \dots, l$. (2.2.17)

Then, relabelling the even labelled variables as

$$\{k_{2s}, i_{2s}\} \hookrightarrow \{k'_s, i'_s\} \quad \text{for} \quad s = m+1, \dots, l \quad \text{and} \quad i_{2m+1} \hookrightarrow i'_m \tag{2.2.18}$$

one gets that

$$\mathbf{\Omega}_{l;m} = \sum_{\substack{\{i_s\}_m^l \\ i_s=1}}^2 \sum_{\substack{\{k_s\}_{m+1}^l \\ k_s=1}}^2 \prod_{s=m+1}^l \left\{ \mathsf{E}_{2s}^{i_sk_s} \mathsf{E}_{2s-1}^{i_{s-1}k_s} \right\} \cdot \mathsf{E}_0^{i_l i_m} \cdot \mathsf{e}^{\frac{h}{2T}\varepsilon_{i_m}\delta_{m0}}.$$
(2.2.19)

At this point, one can readily take the trace over the auxiliary space in the case of $\Omega_{N;0}$ leading to

$$\boldsymbol{\omega}_{N;0} = \operatorname{tr}_{\mathfrak{h}_0} \left[\boldsymbol{\Omega}_{N;0} \right] = \sum_{\{i_s,k_s\}_1^N} e^{\frac{h}{2T} \boldsymbol{\varepsilon}_{i_N}} \prod_{s=1}^N \left\{ \mathsf{E}_{2s}^{i_s k_s} \mathsf{E}_{2s-1}^{i_{s-1} k_s} \right\}.$$
(2.2.20)

The dependence on the identity operator on the auxiliary space \mathfrak{h}_0 has been projected out in the elementary matrices appearing above. Finally, since an elementary matrix can be recast as $\mathbf{E}^{ab} = \boldsymbol{e}_a \cdot \boldsymbol{e}_b^t$, one gets

$$\prod_{s=1}^{N} \left\{ \mathsf{E}_{2s}^{i_{s}k_{s}} \mathsf{E}_{2s-1}^{i_{s-1}k_{s}} \right\} = \prod_{s=1}^{N} \left\{ \boldsymbol{e}_{i_{s}}^{(2s)} \boldsymbol{e}_{i_{s-1}}^{(2s-1)} \right\} \cdot \prod_{s=1}^{N} \left\{ \boldsymbol{e}_{k_{s}}^{(2s)} \boldsymbol{e}_{k_{s}}^{(2s-1)} \right\}^{\mathfrak{t}}.$$
(2.2.21)

As a result, the above factorisation allows one to separate the sums over the indices i_s 's and k_s 's leading to (2.2.13)

The equations (2.2.14) follow from direct calculations.

2.2.3 Analysis of the expansion of δt_q

We now establish various properties of the operator O_l arising in (2.2.10). We remark that one has the following representation for the operator W_l (2.2.6)

$$W_{l} = \sum_{i,k=1}^{2} M_{l}^{ik} E_{0}^{ik}, \text{ where } M_{l}^{ik} = \underbrace{\operatorname{id} \otimes \ldots \otimes \operatorname{id}}_{2l-2} \otimes M^{ik} \otimes \underbrace{\operatorname{id} \otimes \ldots \otimes \operatorname{id}}_{2N-2l},$$
(2.2.22)

and

$$\mathbf{M}^{ik} = \sum_{\alpha=1}^{4} \mathbf{v}_{ik;\alpha} \cdot (\mathbf{w}_{ik;\alpha})^{\mathsf{t}}, \qquad (2.2.23)$$

for some explicitly computable vectors $v_{ik;\alpha}$ and $w_{ik;\alpha}$. The latter are normalised such that

$$\|\boldsymbol{v}_{ik;\alpha}\| = \frac{1}{2} \text{ and } \|\boldsymbol{w}_{ik;\alpha}\| \le C_{\boldsymbol{w}} \cdot \left|\frac{\beta}{N}\right|, \qquad (2.2.24)$$

for a constant $C_{w} > 0$ and any $\alpha \in [[1;4]]$. We employ the representations observed above for $v_{ik;\alpha}$ and $w_{ik;\alpha}$ in order to decompose the operator O_{l} along the lines of what has been carried out in the previous subsection.

Lemma 2.2.2. Let $l = (l_1, \ldots, l_n)$. Then the operator O_l defined in (2.2.11) can be decomposed as

$$O_{l} = \sum_{i,\hat{j}_{l}} \sum_{\alpha_{l}} x_{i}^{(\alpha_{l},l)} \cdot \left(y_{i,\hat{j}_{l}}^{(\alpha_{l},l)} \right)^{t}.$$
(2.2.25)

In the above, one sums over the vectors

$$\boldsymbol{\alpha}_{l} = (\alpha_{l_1}, \dots, \alpha_{l_n}) \in [\![1; 4]\!]^n, \tag{2.2.26}$$

and

$$\mathbf{i} = (i_1, \dots, i_N) \in \{1, 2\}^N, \quad \widehat{\mathbf{j}}_{\mathbf{l}} = (j_1, \dots, j_{l_1 - 1}, \widehat{j}_{l_1}, j_{l_1 + 1}, \dots, \widehat{j}_{l_n}, \dots, j_N) \in \{1, 2\}^{N - n}, \tag{2.2.27}$$

where the `indicates the coordinates which are omitted . Furthermore, one has

$$\boldsymbol{x}_{\boldsymbol{i}}^{(\boldsymbol{\alpha}_{l},\boldsymbol{l})} = \mathrm{e}^{\frac{h}{2T}} \boldsymbol{\varepsilon}_{i_{N}} \prod_{\substack{s=1\\ \neq l_{1},\dots,l_{n}}}^{N} \left\{ \boldsymbol{e}_{i_{s}}^{(2s)} \boldsymbol{e}_{i_{s-1}}^{(2s-1)} \right\} \cdot \prod_{r=1}^{n} \boldsymbol{v}_{i_{l_{r}}i_{l_{r-1}};\alpha_{l_{r}}}^{(l_{r})},$$
(2.2.28)

$$\mathbf{y}_{i,\hat{j}_{l}}^{(\boldsymbol{\alpha}_{l},l)} = \prod_{\substack{s=1\\ \neq l_{1},\dots,l_{n}}}^{N} \left\{ \boldsymbol{e}_{j_{s}}^{(2s)} \boldsymbol{e}_{j_{s}}^{(2s-1)} \right\} \cdot \prod_{r=1}^{n} \boldsymbol{w}_{i_{lr}i_{lr-1};\boldsymbol{\alpha}_{lr}}^{(l_{r})}.$$
(2.2.29)

Note that in the above expression for $\mathbf{x}_{i}^{(\alpha_{l},l)}$ we use periodic boundary conditions for the indices of \mathbf{i} , viz. $i_{0} \equiv i_{N}$.

In (2.2.28) and (2.2.29), the notations $\mathbf{v}_{ij;\alpha}^{(l)}$ and $\mathbf{w}_{ij;\alpha}^{(l)}$ mean that we consider the vector $\mathbf{v}_{ij;\alpha}$, resp. $\mathbf{w}_{ij;\alpha}$ appearing on the positions reserved to the spaces $\mathfrak{h}_{2l} \otimes \mathfrak{h}_{2l+1}$ in the tensor-product decomposition of the full vector.

Proof. Starting from the expression (2.2.8) for \mathcal{O}_l we insert the expressions of the operators $\Omega_{l:m}$ and W_l so that

$$\mathscr{O}_{l} = \sum_{\left\{\{i_{s}^{(r)}\}_{s=l_{r}}^{l_{r+1}-1}\right\}_{r=0}^{n}} \sum_{\left\{\{j_{s}^{(r)}\}_{s=l_{r}+1}^{l_{r+1}-1}\right\}_{r=0}^{n}} \sum_{\{q_{l}, p_{t}\}_{1}^{n}} \prod_{r=0}^{n} \prod_{s=l_{r}+1}^{l_{r+1}-1} \left\{E_{2s}^{i_{s}^{(r)}} E_{2s-1}^{(r)}\right\}_{2s-1}^{r} \right\} \prod_{t=1}^{n} \mathbb{M}_{l_{t}}^{q_{t}p_{t}} \times E_{0}^{i_{t}n} E_{0}^{i_{t}n} E_{0}^{q_{t}p_{t}} E_{0}^{i_{t}n-1} E_{0}^{i_{t}n-1}} \dots E_{0}^{q_{1}p_{1}} E_{0}^{i_{t}n-1} E_{0}^{i_{t}n-1} E_{0}^{i_{t}n-1}} \dots E_{0}^{q_{1}p_{1}} E_{0}^{i_{t}n-1} E_{0}^{i_{t}n-1} E_{0}^{i_{t}n-1}} \dots E_{0}^{q_{1}p_{1}} E_{0}^{i_{t}n-1} E_{0}^{i_{t}n-1} E_{0}^{i_{t}n-1}} \dots E_{0}^{i_{t}n-1} E_{0}^{i_{t}n-1}} \dots E_{0}^{i_{t}n-1} E_{0}^{i_{t}n-1}} \dots E_{0}^{i_{t}n-1}} \dots E_{0}^{i_{t}n-1} E_{0}^{i_{t}n-1}} \dots E_{0}^{i$$

upon agreeing on $l_0 = 0$ and $l_{n+1} = N + 1$. The last line can be simplified as follows

$$\mathbf{E}_{0}^{i_{N}^{(n)}i_{l_{n}}^{(n)}}\mathbf{E}_{0}^{q_{n}p_{n}}\mathbf{E}_{0}^{i_{l_{n-1}}^{(n-1)}i_{l_{n-1}}^{(n-1)}}\mathbf{E}_{0}^{q_{n-1}p_{n-1}}\dots\mathbf{E}_{0}^{q_{1}p_{1}}\mathbf{E}_{0}^{i_{l_{1}-1}^{(0)}i_{0}^{(0)}} = \mathbf{E}_{0}^{i_{N}^{(n)}i_{0}^{(0)}}\cdot\prod_{s=1}^{n}\left\{\delta_{i_{l_{s}}^{(s)}q_{s}}\right\}\prod_{s=1}^{n}\left\{\delta_{p_{s}i_{l_{s-1}}^{(s-1)}}\right\}.$$
(2.2.31)

The Kronecker symbols above allow one to compute the sums over the p_t and q_t indices. In order to have a more compact expression it is useful to change the summations variables as

$$i_a = i_a^{(r)}, \text{ if } l_r \le a \le l_{r+1} - 1 \text{ with } a \in [[0; N]],$$
 (2.2.32)

$$j_a = j_a^{(r)}, \text{ if } l_r \le a \le l_{r+1} - 1 \text{ with } a \in [[1;N]] \setminus \{l_1, \dots, l_n\}.$$
 (2.2.33)

Then one has that

$$\mathscr{O}_{\boldsymbol{l}} = \sum_{\{i_a\}_{a=0}^{N}} \sum_{\substack{\{j_a\}_{a=0}^{N}\\ a \neq l_1, \dots, l_n}} \prod_{\substack{s=1\\ \neq l_1, \dots, l_n}}^{n} \left\{ \mathsf{E}_{2s}^{i_s j_s} \mathsf{E}_{2s-1}^{i_{s-1} j_s} \right\} \cdot \prod_{r=1}^{n} \mathsf{M}_{l_r}^{i_{l_r} i_{l_r-1}} \cdot \mathsf{E}_{0}^{i_N i_0} \cdot \mathsf{e}^{\frac{h}{2T} \varepsilon_{i_0}}.$$
(2.2.34)

At this stage, one may readily take the trace over the auxiliary space h_0 . Upon projecting out the dependence on the identity on h_0 , it remains to observe that

$$\prod_{\substack{s=1\\ \neq l_1,\ldots,l_n}}^n \left\{ \mathbf{E}_{2s}^{i_s j_s} \mathbf{E}_{2s-1}^{i_{s-1} j_s} \right\} \cdot \prod_{r=1}^n \mathbf{M}_{l_r}^{i_{l_r} i_{l_{r-1}}}$$

$$= \sum_{\boldsymbol{\alpha}_l} \prod_{\substack{s=1\\ \neq l_1,\ldots,l_n}}^n \left\{ \boldsymbol{e}_{i_s}^{(2s)} \boldsymbol{e}_{i_s}^{(2s-1)} \right\} \prod_{r=1}^n \boldsymbol{v}_{i_{l_r} i_{l_{r-1}}; \boldsymbol{\alpha}_{l_r}} \cdot \left\{ \prod_{\substack{s=1\\ \neq l_1,\ldots,l_n}}^n \left\{ \boldsymbol{e}_{j_s}^{(2s)} \boldsymbol{e}_{j_s}^{(2s-1)} \right\} \prod_{r=1}^n \boldsymbol{w}_{i_{l_r} i_{l_{r-1}}; \boldsymbol{\alpha}_{l_r}} \right\}^{\mathfrak{t}}, \qquad (2.2.35)$$

where $\boldsymbol{\alpha}_l$ is defined in (2.2.26). This entails the claim.

We now build on the expansion (2.2.25) to compute products of various operators. We first discuss the case of two operators and then present the general formula for a string of *M* operators. However, first, we need to introduce some notations. Given two vectors $l \in \mathbb{N}^n$ and $r \in \mathbb{N}^m$, let \mathscr{S}_l and $\mathscr{S}_{l\cap r}$ denote the sets

$$\mathscr{S}_{l} = \{l_{1}, \dots, l_{n}\}, \ \mathscr{S}_{r} = \{r_{1}, \dots, r_{m}\}.$$
 (2.2.36)

We define further

$$\mathscr{S}_{l\cap r} = \mathscr{S}_l \cap \mathscr{S}_r, \ \mathscr{S}_{l\cup r} = \mathscr{S}_l \cup \mathscr{S}_r$$

as well as

$$\mathscr{S}_{l}^{c} = \mathscr{S}_{l} \backslash \mathscr{S}_{l \cap r}, \ \mathscr{S}_{r}^{c} = \mathscr{S}_{r} \backslash \mathscr{S}_{l \cap r}$$

$$(2.2.37)$$

Corollary 2.2.1. Let

$$\mathscr{S}_{l \cup r} = \{t_1, \dots, t_u\}, \text{ with } 1 \le t_1 < \dots < t_u \le N.$$
 (2.2.38)

Then

$$O_{\boldsymbol{l}} \cdot O_{\boldsymbol{r}} = \sum_{\boldsymbol{i}, \boldsymbol{\hat{q}_{r}}} \sum_{\boldsymbol{\alpha}_{l}, \boldsymbol{\beta}_{r}} \left(2 \cosh\left[\frac{h}{2T}\right] \right)^{\delta_{n,0}\delta_{m,0}} \cdot \boldsymbol{x}_{\boldsymbol{i}}^{(\boldsymbol{\alpha}_{l},\boldsymbol{l})} \cdot \left\{ \sum_{\{p_{t_{a}}\}_{a=1}^{u}} e^{\frac{h}{2T}\varepsilon_{p_{t_{a}}}} \prod_{t_{k}\in\mathscr{S}_{l\cap\boldsymbol{r}}} \left(\boldsymbol{w}_{i_{t_{k}}i_{t_{k}-1};\boldsymbol{\alpha}_{t_{k}}}, \boldsymbol{v}_{p_{t_{k}}p_{t_{k-1}}}; \beta_{t_{k}}\right) \right) \\ \times \prod_{t_{k}\in\mathscr{S}_{l}^{c}} \left(\boldsymbol{w}_{i_{t_{k}}i_{t_{k}-1};\boldsymbol{\alpha}_{t_{k}}}, \boldsymbol{e}_{p_{t_{k-1}}} \otimes \boldsymbol{e}_{p_{t_{k}}} \right) \cdot \prod_{t_{k}\in\mathscr{S}_{\boldsymbol{r}}^{c}} \left(\boldsymbol{u}, \boldsymbol{v}_{p_{t_{k}}p_{t_{k-1}}}; \beta_{t_{k}}\right) \right\} \cdot \left(\boldsymbol{y}_{p_{l},\boldsymbol{\hat{q}_{r}}}^{(\boldsymbol{\beta}_{r},\boldsymbol{r})}\right)^{t}.$$
(2.2.39)

Above, we use periodic boundary conditions on the indices of t_a , viz. $t_0 = t_u$, we agree upon

$$\boldsymbol{u} = \boldsymbol{e}_1 \otimes \boldsymbol{e}_1 + \boldsymbol{e}_2 \otimes \boldsymbol{e}_2 \tag{2.2.40}$$

and have set

$$\boldsymbol{p}_{t} = \left(\underbrace{p_{t_{u}}, \dots, p_{t_{u}}}_{t_{1}-1}, \underbrace{p_{t_{1}}, \dots, p_{t_{1}}}_{t_{2}-t_{1}}, \dots, \underbrace{p_{t_{u-1}}, \dots, p_{t_{u-1}}}_{t_{u}-t_{u-1}}, \underbrace{p_{t_{u}}, \dots, p_{t_{u}}}_{N-t_{u}+1}\right).$$
(2.2.41)

Proof. Using (2.2.25) one obviously has

$$O_{l} \cdot O_{r} = \sum_{i,\hat{j}_{l}} \sum_{\alpha_{l}} \sum_{p,\hat{q}_{r}} \sum_{\beta_{r}} x_{i}^{(\alpha_{l},l)} \cdot \left(y_{i,\hat{j}_{l}}^{(\alpha_{l},l)}, x_{p}^{(\beta_{r},r)} \right) \cdot \left(y_{p,\hat{q}_{r}}^{(\beta_{r},r)} \right)^{t}.$$
(2.2.42)

The scalar product $\left(y_{i,\widehat{j}_{l}}^{(\boldsymbol{\alpha}_{l},l)}, x_{p}^{(\boldsymbol{\beta}_{r},r)}\right)$ in the above is computed as

$$\begin{pmatrix} \mathbf{y}_{i,\hat{j}_{l}}^{(\boldsymbol{\alpha}_{l},l)}, \mathbf{x}_{p}^{(\boldsymbol{\beta}_{r},r)} \end{pmatrix} = e^{\frac{\hbar}{2T}\boldsymbol{\varepsilon}_{p_{N}}} \cdot \prod_{\substack{s=1\\s \notin \mathscr{S}_{l \cup r}}}^{N} \left\{ \delta_{j_{s}p_{s-1}} \delta_{p_{s}p_{s-1}} \right\} \prod_{k \in \mathscr{S}_{l \cap r}} \left(\mathbf{w}_{i_{k}i_{k-1};\boldsymbol{\alpha}_{k}}, \mathbf{v}_{p_{k}p_{k-1};\boldsymbol{\beta}_{k}} \right)$$

$$\times \prod_{k \in \mathscr{S}_{l}^{c}} \left(\mathbf{w}_{i_{k}i_{k-1};\boldsymbol{\alpha}_{k}}, \mathbf{e}_{p_{k-1}} \otimes \mathbf{e}_{p_{k}} \right) \cdot \left(\mathbf{e}_{j_{s}} \otimes \mathbf{e}_{j_{s}}, \mathbf{v}_{p_{s}p_{s-1};\boldsymbol{\beta}_{s}} \right).$$

$$(2.2.43)$$

The product over Kronecker symbols allows one to compute most of the sums over the p_a 's and j_a 's occurring in (2.2.42).

• Consider the case when $\mathscr{S}_{l\cup r} \neq \emptyset$.

To start with, consider the product

$$\prod_{\substack{s=1\\s\notin\mathscr{S}_{l\cup r}}}^{N} \left\{ \delta_{j_{s}p_{s-1}} \delta_{p_{s}p_{s-1}} \right\} = \prod_{s=1}^{t_{1}-1} \delta_{p_{s}} \delta_{p_{s-1}} \cdot \prod_{\nu=2}^{u} \prod_{s=t_{\nu-1}+1}^{t_{\nu}-1} \delta_{p_{s}p_{s-1}} \prod_{s=t_{u}+1}^{N} \delta_{p_{s}p_{s-1}}.$$
(2.2.44)

Thus, the string of Kronecker deltas will set

$$p_s = p_{t_v}$$
, for $s \in [t_v; t_{v+1} - 1]$ $v = 1, \dots, u - 1$ and $p_s = p_{t_u}$ for $s \in [1; t_1 - 1] \cup [t_u; N]$. (2.2.45)

We note that the disjoint interval for the p_{t_u} variables comes from the boundary conditions $p_0 = p_N$ on the indices of the *p*. The summation over *p* reduces to one other p_{t_1}, \ldots, p_{t_u} .

Recall that the indices l_1, \ldots, l_n are absent in \hat{j}_l so that the product

$$\prod_{\substack{s=1\\s\notin\mathscr{S}_{l\cup r}}}^{N} \{\delta_{j_s p_{s-1}}\}$$
(2.2.46)

only leaves the variables j_a with, $a \in \mathscr{S}_r^c$ as "free". The last scalar product in (2.2.43) is written in terms of these variables. Hence, by linearity one can pull the summation over each such variable into the corresponding scalar product. This yields the vectors **u** appearing in the last line of (2.2.39).

• Now consider the case when $\mathscr{S}_{l\cup r} = \emptyset$.

The summation over \hat{j}_l can be explicitly performed, while the one over the p_a s reduces to the summation over p_N . Then due the presence of the weight factor $e^{\frac{h}{2T}\varepsilon_{p_N}}$ in (2.2.43), one gets $2\cosh[\frac{h}{2T}]$.

The formula (2.2.39) allows one to compute the trace of the operator product with respect to the space $\mathfrak{h}_{\mathfrak{q}}$. Indeed, one gets

$$\operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}}\left[\mathsf{O}_{\boldsymbol{l}}\cdot\mathsf{O}_{\boldsymbol{r}}\right] = \sum_{\boldsymbol{\alpha}_{\boldsymbol{l}},\boldsymbol{\beta}_{\boldsymbol{r}}} \left\{ \sum_{\{p_{t_{a}}\}_{a=1}^{u}} e^{\frac{h}{2T}} \varepsilon_{p_{t_{a}}} \prod_{t_{k}\in\mathscr{S}_{\boldsymbol{l}}\cap\boldsymbol{r}} \left(\boldsymbol{w}_{i_{t_{k}}i_{t_{k}-1};\boldsymbol{\alpha}_{t_{k}}}, \boldsymbol{v}_{p_{t_{k}}p_{t_{k-1}};\boldsymbol{\beta}_{t_{k}}}\right) \times \prod_{t_{k}\in\mathscr{S}_{\boldsymbol{l}}} \left(\boldsymbol{w}_{i_{t_{k}}i_{t_{k}-1};\boldsymbol{\alpha}_{t_{k}}}, \boldsymbol{e}_{p_{t_{k-1}}}\otimes\boldsymbol{e}_{p_{t_{k}}}\right) \cdot \prod_{t_{k}\in\mathscr{S}_{\boldsymbol{r}}} \left(\boldsymbol{u}, \boldsymbol{v}_{p_{t_{k}}p_{t_{k-1}};\boldsymbol{\beta}_{t_{k}}}\right) \right\}.$$

$$(2.2.47)$$

Following the same strategy, one may generalise the above result to the calculation of any product of O_l for any choice of vectors l. Likewise one may provide an expression for the trace of such product.

Corollary 2.2.2. Let $n_1, \ldots n_M \in \mathbb{N}^*$ be given and consider a vector $\mathbf{l}^{(s)} = (l_1^{(s)}, \ldots, l_{n_s}^{(s)})$ with components $1 \leq l_1^{(s)} < \ldots < l_{n_s}^{(s)} \leq N$. Further we denote

$$\mathscr{S}_{\boldsymbol{l}^{(k)}\cup\boldsymbol{l}^{(k+1)}} = \{t_{1;k+1},\dots,t_{u_{k+1};k+1}\}.$$
(2.2.48)
Then upon denoting $t_{0;k+1} = t_{u_{k+1}:k+1}$, it holds that

$$O_{I^{(1)}} \dots O_{I^{(M)}} = \sum_{\left\{\{p_{i_{a,k}}^{h}\}_{a=1}^{u_{k}}\}} \sum_{k=2}^{M} \sum_{k;n_{k}>0} \sum_{i,\hat{q}_{I^{(M)}}} x_{i}^{(a^{(1)},I^{(1)})} \cdot \left(y_{p_{i},\hat{q}_{I^{(M)}}}^{(a^{(M)},I^{(M)})}\right)^{t} \cdot \left(2\cosh\left[\frac{h}{2T}\right]\right)^{\delta_{n_{1},0}\,\delta_{n_{M},0}} \\ \times \prod_{s=1}^{M-1} \left\{e^{\frac{h}{2T}\mathcal{E}_{p_{l_{u_{s}};s+1}}^{(s+1)}} \cdot \left(2\cosh\left[\frac{h}{2T}\right]\right)^{\delta_{n_{s},0}\,\delta_{n_{s+1},0}} \\ \times \prod_{t_{k;s+1}\in\mathscr{I}_{I^{(s)}\cap I^{(s+1)}}} \left(w_{p_{i_{k;s+1}}^{(s)}p_{i_{k-1;s+1}}^{(s)};\alpha_{i_{k;s+1}}^{(s)}}, v_{p_{i_{k;s+1}}^{(s+1)}p_{i_{k-1;s+1}}^{(s+1)};\beta_{i_{k;s+1}}^{(s+1)}}\right) \\ \times \prod_{t_{k;s}\in\mathscr{I}_{I}^{(s)}\setminus\mathscr{I}_{I^{(s)}\cap I^{(s+1)}}} \left(w_{p_{i_{k;s+1}}^{(s)}p_{i_{k-1;s+1}}^{(s)};\alpha_{i_{k;s+1}}^{(s)}}, e_{p_{i_{k;s+1}}}^{(s+1)}, e_{p_{i_{k;s+1}}}^{(s+1)}\right) \\ \times \prod_{t_{k;s+1}\in\mathscr{I}_{I^{(s+1)}}\setminus\mathscr{I}_{I^{(s)}\cap I^{(s+1)}}} \left(u, v_{p_{i_{k;s+1}}^{(s+1)}p_{i_{k-1;s+1}}^{(s+1)};\alpha_{i_{k;s+1}}^{(s+1)}}, e_{p_{i_{k;s+1}}}^{(s+1)}\right)\right\}.$$

Here one parametrises

$$\boldsymbol{\alpha}^{(k)} = \left(\alpha_{t_{1;k}}^{(k)}, \dots, \alpha_{t_{u_k;k}}^{(k)}\right), \tag{2.2.50}$$

(2.2.51)

and agrees upon

and denotes

$$\boldsymbol{p}_{t} = \left(\underbrace{p_{t_{u_{M},M}}^{(M)}, \dots, p_{t_{u_{M},M}}^{(M)}}_{t_{1,M}-1}, \underbrace{p_{t_{1,M}}^{(M)}, \dots, p_{t_{1,M}}^{(M)}}_{t_{2,M}-t_{1,M}}, \dots, \underbrace{p_{t_{u_{M}-1,M}}^{(M)}, \dots, p_{t_{u_{M}-1,M}}^{(M)}}_{t_{u_{M},M}-t_{u_{M}-1,M}}, \underbrace{p_{t_{u_{M},M}}^{(M)}, \dots, p_{t_{u_{M},M}}^{(M)}}_{N-t_{u_{M},M}+1}\right).$$
(2.2.52)

The representation (2.2.49) allows one to readily take the trace with respect to the space $\mathfrak{h}_{\mathfrak{q}}$ so that one has

 $p_{t_{a;k}}^{(1)} = i_{t_{a;k}}$

$$\begin{aligned} \operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}}\left[\mathsf{O}_{\boldsymbol{l}^{(1)}}\dots\mathsf{O}_{\boldsymbol{l}^{(M)}}\right] &= \sum_{\left\{\{p_{tu_{k}}^{(k)}\}_{a=1}^{u_{k}}\}_{k=1}^{M}}\sum_{k;n_{k}>0}\prod_{s=1}^{M}\left\{e^{\frac{h}{2T}}\varepsilon_{p_{tu_{s}}^{(s+1)}}\cdot\left(2\cosh\left[\frac{h}{2T}\right]\right)^{\delta_{n_{s},0}\delta_{n_{s+1},0}}\right.\\ &\times\prod_{l_{k};s+1\in\mathscr{S}_{\boldsymbol{l}^{(s)}}\cap\boldsymbol{l}^{(s+1)}}\left(\boldsymbol{w}_{p_{l_{k};s+1}^{(s)}p_{l_{k-1};s+1}^{(s)};\alpha_{l_{k};s+1}^{(s)}},\boldsymbol{v}_{p_{l_{k};s+1}^{(s+1)}p_{l_{k-1};s+1}^{(s+1)};\beta_{l_{k};s+1}^{(s+1)}}\right)\\ &\times\prod_{l_{k;s}\in\mathscr{S}_{\boldsymbol{l}^{(s)}}^{(s)}\setminus\mathscr{S}_{\boldsymbol{l}^{(s)}\cap\boldsymbol{l}^{(s+1)}}}\left(\boldsymbol{w}_{p_{l_{k};s+1}^{(s)}p_{l_{k-1};s+1}^{(s)};\alpha_{l_{k};s+1}^{(s)}},\boldsymbol{e}_{p_{l_{k-1};s}^{(s+1)}},\boldsymbol{e}_{p_{l_{k};s}^{(s+1)}}\right)\\ &\times\prod_{l_{k;s+1}\in\mathscr{S}_{\boldsymbol{l}^{(s)}}\setminus\mathscr{S}_{\boldsymbol{l}^{(s)}\cap\boldsymbol{l}^{(s+1)}}}\left(\boldsymbol{u},\boldsymbol{v}_{p_{l_{k};s+1}^{(s+1)}p_{l_{k-1};s+1}^{(s+1)};\alpha_{l_{k};s+1}^{(s+1)}},\alpha_{l_{k};s+1}^{(s+1)}\right)\right\}.\end{aligned}$$

Equation (2.2.53) is a key tool in the estimates arising in the subsection to come.

