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# Separation of Variables and Correlation Functions of Quantum Integrable Systems

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# Separation of Variables and Correlation Functions of Quantum Integrable Systems

**Thèse de doctorat de l'université Paris-Saclay**

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par**

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# Abstract

The aim of this thesis is to develop an approach to the computation of the correlation functions of quantum integrable lattice models within the quantum version of the Separation of Variables (SoV) method. SoV is a powerful method which applies to a wide range of quantum integrable models with various boundary conditions. Yet, the problem of computing correlation functions within this framework is still widely open. Here, we more precisely consider two simple models solvable by SoV: the XXX and XXZ Heisenberg chains of spins  $1/2$ , with anti-periodic boundary conditions, or more generally quasi-periodic boundary conditions with a non-diagonal twist. We first review their solution by SoV, which presents some similarities but also crucial differences. Then we study the scalar products of separate states, a class of states that notably contains all the eigenstates of the model. We explain how to obtain convenient determinant representations for these scalar products. We also explain how to generalise these determinant representations in the case of form factors, i.e. of matrix elements of the local operators in the basis of eigenstates. These form factors are of particular interest for the computation of correlation since all correlation functions can be obtained as a sum over form factors. Finally, we consider more general elementary building blocks for the correlation functions, and explain how to recover, in the thermodynamic limit of the model, the multiple integral representations that were previously obtained from the consideration of the periodic models by algebraic Bethe Ansatz.



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# Introduction Générale

Le but de cette thèse est de développer une méthode permettant de calculer les fonctions de corrélation de modèles intégrables quantiques sur réseau solubles par la méthode de séparation des variables quantique (SoV), dans le cadre de la méthode dite de diffusion inverse quantique (QISM). Nous présentons ici brièvement cette méthode dans son contexte historique.

La méthode de diffusion inverse quantique (QISM) a été développée en même temps que la quantification de modèles intégrables classiques solubles par la méthode de diffusion inverse classique (CISM). Il s'agit d'un outil puissant pour résoudre des modèles quantiques intégrables, avec une structure mathématique assez riche.

L'histoire commence en 1967 lorsque Gardner, Greene, Kruskal, et Miura (GGKM) [1] mettent en œuvre la méthode de diffusion inverse (CISM) dans le cadre de l'équation de Korteweg-de Vries (KdV), puis se poursuit avec l'introduction du formalisme de Lax (paire de Lax) [2] en 1969. Cette méthode, considérée initialement comme une simple méthode ingénieuse permettant de résoudre un problème particulier, fut alors généralisée par Zakharov et Shabat [3] à l'étude d'un autre modèle, l'équation de Schrödinger non linéaire (NSE). Un an plus tard, Zakharov et Faddeev montrèrent que l'équation de KdV pouvait être interprétée comme un système hamiltonien complètement intégrable avec une infinité de degrés de liberté, et construisirent les variables d'action-angle correspondantes [4]. De 1972 à 1973, cette méthode fut également appliquée à l'équation de Sine-Gordon, qui est un modèle relativiste. Les variables d'action-angle furent construites pour ce modèle par Takhtajan et Faddeev [5].

Par ailleurs, le formalisme de la paire de Lax avait été remplacé par la condition de courbure nulle, plus puissante [6], le problème spectral de l'opérateur Lax étant remplacé par une équation linéaire auxiliaire, et les données de diffusion pouvant être définies comme le comportement asymptotique du groupe d'holonomie pour un intervalle fini. Dans ce contexte, le problème de l'introduction des variables d'action-angle revient donc au calcul explicite des crochets de Poisson des éléments matriciels de l'holonomie. Ce calcul a été fait pour le modèle Sine-Gordon dans [5], et pour le modèle de Heisenberg ferromagnétique dans [7].

Ainsi, le schéma de la CISM pour une équation non linéaire donnée peut être énoncé en bref comme suit: il faut d'abord spécifier l'opérateur de Lax  $L$  correspondant et déterminer l'holonomie pour l'intervalle fini; la deuxième tâche est d'obtenir les données asymptotiques à grande distance (de l'holonomie); la dernière étape consiste à construire les variables d'action-angle.

La machinerie mathématique des systèmes intégrables classiques étant construite, une question naturelle est de savoir comment quantifier ces systèmes intégrables classiques. A cette époque, la quantification exacte du modèle NSE était connue. Par ailleurs, on savait que les modèles intégrables permettent une interprétation en termes des orbites co-adjointe des algèbres de Lie [8, 9], en particulier dans [10] où la quantification signifie la représentation des éléments correspondants Algèbre de Lie. Fortement motivé par ces faits, le groupe de Leningrad (Fad-



deev *et al.*) s'est engagé dans une quantification de la CISM associée à une quantification du système intégrable correspondant.

Dans un premier travail, Faddeev et Sklyanin [11] conjecturèrent les relations de commutation pour les analogues quantiques des éléments de la matrice d'holonomie asymptotique (monodromie). Ils remarquèrent ensuite que la technique de la matrice de transfert appliquée par Baxter [12] pour les modèles de réseau bidimensionnels en mécanique statistique (qui remonte à l'article d'Onsager sur le modèle d'Ising [13]) présente des similitudes significatives avec les caractéristiques de la monodromie de l'opérateur  $L$ . Sklyanin adapta alors cette idée dans l'étude de NSE quantique [14] en écrivant les relations de commutation pour les éléments de matrice d'un opérateur  $L$  (local) de telle sorte que l'on puisse les utiliser pour obtenir les relations de commutation pour les éléments matriciels de la monodromie (globale).

Une fois la coordonnée spatiale correctement discrétisée et la théorie quantique des champs placée sur réseau, l'opérateur  $L$  local (qui est noté  $L_{n,a}(\lambda)$ ), prenant la forme d'une matrice dans un vecteur auxiliaire space  $V_a$  avec des entités agissant sur l'espace quantique local  $\mathcal{H}_n$ ) peut être interprété comme une holonomie 'infinitésimale' le long du réseau. Pour le modèle de Sine-Gordon (SG), les relations de commutation locales ont été trouvées [15] sous la forme:

$$R_{a,b}(\lambda - \mu)L_{i,a}(\lambda)L_{i,b}(\mu) = L_{i,b}(\mu)L_{i,a}(\lambda)R_{a,b}(\lambda - \mu) \quad (1)$$

$$L_{i,a}(\lambda)L_{j,b}(\mu) = L_{j,b}(\mu)L_{i,a}(\lambda), \quad i \neq j \quad (2)$$

où  $R(\lambda)$  est une matrice scalaire de taille 4 par 4 ne contenant pas d'observables dynamiques et agissant de manière non triviale sur  $V_a \otimes V_b$ .<sup>1</sup> L'opérateur local  $L$  peut être utilisé pour définir la monodromie quantique :

$$T(\lambda) = L_N(\lambda)L_{N-1}(\lambda)\dots L_1(\lambda) = \begin{pmatrix} A(u) & B(u) \\ C(u) & D(u) \end{pmatrix} \quad (3)$$

où les éléments de la matrice  $\{A, B, C, D\}$  sont des opérateurs quantiques globaux. La matrice de monodromie quantique satisfait aux mêmes FCR (1). Ainsi, la tâche de dériver des relations de commutation pour les éléments de matrice de la monodromie (globale) à partir de celles d'un opérateur  $L$  (local) a été accomplie.

On peut voir d'après la monodromie quantique (3) et les FCR (1) que les traces de la monodromie quantique :

$$\mathcal{T}(\lambda) = \text{tr}(T(\lambda)) = A(\lambda) + D(\lambda) \quad (4)$$

commutent entre elles pour différentes valeurs du paramètre spectral  $\lambda$ . Ainsi, cette trace peut être considérée comme une fonction génératrice d'une famille à un paramètre d'opérateurs qui commutent et à laquelle appartient le Hamiltonien (à prouver). Elle fournit donc les intégrales du mouvement, c'est-à-dire la version quantique des variables d'action. Les éléments non diagonaux de la monodromie (9) correspondent quant à eux à la version quantique des variables d'angle. Dans les travaux de Baxter, ces opérateurs hors diagonaux ne sont pas très importants, mais ici ils sont cruciaux. En effet, pour un état propre particulier  $|\Omega\rangle$  (état de référence) de  $\mathcal{T}(\lambda)$  annihilé par  $C(\lambda)$ , l'état de la forme

$$B(\lambda_1)B(\lambda_2)\dots B(\lambda_M) |\Omega\rangle \quad (5)$$

---

<sup>1</sup>Les relations (1) ont été appelées *relations de commutation fondamentales (FCR)* par les auteurs.

est aussi un état propre si les paramètres  $\{\lambda_1, \dots, \lambda_M\}$  satisfont certains systèmes d'équations algébriques. En d'autres termes, les éléments hors diagonaux jouent le rôle d'opérateurs de création et d'annihilation d'un état de pseudo-particules. La correspondance entre le schéma du groupe de Leningrad et les travaux de Baxter peut être décrite comme suit: l'opérateur  $L$  local est un analogue du poids de Boltzmann local; les FCR (1) sont un analogue de la relation triangle-étoile [12, 16]; la trace de la matrice de monodromie quantique est un analogue de la matrice de transfert dans [12]. La QISM a donc une architecture claire et s'avère une méthode efficace, un large éventail de modèles intégrables classiques tels que les équations KdV, NLS, le réseau Toda et la chaîne de Heisenberg pouvant être quantifié dans ce cadre.

En particulier, concernant la quantification de la chaîne de Heisenberg, le groupe de Leningrad a constaté que pour la représentation de spin  $1/2$ , leur travail se connecte remarquablement à la diagonalisation du Hamiltonien effectuée par H. Bethe en 1931 [17]. L'état de référence  $|\Omega\rangle$  coïncide avec la représentation de poids la plus élevée (pseudo vide), et l'état propre (5) coïncide avec l'état à  $M$  magnons avec  $\{\lambda_1, \dots, \lambda_M\}$  satisfaisant les équations de Bethe. La méthode inventée par H. Bethe étant appelée Ansatz de Bethe coordonné, la QISM est ainsi souvent également appelée Ansatz de Bethe algébrique.

On s'est alors rendu compte, en étudiant un système de spin supérieur [18, 19, 20], que la relation fondamentale de commutation (1) et le choix concret de l'opérateur  $L$  correspondent à la représentation d'une algèbre universelle  $\mathcal{A}$  déterminée par un objet  $R(\lambda)$ . Par exemple dans le cas où l'espace auxiliaire coïncide avec l'espace quantique local, cet objet  $R(\lambda)$  obéit à la même relation obtenue par C.N. Yang [21] et Baxter [12, 16] qui est maintenant connue sous le nom d'équation de Yang-Baxter.

Au fur et à mesure que la QISM se développait, Kulish et Reshetikhin ont trouvé la forme correcte de l'opérateur  $L$  local pour la chaîne de spin  $XXZ$  de Heisenberg ainsi que les relations de commutation entre ses éléments de matrice [22]. Il était clair que ces éléments de matrice forment une algèbre  $\mathfrak{sl}(2)$  déformée dépendant d'un paramètre d'anisotropie. Sklyanin a étudié le modèle  $XYZ$  et a proposé une déformation supplémentaire de cette algèbre dans le cas à deux paramètres [23]. Pendant ce temps, Izergin et Korepin a montré que les modèles discrétisés NLS et SG pouvaient être considérés comme les représentations correspondantes des modèles  $XXX$  et  $XXZ$  respectivement [24, 20].

Plus tard, Drinfeld [25, 26] et Jimbo [27] ont généralisé indépendamment le cas  $\mathfrak{sl}(2)$  à toute algèbre de Lie semi-simple et l'ont interprété comme une classe spéciale d'Algèbres de Hopf. C'est à ce moment-là que l'étude du «groupe quantique» a commencé.

Il convient également de mentionner que l'Ansatz de Bethe coordonné avait déjà, dans les années suivant l'article fondateur de Bethe en 1931, fourni une nouvelle perspective permettant l'étude d'une large classe de systèmes quantiques. Bien que limité à la dimension  $1 + 1$ , il avait conduit à de nouveaux développements (tels que les méthodes de l'Ansatz de Bethe thermodynamique (TBA), de l'Ansatz de Bethe asymptotique, etc. [28, 29, 30]) qui jouent un rôle important dans la physique de la matière condensée [31] ainsi que dans les théories des champs conformes [32]. Au début du 21ème siècle, il a été étonnamment découvert que la chaîne de spin unidimensionnelle Heisenberg  $XXX$  apparaît dans une limite spéciale du système intégrable AdS/CFT [33, 34, 35]. Depuis lors, l'intégrabilité a été intensivement étudiée dans le cadre des théories des champs de jauge supersymétriques et la théorie des cordes.

Le schéma général pour construire les variables d'action-angle pour les systèmes complète-

ment intégrables est de trouver la transformation canonique à travers une généralisation de la méthode de Hamilton-Jacobi d'intégration des équations canoniques. Et dans ce schéma, pendant longtemps, la seule méthode fructueuse pour intégrer l'équation de Hamilton-Jacobi en mécanique analytique classique était celle de la séparation des variables (SoV) [36].

Cependant, avec l'apparition de la CISM, le rôle indispensable joué par la SoV dans la résolution des systèmes intégrables classiques a semblé être dépassé. En effet, la CISM semblait permettre a priori de s'attaquer à une gamme beaucoup plus large de systèmes intégrables classiques. Néanmoins, après une nouvelle étude dans le cadre de la CISM, il s'avère que la SoV est loin d'être dépassé. De plus, cela peut rester la méthode la plus universelle pour résoudre des modèles intégrables [37].

Un objet central dans le traitement moderne de la CISM est la dite *courbe spectrale* [38]. Celle-ci correspond au domaine des zéros du polynôme caractéristique d'une matrice  $N \times N$  de Lax  $L(\lambda)$ . Si nous considérons la valeur propre  $z(\lambda)$  et l'opérateur Lax  $L(\lambda)$  comme des fonctions d'un paramètre complexe  $\lambda$ , alors l'équation caractéristique les définit comme des fonctions sur la surface de Riemann à  $N$  feuillets paramétrée localement par  $\lambda$ . La manière standard de construire les variables d'action-angle est d'utiliser les pôles de la fonction de *Baker-Akhiezer*. Et cela s'avère être équivalent à une séparation de variables [37]. La fonction de *Baker-Akhiezer*  $\Omega(\lambda)$  est définie comme le vecteur propre de  $L(\lambda)$ :

$$L(\lambda)\Omega(\lambda) = z(\lambda)\Omega(\lambda). \quad (6)$$

Pour une grande classe de modèles intégrables, la recette magique de Sklyanin "Prenez les pôles de la fonction de Baker-Akhiezer correctement normalisée et les valeurs propres correspondantes de l'opérateur Lax et alors vous obtenez SoV" [37] fonctionne.