2.2.4 Spectral radius of δt_q

In this subsection, we use the previous results to obtain an estimate, uniform in N, on the spectral radius of δt_q .

Proposition 2.2.1. There exists an N-independent constant C > 0 such that the spectral radius of the operator δt_q appearing in the decomposition of the quantum transfer matrix (2.2.10) is bounded as

$$r_{S}(\delta t_{\mathfrak{q}}) \leq C \cdot |\beta|. \tag{2.2.54}$$

Furthermore, there exist constants C, C' > 0 *such that for any* $n \in \mathbb{N}$ *,*

$$\left| \operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}} \left[\boldsymbol{\omega}_{N;0} \cdot \left(\delta \mathfrak{t}_{\mathfrak{q}} \right)^{n} \right] \right| \leq C' \cdot \left(C \cdot |\boldsymbol{\beta}| \right)^{n}.$$
(2.2.55)

where $\boldsymbol{\omega}_{N;0}$ was introduced in (2.2.11).

More generally, there exist constants C, C' > 0 such that, for any $l_1, \ldots, l_n \in \mathbb{N}$,

$$\left|\operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}}\left[\boldsymbol{\omega}_{N:0}\cdot\left(\delta \mathsf{t}_{\mathfrak{q}}\right)^{l_{1}}\cdot\boldsymbol{\omega}_{N;0}\cdots\boldsymbol{\omega}_{N;0}\cdot\left(\delta \mathsf{t}_{\mathfrak{q}}\right)^{l_{n}}\right]\right| \leq (C')^{n}\cdot\prod_{a=1}^{n}\left(C\cdot\left|\boldsymbol{\beta}\right|\right)^{l_{a}}.$$
(2.2.56)

Proof. It follows from the definition of δt_q given in (2.2.11) that

$$\left(\delta t_{\mathfrak{q}}\right)^{M} = \sum_{\substack{\{n_{s}\}_{s=1}^{M} \\ n_{s}=1 \\ \boldsymbol{l}^{(s)} \in \mathscr{L}_{N}^{(n_{s})}}} \sum_{\substack{\{\boldsymbol{l}^{(s)}\}_{s=1}^{M} \\ \boldsymbol{\ell}^{(s)} \in \mathscr{L}_{N}^{(n_{s})}}} O_{\boldsymbol{l}^{(1)}} \cdots O_{\boldsymbol{l}^{(M)}}.$$
(2.2.57)

where $\mathscr{L}_{N}^{(n_{s})}$ is defined as in (2.2.9). The expression for the product of operators $O_{l^{(1)}} \cdots O_{l^{(M)}}$ given in (2.2.49) leads to the bound

$$\| \mathbf{O}_{\boldsymbol{l}^{(1)}} \cdots \mathbf{O}_{\boldsymbol{l}^{(M)}} \| \leq \sum_{\left\{ \{ p_{lu_{k}}^{(k)} \}_{a=1}^{u_{k}} \right\}_{k=2}^{M}} \sum_{\boldsymbol{k}; n_{k} > 0} \sum_{\boldsymbol{i}, \hat{\boldsymbol{q}}_{\boldsymbol{l}^{(M)}}} \| \mathbf{x}_{\boldsymbol{i}}^{(\boldsymbol{\alpha}^{(1)}, \boldsymbol{l}^{(1)})} \| \cdot \| \left(\mathbf{y}_{\boldsymbol{p}_{\boldsymbol{i}}, \hat{\boldsymbol{q}}_{\boldsymbol{l}^{(M)}}}^{(\boldsymbol{\alpha}^{(M)}, \boldsymbol{l}^{(M)})} \right)^{\mathsf{t}} \|$$

$$\times \prod_{s=1}^{M-1} \left\{ e^{\frac{h}{2T} \varepsilon_{\boldsymbol{p}_{tu_{s}}; s+1}} \cdot \prod_{t_{k}; s \in \mathscr{S}_{\boldsymbol{l}^{(s)}}} \| \mathbf{w}_{\boldsymbol{p}_{t_{k}; s+1}}^{(s)} \boldsymbol{p}_{t_{k-1}; s+1}^{(s)}; \boldsymbol{\alpha}_{t_{k}; s+1}^{(s)}} \| \cdot \prod_{t_{k}: s+1 \in \mathscr{S}_{\boldsymbol{l}^{(s+1)}}} \left\{ 2 \| \mathbf{v}_{\boldsymbol{p}_{t_{k}; s+1}}^{(s+1)} \boldsymbol{p}_{t_{k-1}; s+1}^{(s+1)}; \boldsymbol{\beta}_{t_{k}; s+1}}^{(s+1)} \| \right\} \right\}.$$

$$(2.2.58)$$

Here we took into account that $n_k > 0$ for any k and $|| \mathbf{u} || = 2$. Thus, upon recalling the estimates (2.2.24) on $\mathbf{w}_{ij;\alpha}$ and $\mathbf{v}_{ij;\alpha}$ and the expression for the vectors $\mathbf{x}_i^{(\alpha,l)}$ and $\mathbf{y}_{p,\hat{q}_{r_m}}^{(\alpha,l)}$, one obtains

$$\sum_{\boldsymbol{i}} \|\boldsymbol{x}_{\boldsymbol{i}}^{(\boldsymbol{\alpha}^{(1)},\boldsymbol{l}^{(1)})}\| \leq \frac{2^{N}}{2^{n_{1}}} \cdot \cosh\left(\frac{h}{2T}\right) \quad \text{and} \quad \sum_{\boldsymbol{\hat{q}}_{\boldsymbol{l}}(M)} \|\boldsymbol{y}_{\boldsymbol{p},\boldsymbol{\hat{q}}_{\boldsymbol{l}}(M)}^{(\boldsymbol{\alpha}^{(M)},\boldsymbol{l}^{(M)})}\| \leq \frac{2^{N}}{2^{n_{M}}} \cdot \left(\frac{C_{\boldsymbol{w}}|\boldsymbol{\beta}|}{N}\right)^{n_{M}}.$$
(2.2.59)

Therefore

$$\||\mathsf{O}_{\boldsymbol{l}^{(1)}}\dots\mathsf{O}_{\boldsymbol{l}^{(M)}}\|| \leq \prod_{k=1}^{M} \{4^{n_k}\} \cdot 2^{2N-n_M-n_1} \cdot \cosh\left(\frac{h}{2T}\right) \cdot \left(\frac{C_{\boldsymbol{w}}|\boldsymbol{\beta}|}{N}\right)^{n_M} \cdot \prod_{s=1}^{M-1} \left\{2^{u_s} \cosh\left(\frac{h}{2T}\right) \cdot \left(\frac{C_{\boldsymbol{w}}|\boldsymbol{\beta}|}{N}\right)^{n_s}\right\}.$$

Since $u_k \leq n_k + n_{k+1}$, this eventually leads to

$$\||\mathsf{O}_{\boldsymbol{l}^{(1)}}\dots\mathsf{O}_{\boldsymbol{l}^{(M)}}\|| \le 2^{2N} \cdot \left[\cosh\left(\frac{h}{2T}\right)\right]^M \cdot \prod_{s=1}^M \left\{16, \frac{C_{\boldsymbol{w}}|\boldsymbol{\beta}|}{N}\right\}^{n_s}.$$
(2.2.60)

Inserting the latter bound into the series and using the bound

$$\sum_{1 \le l_1 < \dots < l_n \le N} 1 \le \frac{1}{n!} \sum_{l_1, \dots, l_n = 1}^N 1 = \frac{N^n}{n!}$$
(2.2.61)

leads to the estimate

$$\|\|(\delta \mathsf{t}_{\mathfrak{q}})^{M}\|\| \leq 2^{2N} \cdot \left[\cosh(\frac{h}{2T})\right]^{M} \cdot \sum_{\substack{\{n_{s}\}_{s=1}^{M}\\n_{s}=1}}^{N} \prod_{s=1}^{M} \left\{16 \cdot \frac{C_{\boldsymbol{w}}|\boldsymbol{\beta}|}{n_{s}!}\right\}^{n_{s}} \leq 2^{2N} \cdot \left\{\cosh\left(\frac{h}{2T}\right) \left(e^{|\boldsymbol{\beta}|\tilde{C}}-1\right)\right\}^{M},$$

for some N-independent constant $\widetilde{C} > 0$. Hence, one gets

$$r_{\mathcal{S}}(\delta t_{\mathfrak{q}}) = \limsup_{M \to \infty} \left\{ \| (\delta t_{\mathfrak{q}})^M \| \|^{\frac{1}{M}} \right\} \le \cosh\left(\frac{h}{2T}\right) \left(e^{|\beta|\widetilde{C}} - 1 \right).$$
(2.2.62)

This readily entails the bound (2.2.54).

The second bound (2.2.55) is obtained by using (2.2.53) and specialising the dimension n_1 associated with the vector $l^{(1)}$ to zero. The strategy yields (2.2.56) as well.

2.2.5 Rigorous estimates on the dominant and sub-leading Eigenvalues of the quantum transfer matrix

Since the quantum transfer matrix $t_q(0)$ has real-valued entries, its characteristic polynomial has real coefficients what entails that the Eigenvalues of the quantum transfer matrix are either real or appear in complex conjugate pairs. The estimates (2.2.55) obtained in the previous section and the expansion (2.2.10) are enough to obtain a precise estimate on the maximal Eigenvalue and on the sub-dominant ones. These results play an important role, in a later chapter, in the identification of the dominant Eigenvalue among those obtained through the Bethe Ansatz approach to the spectrum of $t_q(0)$.

Proposition 2.2.2. The largest modulus Eigenvalue $\widehat{\Lambda}_{max}$ of the quantum transfer matrix $t_q(0)$ is non-degenerate, real and satisfies the estimate

$$\widehat{\Lambda}_{\max} = 2 + \mathscr{O}(T^{-1}), \qquad (2.2.63)$$

with a uniformly in N remainder. All the other Eigenvalues $\widehat{\Lambda}_a, a = 1, \dots, 2^{2N} - 1$, repeated according to their multiplicities, satisfy

$$\widehat{\Lambda}_a = \mathscr{O}(T^{-1}) \tag{2.2.64}$$

uniformly in N.

Proof. Proposition 2.2.1 ensures that the operator δt_q appearing in $t_q(0) = \boldsymbol{\omega}_{N;0} + \delta t_q$ has its spectral radius such that

$$r_{\mathcal{S}}(\delta t_{\mathfrak{q}}) = \mathscr{O}(T^{-1}), \qquad (2.2.65)$$

uniformly in *N*. Then, $\lambda - \delta t_q$ is invertible for any $\lambda \notin \sigma(\delta t_q)$, the spectrum of δt_q . Thus, for $\lambda \notin \sigma(\delta t_q)$, it holds that

$$\det\left[\lambda - \mathsf{t}_{\mathfrak{q}}\right] = \det\left[\lambda - \delta\mathsf{t}_{\mathfrak{q}}\right] \cdot \det\left[\mathrm{id} - (\lambda - \delta\mathsf{t}_{\mathfrak{q}})^{-1} \cdot \boldsymbol{\omega}_{N;0}\right] = \det\left[\lambda - \delta\mathsf{t}_{\mathfrak{q}}\right] \cdot \left\{1 - (\boldsymbol{w}, [\lambda - \delta\mathsf{t}_{\mathfrak{q}})^{-1}]\boldsymbol{v}\right\} \quad (2.2.66)$$

where the explicit expression for $\boldsymbol{\omega}_{N;0}$ from Lemma 2.2.1 was used. At this point, we note that the estimates (2.2.56) from Proposition 2.2.1 can be recast as

$$\left| (\boldsymbol{w}, (\delta t_{\mathfrak{q}})^n \boldsymbol{v}) \right| \le \left(\frac{C}{T}\right)^n$$
 (2.2.67)

for some *N*-independent constant C > 0. The bound (2.2.67) ensures that the series

$$\mathscr{S}(\lambda) = \frac{1}{\lambda} \sum_{n \ge 0} \left(\mathbf{w}, \left(\frac{\delta t_{\mathfrak{q}}}{\lambda} \right)^n \mathbf{v} \right)$$
(2.2.68)

converges uniformly on the set $\{\lambda \in \mathbb{C} : |\lambda| > C(1+\varepsilon)T^{-1}\}$, this for any $\varepsilon > 0$ and fixed. Furthermore, since the series

$$\frac{1}{\lambda} \sum_{n \ge 0} \left(\frac{\delta t_{\mathfrak{q}}}{\lambda} \right)^n \tag{2.2.69}$$

converges in the operator norm to $[\lambda - \delta t_q]^{-1}$ on the set

$$\left\{ \lambda \in \mathbb{C} : |\lambda| > |||\delta t_{\mathfrak{q}}||| \right\}, \tag{2.2.70}$$

one has that $\mathscr{S}(\lambda) = (\mathbf{w}, [\lambda - \delta t_q]^{-1} \mathbf{v})$ on this set. Thus, since $\lambda \mapsto [\lambda - \delta t_q]^{-1}$ is analytic on $\mathbb{C} \setminus \sigma(\delta t_q)$, by uniqueness of the analytic continuation, it holds that

$$\mathscr{S}(\lambda) = (\boldsymbol{w}, [\lambda - \delta t_{\mathfrak{q}}]^{-1} \boldsymbol{v}), \text{ for any } |\lambda| > C \cdot (1 + \varepsilon) \cdot T^{-1}.$$
(2.2.71)

The bound (2.2.67) also entails that

$$\mathscr{S}(\lambda) = \frac{1}{\lambda} \cdot \underbrace{(\mathbf{w}, \mathbf{v})}^{= 2\cosh(\frac{\hbar}{2T})} + \mathscr{O}\left(\frac{1}{T\lambda^2}\right)$$
(2.2.72)

with a differentiable remainder.

Define the disk

$$\mathscr{D}_{2,\frac{C}{T}} = \left\{ \lambda \in \mathbb{C} : |\lambda - 2| < \frac{C}{T} \right\}.$$
(2.2.73)

and $\partial \mathscr{D}_{2,\frac{C}{T}}$ its canonically oriented boundary. Let $\mathscr{S}_0(\lambda) = 2/\lambda$. Then, using (2.2.72), it is easy to see that for some C > 0 large enough

$$|\mathscr{S}(\lambda) - \mathscr{S}_{0}(\lambda)| < |1 - \mathscr{S}_{0}(\lambda)|, \text{ for } \lambda \in \partial \mathscr{D}_{2,\frac{C}{T}}.$$
(2.2.74)

Since $1 - \mathscr{S}_0(\lambda)$ admits a unique zero in $\mathscr{D}_{2,\frac{C}{T}}$ at $\lambda = 2$ and since $1 - \mathscr{S}_0(\lambda)$ does not vanish on $\partial \mathscr{D}_{2,\frac{C}{T}}$, it follows by Rouché's theorem (see Theorem B.3.1) that $1 - \mathscr{S}(\lambda)$ admits a unique zero in $\mathscr{D}_{2,\frac{C}{T}}$. An analogous reasoning based on the bound (2.2.67) and applied to the domain $\mathbb{C} \setminus \{\mathscr{D}_{2,\frac{C}{T}} \cup \mathscr{D}_{0,\frac{C'}{T}}\}$ with C' > 0 large enough implies that $1 - \mathscr{S}(\lambda)$ has no zeroes in this domain. Thus, since the zeroes of $\lambda \mapsto \det [\lambda - \delta t_q]$ belong to the spectrum $\sigma(\delta t_q)$ of the operator δt_q and since $\sigma(\delta t_q) \subset \mathscr{D}_{0,\frac{C'}{T}}$ for some C'', it follows that the characteristic polynomial $\det [\lambda - t_q]$ has:

- (i) a simple zero in the disk $\mathscr{D}_{2,\frac{C}{T}}$;
- (ii) all its other zeroes contained in the disk $\mathscr{D}_{0 \tilde{\underline{c}}}$;

with constants C, \tilde{C} being *N*-independent. This entails the claim.

2.3 Exchangeability of the thermodynamic and Trotter limits

In this section we prove the exchangeability of the thermodynamic and Trotter limits. An ingredient of the proof is a lemma given in [155] reproduced here.

Lemma 2.3.1. [155] Let $a_{N,L}$ be a sequence in \mathbb{C} such that

- for any $L \in \mathbb{N}$, $\lim_{N \to \infty} a_{N,L} = \alpha_L$;
- $\lim_{L\to\infty} \alpha_L = \alpha$;
- $\lim_{L\to\infty} a_{N,L} = z_N$, with a convergence holding uniformly in N.

Then, $\lim_{N\to\infty} z_N$ exists and equals α .

Proof. Let d(x,y) = |x - y|. From the second point one has there exists $L_0 \ge 1$ such that

$$d(\alpha_L, \alpha) < \frac{\varepsilon}{3}$$
 for $L > L_0$. (2.3.1)

From the condition of uniform convergence it follows that there exists $L_1 \ge 1$ such that

$$d(a_{N,L}, z_N) < \frac{\varepsilon}{3}$$
 for $L > L_1$. (2.3.2)

Then from the first point, take $L > \max(L_0, L_1)$. Then there exits $N_0 \ge 1$ such that one has

$$d(a_{N,L},\alpha_L) < \frac{\varepsilon}{3}, \quad \text{for} \quad N > N_0. \tag{2.3.3}$$

Therefore

$$d(z_N, \alpha) = d(z_n, a_{N,L}) + d(a_{N,L}, \alpha_L) + d(\alpha_L, \alpha) < \varepsilon.$$
(2.3.4)

This entails the claim.

The proof of the exchangeability of the limits relies on the existence of the thermodynamic limit for the *per*-site free energy which has been established in Theorem 2.1.1.

Theorem 2.3.1. There exists $T_0 > 0$ such that, for any $T > T_0$ it holds,

$$\lim_{L \to \infty} \lim_{N \to \infty} \frac{1}{L} \ln \operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}}[\mathfrak{t}_{\mathfrak{q}}^{L}(0)] = \lim_{N \to \infty} \lim_{L \to \infty} \frac{1}{L} \ln \operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}}[\mathfrak{t}_{\mathfrak{q}}^{L}(0)].$$
(2.3.5)

Proof. The aim is to apply Lemma 2.3.1 to the sequence

$$\tau_{N,L} = \frac{1}{L} \ln \operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}} [\mathfrak{t}_{\mathfrak{q}}^{L}].$$
(2.3.6)

The equality

$$\lim_{N \to \infty} \tau_{N,L} = \frac{1}{L} \ln \operatorname{tr}_{\mathfrak{h}_{XXZ}} \left[e^{-\frac{1}{T} H_{XXZ}} \right]$$
(2.3.7)

follows from the handlings of the algebraic Bethe Ansatz carried out in Subsection 2.1.3. Furthermore, Theorem 2.1.1 established the existence of the limit

$$f_{\rm XXZ} = -T \cdot \lim_{L \to \infty} \frac{1}{L} \ln \operatorname{tr}_{\mathfrak{h}_{\rm XXZ}} \left[e^{-\frac{1}{T} H_{\rm XXZ}} \right].$$
(2.3.8)

Hence, it holds $\lim_{L\to\infty} \lim_{N\to\infty} \frac{1}{L} \ln \operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}}[\mathfrak{t}_{\mathfrak{q}}^{L}(0)] = -\frac{f_{XXZ}}{T}$.

So, it remains to show that $\lim_{L\to\infty} \frac{1}{L} \ln \operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}}[\mathfrak{t}_{\mathfrak{q}}^{L}(0)]$ exists and that convergence holds uniformly in *N*. Upon following the notations and conclusions of Proposition 2.2.2, one has that for *T* large enough

$$\operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}}\left[\operatorname{t}^{L}_{\mathfrak{q}}(0)\right] = \widehat{\Lambda}^{L}_{\max} + \sum_{a=1}^{2^{2N}-1} \widehat{\Lambda}^{L}_{a}.$$
(2.3.9)

Since $\widehat{\Lambda}_{\max} = 2 + \mathcal{O}(T^{-1})$ and that $\widehat{\Lambda}_a = \mathcal{O}(T^{-1})$ for all $a = 1, \dots, 2^{2N} - 1$ by virtue of Proposition 2.2.2, it is clear that $\lim_{L \to \infty} \tau_{N,L} = \ln \widehat{\Lambda}_{\max}$.

In order to establish the uniformness in N of this convergence, one should provide sharp bounds on the sum over the sub-dominant Eigenvalues. Let \mathfrak{P} denote the projector onto the Eigenspaces of $t_q(0)$ associated with the subdominant Eigenvalues. Then, it holds that

$$\operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}}\left[(\mathfrak{Pt}_{\mathfrak{q}}(0)\mathfrak{P})^{L}\right] = \sum_{a=1}^{2^{2N}-1} \widehat{\Lambda}_{a}^{L}.$$
(2.3.10)

We know that $\lambda \mapsto (\lambda - t_q(0))^{-1}$ is an analytic function on $\mathbb{C} \setminus \sigma(\delta t_q)$ thus, as *per* Proposition 2.2.2, it is licit to write the following integral defining \mathfrak{P}

$$\mathfrak{P} = \oint_{\partial \mathscr{D}_{0,1}} \frac{d\lambda}{2\pi \mathrm{i}} \frac{1}{\lambda - \mathsf{t}_{\mathfrak{q}}(0)}.$$
(2.3.11)

By using that \mathfrak{P} is a projector, *viz*. $\mathfrak{P}^2 = \mathfrak{P}$, and the cyclicity of the trace, one gets

$$\operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}}\left[(\mathfrak{Pt}_{\mathfrak{q}}(0)\mathfrak{P})^{L}\right] = \operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}}\left[(\mathfrak{Pt}_{\mathfrak{q}}(0))^{L}\right].$$
(2.3.12)

We recall that $t_q(0) = \boldsymbol{\omega}_{N;0} + \delta t_q$ with $r_S(\delta t_q) = \mathcal{O}(T^{-1})$ as established in Proposition 2.2.1. This ensures that the operator $\lambda - \delta t_q$ is invertible for any $\lambda \in \partial \mathcal{D}_{0,1}$, hence leading to the representation

$$\frac{1}{\lambda - \mathsf{t}_{\mathfrak{q}}(0)} = \frac{1}{\mathrm{id} - [\lambda - \delta \mathsf{t}_{\mathfrak{q}}]^{-1} \cdot \boldsymbol{\omega}_{N;0}} \cdot \frac{1}{\lambda - \delta \mathsf{t}_{\mathfrak{q}}}.$$
(2.3.13)

Furthermore,

$$[\boldsymbol{\lambda} - \boldsymbol{\delta} \boldsymbol{t}_{\mathfrak{q}}]^{-1} \cdot \boldsymbol{\omega}_{N;0} = \boldsymbol{u} \cdot \boldsymbol{w}^{\mathfrak{t}}, \text{ with } \boldsymbol{u} = [\boldsymbol{\lambda} - \boldsymbol{\delta} \boldsymbol{t}_{\mathfrak{q}}]^{-1} \cdot \boldsymbol{v}, \qquad (2.3.14)$$

and by virtue of (2.2.71) and (2.2.72), one has $(\boldsymbol{w}, \boldsymbol{u}) = 2 \cdot \lambda^{-1} + \mathcal{O}(T^{-1})$ uniformly in $\lambda \in \partial \mathcal{D}_{0,1}$ and in *N*. Then, one easily verifies that

$$\frac{1}{\mathrm{id} - [\lambda - \delta t_{\mathfrak{q}}]^{-1} \cdot \boldsymbol{\omega}_{N;0}} = \mathrm{id} + \frac{1}{1 - \mathscr{S}(\lambda)} [\lambda - \delta t_{\mathfrak{q}}]^{-1} \cdot \boldsymbol{\omega}_{N;0}$$
(2.3.15)

with $\mathscr{S}(\lambda)$ defined as in (2.2.71). This leads to

$$\mathfrak{P} = \oint_{\partial \mathscr{D}_{0,1}} \frac{d\lambda}{2\pi i} \left\{ i d + \frac{1}{1 - \mathscr{S}(\lambda)} [\lambda - \delta t_{\mathfrak{q}}]^{-1} \cdot \boldsymbol{\omega}_{N;0} \right\} \cdot \frac{1}{\lambda - \delta t_{\mathfrak{q}}}.$$
(2.3.16)

It is established in the proof of Proposition 2.2.2 that $1 - \mathscr{S}(\lambda)$ admits a unique zero in $\mathbb{C} \setminus \mathscr{D}_{0,1}$ which corresponds to $\widehat{\Lambda}_{max}$. Furthermore $(\lambda - \delta t_q)^{-1}$ is analytic on $\mathbb{C} \setminus \mathscr{D}_{0,1}$. Hence, by taking the integral defining \mathfrak{P} in terms of the residues of the poles outside of $\mathscr{D}_{0,1}$, one obtains

$$\mathfrak{P} = \mathrm{id} + \frac{[\widehat{\Lambda}_{\max} - \delta t_{\mathfrak{q}}]^{-1} \cdot \boldsymbol{\omega}_{N;0} \cdot [\widehat{\Lambda}_{\max} - \delta t_{\mathfrak{q}}]^{-1}}{\mathscr{S}'(\widehat{\Lambda}_{\max})}.$$
(2.3.17)

Finally, one has the decomposition

$$\mathfrak{Pt}_{\mathfrak{q}}(0) = \mathfrak{I}_{0} + \delta \mathfrak{I} \quad \text{with} \quad \begin{cases} \mathfrak{I}_{0} = \mathfrak{P} \cdot \boldsymbol{\omega}_{N;0} \\ \delta \mathfrak{I} = \mathfrak{P} \cdot \delta \mathfrak{t}_{\mathfrak{q}} \end{cases}$$
(2.3.18)

which entails the expansion

$$\operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}}\left[(\mathfrak{Pt}_{\mathfrak{q}}(0)\mathfrak{P})^{L}\right] = \sum_{n=0}^{L} \sum_{\boldsymbol{l}\in\mathscr{L}_{L}^{(n)}} \operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}}\left[\mathfrak{I}_{0}^{l_{1}-1} \cdot \delta\mathfrak{I} \cdot \mathfrak{I}_{0}^{l_{2}-l_{1}-1} \cdot \delta\mathfrak{I} \cdots \mathfrak{I}_{0}^{l_{n}-l_{n-1}-1} \cdot \delta\mathfrak{I} \cdot \mathfrak{I}_{0}^{L-l_{n}}\right].$$
(2.3.19)

Here $l = (l_1, \ldots, l_n)$ and $\mathscr{L}_L^{(n)}$ is as introduced in (2.2.9). In order to provide estimates for the summand, it is convenient to first recast \mathfrak{I}_0 . By using $\mathscr{S}(\widehat{\Lambda}_{\max}) = 1$, one obtains that

$$-\mathscr{S}'(\widehat{\Lambda}_{\max}) = \frac{1}{\widehat{\Lambda}_{\max}} \cdot (1 + s_T)$$
(2.3.20)

with

$$s_T = \frac{1}{\widehat{\Lambda}_{\max}} \sum_{n \ge 1} n\left(\boldsymbol{w}, [\widetilde{\delta} \mathbf{t}_{\mathfrak{q}}]^n \boldsymbol{v} \right) \quad \text{and} \quad \widetilde{\delta} \mathbf{t}_{\mathfrak{q}} = \frac{\delta \mathbf{t}_{\mathfrak{q}}}{\lambda}.$$
(2.3.21)

The estimates (2.2.55) and (2.2.63) entail that $s_T = \mathcal{O}(T^{-1})$ uniformly in *N*. Furthermore, one has the rewriting

$$2\cosh\left(\frac{h}{2T}\right) \cdot (1+s_T)^{-1} = \widehat{\Lambda}_{\max} \cdot (1+w_T)$$
(2.3.22)

where $w_T = \mathcal{O}(T^{-1})$ owing to (2.2.63). This yields

$$\mathfrak{I}_{0} = -\left\{w_{T} + [\mathrm{id} + \boldsymbol{\omega}_{N;0}] \cdot \frac{\widetilde{\delta t}_{\mathfrak{q}}(1 + w_{T})}{\mathrm{id} - \widetilde{\delta t}_{\mathfrak{q}}} - \frac{\widetilde{\delta t}_{\mathfrak{q}}}{\mathrm{id} - \widetilde{\delta t}_{\mathfrak{q}}} \cdot \boldsymbol{\omega}_{N;0} \cdot \frac{\widetilde{\delta t}_{\mathfrak{q}}}{\mathrm{id} - \widetilde{\delta t}_{\mathfrak{q}}} \cdot \frac{1 + w_{T}}{2\cosh(\frac{h}{2T})}\right\} \cdot \boldsymbol{\omega}_{N;0}.$$
(2.3.23)

This representation for \mathfrak{I}_0 is already enough so as to provide estimates for the summands in (2.3.19). Since the operator products appear under the trace, as in the proof of Propostion 2.2.2, one justifies that it is licit to expand all expressions of the form $[\mathrm{id} - \delta t_q]^{-k}$ for $k \in \mathbb{N}$ into some power series in δt_q and to commute the trace with the summation symbols. Upon expanding each factor, writing up the issuing sums, one concludes that bounding the trace

$$\operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}}\left[\mathfrak{I}_{0}^{l_{1}-1}\cdot\delta\mathfrak{I}\cdot\mathfrak{I}_{0}^{l_{2}-l_{1}-1}\cdot\delta\mathfrak{I}\cdots\mathfrak{I}_{0}^{l_{n}-l_{n-1}-1}\cdot\delta\mathfrak{I}\cdot\mathfrak{I}_{0}^{L-l_{n}}\right]$$
(2.3.24)

amounts to dropping the trace symbol and replacing each appearance of the operator $\boldsymbol{\omega}_{N;0}$ in the product contained under the trace by a constant $C_1 > 0$, each appearance of w_T or s_T by $C_2/T > 0$ with a constant $C_2 > 0$, and each appearance of δt_q or δt_q by C_3/T with a constant $C_3 > 0$. This leads to

$$\begin{aligned} \left| \operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}} \left[\mathfrak{I}_{0}^{l_{1}-1} \cdot \delta \mathfrak{I} \cdot \mathfrak{I}_{0}^{l_{2}-l_{1}-1} \cdot \delta \mathfrak{I} \cdots \mathfrak{I}_{0}^{l_{n}-l_{n-1}-1} \cdot \delta \mathfrak{I} \cdot \mathfrak{I}_{0}^{L-l_{n}} \right] \right| \\ & \leq \mathscr{Z}_{0}^{l_{1}-1} \cdot \delta \mathscr{Z} \cdot \mathscr{Z}_{0}^{l_{2}-l_{1}-1} \cdot \delta \mathscr{Z} \cdots \mathscr{Z}_{0}^{l_{n}-l_{n-1}-1} \cdot \delta \mathscr{Z} \cdot \mathscr{Z}_{0}^{L-l_{n}} \end{aligned} \tag{2.3.25}$$

where

$$\mathscr{Z}_{0} = C_{1} \cdot \left\{ \frac{C_{2}}{T} + \frac{C_{3}}{T - C_{3}} \cdot (1 + C_{1}) \cdot \left(1 + \frac{C_{2}}{T}\right) + C_{1} \cdot \left(\frac{C_{3}}{T - C_{3}}\right)^{2} \cdot \left(1 + \frac{C_{2}}{T}\right) \right\}$$
(2.3.26)

and

$$\delta \mathscr{Z} = \left\{ 1 - |\widehat{\Lambda}_{\max}|^{-1} \cdot \frac{(1 - \frac{C_3}{T})^{-1} \cdot C_1 \cdot (1 - \frac{C_3}{T})^{-1}}{(1 - \frac{C_2}{T})} \right\} \cdot \frac{C_3}{T}.$$
(2.3.27)

This immediately leads to the estimate

$$\left| \operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}} \left[\mathfrak{I}_{0}^{l_{1}-1} \cdot \delta \mathfrak{I} \cdot \mathfrak{I}_{0}^{l_{2}-l_{1}-1} \cdot \delta \mathfrak{I} \cdots \mathfrak{I}_{0}^{l_{n}-l_{n-1}-1} \cdot \delta \mathfrak{I} \cdot \mathfrak{I}_{0}^{L-l_{n}} \right] \right| \leq (C')^{L-l_{n}} \cdot \left(\frac{C}{T} \right)^{L}$$
(2.3.28)

for some C, C' > 0. Thus one has that

$$\left| \operatorname{tr}_{\mathfrak{h}_{\mathfrak{q}}} \left[(\mathfrak{Pt}_{\mathfrak{q}}(0)\mathfrak{P})^{L} \right] \right| \leq \sum_{n \geq 0} \frac{L^{n}}{n!} \cdot (C')^{L-l_{n}} \cdot \left(\frac{C}{T}\right)^{L} = \left(\frac{CC' \mathrm{e}^{\frac{1}{C'}}}{T}\right)^{L}.$$
(2.3.29)

This bound allows one to obtain the estimate

$$\left|\tau_{N,L} - \ln\widehat{\Lambda}_{\max}\right| = \frac{1}{L} \left|\ln\left[1 + (\widehat{\Lambda}_{\max})^{-L} \cdot \sum_{a=1}^{2^{2N}-1} \widehat{\Lambda}_{a}^{L}\right]\right| \le \frac{1}{L} \cdot \left(\frac{C''}{T}\right)^{L}$$
(2.3.30)

for some *N*-independent constant C'' > 0, hence ensuring a uniform in *N* convergence of $\tau_{N,L}$ to $\ln \widehat{\Lambda}_{max}$ when $L \to \infty$. One is then able to conclude by virtue of Suzuki's lemma.

Corollary 2.3.1. The per-site free energy of the XXZ chain is then expressed as

$$f_{\rm XXZ} = -T \lim_{N \to \infty} \ln \widehat{\Lambda}_{\rm max}$$
(2.3.31)

Proof. This is a direct consequence of Theorem 2.3.1, Proposition 2.2.2 and the discussions given in (2.1.57)-(2.1.60).

Chapter 3

Non-linear integral equation approach to the thermodynamics of the XXZ chain

The quantum transfer matrix formalism allows one to effectively describe pertinent observables, namely the free energy or correlation lengths at finite temperatures. As initially shown in [31, 32, 91, 92, 94] this approach exhibits a crucial feature in that it enables one to access the spectrum of the quantum transfer matrix by solving a *single* non-linear integral equation. Therefore, in order to rigorously describe the thermodynamics of the quantum integrable models one needs to characterise this non-linear integral equation rigorously and establish its solvability. Its solution then appears in the integrand of the integral representations of the aforementioned physical quantities. We will rigorously establish that there exists a unique solution to the non-linear integral equation and that one can take the Trotter limit to infinity at the level of the non-linear integral equation at temperatures high enough.

Section 3.1 unfolds with a review of the algebraic Bethe Ansatz approach to the diagonalisation of the quantum transfer matrix leading to the introduction of the auxiliary function and of the non-linear integral equation it satisfies [31, 32, 91, 92, 94]. We then discuss the properties of this auxiliary function in order to write down the non-linear integral equation pertaining to our problem. This formalism enables one to then take the Trotter limit formally as indicated in [31, 32, 91, 92, 94]. Having introduced enough material, we establish the existence and uniqueness of the solution to the non-linear integral equation in Section 3.2 in the high temperature regime. In the wake of doing so we introduce a few auxiliary results necessary to this analysis at high temperature. Finally, we prove that one can indeed take the Trotter limit on the level of the non-linear integral equation.

3.1 Derivation of the non-linear integral equation

3.1.1 The algebraic Bethe Ansatz approach to the quantum transfer matrix

One constructs the Eigenstates of the quantum transfer matrix through the Bethe Ansatz approach following [59, 91, 92, 158]. The quantum monodromy matrix (2.1.54) can be expressed as 2×2 matrix

$$T_{q}(\lambda) = \begin{pmatrix} A_{q}(\lambda) & B_{q}(\lambda) \\ C_{q}(\lambda) & D_{q}(\lambda) \end{pmatrix}_{[0]}$$
(3.1.1)

whose entries are operators acting on the space $\mathfrak{h}_{\mathfrak{q}} = \bigotimes_{k=1}^{2N} \mathfrak{h}_{a_k}$ with $\mathfrak{h}_{a_k} \simeq \mathbb{C}^2$. The quantum monodromy matrix also corresponds to a representation of the Yang-Baxter algebra (2.1.26). The reference pseudo-vacuum for the quantum transfer matrix $|0\rangle_{\mathfrak{q}}$ on $\mathfrak{h}_{\mathfrak{q}}$ takes the form

$$|0\rangle_{\mathfrak{q}} = \underbrace{\boldsymbol{e}_{1} \otimes \boldsymbol{e}_{2} \otimes \cdots \otimes \boldsymbol{e}_{1} \otimes \boldsymbol{e}_{2}}_{2N}$$
(3.1.2)

where $\{e_1, e_2\}$ is the canonical basis of \mathbb{C}^2 as introduced in (2.1.35). Direct calculations show that

$$A_{\mathfrak{q}}(\lambda)|0\rangle_{\mathfrak{q}} = a_{\mathfrak{q}}(\lambda)|0\rangle_{\mathfrak{q}} \quad \text{and} \quad D_{\mathfrak{q}}(\lambda)|0\rangle_{\mathfrak{q}} = \mathsf{d}_{\mathfrak{q}}(\lambda)|0\rangle_{\mathfrak{q}}$$
(3.1.3)

where

$$\mathsf{a}_{\mathfrak{q}}(\lambda) = \left(\frac{\sinh(\lambda + \frac{\beta}{N})}{\sinh(\lambda + \frac{\beta}{N} + \mathrm{i}\zeta)}\right)^{N} \quad \text{and} \quad \mathsf{d}_{\mathfrak{q}}(\lambda) = \left(\frac{\sinh(\lambda - \frac{\beta}{N})}{\sinh(\lambda - \frac{\beta}{N} - \mathrm{i}\zeta)}\right)^{N}.$$
(3.1.4)

The parameter β is as defined in (2.1.52). Analogously to the usual transfer matrix case, the operator $C_q(\lambda)$ annihilates $|0\rangle_q$

$$C_{\mathfrak{q}}(\lambda)|0\rangle_{\mathfrak{q}} = 0 \quad \forall \, \lambda. \tag{3.1.5}$$

When constructing the Eigenstates of the quantum transfer matrix, we generally suppose that *all* the roots $\{\lambda_1, \ldots, \lambda_M\}$ are mutually distinct. This condition may be relaxed allowing for the case where some of the roots are equal. In order to deal with this, we introduce an appropriate notation. Consider *n* complex numbers $z_1, \ldots, z_n \in \mathbb{C}$, distinct or not. If some roots coincide, the total number of roots equal to a given complex number *z* is called their multiplicity and is denoted by k_z . One then defines the set

$$\{z_a\}_{a=1}^n = \{(\lambda, k_{\lambda}) : \lambda \in \{z_1, \dots, z_n\}\}$$
(3.1.6)

in which $\{z_1, \ldots, z_n\}$ stands for the usual set build up from the numbers z_1, \ldots, z_n . The Eigenstates of the quantum transfer matrix are then constructed by a multiple action of B operators

$$|\Psi(\{\lambda_a\}_{a=1}^M)\rangle_{\mathfrak{q}} = \mathsf{B}(\lambda_M)\dots\mathsf{B}(\lambda_1)|0\rangle_{\mathfrak{q}}, \qquad M = 0,\dots 2N.$$
(3.1.7)

 $|\Psi(\{\lambda_a\}_{a=1}^M)\rangle_{\mathfrak{g}}$ is an Eigenvector of the quantum transfer matrix provided the roots $\lambda_1, \ldots, \lambda_M$ are

(i) admissible, namely they should satisfy

-
$$\lambda_a \neq \lambda_b \pm i\zeta \mod i\pi\mathbb{Z}$$
 for any $a \neq b$,
- $\lambda_a \notin \left\{ \pm \frac{\beta}{N}, \pm \frac{\beta}{N} \pm i\zeta \right\}$ for any a ;

(ii) for any a = 1, ..., M solve the set of the Bethe Ansatz equations

$$e^{-\frac{h}{T}}(-1)^{s} \cdot \frac{\partial^{p}}{\partial \xi^{p}} \prod_{k=1}^{M} \left\{ \frac{\sinh(i\zeta - \xi + \lambda_{k})}{\sinh(i\zeta + \xi - \lambda_{k})} \right\} \left\{ \frac{\sinh(\xi - \beta/N)}{\sinh(\xi + \beta/N)} \frac{\sinh(i\zeta + \xi + \beta/N)}{\sinh(i\zeta - \xi + \beta/N)} \right\}_{\substack{|\xi = \lambda_{a}}}^{N}$$
(3.1.8)
$$= -\delta_{p,0}, \quad p = 0, \dots, k_{\lambda_{a}-1}$$

where k_{λ_a} is the multiplicity of λ_a . One adds the subsidiary condition¹ that the derivative does not vanish for $p = k_{\lambda_a}$. Finally s = N - M is called the spin.

Note that if the $\lambda_1, \ldots, \lambda_M$ are such that $\lambda_b \neq \lambda_a$ if $a \neq b$, *viz*. mutually distinct and admissible, the system of Bethe Ansatz equations (3.1.8) reduces to the usually encountered form

$$e^{-\frac{\hbar}{T}}(-1)^{s} \cdot \prod_{k=1}^{M} \left\{ \frac{\sinh(i\zeta - \lambda_{a} + \lambda_{k})}{\sinh(i\zeta + \lambda_{a} - \lambda_{k})} \right\} \left\{ \frac{\sinh(\lambda_{a} - \beta/N)}{\sinh(\lambda_{a} + \beta/N)} \frac{\sinh(i\zeta + \lambda_{a} + \beta/N)}{\sinh(i\zeta - \lambda_{a} + \beta/N)} \right\}^{N} = -1, \ a = 1, \dots, M.$$
(3.1.9)

For a set $\{\lambda_k\}_{k=1}^M$ satisfying (i) - (ii) the vector $\Psi(\{\lambda_k\}_{k=1}^M)$ is an Eigenvector of $t_q(\xi)$

$$\mathbf{t}_{\mathfrak{q}}(\boldsymbol{\xi})|\Psi(\{\boldsymbol{\lambda}_{k}\}_{k=1}^{M})\rangle_{\mathfrak{q}} = \Lambda(\boldsymbol{\xi}|\{\boldsymbol{\lambda}_{k}\}_{k=1}^{M})|\Psi(\{\boldsymbol{\lambda}_{k}\}_{k=1}^{M})\rangle_{\mathfrak{q}}$$
(3.1.10)

¹This may seem to be an unnatural condition but it does indeed play a certain role in the handlings to come.

associated with the Eigenvalue $\Lambda(\xi | \{\lambda_k\}_{k=1}^M)$

$$\begin{aligned} \Lambda(\xi|\{\lambda_k\}_{k=1}^M) &= (-1)^N \cdot e^{\frac{h}{2T}} \cdot \prod_{k=1}^M \left\{ \frac{\sinh(\xi - \lambda_k + i\zeta)}{\sinh(\xi - \lambda_k)} \right\} \cdot \left[\frac{\sinh(\xi + \frac{\beta}{N})\sinh(\xi - \frac{\beta}{N} - i\zeta)}{\sinh^2(-i\zeta)} \right]^N \\ &+ (-1)^N \cdot e^{-\frac{h}{2T}} \cdot \prod_{k=1}^M \left\{ \frac{\sinh(\xi - \lambda_k - i\zeta)}{\sinh(\xi - \lambda_k)} \right\} \cdot \left[\frac{\sinh(\xi - \frac{\beta}{N})\sinh(\xi + \frac{\beta}{N} + i\zeta)}{\sinh^2(-i\zeta)} \right]^N. \end{aligned}$$
(3.1.11)

The Bethe Ansatz equations (3.1.8) cannot be solved explicitly except at the free fermion point when $\zeta = \pi/2$, *viz*. $\Delta = 0$. In the latter case, the model reduces to the XX chain and the Bethe equations decouple, *viz*. reduce to equations in one variable. As follows from the results of the previous chapter, one is interested in accessing the Eigenvalues (in particular the dominant one) of the quantum transfer matrix in the Trotter limit. Working directly at the level of (3.1.9) and (3.1.11) would then demand to study the large-*N* behaviour of the Bethe roots when $N \rightarrow \infty$ in (3.1.9).

In case of the ordinary transfer matrix it has been established that, in the thermodynamic limit, the Bethe roots for the ground state form a dense distribution on a subset of \mathbb{R} [105] and that all observables, such as the low-lying Eigenvalues, can be characterised in this limit in terms of integrals involving solutions to linear integral equations. However, this properly fails in the case of the quantum transfer matrix due to zeroes and poles, present on the left hand side of (3.1.9), which collapse to the same point in the Trotter limit. It turns out that such a setting does not allow for any reasonable study of the large-*N* behaviour of the Bethe roots directly at the level of some direct handlings of the Bethe Ansatz equations. However as pioneered in [31, 32, 91, 92], one may replace this problem by a tractable one based on the use of an *auxiliary* function. Indeed, given a solution $\{\lambda_a\}_{a=1}^M$ to (3.1.8), define a function $\hat{\mathfrak{a}}$ by

$$\widehat{\mathfrak{a}}(\xi|\{\lambda_k\}_{k=1}^M) = e^{-\frac{h}{T}}(-1)^s \prod_{k=1}^M \left\{ \frac{\sinh(\mathrm{i}\zeta - \xi + \lambda_k)}{\sinh(\mathrm{i}\zeta + \xi - \lambda_k)} \right\} \left\{ \frac{\sinh(\xi - \beta/N)}{\sinh(\xi + \beta/N)} \frac{\sinh(\mathrm{i}\zeta + \xi + \beta/N)}{\sinh(\mathrm{i}\zeta - \xi + \beta/N)} \right\}^N.$$
(3.1.12)

 $\hat{\mathfrak{a}}(\xi | \{\lambda_k\}_{k=1}^M)$ is an i π -periodic, meromorphic function on \mathbb{C} that, furthermore, is bounded when $\Re(\xi) \to \infty$. The hat symbol on the function \mathfrak{a} is present to indicate the dependence on the Trotter number. This notation will be used for any *N*-dependent quantity encountered throughout the rest of the chapter.

The main point is that, by construction, the Bethe roots correspond to zeroes of $1 + \hat{\mathfrak{a}}$. More precisely, for pairwise distinct roots $\{\lambda_a\}_{a=1}^{M}$ it holds

$$1 + \widehat{\mathfrak{a}}(\lambda_a | \{\lambda_k\}_{k=1}^M) = 0, \qquad a = 1, \dots, M.$$
(3.1.13)

One may read from (3.1.12), the full set of poles, mod $i\pi$, of $\hat{\mathfrak{a}}(\xi | \{\lambda_k\}_{k=1}^M)$. Namely, it has

- an N^{th} -order pole at $\xi = -\beta / N$;
- an N^{th} -order pole at $\xi = \beta / N i\zeta$;
- *M* simple poles in the case of pairwise distinct λ_k at $\lambda_k i\zeta$.

Being bounded in $\Re(\xi) \to \infty$, it follows that $1 + \widehat{\mathfrak{a}}(\xi | \{\lambda_k\}_{k=1}^M)$ has 2N + M zeroes counted with multiplicities in any generic strip of width $i\pi$. Thus, if one would be able to find a different way to characterise $\widehat{\mathfrak{a}}$, then identifying the appropriate zeroes of $1 + \widehat{\mathfrak{a}}$ would enable one to access the Bethe roots. Note that, in such a case, solving the Bethe Ansatz equations would amount to solving equations in *one* variable. Finally and more importantly, one may hope that in such an alternative scheme, one may find a direct characterisation of the physical observables of interest in terms of $\widehat{\mathfrak{a}}$ and that one may directly characterise the large-*N* behaviour of $\widehat{\mathfrak{a}}$. This is precisely the strategy employed in [31, 32, 91, 92, 93].

3.1.2 The non-linear problem at high temperature

We now discuss the construction of the non-linear integral equations which are expected to describe the auxiliary function associated with the Bethe roots describing the dominant Eigenvalue $\widehat{\Lambda}_{max}$ of the quantum transfer matrix or the sub-dominant Eigenvalues of the quantum transfer matrix having finite $\ln \widehat{\Lambda}_a$ when $N \to \infty$. Before introducing our non-linear problem it is necessary to introduce a certain number of notations.

Given a finite set Ω consider a map

$$n: (\Omega, x) \to (\mathbb{Z}, n_x). \tag{3.1.14}$$

The weighted cardinality |A| of the set

$$A = \{(x, n_x) : x \in \Omega\}$$
(3.1.15)

is defined by

$$|A| = \sum_{x \in \Omega} n_x. \tag{3.1.16}$$

Given a function f on the set Ω and A defined in (3.1.15) we agree upon the shorthand notation

$$\sum_{\lambda \in A} f(\lambda) \equiv \sum_{x \in \Omega} n_x f(x) \quad \text{and} \quad \prod_{\lambda \in A} f(\lambda) \equiv \prod_{x \in \Omega} \left\{ f(x) \right\}^{n_x}.$$
(3.1.17)

Further if we are given two sets

$$A = \{(x, n_x) : x \in \Omega_A\} \quad \text{and} \quad B = \{(x, m_x) : x \in \Omega_B\}$$
(3.1.18)

one defines their algebraic sums \oplus and algebraic difference \ominus as

$$A \oplus B = \{(x, n_x + m_x) : x \in \Omega_A \cup \Omega_B\}, \quad A \oplus B = \{(x, n_x - m_x) : x \in \Omega_A \cup \Omega_B\}$$
(3.1.19)

where one understands that n_x, m_x are extended as $n_x = 0$ and respectively $m_x = 0$ on $\Omega_B \setminus \Omega_A$, respectively $\Omega_A \setminus \Omega_B$. We also agree to denote, for two sets Ω_A, Ω_B

$$\Omega_A \ominus \Omega_B \equiv A \ominus B, \quad \text{where} \quad A, B = \{(x, 1) : x \in \Omega_{A, B}\}.$$
(3.1.20)

These notations allow one to express more compactly the sums and products that will be appearing in what follows. For instance, given a function f on $\Omega_A \cup \Omega_B$ our convention lead to

$$\sum_{\lambda \in A \ominus B} f(\lambda) = \sum_{x \in \Omega_A} n_x f(x) - \sum_{y \in \Omega_B} m_y f(y), \qquad \prod_{\lambda \in A \ominus B} f(\lambda) = \frac{\prod_{x \in \Omega_A} \{f(\lambda)\}^{n_x}}{\prod_{y \in \Omega_B} \{f(\lambda)\}^{m_y}}.$$
(3.1.21)

Given a point $x \in \mathbb{C}, \{x\}^{\oplus n}$ denotes the set $\{(x, n)\}$ implying that

$$\sum_{t \in \{x\}^{\oplus n}} f(t) \equiv nf(x). \tag{3.1.22}$$

Finally, we remind that $\zeta_m = \min(\zeta, \pi - \zeta)$ as defined in (2.1.46).

Proposition 3.1.1. Let $\{\lambda_a\}_{a=1}^M$ be an admissible solution to the Bethe Ansatz equations (3.1.8). Define the strip \mathscr{S}_{α} as

$$\mathscr{S}_{\alpha} = \{ z \in \mathbb{C} : |\mathfrak{I}(z)| < \alpha \}.$$
(3.1.23)

Then, there exists a bounded domain $\mathscr{D} \subset \mathscr{S}_{\zeta_{m/2}}$ containing $-\beta/N$, such that the solution $\{\lambda_a\}_{a=1}^M$ allows one to construct a solution $(\widehat{\mathfrak{U}}, \widehat{\mathfrak{X}}, \widehat{\mathscr{Y}})$ to the following non-linear problem.