Une autre raison pour laquelle SoV doit être étudiée plus en profondeur est que dans de nombreux cas, il est possible de construire une séparation de variables dans des systèmes quantiques intégrables de manière analogue.

Peu de temps après l'établissement de la QISM, inspiré par H. Flashka, D.W. Maclaughlin [39] (1976) M. Gutzwiller [40, 41] (1981-1982) et I.V. Komarov [42] (1982), Sklyanin a proposé une version quantique de la séparation des variables dans une série d'articles de 1985 [43, 44, 45]. Cette approche fonctionne également dans le cadre de la QISM. Elle vise à trouver une base dans l'espace de Hilbert sous-jacent dans lequel le problème spectral de la matrice de transfert peut être séparé. Elle réduit ainsi le problème en dimension  $N$  à la résolution de  $N$  problèmes à une dimension. Depuis lors, de nombreux modèles ont été étudiés dans cette approche [46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57]. Une telle base est souvent appelée « base SoV ». Dans l'approche de Sklyanin, la base SoV a été identifiée comme la base propre de l'élément hors diagonale  $B(\lambda)$  de la matrice de monodromie quantique [47, 37]. Et les éléments diagonaux  $A(\lambda)$  et  $D(\lambda)$  agissent comme des opérateurs de shift sur la base qui conduit à la factorisation souhaitée du problème spectral. Il est important de souligner que pour s'assurer que  $B(\lambda)$  a un spectre simple, le modèle doit être déformé en introduisant des paramètres d'inhomogénéité en chaque site du réseau. Retrouver le modèle physique revient alors à prendre la limite homogène, c'est-à-dire que tous les paramètres d'inhomogénéité doivent tendre vers la même valeur.

Une caractéristique intéressante de cette approche est qu'un "état de référence" n'est pas nécessaire, contrairement à l'ABA. Ainsi, elle peut être appliquée à de nombreux modèles avec diverses conditions aux limites (y compris la condition aux limites anti-périodique) qui ne possèdent pas un tel état de référence simple et ne peuvent pas être résolus directement par l'ABA. Pour de tels modèles, la SoV fournit non seulement une caractérisation complète des

valeurs propres et des états propres de la matrice de transfert correspondante, mais aussi la complétude des états propres en conséquence directe. C'est un avantage considérable par rapport à l'ABA pour lequel la complétude est en général un problème compliqué (voir par exemple [58, 59]).

Mentionnons pour terminer cette brève présentation de la SoV qu'une nouvelle version a été proposée récemment dans une série d'articles [60, 61, 62, 63, 64, 65, 66]. Dans cette nouvelle version, la base SoV peut être construite en n'utilisant que la matrice de transfert elle-même. Cela ouvre de nouvelles perspectives pour l'étude d'une classe de modèles beaucoup plus large. Plus important encore, du point de vue théorique, cela apporte un peu de lumière sur la définition de l'intégrabilité quantique. Dernier point mais non le moindre, SoV peut conduire à des constructions de modèles quantiques intégrables qui n'ont pas besoin de l'équation de Yang-Baxter pour définir la structure algébrique [67].

Même si la naissance de l'Ansatz de Bethe remonte à des décennies, le calcul des fonctions de corrélations pour les modèles sur réseau quantiques reste en général un problème difficile. Pendant longtemps, les calculs ont été effectués uniquement pour les fermions libres [13, 68, 69, 70, 71, 72, 73, 74] et les théories des champs conformes [75]. Les premières tentatives d'utilisation de l'Ansatz de Bethe pour le calcul des fonctions de corrélation de la chaîne de spin  $XXX$  de Heisenberg (qui correspond au paramètre d'anisotropie  $\Delta = 1$ ) ne remontent qu'à 1984 [24, 76]. Plus tard, dans les années 1992, une représentation sous forme d'intégrale multiple pour les fonctions de corrélation du modèle  $XXZ$  dans le régime massif ( $\Delta > 1$ ), dans la limite thermodynamique, à température nulle et champ magnétique nul, a été obtenue pour la première fois par l'approche des opérateurs de vertex  $q$ -déformés (utilisant également la technique de la matrice de transfert de coin) [77]. Une telle représentation a également été conjecturée en 1996 [78] pour le régime de masse nulle  $-1 < \Delta \leq 1$  (voir aussi [79]). Une preuve de ces résultats, avec leur extension au champ magnétique non nul, a été obtenue en 1999 [80] en utilisant l'Ansatz de Bethe algébrique et la solution au problème dit de diffusion inverse quantique [81, 82, 83]. Dans cette approche, les fonctions de corrélation en taille finie ont été obtenues en calculant l'action des produits d'opérateurs locaux sur un état propre du Hamiltonien (par exemple l'état fondamental), puis en calculant le produit scalaire résultant. Grâce à une représentation pratique — sous forme d'un déterminant — pour les produits scalaires [84], la limite thermodynamique peut alors être facilement prise.

Ce type de représentation sous forme d'une intégrale multiple explicite a été obtenu en fait, non pour les fonctions de corrélation elles-mêmes, mais pour leurs blocs élémentaires constitutifs. Ces derniers sont définis comme la valeur moyenne dans l'état fondamental de produits de matrices élémentaires  $E^{\epsilon', \epsilon}$ ,  $\epsilon, \epsilon' \in \{1, 2\}$ , d'éléments  $E_{lk}^{\epsilon', \epsilon} = \delta_{l, \epsilon'} \delta_{k, \epsilon}$ , sur  $m$  sites consécutifs de la chaîne [80]. Toute fonction de corrélation arbitraire peut en effet être écrite comme une combinaison linéaire de ces quantités. Une telle représentation intégrale multiple pour les fonctions de corrélation dynamique de la chaîne  $XXZ$  spin-1/2 a été obtenue plus tard dans [85], ainsi que pour la température finie [86, 87, 88].

Une autre approche du calcul des fonctions de corrélation pour les modèles sur réseau quantiques intégrables est l'approche par sommation sur les facteurs de forme. Dans cette approche, un ensemble complet d'états (par exemple les états propres du Hamiltonien) est inséré entre les observables. Et les fonctions de corrélation sont la somme de ces éléments matriciels d'observables. La représentation sous forme de déterminant des facteurs de forme de la chaîne de

taille finie a été obtenue dans [81], ce qui avait permis le calcul de l'aimantation spontanée dans [89], puis conduit à de nombreuses applications dans le calcul des fonctions de corrélation et des facteurs de structure selon la méthode mentionnée ci-dessus, soit numériquement [90, 91, 92, 93], soit analytiquement [94, 85, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104].

Mentionnons qu'il existe aussi une approche alternative à ce problème du calcul des fonctions de corrélation, développée notamment dans [105, 106, 107, 108, 109, 110, 111, 112, 113].

Ainsi, nous avons vu que l'approche SoV est une approche fructueuse permettant de résoudre les problèmes spectraux des matrices de transfert et des Hamiltoniens des modèles quantiques sur réseau avec diverses conditions aux limites. Cependant, le problème du calcul des fonctions de corrélation dans cette approche reste encore largement ouvert. C'est dans ce but que nous avons rédigé cette thèse, dans laquelle nous considérons ce problème dans le cadre de deux modèles simples: les chaînes de spins 1/2 de Heisenberg XXX (isotrope) et XXZ (partiellement anisotrope) avec conditions aux limites anti-périodiques. L'intérêt de l'étude de ces modèles, outre le fait qu'ils sont parmi les plus simples (et les plus étudiés) solubles par QISM, est qu'il est possible de comparer directement nos résultats avec le cas périodique soluble par Ansatz de Bethe: notamment, à la limite thermodynamique, nous nous attendons à retrouver les mêmes expressions pour les fonctions de corrélation.

L'approche SoV fournit naturellement une représentation sous forme de déterminant pour les produits scalaires entre les états séparés (l'ensemble des états propres de la matrice de transfert est inclus dans l'ensemble des états séparés): le déterminant qui apparaît est celui de la somme de deux matrices de Vandermonde généralisées "habillées". Cependant, cette représentation n'est pas pratique pour prendre la limite homogène. Rappelons que pour garantir à l'opérateur  $B(\lambda)$  d'avoir un spectre simple, le modèle physique doit être déformé par l'introduction d'un ensemble de paramètres d'inhomogénéité. Lors du calcul des fonctions de corrélation, il faut bien sûr pouvoir prendre la limite homogène pour récupérer le modèle physique. Ceci suppose tout d'abord de pouvoir reformuler la caractérisation du spectre de la matrice de transfert qui, dans le cadre de SoV, s'exprime en termes d'un système d'équations discrètes faisant intervenir les paramètres d'inhomogénéité, de façon plus commode, typiquement en termes d'une équation fonctionnelle "à la Baxter" (ou équation  $T-Q$ ) de laquelle peuvent être déduites les équations de Bethe: ceci est aisé dans le cas XXX anti-périodique [114], mais un peu moins direct dans le cas XXZ [115]. Ceci suppose ensuite de pouvoir reformuler les représentations pour les produits scalaires, idéalement en termes des racines de Bethe (ou autrement dit, des racines de la fonction  $Q$  solution de l'équation  $T-Q$ ) comme dans le cas périodique [84]. Une première étape dans ce sens a été résolue dans [114] dans le cas d'un modèle particulièrement simple, la chaîne de spins XXX avec conditions aux limites anti-périodiques, pour laquelle une représentation sous forme de déterminant plus pratique, similaire à celle de [84], a été obtenue pour les produits scalaires et les facteurs de forme à partir de la représentation SoV par une suite de transformations algébriques. Cette nouvelle représentation permet de prendre facilement la limite homogène, et ouvre la porte au calcul des fonctions de corrélation au sein du SoV pour ce modèle simple.

Dans cette thèse, nous poursuivons le calcul des fonctions de corrélation de la chaîne XXX anti-périodique, et montrons explicitement que, au moins pour ce modèle simple, il est possible d'effectuer le calcul jusqu'au bout, c'est-à-dire jusqu'à la limite thermodynamique, exclusivement dans le cadre de la SoV. Plus précisément, nous calculons l'action successive des opérateurs locaux sur les états séparés. Cette action peut s'écrire comme une somme multiple sur les

paramètres d'inhomogénéité. Nous montrons, à l'aide d'intégrales de contour, que ces sommes peuvent être réécrite comme des sommes sur les racines du polynôme  $Q$  (ou racines de Bethe), comme dans le cas périodique soluble par Ansatz de Bethe, avec toutefois des contributions supplémentaires par rapport au cas périodique. Nous montrons explicitement comment il est possible de prendre la limite thermodynamique dans chaque terme de la somme. Nous montrons plus précisément que les termes supplémentaires s'annulent à la limite thermodynamique, et que nous retrouvons, dans cette limite, le résultat obtenu dans [80] pour les fonctions de corrélation de la chaîne périodique. Ceci est également vrai pour une chaîne quasi-périodique avec un twist non-diagonal quelconque: nous montrons ainsi explicitement que, comme on peut s'y attendre, la limite thermodynamique des fonctions de corrélation de la chaîne de spins XXX ne dépend pas du twist. Ce résultat est publié dans [116].

Nous abordons également l'étude du calcul des fonctions de corrélation dans le cas de la chaîne de spins XXZ anti-périodique. Contrairement à ce qui se passe dans le cas périodique, l'étude du cas XXZ présente des différences importantes avec le cas XXX. En effet, la fonction  $Q$ , solution de l'équation  $T$ - $Q$  avec la valeur propre de la matrice de transfert, n'est pas un simple polynôme trigonométrique de même forme que pour la chaîne périodique, mais a en fait une période double [117, 115]. Ce doublement de la période fait que les transformations algébriques utilisées dans [114] pour calculer les produits scalaires et facteurs de forme de la chaîne XXX ne s'appliquent pas directement au cas XXZ. Dans cette thèse, nous proposons donc une méthode alternative pour calculer les produits scalaires et facteurs de forme dans le cas XXZ à partir des formules naturellement issues de l'étude du modèle par SoV. Nous obtenons de nouvelles représentations, sous forme de déterminant dont les lignes et colonnes sont labellées par les racines de  $Q$ , avec néanmoins une forme différente de celle de [84]. Ces résultats sont publiés dans [118]. Le calcul des fonctions de corrélation elles-mêmes est aussi plus compliqué que dans le cas XXX du fait de ce doublement de la période dans  $Q$ : l'action successive des opérateurs locaux comporte des termes supplémentaires par rapport au cas périodique qui sont de nature différente par rapport au cas XXX, et plus compliqués à traiter. De fait, nous n'avons encore pas totalement résolu ce problème. Mais si nous supposons que ces termes supplémentaires s'annulent à la limite thermodynamique, nous retrouvons également, en prenant la limite thermodynamique des autres termes, la représentation sous forme d'intégrales multiples obtenue dans le cas périodique [80].



# Introduction

This thesis aims to use the quantum version of the Separation of Variables (SoV) method to develop an approach to the computation of the correlation functions of quantum lattice models which are solvable in the Quantum Inverse Scattering Method (QISM) framework.

The Quantum Inverse Scattering Method (QISM) was developed along with the quantisation of classical integrable models in the inverse scattering method framework. It is not only a powerful tool in solving quantum integrable models, but also manifests a rather rich mathematical structure.

The story begins in 1967 when Gardner, Greene, Kruskal, and Miura (GGKM) [1] first implemented the Inverse Scattering Method (ISM) using the KdV equation to solve the one-dimensional Schrödinger equation. Later in 1969, Lax [2] reformulated this method by introducing the so-called  $L$ -operator (Schrödinger operator) and wrote the KdV equation in the fashion of the Lax equation. The Lax equation shows that the KdV evolution is given by a similar transformation of  $L$ , thus the spectral of  $L$  is isotropic, i.e. independent of time. This method had been considered as merely an ingenious method to solve a particular problem until Zakharov and Shabat [3] applied this Inverse Scattering Method to the non-linear Schrödinger equation (NSE). One year later, Zakharov and Faddeev treated the KdV equation as a completely integrable Hamiltonian system with infinitely many degrees of freedom and constructed the action-angle variables [4]. During 1972-1973, this method was applied to the Sine-Gordon equation, which is a relativistic model. The action-angle variables were constructed for this model by Takhtajan and Faddeev [5].

In the meanwhile, Novikov, Zakharov, and Shabat in [6] replaced the Lax scheme with the more powerful zero-curvature condition. Then the spectral problem of the Lax operator is substituted by an auxiliary linear equation, and the scattering data can be defined as the asymptotic behaviour of the holonomy group for a finite interval. The problem of introducing the action-angle variables thus amounts to the explicit calculation of the Poisson brackets of the matrix elements of the holonomy. This calculation was done in the Sine-Gordon model [5] and in the Heisenberg ferromagnetic equation in [7].