Find

(i) a piecewise continuous function $\widehat{\mathfrak{U}}$ on $\partial \mathscr{D}$;

(ii) a set
$$\widehat{\mathfrak{X}} = \{\widehat{x}_a\}_1^{|\widehat{\mathfrak{X}}|}$$
 with $\widehat{x}_a \in \mathscr{D} \setminus \{-\frac{\beta}{N}, \frac{\beta}{N}\}$, for $a = 1, \dots, |\widehat{\mathfrak{X}}|$;

(iii) a set $\widehat{\mathscr{Y}} = \{\widehat{y}_a\}_{a=1}^{|\mathscr{Y}|}$ with $\widehat{y}_a \in \mathscr{S}_{\pi/2} \setminus \overline{\mathscr{D}}$ and $\{\widehat{y}_1, \dots, \widehat{y}_{|\widehat{\mathscr{Y}}|}\}$ being an admissible set;

such that

(a) $e^{\hat{\mathfrak{U}}}$ extends to a meromorphic, $i\pi$ -periodic function on \mathbb{C} whose only poles in \mathscr{D} build up exactly the set

$$\widehat{\mathscr{Y}}_{sg} = \left\{ (y - i \operatorname{sgn}(\pi - 2\zeta) \cdot \zeta_{m}, k_{y}) : (y, k_{y}) \in \widehat{\mathscr{Y}} \quad and \quad y - i \operatorname{sgn}(\pi - 2\zeta) \cdot \zeta_{m} \in \mathscr{D} \right\},$$
(3.1.24)

the order of the pole at y being given by the multiplicity k_y of $(y, k_y) \in \widehat{\mathscr{Y}}$;

(b) $1 + e^{\widehat{\mathfrak{U}}}$ does not vanish on $\partial \mathscr{D}$;

(c) for any $(x,k_x) \in \widehat{\mathfrak{X}}$ and $(y,p_y) \in \widehat{\mathscr{Y}}$, with multiplicity k_x and p_y

$$\partial_{\xi}^{r} \{ e^{\mathfrak{U}(\xi)} \}_{\xi = \widehat{x}} = -\delta_{r,0}, \quad r = 0, \dots, k_{x} - 1, \partial_{\xi}^{r} \{ e^{\widehat{\mathfrak{U}}(\xi)} \}_{\xi = \widehat{y}} = -\delta_{r,0}, \quad r = 0, \dots, p_{y} - 1$$
(3.1.25)

and the derivatives do not vanish for $r = k_x$ and $r = p_y$ respectively;

(d) $e^{\hat{u}}$ is subject to monodromy constraint

$$\oint_{\partial \mathscr{D}} \frac{du}{2i\pi} \frac{\widehat{\mathfrak{U}}'(u)}{1 + e^{-\widehat{\mathfrak{U}}(u)}} = -s - |\widehat{\mathscr{Y}}| - |\widehat{\mathscr{D}}_{sg}| + |\widehat{\mathfrak{X}}|$$
(3.1.26)

for some $s \in \mathbb{Z}$;

(e) $\widehat{\mathfrak{U}}$ solves the non-linear integral equation

$$\widehat{\mathfrak{U}}(\xi) = -\frac{h}{T} + \mathfrak{w}_N(\xi) - i\pi s + i\sum_{y\in\widehat{\mathbb{Y}}_{\kappa}} \theta_+(\xi - y) + \oint_{\partial\mathscr{D}} du K(\xi - u) \cdot \mathscr{L}n[1 + e^{\widehat{\mathfrak{U}}}](u)$$
(3.1.27)

where $\theta(\xi)$ is defined in (2.1.46) and $K(\xi)$ is defined as

$$K(\xi) = \frac{\theta'(\xi)}{2\pi} = \frac{\operatorname{sgn}(\pi - 2\zeta)}{2i\pi} \left\{ \operatorname{coth}(\xi - i\zeta_m) - \operatorname{coth}(\xi + i\zeta_m) \right\}$$
(3.1.28)

and where for $v \in \partial \mathcal{D}$, one has

$$\mathscr{L}\mathbf{n}\left[1+\mathbf{e}^{\widehat{\mathfrak{U}}}\right](\nu) = \int_{\kappa}^{\nu} du \, \frac{\widehat{\mathfrak{U}}'(u)}{1+\mathbf{e}^{-\widehat{\mathfrak{U}}(u)}} + \ln\left[1+\mathbf{e}^{\widehat{\mathfrak{U}}(\kappa)}\right]. \tag{3.1.29}$$

Here, κ is some point on $\partial \mathcal{D}$ and the integral is taken, in the positive direction along $\partial \mathcal{D}$, from κ to v. The function "ln" appearing above corresponds to the principal branch of the logarithm extended to \mathbb{R}^- with the convention $\arg(z) \in [-\pi; \pi[$.

Also, we have set

$$\mathfrak{w}_{N}(\xi) = N \ln\left(\frac{\sinh(\xi - \beta/N)\sinh(\xi + \beta/N - i\zeta)}{\sinh(\xi + \beta/N)\sinh(\xi - \beta/N - i\zeta)}\right).$$
(3.1.30)

The sets appearing in the non-linear integral equation (3.1.27) are defined as

$$\widehat{\mathbb{Y}}_{\kappa} = \widehat{\mathbb{Y}} \ominus \{\kappa\}^{\oplus (s+|\widehat{\mathbb{Y}}|)} \quad with \quad \widehat{\mathbb{Y}} = \widehat{\mathscr{Y}} \oplus \{\widehat{\mathscr{Y}}_{sg} - i\zeta\} \ominus \widehat{\mathfrak{X}}.$$
(3.1.31)

where we employed the conventions introduced in (3.1.19) and (3.1.22). Finally, (3.1.27) also builds on the summation convention (3.1.21)-(3.1.22).

Reciprocally, any solution to the above non-linear problem will give rise to an admissible solution of the Bethe Ansatz equations (3.1.8).

Proof. Let $\{\lambda_a\}_{a=1}^M$ be an admissible distribution of roots solving the Bethe Ansatz equations (3.1.8). One introduces an auxiliary function $\hat{\mathfrak{a}}(\xi | \{\lambda_k\}_{k=1}^M)$ as in (3.1.12). Obviously, by definition of the Bethe roots, it holds that

 $\left(\partial_{\xi}^{k_{\lambda_a}} \widehat{\mathfrak{a}}\right) (\lambda_a | \{\lambda_k\}_{k=1}^M) \neq 0.$

$$\left(\partial_{\xi}^{p}\widehat{\mathfrak{a}}\right)\left(\lambda_{a}|\{\lambda_{k}\}_{k=1}^{M}\right) = -\delta_{p,0}, \quad \text{for} \quad a = 1, \dots, M \quad \text{and} \quad p = 1, \dots, k_{\lambda_{a}} - 1 \tag{3.1.32}$$

(3.1.33)

where k_{λ_a} is the multiplicity of the root λ_a , while



Figure 3.1: The contour $\partial \mathcal{D}$ includes the Bethe roots, which are expected to lie on the curve Γ_{λ_a} with an accumulation point at the origin and the pole at $-\beta/N$. It also contains the hole roots represented by the circle \circ . The crosses \times represent the particles roots.

Since the total order of the poles of \hat{a} in a fundamental strip of width π is M + 2N and that

$$\lim_{\Re(\lambda)\to\infty} \mathfrak{a}(\lambda|\{\lambda_k\}_{k=1}^M) = \mathrm{e}^{-\frac{h}{T}+2\mathrm{i}\zeta(N-M)},\tag{3.1.34}$$

the function $1 + \hat{\mathfrak{a}}$ admits 2N more zeroes, counted with multiplicities, in a strip of width π . Therefore one can choose a domain \mathscr{D} (see Figure 3.1) in $\mathscr{S}_{\zeta_m/2}$ such that

- the *N*-fold pole at $-\frac{\beta}{N}$ of $\hat{\mathfrak{a}}$ is contained in \mathscr{D} ;
- $1 + \hat{\mathfrak{a}} \neq 0$ on $\partial \mathcal{D}$, and also, has no poles on this boundary;
- $\overline{\mathscr{D}}$ is bounded.

Aside to the Bethe roots, there exists zeroes of the $1 + \hat{\mathfrak{a}}$ in \mathscr{D} which are not Bethe roots. These roots, which we will call hole roots, are denoted by \hat{x}_a . They are depicted by the circles in Figure 3.1. They build up the set $\hat{\mathfrak{X}}$ defined as

$$\widehat{\mathfrak{X}} = \left\{ (x, k_x) : x \in \mathscr{D} \text{ with } x \notin \{\lambda_k\}_{k=1}^M \text{ and } 1 + \widehat{\mathfrak{a}}(x | \{\lambda_k\}_{k=1}^M) = 0 \right\} \equiv \{\widehat{x}_a\}_{a=1}^{|\mathfrak{X}|}.$$
(3.1.35)

If one has a root which coincide with a zero of $1 + \hat{a}$ with order higher than one, then the root should be repeated according to its multiplicity.

The particle roots \hat{y}_a are those Bethe roots which lie on the outside of contour $\partial \mathcal{D}$. They are depicted by the crosses in Figure 3.1. The root \hat{y}_a should be repeated according to the multiplicity of the corresponding Bethe root. The particle roots build up the set

$$\widehat{\mathscr{Y}} = \{\widehat{y}_a\}_1^{|\widehat{\mathscr{Y}}|} = \{(y, k_y) \in \{\lambda_a\}_{a=1}^M : y \notin \overline{\mathscr{D}} \text{ mod } i\pi\mathbb{Z}\}.$$
(3.1.36)

Since the Bethe roots are admissible it follows that that the set $\widehat{\mathscr{Y}}$ must be admissible as well. The particle roots are partitioned as $\widehat{\mathscr{Y}} = \{\widehat{\mathscr{Y}}_{sg} - i\zeta\} \oplus \widehat{\mathscr{Y}}_{r}$ where $\widehat{\mathscr{Y}}_{sg}$ is defined exactly as in (3.1.24) and corresponds to the singular roots ensemble. This set characterises the poles of $\widehat{\mathfrak{a}}$ in \mathscr{D} . Finally the set $\widehat{\mathscr{Y}}_{r}$ gathers all the remaining elements of $\widehat{\mathscr{Y}}$.

Following the strategy developed by Destri and de Vega in [31] one may express a logarithm $\widehat{\mathfrak{U}}$ of $\widehat{\mathfrak{a}}$. We introduce

$$\widehat{\mathfrak{U}} = -\frac{h}{T} + \mathfrak{w}_N(\xi) - i\pi s + i\sum_{k=1}^M \theta(\xi - \lambda_k) + N \ln\left[\frac{\sinh(\xi + \beta/N + i\zeta)}{\sinh(i\zeta - \xi - \beta/N)}\right]$$
(3.1.37)

with $\mathfrak{w}_N(\xi)$ defined in (3.1.30) and $\theta(\xi)$ defined as in (2.1.46). We see that (3.1.37) obviously satisfies

$$\mathfrak{a}(\xi|\{\lambda_k\}_1^M) = e^{\widehat{\mathfrak{U}}(\xi)}.$$
(3.1.38)

By defining the set $\widehat{\mathscr{X}}$ built up from the Bethe roots $\{\lambda_a\}_1^M$

$$\widehat{\mathscr{X}} = \{ (\lambda_a, k_{\lambda_a}) \in \{\lambda_a\}_{a=1}^M : \lambda_a \in \overline{\mathscr{D}} \}$$
(3.1.39)

one can recast the sum over the Bethe roots by means of the residue formula. One has

$$\oint_{\partial \mathscr{D}} \frac{du}{2\pi} \theta(\xi - u) \cdot \frac{\widehat{\mathfrak{a}'}(u|\{\lambda_k\}_{k=1}^M)}{1 + \widehat{\mathfrak{a}}(u|\{\lambda_k\}_{k=1}^M)} = i \sum_{\lambda \in \widehat{\mathscr{X}}} \theta(\xi - \lambda) - iN \cdot \theta(\xi - \beta/N) + i \sum_{\widehat{x} \in \widehat{\mathfrak{X}}} \theta(\xi - \widehat{x}) - i \sum_{y \in \widehat{\mathscr{D}}_{sg}} \theta(\xi - \widehat{y} + i\zeta).$$
(3.1.40)

By using that

$$\sum_{\lambda \in \widehat{\mathscr{F}}} \theta(\xi - \lambda) = \sum_{k=1}^{M} \theta(\xi - \lambda_k) - \sum_{\widehat{y} \in \widehat{\mathscr{Y}}} \theta(\xi - \widehat{y}), \qquad (3.1.41)$$

one then has the following representation

$$\widehat{\mathfrak{U}}(\xi) = -\frac{h}{T} + \mathfrak{w}_{N}(\xi) - i\pi s - i\sum_{\widehat{x}\in\widehat{\mathfrak{X}}} \theta(\xi-\widehat{x}) + i\sum_{y\in\widehat{\mathscr{Y}}_{sg}} \theta(\xi-\widehat{y}+i\zeta) + i\sum_{\widehat{y}\in\widehat{\mathscr{Y}}} \theta(\xi-\widehat{y}) + \oint_{\partial\mathscr{D}} \frac{du}{2\pi} \theta(\xi-u) \cdot \frac{\widehat{\mathfrak{a}'}(u|\{\lambda_k\}_{k=1}^M)}{1+\widehat{\mathfrak{a}}(u|\{\lambda_k\}_{k=1}^M)}.$$
(3.1.42)

For definiteness the function θ above should be understood in the sense of + boundary values. Equation (3.1.42) may then be simplified into

$$\widehat{\mathfrak{U}}(\xi) = -\frac{h}{T} + \mathfrak{w}_N(\xi) - i\pi s + i\sum_{\widehat{y}\in\widehat{\mathfrak{Y}}} \theta(\xi - \widehat{y}) + \oint_{\partial\mathscr{D}} \frac{du}{2\pi} \theta(\xi - u) \cdot \frac{\mathfrak{U}'(u)}{1 + e^{-\widehat{\mathfrak{U}}(u)}}$$
(3.1.43)

where the set $\widehat{\mathbb{Y}}$ is defined in (3.1.31).

It remains to recast the integral term. Defining the ante-derivative of $\frac{\widehat{\mathfrak{U}}'(u)}{1+e^{-\widehat{\mathfrak{U}}(u)}}$ as in (3.1.29), one obtains by an integration by parts that

$$\oint_{\partial \mathscr{D}} \frac{du}{2\pi} \theta(\xi - u) \cdot \frac{\widehat{\mathfrak{U}'(u)}}{1 + e^{-\widehat{\mathfrak{U}}(u)}} = \oint_{\partial \mathscr{D}} du K(\xi - u) \cdot \mathscr{L}n(1 + e^{\widehat{\mathfrak{U}}})(u) + \frac{1}{2\pi} \left[\theta(\xi - u) \mathscr{L}n(1 + e^{\widehat{\mathfrak{U}}})(u) \right]_{\kappa^+}^{\kappa^-} \quad (3.1.44)$$

where $K(\xi)$ is defined in (3.1.28) and $\mathscr{L}n$ is defined in (3.1.29). κ^{\pm} corresponds to the point $\kappa \in \partial \mathscr{D}$ approached from the left/right direction along $\partial \mathscr{D}$ (see Figure 3.2). Then since $u \mapsto \theta(\xi - u)$ is smooth on $\partial \mathscr{D}$, it follows that

$$\left[\theta(\xi - u) \mathscr{L} \mathbf{n}(1 + e^{\widehat{\mathfrak{U}}})(u) \right]_{\kappa^{+}}^{\kappa^{-}} = \theta(\xi - \kappa) \oint_{\partial \mathscr{D}} du \frac{\widehat{\mathfrak{U}}'(u)}{1 + e^{-\widehat{\mathfrak{U}}(u)}}$$

$$= -2\pi \mathbf{i}(\mathbf{s} + |\widehat{\mathbb{Y}}|) \cdot \theta(\xi - \kappa)$$

$$(3.1.45)$$

with $\widehat{\mathbb{Y}}$ as in (3.1.31).

Finally, by construction, since for any $(\hat{y}, p_y) \in \widehat{\mathscr{Y}}, \hat{y}$ is a Bethe root. The equation

$$\partial_{\xi}^{r} \{ e^{\widehat{\mathfrak{U}}(\xi)} \}_{\xi = \widehat{y}} = -\delta_{r,0}, \qquad r = 0, \dots, p_{y} - 1,$$
(3.1.46)

with the derivative not vanishing at $r = p_y$, is just a rewriting of (3.1.8). The same equation with $(\hat{x}, k_x) \in \hat{\mathfrak{X}}$ and the derivative not equal to zero at $r = k_x$ is just a restatement of the fact that \hat{x} is a root of $1 + e^{\hat{\mathfrak{U}}}$ of finite multiplicity k_x , what is ensured by the meromorphicity of $e^{\hat{\mathfrak{U}}}$ on \mathcal{D} .

By virtue of the above discussion the monodromy integral takes the value

$$\oint_{\partial \mathscr{D}} \frac{du}{2\pi i} \frac{\widehat{\mathfrak{U}}'(u)}{1 + e^{-\widehat{\mathfrak{U}}(u)}} = M - N - |\widehat{\mathscr{Y}}| - |\widehat{\mathscr{Y}}_{sg}| + |\mathfrak{X}|$$
(3.1.47)

where we set s = N - M.

We now establish the reverse statement, namely that a solution to the non-linear problem gives rise to an admissible solution to the Bethe Ansatz equations (3.1.8). Thus, let $\widehat{\mathfrak{U}}$ be a solution to the non-linear problem (3.1.27). The construction of the non-linear integral equation satisfied by $\widehat{\mathfrak{U}}$ ensures that $\widehat{\mathfrak{a}} = e^{\widehat{\mathfrak{U}}}$ can be meromorphically continued to an $i\pi$ -periodic function on \mathbb{C} by the formula

$$\widehat{\mathfrak{a}}(\xi) = (-1)^{s} \cdot \prod_{\varepsilon = \pm} \left[1 + e^{\widehat{\mathfrak{U}}(\xi - i\varepsilon\zeta_{m})} \right]^{\varepsilon \operatorname{sgn}(\pi - 2\zeta) \mathbf{1}_{\mathscr{D}}(\xi - i\varepsilon\zeta_{m})} \cdot \prod_{y \in \widehat{\mathbb{Y}}_{\kappa}} \left\{ \frac{\sinh(i\zeta + y - \xi)}{\sinh(i\zeta + \xi - y)} \right\} \times \left(\frac{\sinh(\xi - \beta/N)\sinh(\xi + \beta/N - i\zeta)}{\sinh(\xi + \beta/N)\sinh(\xi - \beta/N - i\zeta)} \right)^{N} \cdot \exp\left\{ -\frac{h}{T} + \oint_{\partial \mathscr{D}} du K(\xi - u) \cdot \mathscr{L}n[1 + e^{\widehat{\mathfrak{U}}}](u) \right\}.$$
(3.1.48)



Figure 3.2: We represent the contour with a cut at κ . The integration of the logarithm ln is taken from κ to u.

Here, $\mathbf{1}_A$ stands for the indicator function of the set A. The function $\hat{\mathfrak{a}}$ admits an N^{th} order pole at $-\frac{\beta}{N}$ and poles at $\widehat{\mathscr{Y}}$ with multiplicity given by p_y for any $(\widehat{y}, p_y) \in \widehat{\mathscr{Y}}$. Since $1 + \hat{\mathfrak{a}}$ is meromorphic on an open neighbourhood of $\partial \mathscr{D}$ this means that $1 + \hat{\mathfrak{a}}$ has a finite number of zeroes on \mathscr{D} . We denote these zeroes, repeated according to their multiplicities, as $z_1, \ldots, z_{|\widehat{\mathscr{X}}|}$ and further set

$$\widehat{\mathscr{T}} = \{z_a\}_{a=1}^{|\widehat{\mathscr{T}}|}.\tag{3.1.49}$$

By a residue calculation one can compute the difference between the number of zeroes $|\widehat{\mathscr{D}}|$ and the total number of poles $|\widehat{\mathscr{D}}_{sg}| + N$ of $\widehat{\mathfrak{a}}$ on \mathscr{D} , counted with multiplicities, as

$$-N + |\widehat{\mathscr{Z}}| - |\widehat{\mathscr{P}}_{sg}| = \oint_{\partial \mathscr{D}} \frac{du}{2i\pi} \frac{\widehat{\mathfrak{a}'}(u)}{1 + \widehat{\mathfrak{a}}(u)}.$$
(3.1.50)

The right hand side is the monodromy condition (3.1.26) what leads to the constraint on the number of zeroes on \mathcal{D} , counted with multiplicities,

$$|\widehat{\mathscr{X}}| = |\widehat{\mathfrak{X}}| - |\widehat{\mathscr{Y}}| + N + s.$$
(3.1.51)

We perform an integration by parts in the integral occuring in (3.1.27) leading to

$$\oint_{\partial \mathscr{D}} du K(\xi - u) \mathscr{L} \mathbf{n}(1 + \mathbf{e}^{\widehat{\mathfrak{U}}})(u) = \oint_{\partial \mathscr{D}} \frac{du}{2\pi} \theta(\xi - u) \cdot \frac{\widehat{\mathfrak{U}}'(u)}{1 + \mathbf{e}^{-\widehat{\mathfrak{U}}(u)}} + \mathbf{i}(s + |\widehat{\mathbb{Y}}|) \cdot \theta(\xi - \kappa)$$
(3.1.52)

by the monodromy conditions. Then, taking the remaining integral by residues, it holds that

$$\widehat{\mathfrak{U}} = -\frac{h}{T} + \mathfrak{w}_N(\xi) - i\pi s + i\sum_{y\in\widehat{\mathfrak{V}}} \theta(\xi - y) - iN \cdot \theta\left(\xi + \frac{\beta}{N}\right) - i\sum_{y\in\widehat{\mathscr{Y}}_{sg}} \theta(\xi - y + i\zeta) + i\sum_{z\in\widehat{\mathscr{X}}} \theta(\xi - z). \quad (3.1.53)$$

We set M = N - s and we introduce the set $\{\lambda_a\}_{a=1}^M = \widehat{\mathscr{L}} \oplus \widehat{\mathscr{T}} \ominus \widehat{\mathfrak{X}}$. This ensures that

$$\widehat{\mathfrak{a}}(\xi) = e^{-\frac{h}{T}} (-1)^{s} \prod_{k=1}^{M} \left\{ \frac{\sinh(\mathrm{i}\zeta - \xi + \lambda_{k})}{\sinh(\mathrm{i}\zeta + \xi - \lambda_{k})} \right\} \left\{ \frac{\sinh(\xi - \beta/N)}{\sinh(\xi + \beta/N)} \frac{\sinh(\mathrm{i}\zeta + \xi + \beta/N)}{\sinh(\mathrm{i}\zeta - \xi + \beta/N)} \right\}^{N}.$$
(3.1.54)

We now proceed to discuss the admissibility of the roots $\{\lambda_a\}_{a=1}^M$. By construction, those roots solve the Bethe equations (3.1.8).

Since the roots z_a forming the set \mathscr{Z} (3.1.49) satisfy to $z_a \in \mathscr{D} \subset \mathscr{S}_{\zeta_m/2}$, the roots z_a are admissible. By the properties of the solutions to the non-linear integral equation, the roots in $\widehat{\mathscr{Y}}$ are also admissible. Thus the only possibility for $\{\lambda_a\}_{a=1}^M$ to be a non-admissible set of solution is if there exists a root z_a such that $z_a = y_b \pm i\zeta \mod i\pi\mathbb{Z}$ for some $y \in \widehat{\mathscr{Y}}$. We study the possibility of realising any of these two choices. If $z_a = y_b - i\zeta$ in a first instance, then by definition the $y_b - i\zeta$ is a singular root so that it corresponds to a pole of $\hat{\mathfrak{a}}$ on \mathscr{D} . These obviously cannot generate the zeroes of $1 + \hat{\mathfrak{a}}$. Hence one is left with the second possibility which is that for some $(\lambda_b, k_{\lambda_b}) \in \widehat{\mathscr{Y}}$ one has

$$z_a = \lambda_b + i \operatorname{sgn}(\pi - 2\zeta) \zeta_{\mathrm{m}}.$$
(3.1.55)

However, it holds

$$\widehat{\mathfrak{a}}(\lambda_{b} + \mathrm{i}\,\mathrm{sgn}(\pi - 2\zeta)\zeta_{\mathrm{m}} + \varepsilon) = \mathrm{e}^{-\frac{h}{T}}(-1)^{s} \left[\frac{\sinh(\varepsilon)}{\sinh(2\mathrm{i}\zeta + \varepsilon)} \right]^{k_{b}} \prod_{\substack{k=1\\\lambda_{k}\neq\lambda_{b}}}^{M} \left\{ \frac{\sinh(\lambda_{k} - \lambda_{b} + \varepsilon)}{\sinh(2\mathrm{i}\zeta + \lambda_{b} - \lambda_{k} + \varepsilon)} \right\} \times \left[\frac{\sinh(\lambda_{b} - \beta/N + \mathrm{i}\zeta + \varepsilon)\sinh(2\mathrm{i}\zeta + \lambda_{b} + \beta/N + \varepsilon)}{\sinh(\lambda_{b} + \beta/N + \mathrm{i}\zeta + \varepsilon)\sinh(-\lambda_{b} + \beta/N - \varepsilon)} \right]^{N}.$$
(3.1.56)

If $\lambda_b + isgn(\pi - 2\zeta)\zeta_m$ is to be a zero of $1 + \hat{a}$, then the right hand side of (3.1.56) cannot vanish in the $\varepsilon \to 0^+$ limit. Thus the sinh(ε) prefactor has to be compensated by some ε^{-1} behaviour issuing from other terms in the expression. By definition of $\widehat{\mathscr{Y}}$ being admissible, the last line of (3.1.56) cannot blow up in the $\varepsilon \to 0$ limit. Hence we are left with the only possibility that $2i\zeta + \lambda_b - \lambda_k$ vanishes for some $\lambda_a \neq \lambda_b$. Then, upon replacing λ_b from the latter argument in (3.1.55) we end up with $z_a = \lambda_k - i \operatorname{sgn}(\pi - 2\zeta)\zeta_m$ which contradicts the previous argument. This concludes the proof of Proposition 3.1.1.

In the discussion above we can note that a given set of admissible Bethe roots $\{\lambda_a\}_{a=1}^M$ allows for a very large freedom of selecting the domain \mathscr{D} . Choosing different domains may lead to different solutions sets $\widehat{\mathfrak{X}}$ and $\widehat{\mathscr{V}}$. Thus, it seems apparent that different non-linear problems given in Proposition 3.1.1 may lead to exactly the same solutions of the Bethe Ansatz equations. Therefore, it is reasonable to fix the domain \mathscr{D} once and for all and look for solutions giving rise to different sets $\widehat{\mathfrak{X}}$ and $\widehat{\mathscr{Y}}$.

In Subsection 2.2.4 of Chapter 2 we have rigorously demonstrated in Proposition 2.2.2 that the quantum transfer matrix admits a real, non-degenerate dominant Eigenvalue $\widehat{\Lambda}_{max}$. It was argued in the literature [31, 32, 59, 91, 92, 101] that this largest Eigenvalue $\widehat{\Lambda}_{max}$ is described by a solution $\{\lambda_a^{\max}\}_{a=1}^N$ to the Bethe equations containing N distinct admissible Bethe roots. Denote $\widehat{\mathfrak{a}}_{max}(\xi)$ as the auxiliary function associated with the largest Eigenvalue of the quantum transfer matrix. One may then use $\widehat{\mathfrak{a}}_{max}$ to fix the domain \mathscr{D} arising in the non-linear problem. Normally the domain \mathscr{D} is chosen to contain only the Bethe roots $\{\lambda_a^{\max}\}_{a=1}^N$ and no other zero of $1 + \widehat{\mathfrak{a}}_{max}(\xi)$ as well as the N-fold pole at $-\beta/N$. No other pole of $1 + \widehat{\mathfrak{a}}_{max}(\xi)$ is contained in \mathscr{D} . Then one studies the non-linear problem associated with this domain \mathscr{D} and involving the sets $\widehat{\mathfrak{X}}$ and $\widehat{\mathscr{V}}$. Its solution describes, if existing, the auxiliary function associated with Bethe roots characterising the Eigenvalues of the quantum transfer matrix form the domain one.