Thus the scheme of the CISM for a given non-linear equation can be stated in short as follows: one needs to first specify the corresponding  $L$ -operator and determine the holonomy for the finite interval; the second task is to obtain the large distance asymptotic data (of the holonomy); the last step is to construct the action-angle variables.

Since the mathematical machinery for the classical integrable systems has been built, a natural question would be how to quantise those classical integrable systems. At that time, the exact quantisation of the NSE model was known. And meanwhile, it was known that integrable models allow an interpretation in terms of the co-adjoint orbits of the Lie algebras [8, 9], especially in [10] where the quantisation means the representation of the corresponding Lie algebra. Highly motivated by these facts, the Leningrad group (Faddeev *et al.*) believed that



a quantum version of the ISM to quantise the corresponding integrable system was feasible.

The first work was done by Faddeev and Sklyanin in [11] by conjecturing the commutation relations for the quantum analogues of the matrix elements of the asymptotic holonomy (monodromy). Soon enough they noticed that the transfer matrix technique applied by Baxter [12] for the two-dimensional lattice models in classical statistical mechanics (which dates back to Onsager's paper on the Ising model [13]) has significant similarities to those characteristics of the monodromy of the  $L$ -operator. Sklyanin adapted this idea in the study of the quantum NSE in [14] by writing down the commutation relations for the matrix elements of a (local)  $L$ -operator such that one can use them to obtain the commutation relations for the matrix elements of the (global) monodromy.

After the space coordinate is properly discretised and the quantum field theory is put in a lattice, the local  $L$ -operator (which is denoted as  $L_{n,a}(\lambda)$ , taking matrix form in an auxiliary vector space  $V_a$  with entities act on local quantum space  $\mathcal{H}_n$ ) can be interpreted as an 'infinitesimal' holonomy along the lattice. For the Sine-Gordon (SG) model, the local commutation relations were found [15] in the form:

$$R_{a,b}(\lambda - \mu)L_{i,a}(\lambda)L_{i,b}(\mu) = L_{i,b}(\mu)L_{i,a}(\lambda)R_{a,b}(\lambda - \mu) \quad (7)$$

$$L_{i,a}(\lambda)L_{i,b}(\mu) = L_{i,b}(\mu)L_{i,a}(\lambda), \quad i \neq j \quad (8)$$

where  $R(\lambda)$  is a 4 by 4 scalar matrix containing no dynamical observables acting non-trivially on  $V_a \otimes V_b$ .<sup>2</sup> The local  $L$ -operator can be used to define the quantum monodromy:

$$T(\lambda) = L_N(\lambda)L_{N-1}(\lambda)\dots L_1(\lambda) = \begin{pmatrix} A(u) & B(u) \\ C(u) & D(u) \end{pmatrix}, \quad (9)$$

where the matrix elements  $\{A, B, C, D\}$  are some global quantum operators. The quantum monodromy matrix satisfies the same FCR (7). Thus the task of deriving commutation relations for the matrix elements of the (global) monodromy from those of a (local)  $L$ -operator has been accomplished.

It can be seen from the quantum monodromy (9) and the FCR (7) that the trace of the quantum monodromy:

$$\mathcal{T}(\lambda) = \text{tr}(T(\lambda)) = A(\lambda) + D(\lambda) \quad (10)$$

commutes with each other for arbitrary different spectral parameters. Thus it can be considered as a generating function for a one-parameter family of mutually commuting operators to which the Hamiltonian belongs (to be proved). Thus this trace provides the commuting integral of motions, i.e. the quantum version of action variables. The off-diagonal elements in the monodromy (9) are the quantum version of angle variables. In Baxter's work, these off-diagonal operators are not very important however here they are crucial. Indeed, for a particular eigenstate  $|\Omega\rangle$  (reference state) of  $\mathcal{T}(\lambda)$  annihilated by  $C(\lambda)$ , the state of the form

$$B(\lambda_1)B(\lambda_2)\dots B(\lambda_M)|\Omega\rangle \quad (11)$$

is also an eigenstate if the parameters  $\{\lambda_1, \dots, \lambda_M\}$  satisfy some systems of algebraic equations. In other words, the off-diagonal elements play a role as creation and annihilation operators of some particle state. The correspondence between the Leningrad group's scheme and Baxter's

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<sup>2</sup>The relation (7) was called the Fundamental Commutation Relations (FCR) by the authors.

work can be described as follows: the local  $L$ -operator is an analogue to the local Boltzmann weight; the FCR (7) is an analogue to the star-triangular relation [12, 16]; the trace of the quantum monodromy matrix is an analogue to the transfer matrix in [12]. Thus the architecture of the QISM is already quite clear. And quite effectively, a wide range of classical integrable models such as the KdV, the NLS, the Toda lattice, and the Heisenberg magnet can be quantised within this framework.

Particularly, in the quantisation of the Heisenberg magnet, the Leningrad group found that for the spin 1/2 representation, their work remarkably connects to the work done by H. Bethe in 1931 [17] while diagonalising the Hamiltonian of the Heisenberg spin chain. The reference state  $|\Omega\rangle$  coincides with the highest weight representation (pseudo vacuum), and the eigenstate (11) coincides with the  $M$ -magnon state with  $\{\lambda_1, \dots, \lambda_M\}$  satisfying the Bethe equations. The method invented by H. Bethe is called the Coordinate Bethe Ansatz. As a consequence, the QISM is also often referred to as the Algebraic Bethe Ansatz.

It was then realised through studying a higher spin system [18, 19, 20] that the Fundamental Commutation Relation (7) and the concrete choice of  $L$ -operator correspond to the representation of a universal algebra  $\mathcal{A}$  determined by some object  $R(\lambda)$ . For example in the case where the auxiliary space coincides with the local quantum space, this object  $R(\lambda)$  obeys the same relation obtained by C.N.Yang [21] and Baxter [12, 16] which is now known as the Yang-Baxter equation.

As the QISM developed further, Kulish and Reshetikhin found the correct form of the local  $L$ -operator for the  $XXZ$  Heisenberg spin chain as well as the commutation relations between its matrix elements [22]. It was clear that those matrix elements form a deformed  $\mathfrak{sl}(2)$  algebra depending on one anisotropy parameter. Sklyanin studied the  $XYZ$  model and proposed a further deformation of this algebra to the two-parameter case [23]. Meanwhile, Izergin and Korepin showed that the discretised NLS and SG models could be considered as the corresponding representations of the  $XXX$  and the  $XXZ$  models respectively [24, 20]. Later on, Drinfeld [25, 26] and Jimbo [27] independently generalised the  $\mathfrak{sl}(2)$  case to any semi-simple Lie algebra and interpreted it as a special class of Hopf algebras. It was at that time, the study of the "quantum group" got started.

It is also worth mentioning that once the Coordinate Bethe Ansatz was proposed in 1931, it immediately provided a new perspective to study a large class of quantum systems. Though restricted to 1 + 1 dimension, it led to many useful tools (such as the Thermodynamic Bethe Ansatz method (TBA), Asymptotic Bethe Ansatz, etc. [28, 29, 30]) that play an important role in the condensed matter physics [31] as well as the conformal field theories [32]. At the beginning of the 21st century, it was surprisingly found that the one-dimensional Heisenberg  $XXX$  spin chain appears in a special limit of the AdS/CFT integrable system [33, 34, 35], since then integrability was intensively studied in the supersymmetric gauge field theories and string theory.

The general scheme to construct the action-angle variables for the completely integrable systems is to find the canonical transformation through a generalisation of the Hamilton-Jacobi method of integrating the canonical equations. And in this scheme the only successful method of integrating the Hamilton-Jacobi equation in classical analytical mechanics is that of separation of variables (SoV) [36]. However, after the establishment of the QISM, the indispensable role that the SoV plays in solving classical integrable system seemed to be taken over by it. The

CISM empowers us to tackle a much larger range of classical integrable systems. Nonetheless, after a further study in the CISM framework, it is pointed out that SoV is far from out of date. Moreover, it may remain the most universal method of solving integrable models [37].

A central object in the modern treatment of the CISM is the so-called spectral curve [38]. Roughly speaking, a spectral curve is a locus of zeros of the characteristic polynomial of a  $N \times N$  Lax matrix  $L(\lambda)$ . If we regard the eigenvalue  $z(\lambda)$  and the Lax operator  $L(\lambda)$  as functions of a complex parameter  $\lambda$ , then the characteristic equation defines them as functions on the  $N$ -sheeted Riemann surface locally parametrised by  $\lambda$ . The standard way to construct the action-angle variables is to use the poles of the *Baker-Akhiezer* function. And it turns out to be equivalent to a separation of variables [37].

The *Baker-Akhiezer* function  $\Omega(\lambda)$  is defined as the eigenvector of  $L(\lambda)$ :

$$L(\lambda)\Omega(\lambda) = z(\lambda)\Omega(\lambda). \quad (12)$$

Then for a large class of integrable models, Sklyanin's magical recipe "Take the poles of the properly normalised Baker-Akhiezer function and the corresponding eigenvalues of the Lax operator and then you obtain SoV" [37] works. Another reason why SoV needs to be studied more thoroughly is that in many cases, it is possible to construct a separation of variables in quantum integrable systems analogously.

Not long after the QISM was established, inspired by H.Flashka, D.W.Maclaughlin [39] (1976) M.Gutzwiller [40, 41](1981-1982) and I.V.Komarov [42] (1982), Sklyanin proposed a quantum version of the separation of variables in a series of papers from 1985 [43, 44, 45].

This approach works also within the QISM framework. It aims to find a basis in the underlying Hilbert space in which the spectrum problem of the transfer matrix can be separated. It thus reduces the  $N$ -dimensional problem to  $N$  one-dimensional problem. Since then many models were studied in this approach [46, 47, 48, 49, 50, 51, 52, 53, 54, 119, 120, 121, 122, 123, 124, 55, 56, 57]. Such a basis is often referred to as the "SoV basis". In Sklyanin's approach, the SoV basis was identified with the eigenbasis of the off-diagonal element  $B(\lambda)$  in the quantum monodromy matrix [47, 37]. And the diagonal elements  $A(\lambda)$  and  $D(\lambda)$  act as shift operators on the basis which leads to the wanted factorisation of spectrum problem. It is important to point out that to ensure  $B(\lambda)$  has a simple spectrum, the model needs to be deformed by introducing one inhomogeneous parameter to each site of the lattice. And to recover the physical model amounts to taking the homogeneous limit, i.e. all the inhomogeneous parameters are taken to be the same value.

An interesting feature of this approach is that a "reference state" is not needed, unlike in the ABA. Thus it can be applied to many models with various boundary conditions (including the anti-periodic boundary condition) which do not possess such simple reference state and cannot be solved by the ABA directly. For such models, the SoV provides not only a full characterisation of the corresponding transfer matrix eigenvalues and eigenstates, but also the completeness of the eigenstates as a direct consequence. This is a considerable advantage with respect to the ABA for which completeness is in general a complicated issue (see for instance [58, 59]).

And another motivation to study the quantum SoV is the possibility that the SoV basis can be constructed by using only the transfer matrix itself in a new version of the SoV proposed in a series of papers [60, 61, 62, 63, 64, 65, 66]. This opens a new door to the investigation of a much larger class of models. More importantly, in the theoretical point of view, it throws some light upon the definition of quantum integrability. Last but not the least, SoV can lead

to constructions of quantum integrable models that do not need the Yang-Baxter equation as defining algebraic structure [67].

Even though decades have passed since the birth of the Bethe Ansatz, the computation of the correlations functions for quantum lattice models is in general still a difficult problem. For a long time, the computations were done only for free fermions [13, 68, 69, 70, 71, 72, 73, 74] and conformal field theories [75]. Not until 1984 had the first attempts to use the Bethe Ansatz for the  $XXZ$  Heisenberg spin chain (which corresponds to the anisotropy parameter  $\Delta = 1$ ) [24, 76] been made. Later in 1994, the multiple integral representation of the correlation functions for the  $XXZ$  model in the thermodynamic limit at zero temperature and zero magnetic field was obtained for the first time from the q-vertex operator approach (also using corner transfer matrix technique) in the massive regime:  $\Delta > 1$  in 1992 [77] and conjectured in 1996 [78] for the massless regime:  $-1 < \Delta \leq 1$  (see also [79]). Proof of these results together with their extension to the non-zero magnetic field was obtained in 1999 [80] using the Algebraic Bethe Ansatz and the solution to the so-called quantum inverse scattering problem [82, 83]. In this approach, the finite correlation functions were computed by first acting operator products on an eigenstate of the Hamiltonian (for example the ground state) and then computing the resulting scalar product. With the help of a convenient determinant representation for scalar products [84], the thermodynamic limit can be easily taken.

The explicit multiple integral representation was obtained for the so-called elementary building blocks which are defined as the ground state mean value of any product of the local elementary  $2 \times 2$  matrices  $E_{lk}^{\epsilon', \epsilon} = \delta_{l, \epsilon'} \delta_{k, \epsilon}$  [80]. Any arbitrary correlation function can be written as a linear combination of these quantities. With these results, the spontaneous magnetisation was obtained in [89]. Such multiple integral representation for dynamical correlation functions of the  $XXZ$  spin-1/2 chain was obtained later in [85], as well as for finite temperature [86, 87, 88].

Another approach to computing the correlation functions for quantum integrable lattice models is the form factor approach. In this approach, a complete set of states (for example the eigenstates of the Hamiltonian) are inserted between observables. And the correlation functions are the sum of these matrix elements of observables. The determinant representation for the form factors of finite size chain for the  $XXZ_{1/2}$  model was obtained in [81], which leads to many applications in computing the correlation functions and structure factors, either numerically [90, 91, 92, 93] or analytically [94, 85, 95, 96, 97, 98, 99, 100, 101, 102, 103, 125, 126, 104]. See also [105, 106, 107, 108, 109, 110, 111, 112, 113] for an alternative approach to this problem.

The SoV approach is successful in solving the spectrum problems of the transfer matrices and the Hamiltonians of the quantum lattice models with various boundary conditions. However, the problem of computing the correlation functions within the quantum SoV approach is still widely open. It is for this purpose that we wrote this thesis. The SoV approach naturally provides a determinate representation for the scalar products between the separate states (the set of eigenstates of the transfer matrix are included in the set of separate states) — a determinate of the sum of two "dressed" generalised Vandermonde matrices. However, this representation is not convenient for taking the homogeneous limit. Recall that to ensure the operator  $B(\lambda)$  to have a simple spectrum in the underlying lattice model, the physical model has to be deformed by introducing a set of inhomogeneous parameters. In the computation of

correlation functions, one needs to take the homogeneous limit to recover the physical model. In [114] a more convenient determinant representation was first obtained for the scalar products and the form factors in the anti-periodic  $XXX$  model through a sequence of algebraic transformations. This new representation allows us easily to take the homogeneous limit. This gives the hope to develop an approach to the computation of the correlation functions within the SoV .

The thesis is organised as follows:

In Chapter 1 we use the  $XXZ$  spin chain to present very roughly the QISM framework, recall how the scalar product and the correlation functions were computed in the Algebraic Bethe Ansatz (ABA) method. In the last section, we briefly recall how the SoV basis was explicitly constructed and how the eigenstate of the (twisted) transfer matrix was obtained.

In Chapter 2 we present our results of the analysis of the configuration of Bethe roots for the ground state in the thermodynamic limit for both  $XXX$  and  $XXZ$  anti-periodic chains.

In Chapter 3 we recall the core of the method to obtain the determinant representation for the scalar product and the form factors for the anti-periodic  $XXX$  chain in the framework of the SoV. And we present our results for the anti-periodic  $XXZ$  chain.

In Chapter 4 we present our results of the computation of the correlation functions for both  $XXX$  and  $XXZ$  anti-periodic spin chains of finite size and give an explicit multiple summation representation for the finite-size elementary building blocks.

In Chapter 5 we analyse the vanishing and non-vanishing terms in the multiple summation representation in the thermodynamic limit and explain how to recover the multiple integral representation for the elementary building blocks.

# Chapter 1

## The $XXZ$ spin chain in the QISM framework

### 1.1 The general algebraic framework

The classical integrability is well defined in the Liouville's sense. The system needs the phase space to be a  $2N$ -dimensional Poisson manifold with  $N$  integral of motions in involution:

$$\{I_n, I_m\} = 0. \quad (1.1)$$

And together with this definition, it provides a systematic way to find the set of integral of motions  $\{I_n\}_{n=1}^N$  through a canonical transformation:

$$(x_j, p_j) \mapsto (I_j, \varphi_j), \quad (1.2)$$

where  $(I_j, \varphi_j), j = 1, \dots, N$  are the well known action-angle variables. Unfortunately, although the definition is precise and even prescribes a systematic way to solve the underlying classical integrable system, in practice only within few systems we can perform such operation. Among all other efforts, the classical inverse scattering method (CISM) is an effective way to solve the problem.

However, in the quantum case, the definition is controversial [127, 128, 129]. A common feature of those systems is that they possess a "enough" number of mutually commuting conserved quantities:

$$[I_n, I_m] = 0. \quad (1.3)$$

But once a physical model is given, to find such a set of operators seems difficult at first sight. Luckily, the quantum inverse scattering method (QISM) offers a pure algebraic framework to construct a one-parameter set of integral of motions. The idea is to embed the set of integral of motions  $\{I_n\}$  into a larger algebra  $\mathcal{A}$ . After having figured out the structure of  $\mathcal{A}$ , i.e. the commutation relations between generators of  $\mathcal{A}$ , we can solve the system algebraically like in quantum mechanics. However, unlike the Lie algebra in quantum mechanics, the longed algebra  $\mathcal{A}$  turns out to be a "quantum group". In fact, the study of the quantum groups was inspired by the QISM.

The algebraic structure of  $\mathcal{A}$  is determined by the so-called  $R$  matrix. In the language of Hopf algebra, this matrix is an invertible element that satisfies a set of conditions. One of

these conditions happens to be, at the representation level, a relation that was independently highlighted by Yang [21] and Baxter [16] which is now called Yang-Baxter equation :

$$R_{12}(\lambda_1 - \lambda_2)R_{13}(\lambda_1 - \lambda_3)R_{23}(\lambda_2 - \lambda_3) = R_{23}(\lambda_2 - \lambda_3)R_{13}(\lambda_1 - \lambda_3)R_{12}(\lambda_1 - \lambda_2), \quad (1.4)$$

where  $\lambda_1, \lambda_2, \lambda_3 \in \mathbb{C}$ , and the notation  $R_{i,j}$  means that it acts non-trivially on the  $i$ th and  $j$ th space of a tensor product of vector spaces  $\bigotimes_{i=1}^3 V_i$ .

Among the family of quantum integrable lattice models that can be considered in the QISM framework, the spin chains are of particular interest for several reasons. Firstly, for simplicity they are often used to illustrate the framework of the QISM. In fact, one can think of the spin chains as the "harmonic oscillator" in the study of quantum field theory. Although the spin chains are the simplest non-trivial example, there are many subtleties in the computation of correlation functions. It took many years to study the seemingly simple case (the  $XXZ_{1/2}$  chain with periodic boundary condition) [130]. Secondly, many theoretical results can be seen in the experiments [131]. Thirdly, due to the rise of interest in studying the quantum interaction quench, spin chains are often used to understand the dynamics in interacting integrable models (see for example in [132, 133, 134, 135]). Since this thesis aims to develop an approach to computing correlation functions for the anti-periodic  $XXX$  and  $XXZ$  spin-1/2 chains, from now on we will use spin chains to briefly recall the QISM.

The Hamiltonian of the quantum Heisenberg spin chain is defined as follows[29]:

$$H = \sum_{n=1}^N \sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \Delta (\sigma_n^z \sigma_{n+1}^z - 1) \quad (1.5)$$

where  $\Delta = \cosh \eta$  is the anisotropy parameter and in the case  $\Delta = 1$  the model becomes the  $XXX_{1/2}$  spin chain. The positive integer  $N$  denotes the length of the chain. The total quantum space of states will be denoted as  $\mathcal{H}$ , and to each site  $n$ , the local quantum space of states is labelled by  $\mathcal{H}_n$ . In the spin-1/2 case we obviously have  $\mathcal{H}_i \cong \mathbb{C}^2$ , so the total quantum space is apparently  $\mathcal{H} = \bigotimes_{n=1}^N \mathcal{H}_n = \mathbb{C}^{2^N}$ . The local spin operators  $\sigma_n^{x,y,z}$  acts non-trivially as the corresponding Pauli matrices on the corresponding local quantum space. And here we impose the quasi-periodic boundary condition:

$$\sigma_{N+1}^\alpha = K \sigma_1^\alpha K, \quad \forall \alpha = x, y, z, \quad (1.6)$$

with

$$K = \begin{pmatrix} \mathbf{a} & \mathbf{b} \\ \mathbf{c} & \mathbf{d} \end{pmatrix} \quad (1.7)$$

which is a  $2 \times 2$  invertible numeric matrix satisfying  $[K \otimes K, R] = 0^1$ . Each site  $i$  of the chain is associated with an operator  $L_{i,a}(\lambda)$ , which is a matrix of local operators at site  $i$ . The operator  $L_{i,a} \in \text{End}(V_a \otimes \mathcal{H}_i)$  acts on the representation of the local quantum space and the matrix form lives in the representation of an auxiliary space  $V_a$ . Moreover, this operator satisfies

$$R_{a,b}(\lambda - \mu)L_{i,a}(\lambda)L_{i,b}(\mu) = L_{i,b}(\mu)L_{i,a}(\lambda)R_{a,b}(\lambda - \mu) \quad (1.8)$$

---

<sup>1</sup>In the  $XXX$  case ( $\Delta = 1$ ), any invertible matrix  $K$  satisfies this condition, whereas in the  $XXZ$  case, only a diagonal matrix  $K$ , or the product of  $\sigma^x$  by a diagonal matrix satisfies this condition.

The operator  $L(\lambda)$  has the so-called "co-multiplication" property, i.e. the operator  $L_{(i,i+1),a}(\lambda) \in \text{End}(V_a \otimes \mathcal{H}_i \otimes \mathcal{H}_{i+1})$  is simply the product of two local  $L$ -operators

$$L_{(i,i+1),a}(\lambda) = L_{i,a}(\lambda)L_{i+1,a}(\lambda), \quad (1.9)$$

and it also satisfies the relation (1.8). From now on without causing any confusion, the auxiliary space subscript  $a$  for the  $L$ -operator will be omitted.

Since we only study the so-called fundamental model in this thesis, we can restrict ourselves to  $V_a \cong \mathbb{C}^2$ . Then  $R$  matrix which lives in  $\text{End}(V_a \otimes V_b)$  is a  $4 \times 4$  matrix:

$$R(\lambda) = \begin{pmatrix} \varphi(\lambda + \eta) & 0 & 0 & 0 \\ 0 & \varphi(\lambda) & \varphi(\eta) & 0 \\ 0 & \varphi(\eta) & \varphi(\lambda) & 0 \\ 0 & 0 & 0 & \varphi(\lambda + \eta) \end{pmatrix} \quad (1.10)$$

where the function form  $\varphi$  is different for two models concerned:

$$\varphi(\lambda) = \lambda \quad \text{for the } XXX \text{ case}, \quad (1.11)$$

$$\varphi(\lambda) = \sinh \lambda \quad \text{for the } XXZ \text{ case}. \quad (1.12)$$

And  $L_i(\lambda)$  can be written as a  $2 \times 2$  matrix:

$$L_i(\lambda) = \begin{pmatrix} \varphi(\lambda + \eta\sigma_i^z) & \varphi(\eta)\sigma_i^- \\ \varphi(\eta)\sigma_i^+ & \varphi(\lambda - \eta\sigma_i^z) \end{pmatrix}. \quad (1.13)$$

After the local  $L$ -operators are defined, the next step is to build up the so-called quantum monodromy matrix which acts "globally" on the chain:

$$T_a(\lambda) = L_N(\lambda)L_{N-1}(\lambda)\dots L_1(\lambda) = \begin{pmatrix} A(u) & B(u) \\ C(u) & D(u) \end{pmatrix}_a \quad (1.14)$$

where  $\{A, B, C, D\}$  are global operators acting on the total quantum space  $\mathcal{H}$ . Notice that as mentioned at the beginning of this chapter, they are the generators of the embedded algebra  $\mathcal{A}$ —Yang-Baxter algebra. Their commutation relations between each other are governed by:

$$R_{a,b}(\lambda - \mu)T_a(\lambda)T_b(\mu) = T_b(\mu)T_a(\lambda)R_{a,b}(\lambda - \mu) \quad (1.15)$$

where

$$T_a(\lambda) = T(\lambda) \otimes \mathbb{I}, \quad T_b(\lambda) = \mathbb{I} \otimes T(\lambda). \quad (1.16)$$

The  $R$ -matrix is the solution to the Yang-Baxter equation (1.4) and thus plays a role as structure constant as in Lie algebra.

The complete set of commutation relations between the generators of the algebra can be found in many literatures (for example in [136]) while here we only list some of them:

$$\begin{aligned} [B(\lambda), B(\mu)] &= [A(\lambda), A(\mu)] = [C(\lambda), C(\mu)] = [D(\lambda), D(\mu)] = 0 \\ [C(\lambda), B(\mu)] &= \frac{\varphi(\eta)}{\varphi(\lambda - \mu)} (A(\mu)D(\lambda) - A(\lambda)D(\mu)) \\ A(\lambda)B(\mu) &= \frac{\varphi(\lambda - \mu - \eta)}{\varphi(\lambda - \mu)} B(\mu)A(\lambda) + \frac{\varphi(\eta)}{\varphi(\lambda - \mu)} B(\lambda)A(\mu) \\ D(\lambda)B(\mu) &= \frac{\varphi(\lambda - \mu + \eta)}{\varphi(\lambda - \mu)} B(\mu)D(\lambda) - \frac{\varphi(\eta)}{\varphi(\lambda - \mu)} B(\lambda)D(\mu) \end{aligned} \quad (1.17)$$



**Remark 1.1.** In the quadratic relation (1.4), obviously the Yang-Baxter algebra only depends on the spectral parameters  $\lambda, \mu$  by their difference  $\lambda - \mu$ . Together with the co-multiplication property of  $L$ -operators the model can be deformed by introducing a set of parameters called inhomogeneities  $\xi_i$ , associated with each site  $i$ .

The monodromy matrix of the inhomogeneous chain is defined as

$$T_a(\lambda, \{\xi_1, \dots, \xi_N\}) = L_N(\lambda - \xi_N)L_{N-1}(\lambda - \xi_{N-1})\dots L_1(\lambda - \xi_1) = \begin{pmatrix} A(u) & B(u) \\ C(u) & D(u) \end{pmatrix}_a. \quad (1.18)$$

Among the set of generators, the twisted transfer matrix is defined as the partial trace of the twisted monodromy matrix over the auxiliary space:

$$\mathcal{T}_K(\lambda) = \text{tr}_a [KT_a(\lambda)]. \quad (1.19)$$

It is easy to see from the set of commutation rules (1.17) that

$$[\mathcal{T}_K(\lambda), \mathcal{T}_K(\mu)] = 0 \quad \forall \lambda, \mu \in \mathbb{C}. \quad (1.20)$$

Thus the twisted transfer matrix generates  $N$  independent mutually commuting operators. It is important to point out that the transfer matrix commutes with the Hamiltonian (1.5):

$$[H, \mathcal{T}_K(\lambda)] = 0, \quad \forall \lambda \in \mathbb{C}. \quad (1.21)$$

Namely the mutually commuting one-parameter family of operators all commute with the Hamiltonian. Therefore, they are the conserved quantities. Moreover, the Hamiltonian (1.5) can be expressed in terms of the transfer matrix after taking the homogeneous limit:

$$\xi_1, \dots, \xi_N \rightarrow \eta/2 \quad (1.22)$$

as the log derivative evaluating at a special point

$$H = 2 \sinh(\eta) \left. \frac{\partial}{\partial \lambda} \log \mathcal{T}_K(\lambda) \right|_{\lambda=\frac{\eta}{2}} - 2N \cosh \eta. \quad (1.23)$$

Thus the spectrum problem of the Hamiltonian can be solved by solving the spectrum problem of the associated transfer matrix.

Another important object in the Yang-Baxter algebra is the so-called quantum determinant:

$$\begin{aligned} \det_q T(\lambda) &= a(\lambda)d(\lambda - \eta) = A(\lambda)D(\lambda - \eta) - B(\lambda)C(\lambda - \eta) \\ &= D(\lambda)A(\lambda - \eta) - C(\lambda)B(\lambda - \eta) \end{aligned} \quad (1.24)$$

where

$$a(\lambda) = \prod_{n=1}^N \varphi(\lambda + \eta - \xi_n), \quad d(\lambda) = \prod_{n=1}^N \varphi(\lambda - \xi_n) \quad (1.25)$$

which is a central element in the Yang-Baxter algebra and commutes with the transfer matrix particularly. So far, given a solution to the Yang-Baxter equation (1.4), one can determine the corresponding Yang-Baxter algebra. And the family of mutually commuting operators (transfer matrix) can be constructed on it.