3.1.3 The formal infinite Trotter limit

The main advantage of the non-linear integral equation based approach is that it allows one to formally take the Trotter limit directly [31, 32, 59, 91, 92, 93]. For this one *assumes* that

- $\widehat{\mathfrak{U}}$ converges pointwise to \mathfrak{U} when $N \to \infty$ on $\partial \mathscr{D}$;
- all the properties of the non-linear problem are conserved under this limit in particular that

for any
$$a$$
, $\widehat{x}_a \to x_a$, with $\mathfrak{X} = \{x_a\}_1^{|\mathfrak{X}|}$, $\widehat{y}_a \to y_a$, with $\mathscr{Y} = \{y_a\}_1^{|\mathscr{Y}|}$ (3.1.57)

One has that the infinite Trotter limit of \mathfrak{w}_N is

$$\mathfrak{w}_{N}(\xi) \xrightarrow[N \to \infty]{} -2\beta \cdot [\operatorname{coth}(\xi) - \operatorname{coth}(\xi - \mathrm{i}\zeta)] = \frac{2J \sin^{2}(\zeta)}{T \sinh(\xi) \sinh(\xi - \mathrm{i}\zeta)}.$$
(3.1.58)

Upon implementing the above assumptions on the level of (3.1.27), one can write down the following nonlinear integral equation satisfied by the limit function

$$\mathfrak{U}(\xi) = -\frac{1}{T}e_0(\xi) - \mathrm{i}\pi s + \mathrm{i}\sum_{y\in\mathbb{Y}_k}\theta(\xi-y) + \oint_{\partial\mathscr{D}}du\,K(\xi-u)\cdot\mathscr{L}\mathrm{n}\big[1+\mathrm{e}^{\mathfrak{U}}\big](u) \tag{3.1.59}$$

where

$$e_0(\xi) = h - \frac{2J\sin^2(\zeta)}{\sinh(\xi)\sinh(\xi - i\zeta)}.$$
 (3.1.60)

Furthermore the set \mathbb{Y}_{κ} in (3.1.59) is given by

$$\mathbb{Y}_{\kappa} = \mathbb{Y} \ominus \{\kappa\}^{\oplus (s+|\mathbb{Y}|)} \quad \text{with} \quad \mathbb{Y} = \mathscr{Y} \oplus \{\mathscr{Y}_{sg} - i\zeta\} \ominus \mathfrak{X}$$
(3.1.61)

where

$$\mathfrak{X} = \{x_a\}_{a=1}^{|\mathfrak{X}|} \quad \text{and} \quad \mathscr{Y} = \{y_a\}_{a=1}^{|\mathscr{Y}|}.$$
(3.1.62)

The non-linear integral equation at infinite Trotter number is to be supplemented with the constraints

$$\oint_{\partial \mathscr{D}} \frac{du}{2i\pi} \frac{\mathfrak{U}'(u)}{1 + e^{-\mathfrak{U}(u)}} = |\mathfrak{X}| - |\mathscr{Y}| - |\mathscr{Y}_{sg}| - s, \qquad (3.1.63)$$

and

$$\left\{ \partial_{\xi}^{r} e^{\mathfrak{U}(\xi)} \right\}_{\left| \xi = x_{a} \right|} = -1, \quad \text{for} \quad (x_{a}, k_{x_{a}}) \in \mathfrak{X}, \quad r = 0, \dots, k_{x_{a}} - 1,$$

$$\left\{ \partial_{\xi}^{r} e^{\mathfrak{U}(\xi)} \right\}_{\left| \xi = y_{a} \right|} = -1, \quad \text{for} \quad (y_{a}, k_{y_{a}}) \in \mathscr{Y}, \quad r = 0, \dots, p_{y_{a}} - 1$$

$$(3.1.64)$$

where k_{x_a} and p_{y_a} are respectively the multiplicity of hole roots x_a and the particle roots y_a .

3.2 Existence and uniqueness of the solutions of the non-linear integral equations for high temperatures

In the previous section we have constructed a non-linear problem whose solution remains to be characterised. We now develop the framework for proving the existence and uniqueness of the solution to the non-linear integral equation (3.1.27) describing $\hat{\mathfrak{U}}$.

3.2.1 The zeroes of functions pertaining to the dominant contribution of the auxiliary function at high temperature

We start by introducing the following definition which will be useful in singling out a specific class of particle and hole set. We remind that $\mathscr{D}_{z_0,r}$ is the disk of center z_0 and radius r while \mathscr{S}_{α} is the strip of width α around \mathbb{R} .

Definition 3.2.1. Choose $\alpha, \varepsilon, \rho > 0$. The sets \mathfrak{X} and \mathscr{Y} are said to belong to the class $\mathscr{C}^{\varepsilon}_{\alpha,\rho}$ with cardinalities n_x and n_y if

- $\mathfrak{X} = \{x_a\}_{a=1}^{|\mathfrak{X}|} \subset \mathscr{D}_{0,\varepsilon}$ with $|\mathfrak{X}| = n_x$ and all x'_a s are pairwise distinct;
- $\mathscr{Y} \subset \mathscr{S}_{\frac{\pi}{2}} \setminus \{\mathscr{D}_{0,\varepsilon} \bigcup \cup_{v=\pm} \mathscr{D}_{vi\zeta_m,\alpha}\} \text{ and } |\mathscr{Y}| = n_y \text{ and the } y'_a s \text{ are pairwise distinct;}$
- the elements of \mathcal{Y} are subject to the constraint

$$\left| (-1)^{s} \prod_{y \in \mathscr{Y}} \frac{\sinh(\mathrm{i}\zeta + y)}{\sinh(\mathrm{i}\zeta - y)} + 1 \right| > \rho.$$
(3.2.1)

We note that for $\varepsilon < \alpha$ all the sets \mathfrak{X} and \mathscr{Y} in the class $\mathscr{C}^{\varepsilon}_{\alpha,\rho}$ are such that there are *no* singular roots \mathscr{Y}_{sg} within the disc $\mathscr{D}_{0,\varepsilon}$, *viz.* $y - i\zeta \notin \mathscr{D}_{0,\varepsilon} \mod i\pi\mathbb{Z}$, for any $y \in \mathscr{Y}$. The following lemma sets the ground for identifying the dominant term, when $T \to \infty$, in the non-linear integral equation (3.1.27).

Lemma 3.2.1. Fix integers $n_x, n_y \ge 0$ and the relative integer n_{κ} . Let $\alpha, \rho > 0$ be given. Then, there exists $\varepsilon > 0$ with $\alpha/2 > \varepsilon > 0$ such that

- for any $\mathfrak{X}, \mathscr{Y}$ in the class $\mathscr{C}^{\varepsilon}_{\alpha, \rho}$ with cardinalities n_x, n_y ,
- for any $\kappa \in \overline{\mathscr{D}}_{0,\varepsilon}$,

the function 1 + f *with*

$$f(\lambda) = (-1)^{s} \prod_{\substack{y \in \mathscr{Y} \\ \ominus \{\mathfrak{X} \oplus \{\kappa\}^{\oplus n_{\kappa}}\}}} \frac{\sinh(i\zeta + y - \lambda)}{\sinh(i\zeta + \lambda - y)},$$
(3.2.2)

has no zeroes inside of $\overline{\mathcal{D}}_{0,\varepsilon}$ and, uniformly in $\overline{\mathcal{D}}_{0,\varepsilon}$, is subject to the lower bound

$$\left|1+f(\lambda)\right| \ge \frac{\rho}{2}.\tag{3.2.3}$$

Proof. The function 1 + f is recast in a way which enables us to infer bounds later on:

$$1 + f(\lambda) = \left[(-1)^s \prod_{y \in \mathscr{Y}} \frac{\sinh(i\zeta + y)}{\sinh(i\zeta - y)} + 1 \right] e^{u(\lambda)} + 1 - e^{u(\lambda)}$$
(3.2.4)

with

$$u(\lambda) = i \sum_{y \in \mathscr{Y}} \left[\widetilde{\theta}(\lambda - y) - \widetilde{\theta}(-y) \right] - i \sum_{x \in \mathfrak{X} \oplus \{\kappa\}^{n_{\kappa}}} \widetilde{\theta}(\lambda - x).$$
(3.2.5)

Here, the function $\tilde{\theta}(\lambda - y)$ corresponds to a branch of the logarithm defining θ picked in such a way that $\lambda \mapsto \theta(\lambda - y)$ can be extended to a holomorphic function on the domain $\mathcal{D}_{0,\varepsilon}$. We point out that this branch may change for different choices of $y \in \mathscr{Y}$. This choice is possible since the singular roots do not exists due to $\mathscr{Y} \subset \mathscr{B}_{\alpha,\varepsilon}$ where

$$\mathscr{B}_{\alpha,\varepsilon} = \mathscr{S}_{\frac{\pi}{2}} \setminus \left\{ \mathscr{D}_{0,\varepsilon} \bigcup \cup_{\nu=\pm} \mathscr{D}_{\nu i \zeta_{m},\alpha} \right\}$$
(3.2.6)

for $\varepsilon > 0$ small enough.

Observe that if $0 < \varepsilon < \alpha/2$ and α is small enough, then for any $\lambda \in \mathcal{D}_{0,\varepsilon}$,

$$y \in \mathscr{B}_{\alpha,\varepsilon} \implies \lambda - y \in \mathscr{S}_{\frac{\pi}{2} + \varepsilon} \setminus \{ \cup_{\nu = \pm} \mathscr{D}_{\nu i \zeta_{m}, \alpha - \varepsilon} \}.$$
(3.2.7)

By the mean value theorem and the $i\pi$ -periodicity of K, one has that

$$|u(\lambda)| \le |\lambda| \sum_{y \in \mathscr{Y}} \sup_{s \in \mathscr{D}_{0,\varepsilon}} |\widetilde{\theta}(s-y)| + 2\pi |\lambda| \sum_{x \in \mathfrak{X} \oplus \{\kappa\}^{n_{\kappa}}} \sup_{t \in [0;1]} |K[(1-t)s + t(\lambda - x)]|.$$
(3.2.8)

Inferring the bounds

$$|u(\lambda)| \leq \varepsilon |\mathscr{Y}| \sup_{s \in \mathscr{D}_{0,\varepsilon}} \sup_{w \in \mathscr{B}_{\alpha,\varepsilon}} |2\pi K(s-w)| + 2\varepsilon (|\mathfrak{X}| + |n_{\kappa}|) \sup_{s \in \mathscr{D}_{0,2\varepsilon}} |2\pi K(s)|$$

$$\leq 4\pi \varepsilon (|\mathscr{Y}| + |\mathfrak{X}| + |n_{\kappa}|) \sup_{w \in \mathscr{B}_{\frac{\alpha}{2},0}} |2\pi K(w)|.$$
(3.2.9)

The above estimates ensure the existence of an ε -independent constant C > 0 such that

$$|1+f(\lambda)| \ge |\rho e^{-|u(\lambda)|} - |u(\lambda)|e^{|u(\lambda)|}| \ge \rho e^{\varepsilon C} - \varepsilon C e^{\varepsilon C} \ge \frac{\rho}{2}$$
(3.2.10)

where $\rho > 0$ is a constant and provided ε is small enough.

The above lemma allows one to introduce a certain function \mathfrak{U}_{∞} which will satisfy the "leading form", when $T \to \infty$, of the non-linear integral equation (3.1.27).

Corollary 3.2.1. For given $n_x, n_y \in \mathbb{N}$ there exists $\varepsilon > 0$ such that for any \mathfrak{X} and \mathscr{Y} in the class $\mathscr{C}^{\varepsilon}_{\alpha,\rho}$ with cardinalities n_x, n_y and, for any $\kappa \in \partial \mathscr{D}_{0,\varepsilon}$, the function

$$\mathfrak{U}_{\infty}(\xi) = -i\pi s + i\sum_{y\in\mathbb{Y}_{\kappa}} \theta(\xi - y)$$
(3.2.11)

where

$$\mathbb{Y}_{\kappa} = \mathscr{Y} \ominus \big\{ \mathfrak{X} \oplus \big\{ \kappa \big\}^{\oplus (s+|\mathscr{Y}|+|\mathscr{Y}_{sg}|-|\mathfrak{X}|)} \big\},$$
(3.2.12)

has no zeroes on $\overline{\mathscr{D}}_{0,\varepsilon}$, satisfies to the lower bound

$$\left|1 + e^{\mathfrak{U}_{\infty}}\right| \ge \frac{\rho}{2} \quad on \quad \overline{\mathscr{D}}_{0,\varepsilon} \tag{3.2.13}$$

and solves the non-linear integral equation for $\xi \in \mathscr{S}_{\zeta_{m/2}}$

$$\mathfrak{U}_{\infty}(\xi) = -i\pi s + i\sum_{y\in\mathbb{Y}_{\kappa}} \theta(\xi-y) + \oint_{\partial\mathcal{D}_{0,\varepsilon}} du K(\xi-u)\mathscr{L}\mathbf{n}[1+e^{\mathfrak{U}_{\infty}}](u)$$
(3.2.14)

where the logarithm is defined as

$$\mathscr{L}\mathbf{n}\left[1+\mathrm{e}^{\mathfrak{U}_{\infty}}\right](u) = \int_{\kappa}^{u} ds \, \frac{\mathfrak{U}_{\infty}'(s)}{1+\mathrm{e}^{\mathfrak{U}_{\infty}(s)}} + \ln\left[1+\mathrm{e}^{-\mathfrak{U}_{\infty}(\kappa)}\right] \tag{3.2.15}$$

and the integral runs along $\partial \mathcal{D}_{0,\varepsilon}$ from κ to u.

Finally, \mathfrak{U}_{∞} satisfies the zero monodromy condition

$$\oint_{\partial \mathscr{D}_{0,\varepsilon}} \frac{ds}{2i\pi} \frac{\mathfrak{U}'_{\infty}(s)}{1 + e^{-\mathfrak{U}_{\infty}(s)}} = 0.$$
(3.2.16)

Proof. The lower bound is a consequence of Lemma 3.2.1 and entails that $1 + e^{\mathfrak{U}_{\infty}}$ has no zeroes on $\overline{\mathfrak{D}}_{0,\varepsilon}$. This entails the zero monodromy condition.

Finally, the well-definedness of the non-linear integral equation (3.2.14) follows from the fact that the logarithm $\mathscr{L}n[1+e^{\mathfrak{U}_{\infty}}]$ can be analytically continued to a function on $\overline{\mathscr{D}}_{0,\varepsilon}$ since $1+e^{\mathfrak{U}_{\infty}}$ has no zeroes on $\overline{\mathscr{D}}_{0,\varepsilon}$ and is holomorphic there. The map $(\xi, u) \mapsto K(\xi - u)$ is holomorphic on $\mathscr{S}_{\zeta_{m/2}} \times \mathscr{D}_{0,\varepsilon}$ so that

$$\oint_{\mathscr{D}_{0,\varepsilon}} du K(\xi - u) \mathscr{L}\mathbf{n} \big[1 + \mathbf{e}^{\mathfrak{U}_{\infty}} \big](u) = 0.$$
(3.2.17)

3.2.2 Operatorial form of the non-linear integral equation

For given sets $\mathfrak{X}, \mathscr{Y}$, let $\mathfrak{U}_{\infty}(\xi)$ be as in (3.2.11) and introduce

$$\mathscr{L}(v,x) = \frac{1}{1 + e^{-\mathfrak{U}_{\infty}(v) - x}}$$
(3.2.18)

and for $\lambda \in \mathscr{S}_{\zeta_m/2}$ set

$$\overline{\omega}_N(\lambda) = h - T \mathfrak{w}_N(\lambda) \tag{3.2.19}$$

and given $\varepsilon > 0$, define

$$\chi_{N;\varepsilon}(\lambda) = -\oint_{\partial \mathscr{D}_{0,\varepsilon}} du \, \frac{K(\lambda-u)}{1+\mathrm{e}^{-\mathfrak{U}_{\infty}(u)}} \cdot \overline{\sigma}_{N}(u). \tag{3.2.20}$$

Given $\gamma \in O(\mathscr{S}_{\zeta_m/2})$ we denote by

$$G[\gamma](v,t) = \gamma(v)\gamma'(v)\partial_2 \mathscr{L}\left(v,\frac{t\gamma(v)}{T}\right) + (1-t)\gamma^2(v)\mathfrak{U}_{\infty}'(v)\partial_2^2 \mathscr{L}\left(v,\frac{t\gamma(v)}{T}\right).$$
(3.2.21)

where the derivatives of \mathscr{L} are taken with respect to its second variable. Finally, given $\gamma \in O(\mathscr{S}_{\zeta_m/2})$ we define the map $O_{T,N}$

$$O_{T,N}[\gamma](\lambda) = \chi_{N;\varepsilon}(\lambda) + \frac{1}{T} \oint_{\partial \mathscr{D}_{0,\varepsilon}} du K(\lambda - u) \int_{\kappa}^{u} dv \int_{0}^{1} dt \, G[\gamma - \overline{\omega}_{N}](v,t).$$
(3.2.22)

Note that, in (3.2.22), the integration variable *v* runs along $\partial \mathcal{D}_{0,\varepsilon}$ from κ to *u*. For further reasonings, we introduce the space

$$\mathfrak{B}_r = \left\{ \xi \in O(\mathscr{S}_{\zeta_{\mathfrak{m}/2}}) : \| \xi \|_{L^{\infty}(\mathscr{S}_{\zeta_{\mathfrak{m}/2}})} \leq r \right\} \text{ with } \| g \|_{L^{\infty}(U)} = \operatorname{esssup}_{u \in U} |g(u)|.$$
(3.2.23)

Montel's theorem ensures that, for any r > 0, \mathfrak{B}_r is a complete metric space with respect to the distance

$$d(f,g) = \| f - g \|_{L^{\infty}(\mathscr{S}_{\zeta_{\mathrm{m}}/2})}.$$
(3.2.24)

We proceed to establish that, at least for T, N large enough, the operator $O_{T,N}$ is well defined on a functional space \mathfrak{B}_r , for a specific value of r, and admits a unique fixed point. The main point, though, is that one may put in one-to-one correspondence the problem of solving the non-linear integral equation (3.1.27), for arbitrary sets \mathfrak{X} and \mathscr{Y} in a $\mathscr{C}^{\varepsilon}_{\alpha,\rho}$ class, with the one of finding the fixed points of $O_{T,N}$.

In the following we set

$$\mathfrak{c} = 2 \parallel \chi_{\infty; \mathfrak{E}} \parallel_{L^{\infty}(\mathscr{S}_{\zeta_{\mathrm{m}}/2})}.$$
(3.2.25)

Proposition 3.2.1. For given $n_x, n_y \in \mathbb{N}$, there exists $T_0 > 0, N_0 \in \mathbb{N}$ and $\varepsilon > 0$ such that for any \mathfrak{X} and \mathscr{Y} in the class $\mathscr{C}^{\varepsilon}_{\alpha,\rho}$ with cardinalities n_x, n_y and for any $\kappa \in \partial \mathscr{D}_{0,\varepsilon}$

- (i) $O_{T,N}$ is well-defined on \mathfrak{B}_{c} , with c as given in (3.2.25);
- (*ii*) $O_{T,N}$ stabilises $\mathfrak{B}_{\mathfrak{c}}$, viz. $O_{T,N}[\mathfrak{B}_{\mathfrak{c}}] \subset \mathfrak{B}_{\mathfrak{c}}$;
- (iii) the solutions $\widehat{\mathfrak{U}}$ to the non-linear integral equation (3.1.27) associated with the sets \mathfrak{X} and \mathscr{Y} is related to the fixed point ξ of the operator $O_{T,N}$ as

$$T \cdot \widehat{\mathfrak{U}} = T \cdot \widehat{\mathfrak{U}}_{\infty} + \xi - \overline{\omega}_N. \tag{3.2.26}$$

Proof. We begin by establishing the third point. Upon making the change of unknown function

$$\widehat{\mathfrak{U}}(\lambda) = \frac{1}{T} \left(\xi(\lambda) - \boldsymbol{\sigma}_N(\lambda) \right) + \mathfrak{U}_{\infty}(\lambda)$$
(3.2.27)

where \mathfrak{U}_{∞} was introduced in (3.2.11), one can recast the non-linear integral equation (3.1.27) in the operatorial form

$$\xi(\lambda) = T \oint_{\partial \mathscr{D}_{0,\varepsilon}} du K(\lambda - u) \cdot \left\{ \mathscr{L}n\left[1 + e^{\mathfrak{U}_{\infty} + \frac{\xi - \sigma_N}{T}}\right](u) - \mathscr{L}n\left[1 + e^{\mathfrak{U}_{\infty}}\right](u) \right\}.$$
(3.2.28)

Note that, just as for $\widehat{\mathfrak{U}}$, (3.2.28) defines $\xi(\lambda)$ not only on $\partial \mathscr{D}_{0,\varepsilon}$ but for all $\lambda \in \mathscr{S}_{\zeta_m/2}$. Then upon recalling the Taylor integral expansion for a function f of class \mathscr{C}^{n+1} defined in a neighbourhood of 0.

$$f(x) = \sum_{k=0}^{n} x^{k} \frac{f^{(k)}(0)}{k!} + \frac{x^{n+1}}{n!} \int_{0}^{1} (1-t)^{n} f^{(n+1)}(tx) dt, \qquad (3.2.29)$$

one may express the function $\mathscr{L}(v, x)$ as

$$\mathscr{L}(v,x) = \mathscr{L}(v,0) + x\partial_2 \mathscr{L}(v,0) + x^2 \int_0^1 dt \,(1-t)\partial_2^2 \mathscr{L}(v,tx), \qquad (3.2.30)$$

where $\mathscr{L}(v,0) = (1 + e^{-\mathfrak{U}_{\infty}(v)})^{-1}$. This allows us to expand (3.2.28) in a way that permits to explicitly write down the presumed linear order in 1/T:

$$\mathscr{L}\mathbf{n}\left[1+\mathrm{e}^{\mathfrak{U}_{\infty}+\frac{\gamma}{T}}\right](u) = \mathscr{L}\mathbf{n}\left[1+\mathrm{e}^{\mathfrak{U}_{\infty}}\right](u) + \frac{1}{T}\left[\frac{\gamma(u)}{1+\mathrm{e}^{-\mathfrak{U}_{\infty}(u)}} - \frac{\gamma(\kappa)}{1+\mathrm{e}^{-\mathfrak{U}_{\infty}(\kappa)}}\right] \\ + \frac{1}{T^{2}}\int_{\kappa}^{u}dv\int_{0}^{1}dt\left\{\gamma(v)\gamma'(v)\partial_{2}\mathscr{L}\left(v,\frac{t\gamma(v)}{Y}\right) + (1-t)\gamma^{2}(v)\mathfrak{U}_{\infty}'(v)\partial_{2}^{2}\mathscr{L}\left(v,\frac{t\gamma(v)}{T}\right)\right\}$$
(3.2.31)

where $\gamma = \xi - \varpi_N$. One plugs this back in (3.2.28) to obtain

$$\begin{aligned} \xi(\lambda) &= -\oint_{\partial \mathscr{D}_{0,\varepsilon}} du K(\lambda - u) \left(\frac{\gamma(u)}{1 + e^{-\mathfrak{U}_{\infty}(u)}} - \frac{\gamma(\kappa)}{1 + e^{-\mathfrak{U}_{\infty}(\kappa)}} \right) \\ &+ \frac{1}{T} \oint_{\partial \mathscr{D}_{0,\varepsilon}} du K(\lambda - u) \int_{\kappa}^{u} dv \int_{0}^{1} dt \left\{ \gamma(v) \gamma'(v) \partial_{2} \mathscr{L}\left(v, \frac{t\gamma(v)}{Y}\right) \right. \\ &+ (1 - t) \gamma^{2}(v) \mathfrak{U}_{\infty}'(v) \partial_{2}^{2} \mathscr{L}\left(v, \frac{t\gamma(v)}{T}\right) \right\} \end{aligned}$$
(3.2.32)

Since $\xi(u)$ is holomorphic on $\partial \mathcal{D}_{0,\varepsilon}$ and $\kappa \in \partial \mathcal{D}_{0,\varepsilon}$, one has that

$$\begin{aligned} \boldsymbol{\xi}(\boldsymbol{\lambda}) &= -\oint_{\partial \mathscr{D}_{0,\varepsilon}} d\boldsymbol{u} K(\boldsymbol{\lambda} - \boldsymbol{u}) \frac{\boldsymbol{\varpi}_{N}(\boldsymbol{u})}{1 + \mathrm{e}^{-\mathfrak{U}_{\infty}(\boldsymbol{u})}} \\ &+ \frac{1}{T} \oint_{\partial \mathscr{D}_{0,\varepsilon}} d\boldsymbol{u} K(\boldsymbol{\lambda} - \boldsymbol{u}) \int_{\kappa}^{\boldsymbol{u}} d\boldsymbol{v} \int_{0}^{1} dt \left\{ \boldsymbol{\gamma}(\boldsymbol{v}) \boldsymbol{\gamma}'(\boldsymbol{v}) \partial_{2} \mathscr{L}\left(\boldsymbol{v}, \frac{t \boldsymbol{\gamma}(\boldsymbol{v})}{Y}\right) \right. \\ &+ (1 - t) \boldsymbol{\gamma}^{2}(\boldsymbol{v}) \mathfrak{U}_{\infty}'(\boldsymbol{v}) \partial_{2}^{2} \mathscr{L}\left(\boldsymbol{v}, \frac{t \boldsymbol{\gamma}(\boldsymbol{v})}{T}\right) \right\} \end{aligned}$$
(3.2.33)

with the first term on the right hand side above corresponding to the definition of $\chi_{N;\epsilon}$ initially introduced. Hence at high enough temperatures, this entails that ξ is a fixed point of $O_{T,N}$:

$$\xi(\lambda) = \mathsf{O}_{T,N}[\xi](\lambda). \tag{3.2.34}$$

Upon tracing the above steps backwards one concludes that any fixed point ξ of $O_{T,N}$ gives rise to a solution \mathfrak{U} of (3.1.27).

The first point of the proposition requires one to establish a few preparatory bounds. As shown in Lemma 3.2.1, uniformly in the parameters forming the sets \mathfrak{X} and \mathscr{Y} , it holds that

$$|1 + e^{\mathfrak{U}_{\infty}(\nu)}| \ge \frac{\rho}{2}$$
 and $|e^{\mathfrak{U}_{\infty}(\nu)}| \le C$ (3.2.35)

for any $v \in \mathscr{D}_{0,\varepsilon}$, provided that $\varepsilon > 0$ is small enough. Then, there exists x_0 such that for any $|x| \le 2x_0$ one has

$$|1 - e^{-x}| \le \frac{\rho}{4}.$$
 (3.2.36)

Thence for any $|x| \leq 2x_0$ and $v \in \mathcal{D}_{0,\varepsilon}$ one has the lower bound

$$\left|1 + e^{-x - \mathfrak{U}_{\infty}(\nu)}\right| \ge \frac{\rho}{4} \left|e^{-\mathfrak{U}_{\infty}(\nu)}\right| \tag{3.2.37}$$

leading to

$$|\mathscr{L}(v,x)| \le \frac{4C}{\rho}.\tag{3.2.38}$$

Since the map $x \mapsto \mathscr{L}(v, x)$ is holomorphic on $\mathscr{D}_{0,2x_0}$ it follows that by virtue of Lemma B.3.1

$$\|\partial_2^k \mathscr{L}(v,\cdot)\|_{L^{\infty}(\mathscr{D}_{0,x_0})} \leq C_k \|\mathscr{L}(v,\cdot)\|_{L^{\infty}(\mathscr{D}_{0,2x_0})} \leq C_k$$
(3.2.39)

for some constants C_k, \widetilde{C}_k uniformly in $v \in \mathcal{D}_{0,\varepsilon}$.

Let $\xi \in \mathfrak{B}_{\mathfrak{c}}$ and define

$$\gamma_{\xi} = \xi - \overline{\omega}_N. \tag{3.2.40}$$

There exists $N_0 \ge 0$ such that for all $N \ge N_0$ the function $\overline{\omega}_N$ is holomorphic in an annulus containing $\partial \mathcal{D}_{0,\varepsilon}$ and $\partial \mathcal{D}_{0,2\varepsilon}$. Thus, for $N \ge N_0$, there exist constants C_k such that

$$\| \gamma_{\xi}^{(k)} \|_{L^{\infty}(\partial \mathscr{D}_{0,\varepsilon})} \leq C'_{k} \| \gamma_{\xi} \|_{L^{\infty}(\partial \mathscr{D}_{0,2\varepsilon})} \leq C'_{k} (\mathfrak{c} + \| \boldsymbol{\varpi}_{N} \|_{L^{\infty}(\partial \mathscr{D}_{0,2\varepsilon})})$$
(3.2.41)

where $\gamma_{\xi}^{(0)} = \gamma_{\xi}$ and $\gamma_{\xi}^{(k)}$ for k > 0 stands for the kth derivative of γ_{ξ} . Due to the bound (??), there exists T_0 such that $T^{-1} \cdot || \gamma_{\xi} ||_{L^{\infty}(\partial \mathcal{D}_{0,\varepsilon})} \leq x_0$ for all $T > T_0$.