## 1.2 A brief review of the periodic case

When  $K$  is the identity matrix (which corresponds to the periodic boundary condition), or more generally a diagonal numeric matrix, the eigenstates of the transfer matrix of the underlying model can be constructed by the Algebraic Bethe Ansatz (ABA). Here we denote the periodic transfer matrix by  $\mathcal{T}(\lambda)$ .

### 1.2.1 A solution of the model by the ABA

For example, for the  $XXZ_{1/2}$  spin chain with periodic boundary condition  $\sigma_{N+1}^\alpha = \sigma_1^\alpha$ , the highest weight vector thus can be chosen as a convenient reference state<sup>2</sup>:

$$|0\rangle = \underbrace{|\uparrow \otimes \uparrow \otimes \uparrow \otimes \dots \otimes \uparrow\rangle}_{N \text{ times}}. \quad (1.26)$$

From the form of the  $L$ -operator (1.13) and the definition of the monodromy matrix, it is easy to see that  $|0\rangle$  is annihilated by  $C(\lambda)$ , and it's an eigenstate of both  $A(\lambda)$  and  $D(\lambda)$  with some functions  $a(\lambda)$  and  $d(\lambda)$  as the eigenvalues, namely:

$$\begin{aligned} C(\lambda) |0\rangle &= 0 & A(\lambda) |0\rangle &= a(\lambda) |0\rangle \\ B(\lambda) |0\rangle &\neq 0 & D(\lambda) |0\rangle &= d(\lambda) |0\rangle. \end{aligned} \quad (1.27)$$

Another good quantum number is the total spin:

$$S^z := \frac{1}{2} \sum_{n=1}^N \sigma_n^z \quad [S^z, \mathcal{T}(\lambda)] = 0. \quad (1.28)$$

$B(\lambda)$  and  $C(\lambda)$  act as the ladder operators in quantum mechanics moving the states from one sector labelled by its total spin  $\ell$  to another, decreasing or increasing by one, where  $N/2 \leq \ell \leq -N/2$ , where  $\Gamma_\ell$  is the set of states in  $\mathcal{H}$  with total spin  $\ell$ .

Often in literature, the reference state is also called the pseudo vacuum. And the following state labelled by  $M$  spectral parameters

$$|\Phi(\{\lambda\})\rangle = \prod_{n=1}^M B(\lambda_n) |0\rangle \quad (1.29)$$

is called the Bethe state or the Bethe vector. The condition on the set of spectral parameters  $\{\lambda_\ell\}_{\ell=1}^M$  for a Bethe state (1.29) to be an eigenstate, i.e.

$$\mathcal{T}(\lambda) |\Phi(\{\lambda\})\rangle = (A(\lambda) + D(\lambda)) \prod_{n=1}^M B(\lambda_n) |0\rangle = \tau(\lambda | \lambda_1, \dots, \lambda_M) |\Phi(\{\lambda\})\rangle \quad (1.30)$$

is

$$\frac{d(\lambda_j)}{a(\lambda_j)} = \prod_{\substack{n=1 \\ n \neq j}}^M \frac{\sinh(\lambda_j - \lambda_n - \eta)}{\sinh(\lambda_j - \lambda_n + \eta)}, \quad n = 1, \dots, M. \quad (1.31)$$

---

<sup>2</sup>For models with general boundaries such a reference state is hard to be identified in general.

which is obtained by using the commutation relations (1.17) successively when the operator  $A(\lambda)$  and  $D(\lambda)$  are moved to the right and finally hit the reference state  $|0\rangle$ . Thus  $|\Phi(\{\lambda\})\rangle$  is an eigenstate of the transfer matrix  $\mathcal{T}(\lambda)$  if the set of parameters  $\{\lambda_\ell\}_{\ell=1}^M$  satisfy (1.31).

This set of equations are called the Bethe equations. We call those Bethe state with spectral parameters  $\{\lambda_\ell\}_{\ell=1}^M$  fulfilling the Bethe equations "on-shell" Bethe states. The corresponding eigenvalue of the transfer matrix  $\mathcal{T}(\lambda)$  is

$$\tau(\lambda | \{\lambda_\ell\}) = a(\lambda) \prod_{\ell=1}^M \frac{\sinh(\lambda - \lambda_\ell - \eta)}{\sinh(\lambda - \lambda_\ell)} + d(\lambda) \prod_{\ell=1}^M \frac{\sinh(\lambda - \lambda_\ell + \eta)}{\sinh(\lambda - \lambda_\ell)}. \quad (1.32)$$

Writing down the Bethe equations (1.31) is not the end of the story. To study the thermodynamic properties of the model, one needs to understand the type of solutions that these equations can have, specifically as we take the system size  $N$  to infinity. For example, the Lieb-Liniger model was solved by the Bethe Ansatz [28]. Based on that the thermodynamics of the model were described by Yang and Yang [30], which leads to what is now known as the thermodynamic Bethe Ansatz. In the Lieb-Liniger model the solution to the Bethe equations is real. The Bethe state and a set of quantum numbers  $\{I\}$  are in one-one correspondence. Thus any allowed quantum number that does not belong to the set represents a "hole" on the real line and carries positive energy. The ground state in the thermodynamic limit ( $N \rightarrow +\infty$ ) corresponds to all solutions forming a density  $\rho(\alpha)$  defined as the limit  $\lim_{N \rightarrow +\infty} \frac{1}{N(\alpha_{j+1} - \alpha_j)}$  [137] in the rapidity representation in the real axis obeying the Lieb equation:

$$\rho_{tot}(\alpha) + \int_{-\Lambda}^{+\Lambda} K(\alpha - \beta) \rho_{tot}(\beta) d\beta = \frac{p'_{0,tot}(\alpha)}{2\pi}, \quad (1.33)$$

with some kernel  $K(\lambda)$ . After solving this integral equation one can obtain the density functions [29, 138]:

$$\rho(\alpha) = \frac{1}{2\zeta \cosh\left(\frac{\pi\alpha}{\zeta}\right)} \quad \text{for } -1 < \Delta < 1, \quad (1.34)$$

$$\rho(\alpha) = \frac{1}{2\pi} \sum_{n=-\infty}^{+\infty} \frac{e^{2in\alpha}}{\cosh(n\zeta)} = \frac{1}{2\pi} \frac{\vartheta'_1 \vartheta_3(\alpha, q)}{\vartheta_2 \vartheta_4(\alpha, q)}, \quad q = e^{-\zeta}, \quad (1.35)$$

for  $\Delta > 1$ , where  $\vartheta_i(u, q)$ ,  $i \in \{1, 2, 3, 4\}$  are the Theta functions of nome  $q$  defined as in [139]. In his original paper [17] Bethe noticed the existence of complex solutions to the Bethe equations. These complex solutions form strings and can be interpreted as bound states, having less energy than the sets of individual real magnons. There are examples of solutions that do not approach string complexes in the thermodynamic limit [138]. Nonetheless, the free energy is captured correctly only if the string configurations are taken into account [140]. The assumption that all the thermodynamically relevant solutions to the Bethe equations are built up out of such string configurations is called the string hypothesis.

**Remark 1.2.** *To prove that the Bethe vectors form a complete basis of the representation space is in general a difficult problem. In the case of the XXX and XXZ models, see [58, 59]. There are also works done by using computational algebraic geometry to tackle the problem in the finite case [141].*

### 1.2.2 Computation of correlation functions

After the spectrum problem for the transfer matrix  $\mathcal{T}(\lambda)$  is solved, the next physical quantities to compute are for example the correlation functions in the thermodynamic limit at zero temperature:

$$F_m = \frac{\langle \psi_g | \prod_{j=1}^m \sigma_j^{\alpha_j} | \psi_g \rangle}{\langle \psi_g | \psi_g \rangle}, \quad \alpha_j \in \{+, -, z\}, \quad (1.36)$$

which can be written as a linear combination of the so-called elementary building blocks:

$$F_m(\{\epsilon_j, \epsilon'_j\}) = \frac{\langle \psi_g | \prod_{j=1}^m E_j^{\epsilon'_j, \epsilon_j} | \psi_g \rangle}{\langle \psi_g | \psi_g \rangle}, \quad (1.37)$$

where the local elementary  $2 \times 2$  matrices are defined as  $E_{lk}^{\epsilon'_j, \epsilon_j} = \delta_{l, \epsilon'_j} \delta_{k, \epsilon_j}$ , with  $l, k, \epsilon_j, \epsilon'_j \in \{1, 2\}$ . In general, there are two strategies to compute (1.36). The first is to act an observable  $\mathcal{O}$  on an eigenstate of the Hamiltonian, for example, the ground state  $|\psi_g\rangle$ , then get  $|\tilde{\psi}\rangle = \mathcal{O}|\psi_g\rangle$ , and last compute the resulting scalar product:

$$g_{12} = \langle \psi_g | \tilde{\psi} \rangle. \quad (1.38)$$

In this approach, to compute the elementary building blocks (1.37) in the thermodynamic limit ( $N \rightarrow +\infty$ ), firstly, one needs to characterise the ground state of the Hamiltonian by finding the configuration of Bethe roots corresponding to the lowest energy.

Secondly, note that in (1.37) the elementary  $2 \times 2$  matrices are local operators while the Bethe states are constructed with the "global" operators  $B(u)$ . By solving the so-called quantum inverse problem, the local operators can be reconstructed by the generators of the Yang-Baxter algebra, for example [82]:

$$E_j^{\epsilon'_j, \epsilon_j} = \prod_{k=1}^{j-1} (A + D)(\xi_k) \cdot T_{\epsilon_j, \epsilon'_j}(\xi_j) \cdot \prod_{k=j+1}^N (A + D)(\xi_k), \quad (1.39)$$

where  $T_{\epsilon_j, \epsilon'_j}$  denotes the elements of the monodromy matrix (1.14). Thirdly, one also needs to have a manageable expression for the scalar products of the Bethe states to compute the ratio (1.37) in the thermodynamic limit. This determinant representation was first obtained by Slavnov in [84], and also in [81, 80] where the scalar product between one on-shell Bethe state and an off-shell Bethe vector is denoted as:

$$S_N(\{\mu_j\}, \{\lambda_k\}) = \langle 0 | \prod_{j=1}^N C(\mu_j) \prod_{k=1}^N B(\lambda_k) | 0 \rangle, \quad (1.40)$$

where  $\{\lambda_k\}_{k=1}^N$  satisfy the Bethe equations (1.31) and  $\{\mu_k\}_{k=1}^N$  are  $N$  arbitrary complex numbers. Then:

$$S_N(\{\mu_j\}, \{\lambda_k\}) = S_N(\{\lambda_k\}, \{\mu_j\}) = \frac{\det T(\{\mu_j\}, \{\lambda_k\})}{\det V(\{\mu_j\}, \{\lambda_k\})}, \quad (1.41)$$

where the  $N \times N$  matrices  $T$  and  $V$  are

$$T_{ab} = \frac{\partial}{\partial \lambda_a} \tau(\mu_b, \{\lambda_k\}), \quad V_{ab} = \frac{1}{\sinh(\mu_b - \lambda_a)}, \quad 1 \leq a, b \leq N, \quad (1.42)$$

and  $\tau(\mu_b, \{\lambda_k\})$  is the eigenvalue of the transfer matrix  $\mathcal{T}(\mu_b)$  corresponding to the eigenstate given by  $\prod_{k=1}^N B(\lambda_k) |0\rangle$ .

In the limit  $\mu_j \rightarrow \lambda_j$  for  $j = 1, \dots, N$ , the Gaudin formula is recovered as:

$$S_N(\{\lambda_k\}) = \sinh^N \eta \prod_{\alpha \neq \beta} \frac{\sinh(\lambda_\alpha - \lambda_\beta + \eta)}{\sinh(\lambda_\alpha - \lambda_\beta)} \det \Phi'(\{\lambda_\alpha\}), \quad (1.43)$$

where

$$\Phi'_{ab} = -\frac{\partial}{\partial \lambda_b} \ln \left( \frac{a(\lambda_a)}{d(\lambda_a)} \prod_{\substack{k=1 \\ k \neq a}} b(\lambda_a, \lambda_k) \right). \quad (1.44)$$

With the elements recalled above, the multiple sum representation for the elementary blocks (1.37) was obtained [80]:

$$F_m(\{\epsilon_j, \epsilon'_j\}) = \frac{1}{\prod_{k < l} \sinh(\xi_k - \xi_l)} \sum_{\mathcal{J}} H_{\mathcal{J}}(\lambda_1, \dots, \lambda_{N+m}). \quad (1.45)$$

In the thermodynamic limit, it tends to the multiple integral representation for both massless  $-1 < \Delta < 1$  and massive regimes  $\Delta > 1$  which coincide with the results obtained in [78] and in [79, 78] respectively.

The second strategy to compute (1.36) is to insert a complete set of eigenstates of the Hamiltonian and sum over the resulting form factors:

$$g_{12} = \sum_i \langle \psi_g | \mathcal{O}_1 | i \rangle \cdot \langle i | \mathcal{O}_2 | \psi_g \rangle. \quad (1.46)$$

The determinant representations for the form factors of the finite chain were computed in [81, 89]. And remarkably within this approach for the dynamical spin-spin correlation functions [92, 93, 142], the numerical results have a successful comparison to the neutron scattering experiments [131].

### 1.3 The non-diagonal twisted case: a solution by the SoV

In this thesis, we are interested in developing an approach to computing the correlation functions within the SoV. A good test model to develop this approach is the  $XXZ$  with a non-diagonal twist, which is no longer solvable by the usual Bethe Ansatz but solvable by the SoV. Here we briefly recall the SoV approach. It was first proposed by Sklyanin in a series of papers [37, 46]. The explicit separate basis was constructed for the first time by G.Niccoli in 2012 [143] for the anti-periodic  $XXZ_{1/2}$  chain and later generalised to arbitrary spin in [115] and to

the open  $XXX$  chain [144]. The SoV basis is constructed in Sklyanin's approach by using the operator roots of one of the off-diagonal elements of the transfer matrix, e.g.  $B(\lambda)$  labelled by  $\{\hat{x}_1, \dots, \hat{x}_N\}$ . In this basis the operator roots are diagonal and as a result, so is  $B(\lambda)$ . The other two diagonal elements of the transfer matrix, e.g.  $A(\hat{x}_n)$  and  $D(\hat{x}_n)$  act as a shift operator of the corresponding coordinate  $x_n$ . To make the method work, it needs a sequence of conditions [46, 47]. Without diving into the details, one can see these conditions as a guarantee to ensure that the original physical space is isomorphic to the space that contains the SoV basis, or at least after some symmetrising procedure. The conditions imply that we require  $B(\lambda)$  to have a simple spectrum. To suffice this condition we need to introduce an  $N$ -tuple of parameters  $(\xi_1, \dots, \xi_N) \in \mathbb{C}^N$  and deform the original physical model, i.e. the homogeneous chain into the inhomogeneous chain. Thus throughout the whole chapter, we will work on the inhomogeneous chain. It is important to point out that to compute any physical quantities, we need to come back to the physical model, i.e. when the homogenous limit is taken:  $\xi_n \rightarrow \eta/2, \forall n = 1, \dots, N$ . In general, in the computation of the correlation functions, taking this limit was considered to be difficult. Not until now have we gained more knowledge on how to take the homogeneous limit and further on how to take the thermodynamic limit. More recently a new approach to constructing the SoV basis was proposed in [60]. This new approach overcomes the disadvantage of the usual SoV that needs to identify the operator  $B(\lambda)$  to construct the basis which is highly involved in higher rank models [57]. Instead, the new SoV basis is constructed by the repeated action of the transfer matrix on a generically chosen state of the Hilbert space. Afterwards, the action of the transfer matrix on this basis is given again as local shifts, and thus results in the separation of variables for the spectral problem. Last but not the least, within this new approach, the SoV basis depends only on the transfer matrix. Thus it resembles the fact that in classical integrable systems the complete set of conserved charges defines both the level manifold and the flows on it leading to the construction of the action-angle variables. This approach seems promising to define the quantum integrability.

In this thesis we will use the anti-periodic chains to present our results, i.e. we restrict the twist  $K = \sigma^x$ , to keep notations simple for the future demonstration. Here we also recall the diagonalisation of the anti-periodic transfer matrix:

$$\mathcal{T}_K(\lambda) = \text{tr}_0 [\sigma_0^x T_0(\lambda)] = B(\lambda) + C(\lambda). \quad (1.47)$$

As for the  $XXX$  chain we generalise it to the general  $K$  twisted case in [116]. Note that since  $[K \otimes K, R] = 0$ , the transfer matrix (1.47) satisfies the symmetry:

$$[\Gamma_K, \mathcal{T}_K] = 0, \quad \text{where } \Gamma_K = \bigotimes_{n=1}^N K_n. \quad (1.48)$$

The diagonalisation of the anti-periodic transfer matrix (1.47) was performed in [46, 47] by the separation of variables. Here we briefly recall the main results of this construction (see also [114]). Let us suppose that the inhomogeneity parameters  $\xi_1, \dots, \xi_N$  are generic, or at least that they satisfy the following condition:

**Condition 1.1.** *For the  $XXX$  anti-periodic chain, in order to let  $B(\lambda)$  have simple spectrum, the set of inhomogeneities needs to satisfy:*

$$\xi_i \neq \xi_j \pm h\eta \quad \text{for } h \in \{-1, 0, 1\}, \quad \forall i \neq j \in \{1, \dots, N\}. \quad (1.49)$$

**Condition 1.2.** For the XXZ anti-periodic chain, suppose that  $\eta$  is a generic parameter, i.e. non commensurate with  $i\pi$ , in order to let  $B(\lambda)$  have simple spectrum, the set of inhomogeneities must satisfy:

$$\Xi_i \cap \Xi_j = \emptyset, \quad \text{if } i \neq j, \quad (1.50)$$

where  $\Xi_i = \{\xi_i + k\eta + ik'\pi | k \in \{0, -1\}, k' \in \mathbb{Z}\}$ .

Then, there exist a basis  $\{|\mathbf{h}\rangle, \mathbf{h} = (h_1, \dots, h_N) \in \{0, 1\}^N\}$  of  $\mathcal{H}$  and a basis  $\{\langle \mathbf{h}|, \mathbf{h} = (h_1, \dots, h_N) \in \{0, 1\}^N\}$  of  $\mathcal{H}^*$ :

$$|\mathbf{h}\rangle = \frac{1}{V(\{\xi\})} \prod_{n=1}^N \left( \frac{B(\xi_n)}{a(\xi_n)} \right)^{h_n} |0\rangle, \quad \langle \mathbf{h}| = \frac{1}{V(\{\xi\})} \langle 0| \prod_{n=1}^N \left( \frac{C(\xi_n)}{d(\xi_n - \eta)} \right)^{h_n}, \quad (1.51)$$

where

$$|0\rangle = \bigotimes_{n=1}^N \begin{pmatrix} 1 \\ 0 \end{pmatrix}_n, \quad \langle 0| = \bigotimes_{n=1}^N (1 \ 0)_n \quad (1.52)$$

such that  $D(\lambda)$  is diagonalised and  $B(\lambda), C(\lambda)$  act as shift operators:

$$D(\lambda) |\mathbf{h}\rangle = d_{\mathbf{h}}(\lambda) |\mathbf{h}\rangle = \prod_{n=1}^N \varphi(\lambda - \xi_n^{(h_n)}) |\mathbf{h}\rangle, \quad (1.53)$$

$$C(\lambda) |\mathbf{h}\rangle = \sum_{a=1}^N \delta_{h_a, 1} d(\xi_a^{(1)}) \prod_{b \neq a} \frac{\varphi(\lambda - \xi_b^{(h_b)})}{\varphi(\xi_a^{(h_a)} - \xi_b^{(h_b)})} |T_a^- \mathbf{h}\rangle, \quad (1.54)$$

$$B(\lambda) |\mathbf{h}\rangle = - \sum_{a=1}^N \delta_{h_a, 0} a(\xi_a^{(0)}) \prod_{b \neq a} \frac{\varphi(\lambda - \xi_b^{(h_b)})}{\varphi(\xi_a^{(h_a)} - \xi_b^{(h_b)})} |T_a^+ \mathbf{h}\rangle, \quad (1.55)$$

and

$$\langle \mathbf{h}| D(\lambda) = d_{\mathbf{h}}(\lambda) \langle \mathbf{h}| = \prod_{n=1}^N \varphi(\lambda - \xi_n^{(h_n)}) \langle \mathbf{h}|, \quad (1.56)$$

$$\langle \mathbf{h}| C(\lambda) = \sum_{a=1}^N \delta_{h_a, 0} d(\xi_a^{(1)}) \prod_{b \neq a} \frac{\varphi(\lambda - \xi_b^{(h_b)})}{\varphi(\xi_a^{(h_a)} - \xi_b^{(h_b)})} \langle T_a^+ \mathbf{h}|, \quad (1.57)$$

$$\langle \mathbf{h}| B(\lambda) = - \sum_{a=1}^N \delta_{h_a, 1} a(\xi_a^{(0)}) \prod_{b \neq a} \frac{\varphi(\lambda - \xi_b^{(h_b)})}{\varphi(\xi_a^{(h_a)} - \xi_b^{(h_b)})} \langle T_a^- \mathbf{h}|. \quad (1.58)$$

Here the following notation will be set as the same in [115, 114]

$$\xi_n^{(h_n)} = \xi_n - h_n \eta \quad \text{for } h_n \in \{0, 1\}, \quad (1.59)$$

$$d_{\mathbf{h}}(\lambda) = \prod_{n=1}^N \varphi(\lambda - \xi_n^{(h_n)}), \quad (1.60)$$

and

$$T_a^\pm(h_1, \dots, h_N) = (h_1, \dots, h_a \pm 1, \dots, h_N). \quad (1.61)$$

To determine the action of  $A(\lambda)$  on  $|\mathbf{h}\rangle$  and  $\langle\mathbf{h}|$ , one can use the quantum determinant relation (1.24). By using the first line of (1.24) and (1.53)-(1.55) we obtain:

$$\begin{aligned} A(\lambda) |\mathbf{h}\rangle &= \frac{\det_q T(\lambda) + B(\lambda) C(\lambda - \eta)}{d_{\mathbf{h}}(\lambda - \eta)} |\mathbf{h}\rangle \\ &= \frac{\det_q T(\lambda)}{d_{\mathbf{h}}(\lambda - \eta)} |\mathbf{h}\rangle - \frac{1}{d_{\mathbf{h}}(\lambda - \eta)} \sum_{a=1}^N \delta_{h_{a,1}} d(\xi_a^{(1)}) \prod_{\ell \neq a} \frac{\varphi(\lambda - \eta - \xi_{\ell}^{(h_{\ell})})}{\varphi(\xi_a^{(1)} - \xi_{\ell}^{(h_{\ell})})} \\ &\quad \times \sum_{b=1}^N \delta_{(T_a^- \mathbf{h})_{b,0}} a(\xi_b^{(0)}) \prod_{\ell \neq b} \frac{\varphi(\lambda - \xi_{\ell}^{((T_a^- \mathbf{h})_{\ell})})}{\varphi(\xi_b^{(0)} - \xi_{\ell}^{((T_a^- \mathbf{h})_{\ell})})} |T_b^+ T_a^- \mathbf{h}\rangle. \end{aligned} \quad (1.62)$$

By using the second line of (1.24) and (1.56)-(1.58):

$$\begin{aligned} \langle\mathbf{h}| A(\lambda) &= \langle\mathbf{h}| \frac{\det_q T(\lambda + \eta) + C(\lambda + \eta) B(\lambda)}{d_{\mathbf{h}}(\lambda + \eta)} \\ &= \langle\mathbf{h}| \frac{\det_q T(\lambda + \eta)}{d_{\mathbf{h}}(\lambda + \eta)} - \frac{1}{d_{\mathbf{h}}(\lambda + \eta)} \sum_{a=1}^N \delta_{h_{a,0}} d(\xi_a^{(1)}) \prod_{\ell \neq a} \frac{\varphi(\lambda + \eta - \xi_{\ell}^{(h_{\ell})})}{\varphi(\xi_a^{(0)} - \xi_{\ell}^{(h_{\ell})})} \\ &\quad \times \sum_{b=1}^N \delta_{(T_a^+ \mathbf{h})_{b,1}} a(\xi_b^{(0)}) \prod_{\ell \neq b} \frac{\varphi(\lambda - \xi_{\ell}^{((T_a^+ \mathbf{h})_{\ell})})}{\varphi(\xi_b^{(1)} - \xi_{\ell}^{((T_a^+ \mathbf{h})_{\ell})})} \langle T_b^- T_a^+ \mathbf{h}|. \end{aligned} \quad (1.63)$$

We have

$$\langle\mathbf{h} | \mathbf{k}\rangle = \frac{\delta_{\mathbf{h},\mathbf{k}}}{V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)})}, \quad (1.64)$$

where, for any  $n$ -tuple  $(x_1, \dots, x_n)$ ,  $V(x_1, \dots, x_n)$  denotes the Vandermonde determinant

$$V(x_1, \dots, x_n) = \prod_{\substack{i,j=1 \\ i < j}}^n \varphi(x_j - x_i). \quad (1.65)$$

The so-called separate states can be defined from the SoV basis for arbitrary functions  $\alpha$  and  $\beta$  as follows: <sup>3</sup>

$$\langle\alpha| = \sum_{\mathbf{h} \in \{0,1\}^N} \prod_{n=1}^N \alpha(\xi^{(h_n)}) V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle\mathbf{h}|, \quad (1.66)$$

$$\begin{aligned} |\beta\rangle &= \sum_{\mathbf{h} \in \{0,1\}^N} \prod_{n=1}^N \left\{ \left( -\frac{a(\xi_n)}{d(\xi_n - \eta)} \right)^{h_n} \beta(\xi_n^{(h_n)}) \right\} V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) |\mathbf{h}\rangle \\ &= \sum_{\mathbf{h} \in \{0,1\}^N} \prod_{n=1}^N \beta(\xi_n^{(h_n)}) V(\xi_1^{(1-h_1)}, \dots, \xi_N^{(1-h_N)}) |\mathbf{h}\rangle. \end{aligned} \quad (1.67)$$

<sup>3</sup>where the second line of (1.67) comes from the fact:

$$\prod_{n=1}^N \left( -\frac{a(\xi_n)}{d(\xi_n - \eta)} \right)^{h_n} V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) = V(\xi_1^{(1-h_1)}, \dots, \xi_N^{(1-h_N)}) = V(\xi_1 + h_1\eta, \dots, \xi_N + h_N\eta)$$



The separate states (1.66) or (1.67) are defined up to some global normalisation only by the  $N$  ratios  $\alpha(\xi_j - \eta)/\alpha(\xi_j)$  or  $\beta(\xi_j - \eta)/\beta(\xi_j)$ ,  $1 \leq j \leq N$ , respectively. Thus many different functions  $\alpha$  or  $\beta$  can lead to the same separate states. The eigenstates of the anti-periodic transfer matrix (1.47) happen to be a particular class of separate states defined by the ratios  $Q(\xi_j - \eta)/Q(\xi_j)$ ,  $1 \leq j \leq N$ , with some function  $Q(\lambda)$ . The function  $Q(\lambda)$  turns out to be fixed by the eigenvalue of the transfer matrix (1.47). Up until now, the SoV basis and the separate states are defined generally for both  $XXX$  and  $XXZ$  models. On the contrary, the function forms of  $Q(\lambda)$  turn out to be quite different.

Due to the function form of  $\varphi(\lambda)$  (which is simple polynomial), for the anti-periodic  $XXX$  inhomogeneous chain, the transfer matrix (1.47) is a polynomial of  $\lambda$  of degree  $N - 1$ . So is the eigenvalue<sup>4</sup>. As for the  $XXZ$  case, the determination of function form is more involved and will be discussed later. Denote  $\langle Q_\tau |$  as a left eigenstate of the anti-periodic transfer matrix (1.47) of the form (1.66) corresponding to eigenvalue  $\tau(\lambda)$ . Then the eigenvalue  $\tau(\lambda)$  satisfies the following set of quadratic discrete equations<sup>5</sup>:

$$\tau(\xi_n)\tau(\xi_n - \eta) + a(\xi_n)d(\xi_n - \eta) = 0, \quad \forall n = 1, \dots, N. \quad (1.68)$$

The function  $Q_\tau$  satisfies the following set of conditions<sup>6</sup>:

$$\tau(\xi_n)Q_\tau(\xi_n) + a(\xi_n)Q_\tau(\xi_n - \eta) = 0, \quad (1.69)$$

$$(Q_\tau(\xi_n), Q_\tau(\xi_n - \eta)) \neq (0, 0). \quad (1.70)$$

Similarly for the right eigenstate  $|Q_\tau\rangle$  with eigenvalue  $\tau(\lambda)$ :

$$\tau(\xi_n - \eta)Q_\tau(\xi_n - \eta) - d(\xi_n - \eta)Q_\tau(\xi_n) = 0, \quad (1.71)$$

$$(Q_\tau(\xi_n), Q_\tau(\xi_n - \eta)) \neq (0, 0). \quad (1.72)$$

The conditions (1.68)-(1.69) and (1.71) for the eigenvalue  $\tau(\lambda)$  and the function  $Q_\tau(\lambda)$  are equivalent to the set of  $2N$  discrete version of Baxter's TQ-equations<sup>7</sup>:

$$\tau(\xi_n^{(h_n)})Q_\tau(\xi_n^{(h_n)}) = -a(\xi_n^{(h_n)})Q_\tau(\xi_n^{(h_n)} - \eta) + a(\xi_n^{(h_n)})Q_\tau(\xi_n^{(h_n)} + \eta), \quad (1.73)$$

which characterise the spectrum of the anti-periodic transfer matrix (1.47) and its eigenstates completely.