Having established all the preparatory definitions and bounds we can now infer bounds on the operator $O_{T,N}$ (3.2.22). We have that

$$\| \mathcal{O}_{T,N}[\xi] \|_{L^{\infty}(\mathscr{S}_{\zeta_{m/2}})} \leq \| \chi_{N,\varepsilon} \|_{L^{\infty}(\mathscr{S}_{\zeta_{m/2}})} + \| \frac{1}{T} \oint_{\partial \mathscr{D}_{0,\varepsilon}} du K(*-u) \int_{\kappa}^{u} dv \int_{0}^{1} dt \, G[\gamma_{\xi}](v,t) \|_{L^{\infty}(\mathscr{S}_{\zeta_{m/2}})}$$
(3.2.42)

where $G[\gamma](v,t)$ is defined in (3.2.21) and * stands for the running variable in respect to which the norm is taken. It follows that

$$\| O_{T,N}[\xi] \|_{L^{\infty}(\mathscr{S}_{\zeta_{m}/2})} \leq \| \chi_{N,\varepsilon} \|_{L^{\infty}(\mathscr{S}_{\zeta_{m}/2})} + \frac{4\pi^{2}\varepsilon^{2}}{T} \cdot \| K \|_{L^{\infty}(\mathscr{S}_{\zeta_{m}/2+\varepsilon})} \cdot C_{0}' (\mathfrak{c} + \| \varpi_{N} \|_{L^{\infty}(\partial \mathscr{D}_{0,2\varepsilon})})^{2} \cdot \left\{ C_{1}'\widetilde{C}_{1} + \frac{C_{0}'\widetilde{C}_{2}}{2} \cdot \| \mathfrak{U}_{\infty}' \|_{L^{\infty}(\partial \mathscr{D}_{0,\varepsilon})} \right\}.$$

$$(3.2.43)$$

Then, since $\chi_{N,\mathscr{D}} = \chi_{\infty;\varepsilon} + \mathscr{O}(\frac{1}{TN})$, one can take *T* and *N* large enough so as to get

$$\| \mathsf{O}_{T,N}[\xi] \|_{L^{\infty}(\mathscr{S}_{\zeta_{\mathfrak{m}/2}})} \leq 2 \| \chi_{\infty;\varepsilon} \|_{L^{\infty}(\mathscr{S}_{\zeta_{\mathfrak{m}/2}})}.$$

$$(3.2.44)$$

This entails the claim.

After establishing the basic properties of the the operator $O_{T,N}$, we are in position to prove the existence of its fixed point by showing that the operator $O_{T,N}$ is strictly contractive at high temperature. Before establishing those results, we define the operator O_T , which is:

$$O_T[\xi](\lambda) = \chi_{\infty;\varepsilon}(\lambda) + \frac{1}{T} \oint_{\partial \mathscr{D}_{0,\varepsilon}} du K(\lambda - u) \int_{\kappa}^{u} dv \int_{0}^{1} dt \, G[\xi - e_0](v, t).$$
(3.2.45)

where

$$\chi_{\infty;\varepsilon}(\lambda) = -\oint_{\partial \mathscr{D}_{0,\varepsilon}} du \, \frac{K(\lambda-u)}{1 + \mathrm{e}^{-\mathfrak{U}_{\infty}(u)}} e_0(u). \tag{3.2.46}$$

It is clear that O_T corresponds to the formal Trotter limit of the operator $O_{T,N}$.

Theorem 3.2.2. There exists N_0 , T_0 such that, for any $N > N_0$ and $T > T_0$:

- the operator $O_{T,N}$ admits a unique fixed point in \mathfrak{B}_{c} ;
- the fixed point is continuous in $N \ge N_0$ and converges, when $N \to \infty$, to the unique fixed point of O_T in $\mathfrak{B}_{\mathfrak{c}}$.

The existence of a unique fixed point for O_T is part of the conclusions.

Proof. We start by showing that the operator $O_{T,N}$ is strictly contractive on $\mathfrak{B}_{\mathfrak{c}}$ for temperatures high enough, namely that for any $\xi_1, \xi_2 \in \mathfrak{B}_{\mathfrak{c}}$, it holds

$$\| O_{T,N}[\xi_1] - O_{T,N}[\xi_2] \|_{L^{\infty}(\mathscr{S}_{\zeta_{m/2}})} \le \frac{C}{T} \| \xi_1 - \xi_2 \|_{L^{\infty}(\mathscr{S}_{\zeta_{m/2}})}$$
(3.2.47)

for some constant C > 0. Considering the first term in the function $G[\gamma_{\xi}](v,t)$ (3.2.21), we first remark that

$$\begin{aligned} \gamma_{\xi_{1}}(v)\gamma_{\xi_{1}}'(v)\partial_{2}\mathscr{L}\left(v,\frac{t\gamma_{\xi_{1}}(v)}{T}\right) &-\gamma_{\xi_{2}}(v)\gamma_{\xi_{2}}'(v)\partial_{2}\mathscr{L}\left(v,\frac{t\gamma_{\xi_{2}}(v)}{T}\right) \\ &= \frac{1}{2}\partial_{v}\left[\gamma_{\xi_{1}}^{2}(v)-\gamma_{\xi_{2}}^{2}(v)\right]\partial_{2}\mathscr{L}\left(v,\frac{t\gamma_{\xi_{1}}}{T}\right) + \frac{1}{2}\partial_{v}\left[\gamma_{\xi_{2}}^{2}(v)\right]\left\{\partial_{2}\mathscr{L}\left(v,\frac{t\gamma_{\xi_{1}}(v)}{T}\right) - \partial_{2}\mathscr{L}\left(v,\frac{t\gamma_{\xi_{2}}(v)}{T}\right)\right\}. \end{aligned}$$

$$(3.2.48)$$

Then, one may decompose the first term using

$$\gamma_{\xi_1}^2 - \gamma_{\xi_2}^2 = (\xi_1 - \xi_2)(\xi_1 - \xi_2 - 2\overline{\omega}_N)$$
(3.2.49)

as the difference of first order derivatives of the functions \mathscr{L} . Further, one rewrites by a first order Taylor integral formula

$$\mathscr{L}(v,x) = \mathscr{L}(v,0) + x \int_0^1 \partial_2 \mathscr{L}(v,tx) dt$$
(3.2.50)

leading to

$$\partial_2 \mathscr{L}\left(v, \frac{t\gamma_{\xi_1}(v)}{T}\right) - \partial_2 \mathscr{L}\left(v, \frac{t\gamma_{\xi_2}(v)}{T}\right) = \frac{t}{T} (\xi_1 - \xi_2)(v) \int_0^1 dx \,\partial_2^2 \mathscr{L}\left(v, \frac{t\gamma_{\xi_1}}{T} - \frac{tx}{T} [\gamma_{\xi_1}(v) - \gamma_{\xi_2}(v)]\right).$$
(3.2.51)

We proceed similarly for the second term of (3.2.21), so that, eventually, one gets

$$\begin{split} G[\gamma_{\xi_{1}}](v,t) &- G[\gamma_{\xi_{2}}](v,t) \\ &= \frac{1}{2} \partial_{v} \left\{ (\xi_{1} - \xi_{2})(v)(\xi_{1} + \xi_{2} - 2\varpi_{N})(v) \right\} \partial_{2} \mathscr{L} \left(v, \frac{t\gamma_{\xi_{1}}(v)}{T} \right) \\ &+ \frac{t}{2T} (\xi_{1} - \xi_{2})(v) \partial_{v} \left[\gamma_{\xi_{2}}^{2} \right] \int_{0}^{1} dx \, \partial_{2}^{2} \mathscr{L} \left(v, \frac{t\gamma_{1}}{T} - \frac{tx}{T} \left[\gamma_{\xi_{1}}(v) - \gamma_{\xi_{2}}(v) \right] \right) \\ &+ (1 - t) \mathfrak{U}_{\infty}'(v) \left\{ (\xi_{1} - \xi_{2})(v)(\xi_{1} + \xi_{2} - 2\varpi_{N})(v) \partial_{2} \mathscr{L} \left(v, \frac{t\gamma_{\xi_{1}}(v)}{T} \right) \\ &+ \frac{t}{T} (\xi_{1} - \xi_{2})(v) \gamma_{\xi_{2}}^{2}(v) \int_{0}^{1} dx \, \partial_{2}^{3} \mathscr{L} \left(v, \frac{t\gamma_{1}}{T} - \frac{tx}{T} \left[\gamma_{\xi_{1}}(v) - \gamma_{\xi_{2}}(v) \right] \right) \right\}. \end{split}$$
(3.2.52)

Upon replacing the above in the left hand side of (3.2.47) one can infer bounds by invoking (3.2.39) and (3.2.41). Hence one does get (3.2.47) for some constant C > 0 and so the strict contractivity of $O_{T,N}$ follows provided that T is large enough. Thus, by the Banach fixed point theorem (see Theorem B.4.2), the operator $O_{T,N}$ admits a unique fixed point in $\mathfrak{B}_{\mathfrak{c}}$.

Furthermore, by dominated convergence and the previous bounds, one has that, for any $\xi \in \mathfrak{B}_c$, the map $N \mapsto O_{T,N}[\xi]$ is continuous with a uniform in *N* strict contractivity constant (see Corollary B.4.1). This ensures that the solution is continuous in *N* as well. The claims relative to the operator O_T follow from this continuity. \Box

Chapter 4

Integral representations of thermodynamical quantities

This chapter completes the setting developed in the previous two chapters. More precisely, we provide a way to establish rigorously the integral representation for the free energy of the XXZ chain (2.1.4) in Section 4.2. This is achieved by a rigorous identification of the non-linear integral equation whose solution corresponds to the auxiliary function built up from the solutions to the Bethe Ansatz equations parametrising the dominant Eigenvalue. Of course, the rigorous construction relies on the ideas developed in previous works [31, 32, 91, 92]. Also, by building on the solutions of the non-linear integral equation with particle \mathscr{Y} and hole \mathfrak{X} root sets belonging to the $\mathscr{C}^{\varepsilon}_{\rho,\alpha}$ class, we provide a rigorous characterisation of the sub-leading Eigenvalues of the quantum transfer matrix in the high temperature regime in Section 4.3. In particular such an expression for the sub-dominant Eigenvalue provides an integral representation of the correlation lengths. And finally, in Section 4.4, we rigorously characterise the high temperature behaviour of the particle and hole roots and express the sub-leading Eigenvalues and correlation lengths in terms of the former. Notably, in the large temperature limit the particle roots are described in terms of solutions to the Bethe Ansatz equations for the XXZ spin-1 chain.

4.1 Identification of the dominant Eigenvalue

We now present a framework for constructing the integral representation of the dominant Eigenvalue.

Theorem 4.1.1. There exists $T_0 > 0, N_0 > 0$ and $\varepsilon > 0$ such that, uniformly in $N \ge N_0$ and $T \ge T_0$, the nondegenerate dominant Eigenvalue $\widehat{\Lambda}_{max}$ of the quantum transfer matrix admits the integral representation

$$\widehat{\Lambda}_{\max} = \left(\frac{\sinh(\beta/N + i\zeta)}{\sinh(i\zeta)}\right)^{2N} \exp\left\{\frac{h}{2T} - \oint_{\partial \mathscr{D}_{0,\varepsilon}} \frac{du}{2\pi} \frac{\sin(\zeta)\mathscr{L}n[1 + e^{\widehat{\mathfrak{U}}_{\max}}](u)}{\sinh(u - i\zeta)\sinh(u)}\right\}$$
(4.1.1)

given in terms of the unique solution to the non-linear integral equation on $\mathfrak{B}_{\mathfrak{c}}(3.2.23)$:

$$\widehat{\mathfrak{U}}_{\max}(\xi) = -\frac{h}{T} + \mathfrak{w}_N(\xi) + \oint_{\partial \mathscr{D}_{0,\varepsilon}} du K(\xi - u) \mathscr{L}n\big[1 + e^{\widehat{\mathfrak{U}}_{\max}}\big](u)$$
(4.1.2)

where $\mathcal{L}n$ is defined in (3.1.29) and subject to the zero monodromy condition

$$\oint_{\partial \mathscr{D}_{0,\varepsilon}} \frac{d\lambda}{2i\pi} \frac{\widehat{\mathcal{U}}_{\max}(\lambda)}{1 + e^{-\widehat{\mathcal{U}}_{\max}(\lambda)}} = 0.$$
(4.1.3)

The strategy of the proof is as follows. First, one considers the solution $\widehat{\mathfrak{U}}_{max}$ to the non-linear integral equation (3.1.27) and shows that $1 + e^{\widehat{\mathfrak{U}}_{max}}$ admits exactly *N* distinct simple zeroes inside of $\mathscr{D}_{0,\varepsilon}$. These define

a set of Bethe roots according to Theorem 3.2.2 and hence give rise to an Eigenvector of the quantum transfer matrix and to the associated Eigenvalue. Following [31, 32, 91, 92], one then represents this Eigenvalue in terms of $1 + e^{\widehat{\mathfrak{U}}_{max}}$ and computes its large temperature behaviour. This shows that this Eigenvalue differs from $\widehat{\Lambda}_{max}$ (4.1.1) by $\mathscr{O}(T^{-1})$ and hence coincides with it, owing to Proposition 2.2.2, *c.f.* eq. (2.2.63).

Proof. Let $\widehat{\mathfrak{U}}_{max}$ be the unique solution of (4.1.2). We first provide a precise description of the zeroes of $1 + e^{\widehat{\mathfrak{U}}_{max}}$. Recall that $\widehat{\mathfrak{U}}_{max}$ is expressed as

$$\widehat{\mathfrak{U}}_{\max}(\lambda) = \frac{1}{T} \big(\xi(\lambda) - \boldsymbol{\sigma}_N(\lambda) \big)$$
(4.1.4)

in which $\widehat{\xi}$ is the unique fixed point of $O_{T,N}$, *c.f.* Theorem 3.2.2. As follows from Proposition 3.2.1, $\|\widehat{\xi}\|_{L^{\infty}(\partial \mathscr{D}_{0,\varepsilon})} \leq \frac{C}{T}$, uniformly in *N*. Since $\|\varpi_N\|_{L^{\infty}(\partial \mathscr{D}_{0,\varepsilon})} \leq \frac{C}{T}$, uniformly in *N*, one has that

$$\widehat{\mathfrak{U}}_{\max}(\lambda) = \mathscr{O}(T^{-1}) \tag{4.1.5}$$

uniformly on $\partial \mathcal{D}_{0,\varepsilon}$. Further, we can write that

$$\exp\{\widehat{\mathfrak{U}}_{\max}(\lambda)\} = \left(\frac{\lambda - \beta/N}{\lambda + \beta/N}\right)^N \cdot e^{\frac{1}{T}\widehat{\mathfrak{U}}_{\text{eff}}(\lambda)}$$
(4.1.6)

where we have set

$$\widehat{\mathfrak{U}}_{\rm eff}(\lambda) = \widehat{\mathfrak{U}}_{\rm max}(\lambda) + NT \ln\left(\frac{\sinh(\lambda + \beta/N - i\zeta)}{\sinh(\lambda - \beta/N - i\zeta)}\right) + NT \ln\left(\frac{\sinh(\lambda - \beta/N)}{\sinh(\lambda + \beta/N)}\right) - h \tag{4.1.7}$$

upon defining sinch $(\lambda) = \sinh(\lambda)/\lambda$.

Owing to (4.1.5) we have that $\|\widehat{\mathfrak{U}}_{eff}\|_{L^{\infty}(\partial \mathscr{D}_{0,\varepsilon})} < C$ uniformly in *N* and *T* large enough. This representation shows explicitly that $e^{\widehat{\mathfrak{U}}_{max}}$ admits an *N*th-order pole at $-\beta/N$ and no other singularities on $\mathscr{D}_{0,\varepsilon}$. Hence, the zero monodromy condition

$$\oint_{\partial \mathscr{D}_{0,\varepsilon}} \frac{d\lambda}{2i\pi} \frac{\mathfrak{U}'_{\max}(\lambda)}{1 + e^{-\widehat{\mathfrak{U}}_{\max}(\lambda)}} = 0$$
(4.1.8)

entails that $1 + e^{\widehat{\mathfrak{U}}_{\max}}$ admits *N* zeroes counted with multiplicity, inside of $\mathscr{D}_{0,\varepsilon}$. We now show that these zeroes are simple.

Let z be any such zero. The explicit form for $\widehat{\mathfrak{U}}_{eff}$ given in (4.1.7), leads, upon taking the Nth root, to

$$z - \frac{\beta}{N} = \left(z + \frac{\beta}{N}\right) e^{i\psi_N} \quad \text{with} \quad \psi_N = \frac{1}{N} \left\{ (2p - 1)\pi + \frac{i}{T} \widehat{\mathfrak{U}}_{\text{eff}}(z) \right\}$$
(4.1.9)

for some $p \in Z_N$, where $Z_N = [[-N/2 + 1; N/2]]$ if N is even, $Z_N = [[-(N-1)/2; (N-1)/2]]$ if N is odd. One then readily concludes that

$$z - \frac{\beta}{N} = \frac{2\beta \cdot e^{i\psi_N}}{N \cdot [1 - e^{i\psi_N}]} \quad \text{and} \quad z + \frac{\beta}{N} = \frac{2\beta}{N \cdot [1 - e^{i\psi_N}]}.$$
(4.1.10)

The root z has multiplicity higher or equal to 2 if and only if

$$(1 + e^{\widehat{\mathfrak{U}}_{\max}})'(z) = -\widehat{\mathfrak{U}}'_{\max}(z) = 0.$$
 (4.1.11)

Equations (4.1.9) and (4.1.10) allow one to compute $\widehat{\mathfrak{U}}'_{max}(z)$ explicitly:

$$\begin{aligned} \widehat{\mathfrak{U}}_{\max}'(z) &= 2\frac{N^2}{\beta} \cdot \sin^2\left(\frac{\psi_N}{2}\right) + \frac{1}{T}\widehat{\mathfrak{U}}_{\text{eff}}'(z) \\ &= \frac{\pi^2(2p-1)^2}{2\beta} \left\{ 1 + i\frac{\widehat{\mathfrak{U}}_{\text{eff}}(z)}{\pi T(2p-1)} \right\}^2 \cdot \left(\frac{\sin[\psi_N/2]}{\psi_N/2}\right)^2 + \frac{1}{T}\widehat{\mathfrak{U}}_{\text{eff}}(z). \end{aligned}$$
(4.1.12)

We choose c > 0 small enough, then uniformly in N, T large enough and for any $p \in Z_N$ it holds

$$\Re(\psi_N) \in \left[-\pi(1+c); \pi(1+c)\right] \text{ and } \Im(\psi_N) \in \left[-\frac{c}{T}; \frac{c}{T}\right] \quad viz. \quad \left|\frac{\sin[\psi_N/2]}{\psi_N/2}\right| > C'$$
(4.1.13)

for some N and T independent constant C' > 0. This establishes that $\widehat{\mathfrak{U}}'_{\max}(z) \neq 0$. As a consequence, all the zeroes of $1 + e^{\widehat{\mathfrak{U}}_{\max}}$ on $\mathscr{D}_{0,\varepsilon}$ are simple. We denote these N distinct zeroes by $\{\lambda_a^{(\max)}\}_{a=1}^N$.

By repeating the handlings of Chapter 3, it follows that

$$e^{\widehat{\mathfrak{U}}_{\max}(\xi)} = e^{-\frac{\hbar}{T}} (-1)^{s} \prod_{k=1}^{M} \left\{ \frac{\sinh(\mathrm{i}\zeta - \xi + \lambda_{k}^{(\max)})}{\sinh(\mathrm{i}\zeta + \xi - \lambda_{k}^{(\max)})} \right\} \left\{ \frac{\sinh(\xi - \beta/N)}{\sinh(\xi + \beta/N)} \frac{\sinh(\mathrm{i}\zeta + \xi + \beta/N)}{\sinh(\mathrm{i}\zeta + \xi - \beta/N)} \right\}^{N}.$$
(4.1.14)

Thus $\{\lambda_a^{(\max)}\}_{a=1}^N$ is an admissible, pairwise distinct solution of the Bethe Ansatz equations (3.1.9). Hence, the vector $|\Psi(\{\lambda_a^{(\max)}\}_{a=1}^N)\rangle$ introduced in (3.1.7) gives rise to an Eigenvector of the quantum transfer matrix. The associated Eigenvalue (3.1.11) then can be shown to admit the integral representation (4.1.1) by following [31, 32, 91, 92]. Let's consider (3.1.11)

$$\begin{split} \Lambda(\xi|\{\lambda_k^{(\max)}\}_{k=1}^N) &= (-1)^N \cdot e^{\frac{h}{2T}} \cdot \prod_{k=1}^N \left\{ \frac{\sinh(\xi - \lambda_k^{(\max)} + i\zeta)}{\sinh(\xi - \lambda_k^{(\max)})} \right\} \cdot \left[\frac{\sinh(\xi + \frac{\beta}{N})\sinh(\xi - \frac{\beta}{N} - i\zeta)}{\sinh^2(-i\zeta)} \right]^N \\ &+ (-1)^N \cdot e^{-\frac{h}{2T}} \cdot \prod_{k=1}^N \left\{ \frac{\sinh(\xi - \lambda_k^{(\max)} - i\zeta)}{\sinh(\xi - \lambda_k^{(\max)})} \right\} \cdot \left[\frac{\sinh(\xi - \frac{\beta}{N})\sinh(\xi + \frac{\beta}{N} + i\zeta)}{\sinh^2(-i\zeta)} \right]^N. \end{split}$$

$$(4.1.15)$$

We express the above as

$$\Lambda(\xi|\{\lambda_k^{(\max)}\}_{k=1}^N) = (-1)^N \cdot e^{\frac{\hbar}{2T}} \cdot \prod_{k=1}^N \left\{ \frac{\sinh(\xi - \lambda_k^{(\max)} + i\zeta)}{\sinh(\xi - \lambda_k^{(\max)})} \right\} \times \left[\frac{\sinh(\xi + \frac{\beta}{N})\sinh(\xi - \frac{\beta}{N} - i\zeta)}{\sinh^2(-i\zeta)} \right]^N \cdot \left[1 + e^{\widehat{\mathfrak{U}}_{\max}(\xi)} \right].$$
(4.1.16)

Let ξ be small enough and Γ be a loop around the Bethe roots $\{\lambda_a^{(\max)}\}_{a=1}^N$, the *N*-fold pole $-\beta/N$ and such that

$$u \mapsto \ln\left(\frac{\sinh(\xi - u + i\zeta)}{\sinh(\xi - u)}\right) \tag{4.1.17}$$

is analytic in its interior. Note that ξ lies outside of Γ . Then, it holds that

$$\oint_{\Gamma} \frac{du}{2i\pi} \ln\left(\frac{\sinh(\xi - u + i\zeta)}{\sinh(\xi - u)}\right) \frac{\widehat{\mathfrak{U}}'_{\max}(u)}{1 + e^{-\widehat{\mathfrak{U}}_{\max}(u)}} = \sum_{a=1}^{N} \ln\left(\frac{\sinh(\xi - \lambda_a^{(\max)} + i\zeta)}{\sinh(\xi - \lambda_a^{(\max)})}\right) - N\ln\left(\frac{\sinh(\xi + \beta/N + i\zeta)}{\sinh(\xi + \beta/N)}\right).$$
(4.1.18)

Furthermore, one may carry an integration by parts which, due to the zero monodromy condition of $1 + e^{\hat{\mathfrak{U}}_{max}}$, yields

$$\oint_{\Gamma} \frac{du}{2i\pi} \ln\left(\frac{\sinh(\xi - u + i\zeta)}{\sinh(\xi - u)}\right) \frac{\widehat{\mathfrak{U}}'_{\max}(u)}{1 + e^{-\widehat{\mathfrak{U}}_{\max}(u)}} = \oint_{\Gamma} \frac{du}{2\pi i} e_0(u - \xi) \mathscr{L}n \left[1 + e^{\widehat{\mathfrak{U}}_{\max}}\right](u) \qquad (4.1.19)$$

$$= \oint_{\partial \mathscr{D}_{0,\varepsilon}} \frac{du}{2\pi i} e_0(u - \xi) \mathscr{L}n \left[1 + e^{\widehat{\mathfrak{U}}_{\max}}\right](u) + \mathscr{L}n \left[1 + e^{\widehat{\mathfrak{U}}_{\max}}\right](\xi)$$

where we remind that

$$e_0(\xi) = h - \frac{2J\sin^2(\zeta)}{\sinh(\xi)\sinh(\xi - i\zeta)}.$$
(4.1.20)

The last line in (4.1.19) results from taking the residue at $u = \xi$ since the last contour integral on the right hand side of (4.1.19) does contain the pole at $\xi = u$ and $\mathscr{L}n[1 + e^{\widehat{\mathfrak{U}}_{max}}](u)$ is analytic in the domain delimited by Γ and $\partial \mathscr{D}_{0,\varepsilon}$. By putting all these formulae together one gets

$$\widehat{\Lambda}(\xi|\{\lambda_a^{(\max)}\}_{a=1}^N) = \left(\frac{\sinh(\xi - \beta/N - \mathrm{i}\zeta)}{\sinh(-\mathrm{i}\zeta)}\right)^{2N} \times \exp\left\{\frac{h}{2T} - \oint_{\partial \mathscr{D}_{0,\varepsilon}} \frac{du}{2\pi} \frac{\sin(\zeta)}{\sinh(u - \xi - \mathrm{i}\zeta)\sinh(u - \xi)} \mathscr{L}n\left[1 + \mathrm{e}^{\widehat{\mathfrak{U}}_{\max}}\right](u)\right\}.$$
(4.1.21)

Setting $\xi = 0$ leads to the representation (4.1.1).

A simple residue calculation at u = 0 shows that, due to $\widehat{\mathfrak{U}}_{max} = \mathscr{O}(T^{-1})$ uniformly on on $\partial \mathscr{D}_{0,\varepsilon}$, one has the large-*T* behaviour

$$\oint_{\partial \mathscr{D}_{0,\varepsilon}} \frac{du}{2\pi} \frac{\sin(\zeta)}{\sinh(u - \mathrm{i}\zeta)\sinh(u)} \mathscr{L}\mathrm{n}\big[1 + \mathrm{e}^{\widehat{\mathfrak{U}}_{\max}}\big](u) = -\ln 2 + \mathscr{O}\bigg(\frac{1}{T}\bigg). \tag{4.1.22}$$

Thence, (4.1.21) entails that the Eigenvalue admits the following large-T behaviour

$$\widehat{\Lambda}(0|\{\lambda_a^{(\max)}\}_{a=1}^N) = 2 + \mathscr{O}\left(\frac{1}{T}\right).$$
(4.1.23)

Thus, by Proposition 2.2.2, since $\widehat{\Lambda}_{\max} = 2 + \mathcal{O}(T^{-1})$ and that all other Eigenvalues verify $\widehat{\Lambda}_a = \mathcal{O}(T^{-1})$, $\widehat{\Lambda}(0|\{\lambda_a^{(\max)}\}_{a=1}^N)$ must coincide with $\widehat{\Lambda}_{\max}$.

At this point we have that the largest Eigenvalue of the quantum transfer matrix t_q has been fully characterised in this rigorous framework. We now proceed to compute further quantities associated to the XXZ chain (2.1.1) at finite temperature.