**Remark 1.3.** *In the paper [46, 47] Sklyanin stopped at the discrete Baxter's TQ-equations. Though serving a role of characterising the spectrum problem of the transfer matrix, these equations are explicitly encoded by the inhomogeneous parameters which make it difficult to recover the physical model. Thus it is necessary to reformulate these equations to a form such that the homogeneous limit can be easily taken.*

It is easy to see that for a given function  $\tau(\lambda)$ , any solution  $Q(\lambda)$  to the inhomogeneous functional Baxter's TQ-equation:

$$\tau(\lambda)Q(\lambda) = -a(\lambda)Q(\lambda - \eta) + d(\lambda)Q(\lambda + \eta) + F_Q(\lambda) \quad (1.74)$$

<sup>4</sup>From the fact that the monodromy matrix is a polynomial of degree  $N - 1$  [47].

<sup>5</sup>proof see [143].

<sup>6</sup>From (1.69) one can see that for a given eigenvalue  $\tau(\lambda)$ , indeed only the ratio  $Q(\xi_j - \eta)/Q(\xi_j)$  determines the eigenstate.

<sup>7</sup>This can be seen from the fact that  $a(\xi_n - \eta) = d(\xi_n) = 0, \forall n = 1, \dots, N$ .

with additional term  $F_Q(\lambda)$  vanishing at all points  $\xi_n^{(h_n)}$ ,  $n = 1, \dots, N$ , obviously satisfies the discrete version (1.73) and consequently gives us the eigenstate. However, it is more convenient to use the homogeneous functional Baxter's TQ-equation <sup>8</sup>:

$$\tau(\lambda)Q(\lambda) = -a(\lambda)Q(\lambda - \eta) + d(\lambda)Q(\lambda + \eta) \quad (1.75)$$

to characterise the transfer matrix spectrum and eigenstates. But depending on the models that one considers, to pass from (1.73) directly to (1.75) for characterising the transfer matrix spectrum problem can be difficult. On one hand, the existence of such a solution  $Q(\lambda)$  to (1.75) is not ensured. On the other hand, it also requires to characterise the function form of  $Q(\lambda)$  <sup>9</sup> [115, 146].

### 1.3.1 Complete characterisation of the spectrum and eigenstates in terms of the functional TQ-equation: the $XXX$ case

For the  $XXX$  model the problem of finding the solution  $Q_\tau(\lambda)$  is easy. All the functions appearing are simply polynomials. Thus by interpolation one can find that the form of  $Q_\tau(\lambda)$  is:

$$Q(\lambda) = \prod_{j=1}^R (\lambda - \lambda_j), \quad R \leq N, \quad (1.76)$$

for some set of roots  $\lambda_1, \dots, \lambda_R$  such that  $\lambda_a \neq \xi_b, \forall a \in \{1, \dots, R\}, \forall b \in \{1, \dots, N\}$ . Moreover, for a given eigenvalue  $\tau(\lambda)$  of the transfer matrix (1.47), the polynomial  $Q_\tau(\lambda)$  satisfying these conditions is unique. The corresponding left and right eigenstates of (1.47) with eigenvalue  $\tau(\lambda)$  are obtained in terms of  $Q_\tau$  as the states of the form

$$\langle Q_\tau | = \sum_{\mathbf{h} \in \{0,1\}^N} \prod_{n=1}^N Q_\tau(\xi_n^{(h_n)}) V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle \mathbf{h} |, \quad (1.77)$$

$$\begin{aligned} |Q_\tau\rangle &= \sum_{\mathbf{h} \in \{0,1\}^N} \prod_{n=1}^N \left\{ \left( -\frac{a(\xi_n)}{d(\xi_n - \eta)} \right)^{h_n} Q_\tau(\xi_n^{(h_n)}) \right\} V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) |\mathbf{h}\rangle \\ &= \sum_{\mathbf{h} \in \{0,1\}^N} \prod_{n=1}^N Q_\tau(\xi_n^{(h_n)}) V(\xi_1^{(1-h_1)}, \dots, \xi_N^{(1-h_N)}) |\mathbf{h}\rangle. \end{aligned} \quad (1.78)$$

Hence, from the entireness of  $\tau(\lambda)$  and (1.75), the eigenvalues and eigenstates of the anti-periodic transfer matrix can be characterised in terms of the (admissible) solutions of the Bethe equations:

$$\mathbf{a}_Q(\lambda_j) = 1, \quad j = 1, \dots, R, \quad (1.79)$$

for the roots  $\lambda_1, \dots, \lambda_R$  of  $Q(\lambda)$  where

$$\mathbf{a}_Q(\lambda) = \frac{d(\lambda) Q(\lambda + \eta)}{a(\lambda) Q(\lambda - \eta)}. \quad (1.80)$$

<sup>8</sup>There is also an approach developed keeping the inhomogeneous term  $F_Q(\lambda)$  [145].

<sup>9</sup>The equation (1.75) is more convenient as the entireness condition for  $\tau(\lambda)$  will lead to Bethe-type equations, thus the homogeneous limit and thermodynamic limit can be taken in a standard way. Also, the function form of  $Q(\lambda)$  does not necessarily coincide with the form of  $\tau(\lambda)$ .

**Remark 1.4.** Let  $\tau(\lambda)$  be an eigenvalue of the transfer matrix (1.47). Then the condition (1.68) implies that  $-\tau(\lambda)$  is also an eigenvalue. With the same argument it will lead to the functional equation:

$$\tau(\lambda)\hat{Q}(\lambda) = a(\lambda)\hat{Q}(\lambda - \eta) - d(\lambda)\hat{Q}(\lambda + \eta). \quad (1.81)$$

Since the transfer matrix (1.47) has a simple spectrum and  $\tau(\lambda) = 0$  cannot be an eigenvalue (can be seen from condition (1.68)), the equation (1.81) should be thought of as an independent TQ-equation from (1.75). The two polynomials  $Q_\tau(\lambda)$  and  $\hat{Q}_\tau(\lambda) = Q_{-\tau}(\lambda)$  subjected to the two eigenvalues  $\tau(\lambda)$  and  $-\tau(\lambda)$  satisfy the quantum Wronskian relation:

$$\hat{W}_{Q, \hat{Q}}(\lambda) = d(\lambda), \quad (1.82)$$

where

$$\hat{W}_{Q, \hat{Q}}(\lambda) = \frac{1}{2} \left[ Q(\lambda) \hat{Q}(\lambda - \eta) + \hat{Q}(\lambda) Q(\lambda - \eta) \right]. \quad (1.83)$$

This implies that if  $Q(\lambda)$  is of the form (1.76),  $\hat{Q}(\lambda)$  should be a polynomial of degree  $N - R$ :

$$\hat{Q}(\lambda) = \prod_{j=1}^{N-R} (\lambda - \hat{\lambda}_j). \quad (1.84)$$

Thus the spectrum problem of the anti-periodic transfer matrix (1.47) can alternatively be characterised by  $N - R$  roots  $\{\hat{\lambda}_1, \dots, \hat{\lambda}_{N-R}\}$  of (1.84) if the Bethe equations hold:

$$\mathbf{a}_{\hat{Q}}(\hat{\lambda}_j) = 1, \quad j = 1, \dots, N - R. \quad (1.85)$$

**Remark 1.5.** Moreover, the eigenstates (1.77)-(1.78) can be written in the form of generalised Bethe states as

$$\langle Q_\tau | = (-1)^{RN} \langle \mathbf{1} | \prod_{k=1}^R D(\lambda_k), \quad (1.86)$$

$$|Q_\tau\rangle = (-1)^{RN} \prod_{k=1}^R D(\lambda_k) | \mathbf{1} \rangle, \quad (1.87)$$

where

$$\langle \mathbf{1} | = \sum_{\mathbf{h} \in \{0,1\}^N} V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle \mathbf{h} |, \quad (1.88)$$

$$| \mathbf{1} \rangle = \sum_{\mathbf{h} \in \{0,1\}^N} V(\xi_1^{(1-h_1)}, \dots, \xi_N^{(1-h_N)}) | \mathbf{h} \rangle \quad (1.89)$$

are eigenvectors of the transfer matrix (1.47) with eigenvalue  $-a(\lambda) + d(\lambda)$ . Note that the eigenstates (1.86)-(1.87) can alternatively be written in the form:

$$\langle Q_\tau | = (-1)^N \frac{\prod_{k=1}^R d(\lambda_k)}{\prod_{k=1}^{N-R} d(\hat{\lambda}_k)} \sum_{\mathbf{h}} \prod_{n=1}^N \left[ (-1)^{h_n} \hat{Q}(\xi_n^{(h_n)}) \right] V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle \mathbf{h} | \quad (1.90)$$

$$= (-1)^{RN} \frac{\prod_{k=1}^R d(\lambda_k)}{\prod_{k=1}^{N-R} d(\hat{\lambda}_k)} \langle \mathbf{1}_{\text{alt}} | \prod_{k=1}^{N-R} D(\hat{\lambda}_k), \quad (1.91)$$

$$|Q_\tau\rangle = (-1)^N \frac{\prod_{k=1}^R d(\lambda_k)}{N-R} \sum_{\mathbf{h}} \prod_{n=1}^N \left[ (-1)^{h_n} \widehat{Q}(\xi_n^{(h_n)}) \right] V(\xi_1^{(1-h_1)}, \dots, \xi_N^{(1-h_N)}) |\mathbf{h}\rangle \quad (1.92)$$

$$= (-1)^{RN} \frac{\prod_{k=1}^R d(\lambda_k)}{\prod_{k=1}^{N-R} d(\widehat{\lambda}_k)} \prod_{k=1}^{N-R} D(\widehat{\lambda}_k) |\mathbf{1}_{\text{alt}}\rangle, \quad (1.93)$$

where

$$\langle \mathbf{1}_{\text{alt}} | = \sum_{\mathbf{h} \in \{0,1\}^N} \prod_{n=1}^N (-1)^{h_n} V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle \mathbf{h} |, \quad (1.94)$$

$$|\mathbf{1}_{\text{alt}}\rangle = \sum_{\mathbf{h} \in \{0,1\}^N} \prod_{n=1}^N (-1)^{h_n} V(\xi_1^{(1-h_1)}, \dots, \xi_N^{(1-h_N)}) |\mathbf{h}\rangle, \quad (1.95)$$

are eigenvectors of the anti-periodic transfer matrix (1.47) with eigenvalue  $a(\lambda) - d(\lambda)$ .

Note that the expressions (1.75), (1.76), (1.79), (1.86)-(1.87) and (1.84), (1.81), (1.85) (1.91)-(1.93) are now suitable for the consideration of the homogeneous limit  $\xi_1, \dots, \xi_N \rightarrow \eta/2$  (provided that the homogeneous limit of the states  $\langle \mathbf{1} |, |\mathbf{1}\rangle$  and  $\langle \mathbf{1}_{\text{alt}} |, |\mathbf{1}_{\text{alt}}\rangle$  is well defined). In this limit, one recovers the physical model (1.5). The states  $\langle \Psi_\tau |$  (1.86), (1.91) and  $|\Psi_\tau\rangle$  (1.87), (1.93) are eigenstates of the Hamiltonian with the eigenvalue  $E_\tau$  which can be expressed in terms of the roots of either  $Q_\tau(\lambda)$  or  $\widehat{Q}_\tau(\lambda)$ :

$$E_\tau = \sum_{a=1}^R \frac{2\eta^2}{(\lambda_a - \eta/2)(\lambda_a + \eta/2)} = \sum_{a=1}^{N-R} \frac{2\eta^2}{(\widehat{\lambda}_a - \eta/2)(\widehat{\lambda}_a + \eta/2)}. \quad (1.96)$$

**Remark 1.6.** The spectrum of the Hamiltonian (1.5) obtained from (1.23) is doubly degenerated with energy given in terms of the roots of  $Q_\tau(\lambda)$  or of  $\widehat{Q}_\tau(\lambda) = Q_{-\tau}(\lambda)$  as in (1.96).