4.2 The free energy

In this section we establish an integral representation for the *per*-site free energy (2.1.4) of the XXZ chain. As proven in the beginning of Chapter 2, the *per*-site free energy can be calculated from the Trotter limit of $\ln \hat{\Lambda}_{max}$. Since $\hat{\Lambda}_{max}$ has been identified in Theorem 4.1.1, this leads to the following result

Corollary 4.2.1. There exists $T_0 > 0, \varepsilon > 0$ such that for any $T > T_0$, the per-site free energy of the XXZ chain defined by (2.1.60) admits an integral representation

$$\frac{f_{\text{XXZ}}}{T} = -\frac{h}{2T} + \frac{2J}{T}\cos(\zeta) + \oint_{\partial \mathscr{D}_{0,\varepsilon}} \frac{du}{2\pi} \frac{\sinh(i\zeta)}{\sinh(u - i\zeta)\sinh(u)} \mathscr{L}n[1 + e^{\mathfrak{U}_{\text{max}}}](u)$$
(4.2.1)

in which \mathfrak{U}_{max} corresponds to the unique solution to the non-linear integral equation on $\mathfrak{B}_{\mathfrak{c}}$

$$\mathfrak{U}_{\max}(\xi) = -\frac{e_0(\xi)}{T} + \oint_{\partial \mathscr{D}_{0,\varepsilon}} \frac{du}{2\pi} \frac{\sin(2\zeta)}{\sinh(\xi - u + i\zeta)\sinh(\xi - u - i\zeta)} \mathscr{L}n\big[1 + e^{\mathfrak{U}_{\max}}\big](u)$$
(4.2.2)

where $e_0(\xi)$ is defined in (3.1.60) and the logarithm is defined as in (3.1.29).

The non-linear integral equation is endowed with the zero-monodromy condition

$$\oint_{\partial \mathscr{D}_{0,\varepsilon}} \frac{d\lambda}{2i\pi} \frac{\mathfrak{U}'_{\max}(\lambda)}{1 + e^{-\mathfrak{U}_{\max}(\lambda)}} = 0.$$
(4.2.3)

Finally, the per-site free energy admits the large temperature expansion:

$$\frac{f_{\text{XXZ}}}{T} = -\ln 2 + \frac{J}{T} \{\cos(\zeta)\} + \frac{1}{T^2} \cdot \left\{ \frac{1}{4} \cdot \left[\frac{h^2}{2} + 3J^2 \cdot (1 + 5 \cdot \cos^2(\zeta)) \right] - \frac{3}{2}hJ \cdot \cos(\zeta) \right\} + \mathcal{O}\left(\frac{1}{T^3}\right).$$
(4.2.4)

Proof. It has been established in Theorem 2.3.1 that -

$$-\frac{f_{\rm XXZ}}{T} = \lim_{N \to \infty} \ln \widehat{\Lambda}_{\rm max}.$$
(4.2.5)

Theorem 4.1.1 provides one with the integral representation (4.1.1) for $\widehat{\Lambda}_{max}$. It follows from Theorem 3.2.2 that $\widehat{\mathfrak{U}}_{max}$, converges uniformly on $\partial \mathscr{D}_{0,\varepsilon}$, to the unique solution \mathfrak{U}_{max} of (4.2.2). Thus, by dominated convergence, (4.2.1) follows. The details of the calculations of the high temperature expansion of the *per*-site free energy are given in Appendix D.

We stress that the expression (4.2.1) has already appeared in the literature [91, 92, 31, 32]. The high temperature expansion (4.2.4) was derived from (4.2.1) long ago. Here the results are only stated for completeness. Also, the high temperature expansion was obtained through a different method, up to order $\mathcal{O}(T^{-5})$, in [144] for the XXZ chain in a non-vanishing magnetic field and up to order $\mathcal{O}(T^{-100})$ for the Heisenberg chain at zero magnetic field [148].

4.3 The sub-leading Eigenvalues and the correlation lengths

This section is devoted to the rigorous characterisation of the high temperature behaviour, directly in the Trotter limit, of the sub-dominant Eigenvalues of the quantum transfer matrix. We recall that Proposition 2.2.2 stipulates that any sub-leading Eigenvalue $\hat{\Lambda}_a$ is estimated as $|\hat{\Lambda}_a| \leq C/T$ for some *C* that is *N*-independent. In this section, we will refine these estimates, at least for a certain subset of Eigenvalues. While, in principle, one should start by discussing the finite Trotter number case, we will only focus our discussion on the infinite Trotter number limit of the Eigenvalues $\hat{\Lambda}_a$. The fact that $\lim_{N\to\infty} \hat{\Lambda}_a$ exists may be extracted readily from the results to come, by an application of the implicit function theorem, at least in the well-behaved cases. However, prior to going into such details, we wish to discuss the physical pertinence of the sub-dominant Eigenvalues of the quantum transfer matrix. For example, just as an identification of the largest Eigenvalue allows one to explicitly calculate the *per*-site free energy, the sub-leading Eigenvalues allow one to compute the correlation lengths of the XXZ chain [41, 59, 92, 95, 107, 106, 162].

To discuss this matter, let $|\Psi_0\rangle$ stand for the dominant Eigenstate of the quantum transfer matrix, $|\Psi_a\rangle_1^{N_L}$ be all the Eigenvalues in the spin s = 0 sector and $|\Phi_a\rangle_1^{N_T}$ be all the other Eigenstates in the spin s = 1 sector. Denote by $\widehat{\Lambda}_a^0$, respectively $\widehat{\Lambda}_a^+$, the associated Eigenstates. Then as indicated in [36, 37], within the quantum transfer

approach the longitudinal and transverse two points functions $\langle \sigma_1^z \sigma_{m+1}^z \rangle$ and $\langle \sigma_1^- \sigma_{m+1}^+ \rangle$ can be recast in terms of finite Trotter limit number approximants

$$\langle \sigma_1^z \sigma_{m+1}^z \rangle = \lim_{N \to \infty} \langle \sigma_1^z \sigma_{m+1}^z \rangle_N \quad \text{and} \quad \langle \sigma_1^- \sigma_{m+1}^+ \rangle = \lim_{N \to \infty} \langle \sigma_1^- \sigma_{m+1}^+ \rangle_N.$$
(4.3.1)

The finite Trotter number approximants admit thermal form factor expansions of the form

$$\langle \boldsymbol{\sigma}_{1}^{z}\boldsymbol{\sigma}_{m+1}^{z}\rangle_{N} - \langle \boldsymbol{\sigma}_{1}^{z}\rangle_{N}\langle \boldsymbol{\sigma}_{m+1}^{z}\rangle_{N} = \sum_{a=1}^{N_{M_{L}}}\widehat{A}_{a}^{zz}(\widehat{\boldsymbol{\rho}}_{a}^{(s)}-1)^{2}[\widehat{\boldsymbol{\rho}}_{a}^{(s)}]^{m-1}$$
(4.3.2)

and

$$\langle \sigma_1^- \sigma_{m+1}^+ \rangle_N = \sum_{a=1}^{N_{M_T}} \widehat{A}_a^{-+} (\widehat{\rho}_a^{(s)} - 1)^2 [\widehat{\rho}_a^{(s)}]^m.$$
(4.3.3)

Equations (4.3.2) and (4.3.3) represents the finite-temperature asymptotic expansion of longitudinal and transverse correlation functions at finite Trotter number. \hat{A}_a^{zz} and \hat{A}_a^{-+} corresponds to respective amplitudes of the correlation functions (4.3.2) and (4.3.3) constructed as

$$\widehat{A}_{a}^{zz} = \frac{\langle \Psi_{0} | [\mathbf{A}(0) - \mathbf{D}(0)] | \Psi_{a} \rangle \langle \Psi_{a} | [\mathbf{A}(0) - \mathbf{D}(0)] | \Psi_{0} \rangle}{\langle \Psi_{0} | \Psi_{0} \rangle \langle \Psi_{a} | \Psi_{a} \rangle}$$
(4.3.4)

and

$$\widehat{A}_{a}^{-+} = \frac{\langle \Psi_{0} | \mathsf{B}(0) | \Phi_{a} \rangle \langle \Phi_{a} | \mathsf{C}(0) | \Psi_{0} \rangle}{\widehat{\Lambda}_{\max} \langle \Psi_{0} | \Psi_{0} \rangle \widehat{\Lambda}_{a} \langle \Phi_{a} | \Phi_{a} \rangle}.$$
(4.3.5)

The function $\hat{\rho}_a^{(s)}$ is the ratio of the sub-leading Eigenvalues to the maximal Eigenvalue

$$\widehat{\rho}_{a}^{(s)} = \frac{\widehat{\Lambda}_{a}^{(s)}}{\widehat{\Lambda}_{\max}}.$$
(4.3.6)

It is useful to take the parametrisation

$$\widehat{\rho}_a^{(s)} = \mathrm{e}^{-\frac{1}{\widehat{\xi}_a^{(s)}}} \tag{4.3.7}$$

in which $\hat{\xi}_a^{(s)}$ plays the role of the correlation lengths. Thus correlation lengths control the speed of the exponential decay of two and multi-point correlation functions seen as a function of the distances separating the local operators [36, 37].

The Eigenvalue ratio defining $\hat{\rho}_a^{(s)}$ may be computed from the Bethe Ansatz approach. Indeed by repeating the reasonings outlined in (4.1.15)-(4.1.22) one readily obtains that at least those Eigenvalues of the quantum transfer matrix which can be computed from the Bethe Ansatz admit the following integral representation

$$\ln\widehat{\Lambda}(0|\{\lambda_k\}_{k=1}^M) = -\frac{h}{2T} - 2J\cos(\zeta) + \sum_{y\in\mathscr{Y}} \ln\left\{\frac{\sinh(y-i\zeta)}{\sinh(y)}\right\} - \sum_{x\in\mathfrak{X}} \ln\left\{\frac{\sinh(x-i\zeta)}{\sinh(x)}\right\} + \oint_{\partial\mathscr{D}_{0,\varepsilon}} \frac{du}{2\pi} \cdot \frac{\sin(2\zeta)}{\sinh(u-i\zeta)\sinh(u)} \cdot \mathscr{L}n\left[1 + e^{\widehat{\mathfrak{U}}}\right](u).$$

$$(4.3.8)$$

The latter involves the solutions $(\mathfrak{U}, \mathfrak{X}, \mathscr{Y})$ to the non-linear problem in Section 3.1.2 of Chapter 3. Of course, while the solvability of the non-linear integral equation

$$\mathfrak{U}(\xi) = -\frac{h}{T} + e_0(\xi) - \mathrm{i}\pi s + \mathrm{i}\sum_{y \in \mathbb{Y}_{\kappa}} \theta(\xi - y) + \oint_{\partial \mathscr{D}_{0,\varepsilon}} du \, K(\xi - u) \cdot \mathscr{L}\mathrm{n}\big[1 + \mathrm{e}^{\mathfrak{U}}\big](u) \tag{4.3.9}$$

where

$$e_0(\xi) = h - \frac{2J\sin^2(\zeta)}{\sinh(\xi)\sinh(\xi - i\zeta)}$$
(4.3.10)

for sets $\mathfrak{X}, \mathscr{Y}$ in a $\mathscr{C}^{\varepsilon}_{\alpha,\rho}$ class follows from the setting of Section 2, one still needs to solve the subsidiary conditions to give a meaning to the representation (4.2.1). The non-linear integral equation (4.3.9) is now subject to the additional constraints (3.1.26) on the monodromy of the solution and on the parameters building up the particle-hole sets.

One eventually takes the Trotter limit in (4.3.6) which amounts to taking the $N \rightarrow \infty$ limit at the level of (4.1.1) and (4.3.8) leading to

$$\xi_a = \left[-\ln\left(\frac{\Lambda_a}{\Lambda_{\max}}\right) \right]^{-1}.$$
(4.3.11)

The integral representation in the Trotter limit follows readily and is

$$\rho_{a} = \exp\left\{\sum_{y \in \mathscr{Y}} \ln\left(\frac{\sinh(y - i\zeta)}{\sinh y}\right) - \sum_{x \in \mathfrak{X}} \ln\left(\frac{\sinh(x - i\zeta)}{\sinh x}\right) + \oint_{\partial \mathscr{D}_{0,\varepsilon}} \frac{du}{2\pi} \frac{\sin(2\zeta)}{\sinh(u - i\zeta)\sinh(u)} \mathscr{L}n\left(\frac{1 + e^{\mathfrak{U}}}{1 + e^{\mathfrak{U}_{\max}}}\right)(u)\right\}$$
(4.3.12)

where

$$\rho_a = \mathrm{e}^{-\frac{1}{\xi_a}} \quad \text{and} \quad \rho_a = \lim_{N \to \infty} \widehat{\rho}_a.$$
(4.3.13)

and $\mathcal{L}n$ defined in (3.1.29). In this representation, one can readily compute the large temperature asymptotics of the correlation lengths. Together with the representations of the amplitudes in the infinite Trotter limit (see *e.g.* [36]) admitting large temperature behaviours as well, one can obtain the dominant contribution of the high temperature expansion of the aforementioned two point functions.

4.4 Structure of the zero sets to the particle and hole roots at high temperature

In Chapter 3 we have shown that any choice of sets $\mathfrak{X}, \mathscr{Y}$ in a $\mathscr{C}^{\varepsilon}_{\alpha,\rho}$ class gives rise to a solution to (4.3.9). We now study the solvability of the auxiliary conditions for the subsets of solutions belonging to the class $\mathscr{C}^{\varepsilon}_{\alpha,\rho}$ defined in (3.2.1) with fixed cardinalities n_x and n_y and parameters ε , α and ρ small but finite. Further we discuss the behaviours of the hole and particle roots building up the resulting sets \mathfrak{X} and \mathscr{Y} respectively. In this section we rigorously characterise their behaviours up to the order $\mathscr{O}(T^{-1})$. This analysis allows us to write down the leading large temperature behaviour of the correlation length in terms of the dominant contribution of the particle and hole roots.

4.4.1 A preliminary high temperature analysis

In Proposition 3.2.1 we have established the properties satisfied by the operator $O_{T,N}$ which allowed us to form Theorem 3.2.2 pertaining to the strict contractivity of this operator $O_{T,N}$ at temperatures high enough, this for $\alpha, \rho > 0$ and n_x, n_y fixed. All of this ensures that there exist temperatures $T_0 > 0$ and $\varepsilon > 0$ such that the solution to the non-linear integral equation (4.3.9) can be expressed as

$$\mathfrak{U} = \mathfrak{U}_{\infty} + \frac{1}{T}\mathfrak{b} \tag{4.4.1}$$

with

$$\mathfrak{b} = -e_0 + \chi_{\infty;\varepsilon}(\lambda) + \frac{1}{T} \oint_{\partial \mathscr{D}_{0,\varepsilon}} du K(\lambda - u) \int_{\kappa}^{u} dv \int_{0}^{1} dt \, G[\xi - e_0](v, t)$$
(4.4.2)

where $\chi_{\infty;\varepsilon}(\lambda)$ is defined in (3.2.46). In the above, ξ is the unique fixed point of $O_{T,N}$ (3.2.22) associated with the roots \mathfrak{X} and \mathscr{Y} . The function \mathfrak{b} grasp the structure of the sub-leading corrections in $\frac{1}{T}$ to \mathfrak{U} and is readily seen to be bounded on $\partial \mathscr{D}_{0,\varepsilon}$. We study the solvability of the constraints (3.1.26) assuming that $\mathfrak{X}, \mathscr{Y}$ belong to the class $\mathscr{C}^{\varepsilon}_{\alpha,\rho}$ with cardinalities n_x, n_y .

In what follows, we will show that the particle root of the set \mathscr{Y} , approaches to the leading order in T^{-1} , an element of the solution set of the Bethe Ansatz equation associated with the XXZ spin-1 chain

$$\sigma_{\infty} = \left\{ \mathscr{Y}_{\infty} = \left\{ y_{\infty;a} \right\}_{a=1}^{|\mathscr{Y}|} : \forall a \in [\![1:n_y]\!], \\ (-1)^{s+1} \lim_{u \to y_{\infty;a}} \prod_{b=1}^{n_y} \left\{ \frac{\sinh(i\zeta + y_{\infty;b} - u)}{\sinh(i\zeta + u - y_{\infty;b})} \right\} \cdot \left(\frac{\sinh(i\zeta + u)}{\sinh(i\zeta - u)} \right)^{n_y} = 1 \right\}.$$

$$(4.4.3)$$

The above definition of the solutions sets allows, in principle, for some roots to be located at infinity. Indeed, the limit of some roots going to infinity is well-defined within the prescription used for defining the full solution set σ_{∞} . In order to make the statement about this convergence precise, we introduce a distance between two sets $\mathscr{Y} = \{y_a\}_{a=1}^{n_y}$ and $\mathscr{Y}' = \{y_a\}_{a=1}^{n_y}$ as

$$d(\mathscr{Y},\mathscr{Y}') = \min_{\sigma \in \mathfrak{S}_{n_y}} \bigg\{ \sum_{a=1}^{n_y} |y_a - y'_{\sigma(a)}| \bigg\}.$$
(4.4.4)

Then, the distance of a set \mathscr{Y} of cardinality n_y to σ_{∞} is

$$d(\boldsymbol{\sigma}_{\infty}, \mathscr{Y}) = \min_{\mathscr{Y}_{\infty} \in \boldsymbol{\sigma}_{\infty}} \left\{ d(\mathscr{Y}_{\infty}, \mathscr{Y}) \right\}.$$
(4.4.5)

4.4.2 The particle and hole sets at high temperatures

Proposition 4.4.1. Let $\alpha, \rho > 0$ and $n_x, n_y \in \mathbb{N}$ be fixed. Let \mathfrak{X} and \mathscr{Y} belong to the class $\mathscr{C}^{\varepsilon}_{\alpha,\rho}$ with cardinalities n_x, n_y . Let $T_0 > 0$ and $\varepsilon > 0$ be as in Theorem 4.1.1. Let \mathfrak{U} be the unique solution to the non-linear integral equation (3.1.27).

If the sets $\mathfrak{X} = \{x_a\}_{a=1}^{n_x}$ and $\mathscr{Y} = \{y_a\}_{a=1}^{n_y}$ giving rise to the solution \mathfrak{U} are also such that it holds

$$\oint_{\partial \mathscr{D}} \frac{du}{2i\pi} \frac{\mathfrak{U}'(u)}{1 + e^{-\mathfrak{U}(u)}} = -s - |\mathscr{Y}| + |\mathfrak{X}|$$
(4.4.6)

and the subsidiary conditions

$$e^{\mathfrak{U}(x_a)} = -1, \text{ for any } a = 1, \dots, n_x,$$

 $e^{\mathfrak{U}(y_a)} = -1, \text{ for any } a = 1, \dots, n_y$
(4.4.7)

are satisfied uniformly in T large enough, then necessarily,

- $|\mathfrak{X}| = |\mathscr{Y}| + s;$
- there exists integers $k_a \in \mathbb{Z}$ such that the hole roots admit the high temperature expansion

$$x_a = \frac{-2J\sin(\zeta)}{T\left[(2k_a+1+s)\pi - \sum_{y \in \mathscr{Y}} \theta(-y)\right]} + \mathscr{O}\left(\frac{1}{T^2}\right) \quad a = 1, \dots, n_x;$$
(4.4.8)

• $d(\sigma_{\infty}, \mathscr{Y}) = o(1)$, for $T \to \infty$ and where the control on the remainder only depends on $\varepsilon, \rho, \alpha, n_x, n_y$.

Remark 4.4.1. This entails that, in the high temperature limit, the sub-dominant Eigenvalues of the quantum transfer matrix are parametrised in terms of solutions to a finite length spin-1 chain. The hole roots then converge to 0 at a speed of $\mathcal{O}(T^{-1})$. This convergence may be faster if it happens that the integers k_a goes to infinity with T.

Proof. The expansion of the auxiliary function \mathfrak{U} from (4.4.1) guarantees that

$$\frac{\mathfrak{U}'}{1+\mathrm{e}^{-\mathfrak{U}(\lambda)}} = \frac{\mathfrak{U}'_{\infty}(\lambda)}{1+\mathrm{e}^{-\mathfrak{U}_{\infty}(\lambda)}} + \frac{1}{T}\partial_{\lambda}\left\{\frac{\mathfrak{b}(\lambda)}{1+\mathrm{e}^{-\mathfrak{U}_{\infty}(\lambda)}}\right\} + \mathscr{O}\left(\frac{1}{T^2}\right),\tag{4.4.9}$$

with the T^{-2} remainder being uniform on $\partial \mathcal{D}_{0,\varepsilon}$.

Upon inserting this expansion into the monodromy condition (3.1.26), one has that

$$\oint_{\partial \mathscr{D}_{0,\varepsilon}} \frac{\mathfrak{U}_{\infty}'(\lambda)}{1 + \mathrm{e}^{-\mathfrak{U}_{\infty}(\lambda)}} + \mathscr{O}\left(\frac{1}{T}\right) = |\mathfrak{X}| - |\mathscr{Y}| - s, \tag{4.4.10}$$

since the sets $\mathfrak{X}, \mathscr{Y}$, belonging to the class $\mathscr{C}^{\varepsilon}_{\alpha,\rho}$ with $\varepsilon > 0$ small enough, do not give rise to singular roots. However, due to (3.2.13), the first integral vanishes. Since the right hand side is integer valued, and since the sole dependence on $\mathfrak{X}, \mathscr{Y}$ of the remainder $\mathscr{O}(T^{-1})$ in the left hand side is bounded by $|\mathfrak{X}| + |\mathscr{Y}|$, one concludes that there exits T'_0 large enough such that, for any $T > T'_0$, the sets $\mathfrak{X}, \mathscr{Y}$ belonging to the class $\mathscr{C}^{\varepsilon}_{\alpha,\rho}$ produce solutions to the joint problem (3.1.27) if and only if their cardinalities are subject to the constraint

$$|\mathfrak{X}| = |\mathscr{Y}| + s. \tag{4.4.11}$$

With the above settled, we can now precisely study the structure of the sets \mathfrak{X} and \mathscr{Y} satisfying to the constraint (3.1.26).

The hole roots

We start by determining the elements building up the hole set \mathfrak{X} . The function \mathfrak{b} is meromorphic on $\mathscr{D}_{0,\varepsilon}$ with a simple pole at $\xi = 0$ such that

$$\operatorname{Res}(\mathfrak{b}(\xi)d\xi,\xi=0) = -2iJ\sin(\zeta). \tag{4.4.12}$$

Hence there exists a holomorphic function, on the domain $\mathscr{D}_{0,\varepsilon}$ noted $\mathfrak{b}^{(r)}$, that is bounded uniformly in *T* large enough and such that

$$\mathfrak{b}(\xi) = -\frac{2iJ}{\xi}\sin(\zeta) + \mathfrak{b}^{(r)}(\xi). \tag{4.4.13}$$

Any hole root *x* will then satisfy to the equation

$$\mathfrak{U}(x) = \mathfrak{U}_{\infty}(x) + \frac{\mathfrak{b}(x)}{T} = (2k_x + 1)\mathbf{i}\pi \quad \text{for some } k_x \in \mathbb{Z}.$$
(4.4.14)

Since we have established that $1 + e^{-\mathfrak{U}_{\infty}}$ does not have zeroes on $\mathscr{D}_{0,\varepsilon}$, it holds that

$$d(\mathfrak{U}_{\infty}(\mathscr{D}_{0,\varepsilon}), \mathrm{i}\pi + 2\mathrm{i}\pi\mathbb{Z}) > C_{\rho} \quad \text{for some } C_{\rho} > 0 \tag{4.4.15}$$

and depending on ρ .

Hence any solution to (4.4.14) has to be such that

$$\left|\frac{\mathfrak{b}(x)}{T}\right| > C_{\rho}.\tag{4.4.16}$$

The form of the behaviour around the origin (4.4.13) then entails that Tx has to be uniformly bounded. Thus, one reparametrises

$$x = \frac{u_x}{T} \tag{4.4.17}$$

with u_x bounded in T leading to the equation

$$(2k_x+1)\mathbf{i}\pi = \mathfrak{U}_{\infty}(0) - \frac{2\mathbf{i}J}{u_x}\sin(\zeta) + \mathscr{O}\left(\frac{1}{T}\right).$$
(4.4.18)

Since $(2k_x + 1)i\pi - \mathfrak{U}_{\infty}(0)$ does not vanish due to (4.4.15) it follows that

$$u_x = \frac{-2iJ\sin(\zeta)}{(2k_x + 1)i\pi - \mathfrak{U}_{\infty}(0)} + \mathscr{O}\left(\frac{1}{T}\right)$$
(4.4.19)

with $x = \frac{u_x}{T}$.

The particle roots

The very definition of the class $\mathscr{C}^{\varepsilon}_{\alpha,\rho}$ entails that particle roots $y \in \mathscr{Y}$ are such that $y \pm i\zeta \notin \mathscr{D}_{0,\varepsilon}$. Then, one has

$$e^{\mathfrak{U}(\lambda)} = e^{\mathfrak{U}_{\infty}(\lambda)} \cdot e^{\frac{\mathfrak{b}(\lambda)}{T}} \quad \text{for } \lambda \in \mathscr{S}_{\frac{\pi}{2}} \setminus \big\{ \mathscr{D}_{0,\varepsilon} \bigcup \cup_{\nu=\pm} \mathscr{D}_{\nu i \zeta_{m},\alpha} \big\}$$
(4.4.20)

and thus any root $y \in \mathscr{Y}$ satisfies

$$(-1)^{s+1} \cdot \lim_{u \to y} \left\{ \prod_{y' \in \mathscr{Y} \ominus \mathfrak{X}} \frac{\sinh(\mathrm{i}\zeta + y' - u)}{\sinh(\mathrm{i}\zeta + u - y')} \right\} \cdot \mathrm{e}^{\mathscr{O}(T^{-1})} = 1.$$
(4.4.21)

We note that the limit procedure enables one to have a prescription for treating the roots at infinity and also for regularising potential zeroes and poles which cancels eventually between the numerator and denominator in the product. We have already established in (4.4.19) that

$$x = \mathscr{O}\left(\frac{1}{T}\right) \quad \text{for any } x \in \mathfrak{X}.$$
 (4.4.22)

Thus, the properties of the class $\mathscr{C}^{\varepsilon}_{\alpha,\rho}$ allow to recast (4.4.21) in the form

$$(-1)^{s+1} \lim_{u \to y} \left\{ \prod_{y \in \mathscr{Y}} \left[\frac{\sinh(\mathrm{i}\zeta + y' - u)}{\sinh(\mathrm{i}\zeta + u - y')} \right] \cdot \left(\frac{\sinh(\mathrm{i}\zeta + y)}{\sinh(\mathrm{i}\zeta - y)} \right)^{n_y} \right\} \cdot \mathrm{e}^{\mathscr{O}(T^{-1})} = 1.$$
(4.4.23)

Assume that \mathscr{Y} is a one parameter T family of particle sets solving the constraints (3.1.26) and such that $d(\mathscr{Y}, \sigma_{\infty})$ does not converge to zero as $T \to \infty$. Thus, one may extract a sequence of sets \mathscr{Y}_n associated with a sequence of temperatures $T_n \to \infty$ such that $d(\mathscr{Y}_n, \sigma_{\infty}) > \gamma$ for some $\gamma > 0$. By taking $n \to +\infty$ on the level of the associated equation (4.4.23), one gets that the limiting set $\mathscr{Y}_{\infty} \in \sigma_{\infty}$ which contradicts $d(\mathscr{Y}_n, \sigma_{\infty}) > \gamma$. This entails the claim.

4.4.3 Comments on the hole and particle roots high-*T* behaviours

Observe that the previous analysis indicates that the elements of a particle set, gathered in a vector $\mathbf{y} = (y_1, \dots, y_{|\mathscr{Y}|})$ converge to a zero on

$$\mathscr{S}_{\frac{\pi}{2}} \setminus \{ \mathscr{D}_{0,\varepsilon} \bigcup \cup_{\nu=\pm} \mathscr{D}_{\nu i \zeta_{m},\alpha} \}, \tag{4.4.24}$$

of the map

$$\boldsymbol{f}: \begin{cases} \mathbb{C}^{|\mathscr{Y}|} \to \mathbb{C}^{|\mathscr{Y}|} \\ \boldsymbol{y} \mapsto \boldsymbol{f}(\boldsymbol{y}) \end{cases}$$
(4.4.25)
where

$$\boldsymbol{f}(\boldsymbol{y}) = \left(\boldsymbol{f}_1(\boldsymbol{y}), \dots, \boldsymbol{f}_{|\mathscr{Y}|}(\boldsymbol{y})\right), \tag{4.4.26}$$

with

$$\boldsymbol{f}_{b}(\boldsymbol{y}) = 1 + (-1)^{s} \cdot \prod_{a=1}^{|\mathscr{Y}|} \frac{\sinh(i\zeta + y_{a} - y_{b})}{\sinh(i\zeta + y_{b} - y_{a})} \cdot \left[\frac{\sinh(i\zeta + y_{b})}{\sinh(i\zeta - y_{b})}\right]^{|\mathscr{Y}| + s}.$$
(4.4.27)

In order to refine the information on the rate of convergence of the set \mathscr{Y} to some element of σ_{∞} , one needs to have more information on the behaviour of f around the neighbourhood of its zeroes.

In particular, if

$$\mathbf{y}_{\infty} = \left(y_{\infty;1}, \dots, y_{\infty;|\mathscr{Y}|} \right) \tag{4.4.28}$$

constitutes a zero of f and if the differential $\mathfrak{D}_{\mathbf{y}_{\infty}} f$ of f at \mathbf{y}_{∞} is invertible, then if $\mathbf{y} = (y_1, \dots, y_{|\mathscr{Y}|})$ is the vector built up from the elements of the particle set \mathscr{Y} , and if it holds that

$$\mathbf{y} = \mathbf{y}_{\infty} + o(1), \tag{4.4.29}$$

where the remainder is to be understood coordinate-wise when $T \rightarrow \infty$. Then the implicit function theorem entails that, in fact, one has the estimate

$$y_a = y_{\infty;a} + \mathscr{O}\left(\frac{1}{T}\right). \tag{4.4.30}$$

This allows us to formulate the below corollary relatively to this special case:

Corollary 4.4.1. Under the above assumptions there exists $T_0 > 0$ such that the infinite Trotter limit of a set of sub-leading Eigenvalue Λ_a the quantum transfer matrix has the high temperature expansion

$$\Lambda_a = \frac{1}{T^{n_x}} \cdot (1 + \mathrm{e}^{\mathfrak{U}_{\infty}(0)}) \cdot \prod_{a=1}^{n_x} \left\{ \frac{-2\mathrm{i}J}{(2k_a + 1)\mathrm{i}\pi - \mathfrak{U}_{\infty}(0)} \right\} \cdot \prod_{a=1}^{n_y} \left\{ \frac{\sinh(y_{a;\infty} - \mathrm{i}\zeta)}{\sinh(y_{a;\infty})} \right\} \cdot \left\{ 1 + \mathscr{O}\left(\frac{1}{T}\right) \right\}$$
(4.4.31)

where

$$\mathbf{e}^{\mathfrak{U}_{\infty}(0)} = (-1)^{s} \cdot \prod_{a=1}^{n_{y}} \frac{\sinh(\mathbf{i}\boldsymbol{\zeta} - y_{a;\infty})}{\sinh(\mathbf{i}\boldsymbol{\zeta} + y_{a;\infty})}.$$
(4.4.32)

and $k_a \in \mathbb{Z}$. Consequently, the exponents of the correlation lengths read

$$e^{-\frac{1}{\xi_a}} = \frac{1}{2} \cdot \frac{1}{T^{n_x}} \cdot (1 + e^{\mathfrak{U}_{\infty}(0)}) \cdot \prod_{a=1}^{n_x} \left\{ \frac{-2iJ}{(2k_a + 1)i\pi - \mathfrak{U}_{\infty}(0)} \right\} \cdot \prod_{a=1}^{n_y} \left\{ \frac{\sinh(y_{a;\infty} - i\zeta)}{\sinh(y_{a;\infty})} \right\}.$$
(4.4.33)

Proof. Let $\mathbf{y}_{\infty} = (y_{\infty;1}, \dots, y_{n_y})$ be a vector with pairwise distinct coordinates and such that $y_{\infty;a} \neq 0$ and $\{y_{\infty;a}\}_1^{n_y}$ is an admissible set. Assume that

$$\boldsymbol{f}(\boldsymbol{y}_{\infty}) = \boldsymbol{0} \tag{4.4.34}$$

and that $\mathfrak{D}_{\mathbf{y}_{\omega}} \mathbf{f}$ is invertible. Then given k_1, \ldots, k_{n_y} integers, there exist sets $\mathfrak{X}, \mathscr{Y}$ belonging to a $\mathscr{C}^{\varepsilon}_{\alpha,\rho}$ class for some ε, α and ρ such that $(\mathfrak{U}, \mathfrak{X}, \mathscr{Y})$ solves the non-linear problem (4.3.9) for

$$\mathscr{Y} = \{y_a\}_{a=1}^{n_y} \quad \text{with} \quad y_a = y_{\infty;a} + \mathscr{O}\left(\frac{1}{T}\right)$$

$$\mathfrak{X} = \{x_a\}_{a=1}^{n_x} \quad \text{with} \quad x_a = x_{\infty;a} + \mathscr{O}\left(\frac{1}{T^2}\right), \quad x_{\infty;a} = \frac{-2J\sin(\zeta)}{T\left[(2k_a + 1 + s)\pi - \sum_{y \in \mathscr{Y}} \theta(-y)\right]}.$$
(4.4.35)

The associated Eigenvalue Λ_a (4.3.8) of the quantum transfer matrix in the infinite Trotter limit admits the large temperature expansion

$$\ln \Lambda_{a} = -\frac{h}{2T} - 2J\cos(\zeta) + \sum_{a=1}^{n_{y}} \ln \left\{ \frac{\sinh(y_{\infty;a} + \mathcal{O}(1/T) - i\zeta)}{\sinh(y_{\infty;a} + \mathcal{O}(1/T))} \right\} - \sum_{a=1}^{n_{x}} \ln \left\{ \frac{\sinh(x_{\infty;a}/T + \mathcal{O}(1/T^{2})) - i\zeta)}{\sinh(x_{\infty;a}/T + \mathcal{O}(1/T^{2}))} \right\} - \oint_{\partial \mathscr{D}_{0,\varepsilon}} \frac{du}{2\pi} \cdot \frac{\sin(2\zeta)}{\sinh(u + i\zeta)\sinh(u)} \cdot \mathscr{L}n\left\{ (1 + e^{\mathfrak{U}_{\infty}}) \left[1 + \frac{e^{\mathfrak{U}_{\infty}}}{1 + e^{\mathfrak{U}_{\infty}}} \frac{\mathfrak{b}}{T} + \mathcal{O}\left(\frac{1}{T^{2}}\right) \right] \right\} (u).$$

$$(4.4.36)$$

A direct residue calculation at u = 0 allows to compute the leading high temperature behaviour of the integral above and allows one to recast Λ_a as in (4.4.31).

The $\mathcal{O}(T^{-1})$ expansion for the correlation lengths (4.4.33) follows immediately upon replacing (4.3.8) and (4.1.23) into the expression (4.3.11). This entails the claim.

Chapter 5

Conclusions

In this thesis, we have set the quantum transfer matrix approach to the study of quantum spin chains at finite temperature into a rigorous framework. For temperatures high enough, the conjectures raised in the literature have been rigorously established, namely the exchangeability of the infinite volume and infinite Trotter limit, the existence of non-degenerate, real and maximal in modulus Eigenvalue of the quantum transfer matrix, the welldefinedness of the class of non-linear integral equations characterising the Eigenvalues of the quantum transfer matrix together with the existence and uniqueness of their solutions, and, finally, the rigorous identification of the non-linear integral representation characterising the dominant Eigenvalue of the quantum transfer matrix. The proof we developed allowed us to rigorously frame the integral representation of the *per*-site free energy of the spin-1/2 XXZ chain which was argued in [31] and in [92]. We do trust that these results developed in this thesis lay a firm ground for the rigorous analysis of the correlation functions of the spin-1/2 XXZ chain at finite but sufficiently large temperatures. In particular, in this respect, it would be very interesting to generalise the exchangeability of the limits theorem to the case of the reduced density matrix of a finite sub-segment of the chain. Also, the explicit results relative to the structure of the excited states should allow for a precise analysis of the high temperature behaviour of the form factors series representation of the thermal dynamical correlation functions of the chain. In part, building on the determinant representation for the amplitudes of the transverse correlation functions obtained in [37, 36], one should be able to access their dominant behaviours. We should also stress, that with minor modifications, the exchangeability of the limits theorem that we have established in Chapter 2 should generalise to the case of the higher rank quantum integrable models in their fundamental representations.

Appendices

Appendix A

Notations

A.1 Symbols and set notations

- id_M refers to the $M \times M$ identity matrix.
- The o and \mathcal{O} refer to usual domination relations between functions.
- For integers a < b, $[[a;b]] = \{a, a+1, ..., b\}$
- Define $\mathscr{D}_{z_0,r}$ is the open disk centred on $z_0 \in \mathbb{C}$ of radius *r* as

$$\mathscr{D}_{z_0,r} = \{ z \in \mathbb{C} : |z - z_0| < r \}.$$
(A.1.1)

 $\partial \mathcal{D}_{z_0,r}$ stands for its canonically oriented boundary.

• Define for $\alpha > 0$ the strip \mathscr{S}_{α} is the strip of width α centred around \mathbb{R} as

$$\mathscr{S}_{\alpha} = \{ z \in \mathbb{C} : |\mathfrak{I}(z)| < \alpha \}.$$
(A.1.2)

• δ_{ab} refers to the Kronecker delta symbol with

$$\delta_{ab} = \begin{cases} 1, a = b, \\ 0, a \neq b. \end{cases}$$
(A.1.3)

• $\sigma^x, \sigma^y, \sigma^z$ stands for the Pauli matrices:

$$\sigma^{x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma^{y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma^{z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
(A.1.4)

- Bold letters denotes a vector.
- The superscript ^t_a denotes the partial transposition with respect to the *a*th space while the superscript ^t denotes the global transposition with respect to the full tensor product space.

A.2 Functions

• The indicator function of a subset A of a set X is a function $\mathbf{1}_A : X \to \{0,1\}$ is defined as

$$\mathbf{1}_{A}(x) := \begin{cases} 1, & \text{if } x \in A \\ 0, & \text{if } x \notin A \end{cases}.$$
 (A.2.1)

• sgn is the sign function on $\mathbb R$ defined as

$$\operatorname{sgn}(x) = \begin{cases} -1 \text{ if } x < 0, \\ 0 \text{ for } x = 0, \\ 1 \text{ if } x > 0. \end{cases}$$
(A.2.2)

A.3 Functional calculus

- The spectrum of an operator A, denoted $\sigma(\mathtt{A})$ is the set

$$\sigma(\mathbf{A}) = \big\{ \lambda \in \mathbb{C} : \mathbf{A} - \lambda \text{ id is not invertible} \big\}.$$
(A.3.1)

• The spectral radius of an operator A is

$$r_{S}(A) = \sup\{|\lambda| : \lambda \in \sigma(A)\}$$
(A.3.2)

and $\|\cdot\|$ its norm.

Appendix B

Several theorems of use to the analysis

B.1 Matrix analysis

Lemma B.1.1. For Hermitian matrices A and B, it follows that

$$\left|\ln \operatorname{tre}^{A} - \ln \operatorname{tre}^{B}\right| \leq \left\|A - B\right\| \tag{B.1.1}$$

where $\|\cdot\|$ is the operator norm induced by the canonical scalar product.

B.2 Functional spaces

• Let $U \subset \mathbb{C}$. O(U) stands for the ring of holomorphic functions on U, and for any function f on U, we denote

$$\|f\|_{L^{\infty}(U)} = \operatorname{supess}_{u \in U} |f(u)|.$$
(B.2.1)

• \mathfrak{B}_r is the complete metric space

$$\mathfrak{B}_r = \left\{ \xi \in O(\mathscr{S}_{\zeta_{\mathrm{m}}/2}) : \| \xi \|_{L^{\infty}(\mathscr{S}_{\zeta_{\mathrm{m}}/2})} \leq r \right\}.$$
(B.2.2)

B.3 Complex analysis

In the following U is open in \mathbb{C} .

Theorem B.3.1. (Argument Principle) Let $f \in O(U)$. Consider a compact domain $\Omega \subset U$ and let f be non-vanishing on $\partial \Omega$. Then the number of zeroes N of f on Ω counted with multiplicities, is

$$N = \frac{1}{2\pi i} \oint_{\partial \Omega} dz \frac{f'(z)}{f(z)}.$$
 (B.3.1)

Moreover, let f be a meromorphic function on U containing a compact domain Ω and such that f does not have any zeroes or poles on $\partial \Omega$. Then the difference between the number of zeroes N and the number of poles P of f, counted with multiplicities, is

$$N - P = \frac{1}{2\pi i} \oint_{\partial \Omega} dz \frac{f'(z)}{f(z)}.$$
(B.3.2)

Corollary B.3.1. (*Rouché's theorem*) Let $f, g \in O(U)$ and Ω be a compact domain in U. If

$$|f(z) - g(z)| < |f(z)|$$
(B.3.3)

for all $z \in \partial \Omega$, we have that f and g have the same number of zeroes on Ω .

Lemma B.3.1. (*Cauchy's estimates*) Let $f \in O(U)$ and if $\mathcal{D}(z_0, r) \subset U$. Then

$$\forall n \ge 0, \qquad \left| f^n(z) \right| \le \frac{n!}{r^n} \sup_{\partial \mathcal{D}_{20,r}} |f|. \tag{B.3.4}$$

Theorem B.3.2. (*Montel*) Let $\mathfrak{D} \subset \mathbb{C}$ be a domain. If a family of holomorphic functions on \mathfrak{D} is bounded, then this family is normal.

B.4 Fixed point theory

Definition B.4.1. Let X be a metric space equipped with a distance d. A map

$$f: X \to X \tag{B.4.1}$$

is said to be Lipschitz continuous if there is a $\lambda \ge 0$ such that

$$d(f(x_1), f_{x_2}) \le \lambda d(x_1, x_2), \quad \forall x_1, x_2 \in X.$$
 (B.4.2)

The smallest λ for which the above inequality holds is the Lipschitz constant of f.

If $\lambda \leq 1$ f is said to be non-expansive, if $\lambda < 1$ f is said to be a contraction.

Theorem B.4.2. (*Banach*) Let f be a contraction on a complete metric space X. Then f admits a unique fixed point $x_0 \in X$.

Corollary B.4.1. Let X be a complete metric space and Y a topological space. Let $f : X \times Y \to X$ be a continuous function. Assume that f is a contraction on X uniformly in Y, that is,

$$d(f(x_1, y), f(x_2, y)) \le \lambda d(x_1, x_2), \quad \forall x_1, x_2 \in X, \ y \in Y,$$
(B.4.3)

for some $\lambda < 1$. Then for every fixed point $y \in Y$, the map $x \mapsto f(x, y)$ has a unique fixed point $\psi(y)$.

Moreover the function $y \mapsto \psi(y)$ *is continuous form* Y *to* X*.*

Appendix C

The spin-1 XXZ chain

The XXZ spin-1 chain was first introduced by Fateev and Zamolodchikov [187]. It is described by the Hamiltonian

$$\mathbf{H}_{XXZ}^{(2)} = \sum_{a=1}^{L} \left\{ \sum_{\alpha,\beta \in \{x,y,z\}} \gamma_{\alpha\beta} S_{a}^{\alpha} S_{a}^{\beta} S_{a+1}^{\alpha} S_{a+1}^{\beta} - \sum_{\alpha \in \{x,y,z\}} J_{\alpha} \left[S_{a}^{\alpha} S_{a+1}^{\alpha} + 2(S_{a}^{\alpha})^{2} \right] \right\},$$
(C.0.1)

which acts on the Hilbert space $\mathfrak{h}_{XXZ}^{(2)} \simeq \mathbb{C}^{3L}$ and where the coupling constants $\gamma_{\alpha\beta}$ and J_{α} are expressed as

$$J_{x} = \gamma_{xx} = J_{y} = \gamma_{yy} = 1, \quad J_{z} = \gamma_{zz} = 2\sin^{2}(\zeta)$$

$$\gamma_{xy} = \gamma_{yx} = 1, \quad \gamma_{xz} = \gamma_{zx} = \gamma_{zy} = 2\cos(\zeta) - 1.$$
(C.0.2)

 $\zeta \in]0; \pi[$ parametrises the anisotropy. The spin operator S_a^{α} for $\alpha \in \{x, y, z\}$ acts non-trivially as a spin-1 operator on the a^{th} site

$$S_a^{\alpha} = \underbrace{\operatorname{id} \otimes \cdots \otimes \operatorname{id}}_{a-1} \otimes S^{\alpha} \otimes \underbrace{\operatorname{id} \otimes \cdots \otimes \operatorname{id}}_{L-a}$$
(C.0.3)

where the S^{α} are the below operators on \mathbb{C}^3

$$S^{x} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S^{y} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad S^{z} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$
 (C.0.4)

The Bethe Ansatz equations for the XXZ spin-1 chain take the form

$$\left(\frac{\sinh(\lambda_j - \mathrm{i}\zeta)}{\sinh(\lambda_j + \mathrm{i}\zeta)}\right)^L = \prod_{\substack{k=1\\k\neq j}}^M \frac{\sinh(\lambda_j - \lambda_k - \mathrm{i}\zeta)}{\sinh(\lambda_j - \lambda_k + \mathrm{i}\zeta)}, \quad j = 1, \dots, M$$
(C.0.5)

where *M* is the number of Bethe roots. The existence of a Hamiltonian as the one in (C.0.1) was an important motivation to study further integrable higher spin chains under periodic boundary conditions (see [137]). Following the work of Fateev-Zamolodchikov, the XXX and XXZ spin-1 and higher spin chains were constructed *via* the fusion procedure [111, 112]. The ground state as well as the low-lying excitations of the XXX spin-*s* chain were first characterised by Takhtajan [167] and the Bethe Ansatz equations were first written by Babujian [7] within the Algebraic Bethe Ansatz approach. The ground and low-lying spectrum of the XXZ spin-*s* chain were discussed by Sogo [151], Babujian and Tsvelik [9] and Kirillov and Reshitikhin [85].

Appendix D

Higher orders to the high-*T* **expansion of the free energy**

Proposition D.0.1. *The integral representation of the per-site free energy given in Corollary 4.2.1 leads to the expansion*

$$\frac{f}{T} = -\ln 2 - \frac{J}{T} \cdot \{\cos(\zeta)\} + \frac{1}{T^2} \cdot \left\{\frac{1}{4} \cdot \left[\frac{h^2}{2} + 3J^2 \cdot (1 + 5 \cdot \cos^2(\zeta))\right] - \frac{3}{2}hJ \cdot \cos(\zeta)\right\} + \mathcal{O}\left(\frac{1}{T^3}\right).$$
(D.0.1)

Proof. We start with the following representation for the free energy

$$\frac{f}{T} = -\frac{h}{2T} - \frac{J}{T} \cdot \{\cos(\zeta)\} - \frac{1}{T^2} \cdot \oint_{\partial \mathscr{D}_{0,\varepsilon}} \frac{du}{2i\pi} \cdot \frac{\sinh(i\zeta)}{\sinh(u - i\zeta)\sinh(u)} \cdot \mathscr{L}n[1 + e^{\mathfrak{U}}](u)$$
(D.0.2)

where the function \mathfrak{U} admits an expansion as in (4.4.1). This allows one to express the logarithm in the integrand as

$$\mathscr{L}\mathbf{n}\big[1+\mathrm{e}^{\mathfrak{U}}\big] = \mathscr{L}\mathbf{n}\big[1+\mathrm{e}^{\mathfrak{U}_{\infty}}\big](u) + \mathscr{L}\mathbf{n}\bigg[1+\frac{\mathrm{e}^{\mathfrak{U}_{\infty}}}{1+\mathrm{e}^{\mathfrak{U}_{\infty}}}\frac{\mathfrak{b}}{T} + \frac{\mathrm{e}^{\mathfrak{U}_{\infty}}}{1+\mathrm{e}^{\mathfrak{U}_{\infty}}}\frac{\mathfrak{b}^{2}}{T^{2}} + \mathscr{O}\bigg(\frac{1}{T^{3}}\bigg)\bigg](u). \tag{D.0.3}$$

We now substitute the above into (D.0.2). The first term of (D.0.3) produces the usual $-\ln 2$ contribution. The $\mathcal{O}(T^{-1})$ contribution is calculated by considering the first terms, independent of *T*, from the non-linear integral equation of b in (4.4.2). This term readily produces the $J\cos(\zeta)/T$ contribution. One then obtains the following representation

$$\frac{f}{T} = -\ln 2 - \frac{J}{T} \cdot \{\cos(\zeta)\} - \frac{1}{T^2} \cdot \oint_{\partial \mathscr{D}_{0,\varepsilon}} \frac{du}{2i\pi} \cdot \frac{\sinh(i\zeta)}{\sinh(u - i\zeta)\sinh(u)} \cdot \frac{\mathfrak{b}^2(u)}{8}$$
(D.0.4)

where it remains to characterise the $\mathcal{O}(T^{-2})$ term, *viz*. the integrand in terms of \mathfrak{b}^2 .

We consider the following expansion first

$$\mathfrak{b}^{2}(\xi) = e_{0}^{2}(\xi) - 2e_{0}(\xi) \cdot \chi_{\infty,\varepsilon}(\xi) + \chi_{\infty,\varepsilon}^{2}(\xi)$$
(D.0.5)

which we substitute back in the integrand of (D.0.4) leading to the explicit formula

$$\frac{f}{T} = -\ln 2 - \frac{J}{T} \cdot \{\cos(\zeta)\} - \frac{1}{8T^2} \cdot \oint_{\partial \mathscr{D}_{0,\varepsilon}} \frac{du}{2i\pi} \cdot \frac{\sinh(i\zeta)}{\sinh(u - i\zeta)\sinh(u)} \cdot \{e_0^2 - 2e_0 \cdot \chi_{\infty,\varepsilon} + \chi_{\infty,\varepsilon}^2\}(u).$$
(D.0.6)

At this point the strategy is to simply evaluate the integrand above term-by-term after simplifying completely the terms in the curly brackets of the integrand We expand the terms $\{e_0^2 - 2e_0 \cdot \chi_{\infty,\mathscr{C}} + \chi^2_{\infty,\mathscr{C}}\}(u)$ which leads to

$$\{e_0^2 - 2e_0 \cdot \boldsymbol{\chi}_{\infty,\mathscr{C}} + \boldsymbol{\chi}_{\infty,\mathscr{C}}^2\}(\boldsymbol{\xi}) = \{h^2 - 4hJ \cdot \cosh(i\boldsymbol{\zeta}) + 4J^2 \cdot \cosh^2(i\boldsymbol{\zeta})\}$$

$$-\frac{1}{\sinh(\xi)\sinh(\xi-i\zeta)}\cdot\{4hJ\cdot\sin^2(\zeta)-8J^2\cdot\sin^2(\zeta)\cosh(i\zeta)\}+\frac{4J^2\cdot\sin^4(\zeta)}{\sinh^2(\xi)\sinh^2(\xi-i\zeta)}.$$
(D.0.7)

It remains to substitute back the above in the contour integral and apply the residue theorem term by term. One then has that

$$\begin{aligned} -\frac{1}{8} \cdot \oint_{\partial \mathscr{D}_{0,\varepsilon}} \frac{du}{2i\pi} \cdot \frac{\sinh(\mathrm{i}\zeta)}{\sinh(u-\mathrm{i}\zeta)\sinh(u)} \cdot \{h^2 - 4hJ \cdot \cosh(\mathrm{i}\zeta) + 4J^2 \cdot \cosh^2(\mathrm{i}\zeta)\} \\ &= \frac{1}{8} \cdot \{h^2 - 4hJ \cdot \cosh(\mathrm{i}\zeta) + 4J^2 \cdot \cosh^2(\mathrm{i}\zeta)\}, \\ -\frac{1}{8} \cdot \oint_{\partial \mathscr{D}_{0,\varepsilon}} \frac{du}{2i\pi} \cdot \frac{\sinh(\mathrm{i}\zeta)}{\sinh^2(u-\mathrm{i}\zeta)\sinh^2(u)} \cdot \{4hJ \cdot \sin^2(\zeta) - 8J^2 \cdot \sin^2(\zeta)\cosh(\mathrm{i}\zeta)\} \\ &= -J \cdot \cosh(\mathrm{i}\zeta) \cdot \{h - 2J \cdot \cosh(\mathrm{i}\zeta)\} \end{aligned}$$

and finally

$$-\frac{1}{8} \cdot \oint_{\partial \mathscr{D}_{0,\varepsilon}} \frac{du}{2\mathrm{i}\pi} \cdot \frac{\sinh(\mathrm{i}\zeta)}{\sinh^3(u-\mathrm{i}\zeta)\sinh^3(u)} \cdot \{4J^2 \cdot \sin^4(\zeta)\} = -\frac{3}{4}J^2 \cdot \{3 \cdot \cosh(\mathrm{i}\zeta) + 1\}.$$

Adding all the above contributions entails the claim.

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Rigorous approach to quantum integrable models at finite temperature.

This thesis develops a rigorous framework allowing one to prove the exact representations for various observables in the XXZ Heisenberg spin-1/2 chain at finite temperature. Previously it has been argued in the literature that the per-site free energy or the correlation lengths admit integral representations whose integrands are expressed in terms of solutions of non-linear integral equations. The derivations of such representations relied on various conjectures such as the existence of a real, non-degenerate, maximal in modulus Eigenvalue of the quantum transfer matrix, the exchangeability of the infinite volume limit and the Trotter number limits, the existence and uniqueness of the solutions to the auxiliary non-linear integral equations and finally the identification of the quantum transfer matrix's Eigenvalues with solutions to the non-linear integral equation. We rigorously prove all these conjectures in the high temperature regime. Our analysis also allows us to prove that for temperatures high enough, one may describe a certain subset of sub-dominant Eigenvalues of the quantum transfer matrix described in terms of solutions to a spin-1 chain of finite length.

Keywords: XXZ Heisenberg spin chain, quantum transfer matrix, non-linear integral equations.

Approche rigoureuse aux modèles intégrable quantique à température finie.

Cette thèse développe un cadre rigoureux qui permet de démontrer des représentations exactes associées à divers observables de la chaîne XXZ de Heisenberg de spin 1/2 à température finie. Il a était argumenté dans la littérature que l'énergie libre par site ou les longueurs de corrélations admettent des représentations intégrales où les intégrandes sont exprimées en termes de solutions d'équations intégrales non-linéaires. Les dérivations de ces représentations reposaient sur divers conjectures telles que l'existence d'une valeur propre de la matrice de transfert quantique, réelle, non-dégénérée, de module maximale, de l'échangeabilitée de la limite du volume infinie et du nombre de Trotter à l'infinie, de l'existence et de l'unicité des solutions des equation intégrales non-linéaires auxiliaires et finalement de l'identification des valeurs propers de la matrice de transfert quantiques avec les solutions intégrales non-linéaires. Nous démontrons toutes ces conjectures dans le regime de haute température. Nôtre analyse nous permet aussi de démontrer que pour ces température suffisamment élevées, il est possible d'avoir une description d'un certain sous-ensemble de valeurs propres sous-dominante de la matrice de transfert quantique décrite en terme de solutions d'une chaîne de spin-1 de taille finie.

Mots clés: Chaîne de spin XXZ de Heisenberg, matrice de transfert quantique, équations intégrales nonlinéaires.