**Remark 1.7.** From the quantum Wronskian relation (1.82)-(1.83), one can obtain several relations between the roots  $\lambda_j$ ,  $j = 1, \dots, R$  of  $Q_\tau(\lambda)$  and the roots  $\widehat{\lambda}_j$ ,  $j = 1, \dots, N - R$  of  $\widehat{Q}_\tau(\lambda) = Q_{-\tau}(\lambda)$ . In particular, we have the sum rule:

$$\sum_{n=1}^N (\xi_n - \eta/2) = \sum_{j=1}^R \lambda_j + \sum_{j=1}^{N-R} \widehat{\lambda}_j. \quad (1.97)$$

**Remark 1.8.** The eigenstates  $|Q_\tau\rangle$  of the anti-periodic transfer matrix are also eigenstates of the symmetry operators  $S^x$  (1.99) and  $\Gamma^x$  (1.100):

$$S^x |Q_\tau\rangle = (N - 2R) |Q_\tau\rangle, \quad \Gamma^x |Q_\tau\rangle = (-1)^R |Q_\tau\rangle. \quad (1.98)$$

$$[S^x, \mathcal{T}(\lambda)] = 0, \quad S^x = \sum_{n=1}^N \sigma_n^x, \quad (1.99)$$

$$[\Gamma^x, \mathcal{T}(\lambda)] = 0, \quad \Gamma^x = \bigotimes_{n=1}^N \sigma_n^x = (-i)^N \exp\left[\frac{i\pi}{2} S^x\right]. \quad (1.100)$$

### 1.3.2 Complete characterisation of the spectrum and eigenstates in terms of the functional TQ-equation: the XXZ case

Similarly, as in the XXX case, the transfer matrix spectrum and eigenstates can be completely characterised in terms of a system of discrete equations (1.73) in the inhomogeneity parameters of the model [47, 143]. One of the differences from the XXX case is that the eigenvalue function of the anti-periodic transfer matrix now needs to satisfy the quasi-periodic property:

$$\tau(\lambda + i\pi) = (-1)^{N-1} \tau(\lambda). \quad (1.101)$$

Such a characterisation has been more conveniently reformulated in [115] in terms of the solutions of a functional TQ-equation of Baxter's type (in relation with the eigenvalues of the Q-operator previously constructed by Baxter *et al.* in [117]):

$$\tau(\lambda) Q(\lambda) = -a(\lambda) Q(\lambda - \eta) + d(\lambda) Q(\lambda + \eta). \quad (1.102)$$

As a consequence of (1.101), for a given eigenvalue  $\tau(\lambda)$ , the unique  $Q(\lambda)$  function in the XXZ anti-periodic model is no longer a usual trigonometric polynomial<sup>10</sup>. Instead, it has the form:

$$Q(\lambda) = \prod_{j=1}^N \sinh\left(\frac{\lambda - q_j}{2}\right), \quad q_1, \dots, q_N \in \mathbb{C} \setminus \bigcup_{i=1}^N \Xi_i, \quad (1.103)$$

Then the eigenvalues and eigenstates of the anti-periodic transfer matrix can be fully characterised in terms of the admissible solutions of the Bethe equations for the roots  $q_1, \dots, q_N$  of  $Q(\lambda)$  in the condition that the eigenvalue function  $\tau(\lambda)$  is an entire function:

$$\mathfrak{a}_Q(q_j) = 1, \quad j = 1, \dots, N, \quad (1.104)$$

Alternatively, the transfer matrix spectrum and eigenstates can be equally characterised by another functional TQ-relation since  $-\tau(\lambda)$  is also an eigenvalue:

$$\tau(\lambda) \widehat{Q}(\lambda) = a(\lambda) \widehat{Q}(\lambda - \eta) - d(\lambda) \widehat{Q}(\lambda + \eta), \quad (1.105)$$

with a unique solution:

$$\widehat{Q}(\lambda) = \prod_{j=1}^N \sinh\left(\frac{\lambda - \hat{q}_j}{2}\right), \quad \hat{q}_1, \dots, \hat{q}_N \in \mathbb{C} \setminus \bigcup_{i=1}^N \Xi_i. \quad (1.106)$$

Note that, for a given eigenvalue  $\tau(\lambda)$  of (1.47), the trigonometric polynomials  $Q$  satisfying (1.102) and  $\widehat{Q}$  satisfying (1.105) are simply related by

$$\widehat{Q}(\lambda) = Q(\lambda + i\pi). \quad (1.107)$$

We also recall that these two solutions satisfy the quantum Wronskian relation [115]:

$$\frac{1}{2} \left[ Q(\lambda) \widehat{Q}(\lambda - \eta) + \widehat{Q}(\lambda) Q(\lambda - \eta) \right] = \pm \left(\frac{i}{2}\right)^N d(\lambda), \quad (1.108)$$

---

<sup>10</sup>Here we adopted the terminology usual trigonometric polynomial for the functions of the form:  $\prod_{n=1}^N \sinh(\lambda - \lambda_n)$ .

which implies notably the following sum rule for the roots  $q_1, \dots, q_N$ :

$$\sum_{j=1}^N q_j = \sum_{n=1}^N \left( \xi_n - \frac{\eta}{2} \right) + ik\pi, \quad k \in \mathbb{Z}. \quad (1.109)$$

And this alternative characterisation of eigenvalues and eigenvectors can be reformulated as the Bethe equations:

$$\mathbf{a}_{\widehat{Q}}(\hat{q}_j) = 1, \quad j = 1, \dots, N. \quad (1.110)$$

with admissible solutions  $\hat{q}_1, \dots, \hat{q}_N$  of  $\widehat{Q}(\lambda)$  satisfying (1.105) when  $\tau(\lambda)$  is an entire function.

Due to this reason (1.107), for a given function  $P$ ,  $\epsilon \in \{+, -\}$ , the separate states in the  $XXZ$  case are denoted slightly different with a label  $\epsilon$  indicating the two solutions:

$$\langle P, \epsilon | = \sum_{\mathbf{h} \in \{0,1\}^N} \prod_{n=1}^N \{ \epsilon^{h_n} P(\xi_n^{(h_n)}) \} V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) |\mathbf{h}\rangle, \quad (1.111)$$

$$\begin{aligned} |P, \epsilon\rangle &= \sum_{\mathbf{h} \in \{0,1\}^N} \prod_{n=1}^N \left\{ (-\epsilon)^{-h_n} \left( \frac{a(\xi_n)}{d(\xi_n - \eta)} \right)^{h_n} P(\xi_n^{(h_n)}) \right\} V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) |\mathbf{h}\rangle \\ &= \sum_{\mathbf{h} \in \{0,1\}^N} \prod_{n=1}^N \{ \epsilon^{-h_n} P(\xi_n^{(h_n)}) \} V(\xi_1^{(1-h_1)}, \dots, \xi_N^{(1-h_N)}) |\mathbf{h}\rangle. \end{aligned} \quad (1.112)$$

Thus the one-dimensional left and right eigenspaces of  $\mathcal{T}_K(\lambda)$  (1.47) associated with the eigenvalue  $\tau(\lambda)$  are respectively spanned by the separate states  $\langle Q, + |$  and  $|Q, +\rangle$  where  $Q$  of the form (1.103) satisfies (1.102), or by the separate states  $\langle \widehat{Q}, - |$  and  $|\widehat{Q}, -\rangle$  where  $\widehat{Q}$  of the form (1.106) satisfies (1.105).

The proportionality between the coefficient of  $\langle Q, + |$  and  $\langle \widehat{Q}, - |$ , and of  $|Q, +\rangle$  and  $|\widehat{Q}, -\rangle$  can be computed through the relations:

$$\frac{Q(\xi_n - \eta)}{Q(\xi_n)} = -\frac{\widehat{Q}(\xi_n - \eta)}{\widehat{Q}(\xi_n)} = -\frac{\tau(\xi_n)}{a(\xi_n)}, \quad n = 1, \dots, N, \quad (1.113)$$

so that

$$\langle \widehat{Q}, - | = \prod_{n=1}^N \frac{\widehat{Q}(\xi_n)}{Q(\xi_n)} \langle Q, + |, \quad |\widehat{Q}, -\rangle = \prod_{n=1}^N \frac{\widehat{Q}(\xi_n)}{Q(\xi_n)} |Q, +\rangle. \quad (1.114)$$

**Remark 1.9.** *If  $\tau(\lambda)$  is an eigenvalue of the anti-periodic transfer matrix  $\mathcal{T}_K(\lambda)$  (1.47) with left and right eigenvectors  $\langle Q, + |$  and  $|Q, +\rangle$ ,  $-\tau(\lambda)$  is an eigenvalue of  $\mathcal{T}_K(\lambda)$  (1.47) with left and right eigenvectors  $\langle Q, - |$  and  $|Q, -\rangle$  and vice versa.*

**Remark 1.10.** *Since the transfer matrix (1.47) satisfies the symmetry (1.48) and has a simple spectrum, together with the fact that  $\Gamma_K^2 = 1$ , the eigenstates of the transfer matrix are also the eigenstates of  $\Gamma_K$  with eigenvalue  $\pm 1$ .*

**Remark 1.11.** *We can consider a slightly more general twist  $K = \text{diag}(\kappa, \kappa^{-1}) \cdot \sigma^x$  for  $\kappa \in \mathbb{C} \setminus \{0\}$ . As a result, the separate states (1.111)-(1.112) will be defined with a different normalisation.*



# Chapter 2

## Description of the ground state

To study the correlation functions at zero temperature in the thermodynamic limit, as in the ABA approach, we need to describe the ground state in terms of the solution to the Bethe equations.

Under the natural assumption which has been proved for periodic boundary condition [137] that the Bethe roots will form a distribution in the thermodynamic limit for the ground state, we used a similar method as in [138] and obtained the same integral equation as in the periodic case and thus obtained same roots density for the ground state in the  $XXX$  case. For the  $XXZ$  chain, we obtained a similar result. It is slightly more complicated to summarise here, so we will explain it in the main context.

### 2.1 The $XXX$ case

We now consider the homogeneous limit  $\xi_1, \dots, \xi_N \rightarrow \eta/2$ , and we set for convenience  $\eta = -i$ . The Bethe equations (1.79) then take the form:

$$\left(\frac{i/2 - \lambda_j}{i/2 + \lambda_j}\right)^N \prod_{k=1}^R \frac{i + \lambda_j - \lambda_k}{i - \lambda_j + \lambda_k} = (-1)^{N-R}, \quad j = 1, \dots, R, \quad (2.1)$$

and the energy (1.96) associated with a configuration of the Bethe roots  $\{\lambda_j\}_{1 \leq j \leq R}$  is

$$E(\{\lambda_j\}_{1 \leq j \leq R}) = \sum_{a=1}^R \epsilon(\lambda_a), \quad \text{with} \quad \epsilon(\lambda) = -\frac{2}{\lambda^2 + 1/4}. \quad (2.2)$$

We can show similarly as in [138] that the complex roots appear by pairs  $z, \bar{z}$  for a solution with much more real roots than complex roots<sup>1</sup>.

For the real roots  $\lambda_j$ , it is convenient, as in the periodic case, to rewrite the Bethe equations (2.1) in logarithmic form:

$$\widehat{\xi}_Q(\lambda_j) = \frac{2n_j - N + R}{N} \pi, \quad n_j \in \mathbb{Z}, \quad (2.3)$$

where  $\widehat{\xi}_Q(\lambda)$  is the counting function associated with a configuration of the Bethe roots  $Q$ ,

$$\widehat{\xi}_Q(\lambda) = \frac{i}{N} \log \left( (-1)^{N-R} \mathbf{a}_Q(\lambda) \right) = p(\lambda) + \frac{1}{N} \sum_{k=1}^R \theta(\lambda - \lambda_k) \quad (2.4)$$

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<sup>1</sup>i.e. where the number of real roots is more than twice the number of complex roots.



with

$$p(\lambda) = i \log \left( \frac{i/2 + \lambda}{i/2 - \lambda} \right), \quad p'(\lambda) = \frac{1}{\lambda^2 + 1/4} \quad (2.5)$$

$$\theta(\lambda) = i \log \left( \frac{i - \lambda}{i + \lambda} \right), \quad \theta'(\lambda) = -\frac{2}{\lambda^2 + 1}. \quad (2.6)$$

Note that these Bethe equations are completely similar in their form to the ones that we have in the periodic case, the only difference being in the sign on the right-hand side of (2.1). Hence the analysis of the solution is similar, except that this difference of sign will result in a difference in the allowed set of quantum numbers on the right-hand side of (2.3).

**Remark 2.1.** *We have however a crucial difference here with the periodic case: the SoV approach gives us the completeness of the corresponding Bethe states (at least if we slightly deform the model by inhomogeneity parameters), contrary to the periodic case for which the Bethe states give only  $\mathfrak{su}(2)$  the highest weight vectors. Moreover, we need here a priori to consider all degrees  $R \leq N$  of  $Q$ , in addition to  $R \leq \frac{N}{2}$  as in the periodic case. Let us nevertheless remark that we can avoid considering solutions of the Bethe equations "beyond the equator" (i.e. with  $R > \frac{N}{2}$ ) by constructing the eigenstates associated with polynomials  $Q$  with degree  $R > \frac{N}{2}$  by (1.91)-(1.93), i.e. by using the polynomial  $\widehat{Q}$  which in that case has the degree  $N - R < \frac{N}{2}$ .*

As in the periodic case, we expect that, in the large  $N$  limit, the low-energy states will be given by solutions  $\{\lambda\} \equiv \{\lambda_1, \dots, \lambda_R\}$  of the Bethe equations with an infinite number of real roots (of order  $N/2$ ) and a finite number of complex roots. Let us also suppose that, for such states, the real Bethe roots have a continuous distribution in the thermodynamic limit:

$$\frac{1}{N(\lambda_{j+1} - \lambda_j)} \underset{N \rightarrow \infty}{\sim} \rho(\lambda_j), \quad \text{if } \lambda_j, \lambda_{j+1} \in \mathbb{R}, \quad (2.7)$$

so that we suppose we can, in the leading order in the thermodynamic limit, replace the sums by integrals (see [137] for a proof in the periodic case):

$$\frac{1}{N} \sum_{k=1}^R f(\lambda_k) \underset{N \rightarrow +\infty}{\longrightarrow} \int_{-\infty}^{\infty} f(\lambda) \rho(\lambda) d\lambda, \quad (2.8)$$

for any sufficiently regular function  $f$ . The function  $\rho(\lambda)$  is, therefore, the solution to the integral equation

$$2\pi\rho(\lambda) - \int_{-\infty}^{\infty} \theta'(\lambda - \mu) \rho(\mu) d\mu = p'(\lambda) \quad (2.9)$$

which is the same integral equation as in the periodic case and therefore admits the same solution:

$$\rho(\lambda) = \frac{1}{2 \cosh(\pi\lambda)}. \quad (2.10)$$

Note that we have

$$\widehat{\xi}_Q^l(\lambda) = \frac{i}{N} \frac{\mathfrak{a}'_Q(\lambda)}{\mathfrak{a}_Q(\lambda)} \underset{N \rightarrow \infty}{\longrightarrow} 2\pi\rho(\lambda). \quad (2.11)$$

The function  $p$  (resp.  $\theta$ ) is holomorphic in a band of width  $i$  (resp.  $2i$ ) around the real axis.  $p$  and  $\theta$  (and hence  $\widehat{\xi}$ , as it is the sum of the two) are odd functions of  $\lambda$ . Moreover,

$$p(\lambda) \xrightarrow{\Re(\lambda) \rightarrow \pm\infty} \pm\pi, \quad \text{if } |\Im(\lambda)| < \frac{1}{2}, \quad (2.12)$$

$$\theta(\lambda) \xrightarrow{\Re(\lambda) \rightarrow \pm\infty} \mp\pi, \quad \text{if } |\Im(\lambda)| < 1, \quad (2.13)$$

so that, under the assumption that all roots are *close roots* (i.e. such that  $|\Im(\lambda_k)| < 1$ ,  $k = 1, \dots, R$ ),

$$\widehat{\xi}(\lambda) \xrightarrow{\lambda \rightarrow \pm\infty} \pm \frac{N-R}{N} \pi, \quad \text{for } \lambda \in \mathbb{R}. \quad (2.14)$$

Note that the limit is taken concerning  $\lambda$ , not  $N$ . Hence, if we suppose that the counting function is an increasing function and if all roots are close roots, the allowed set of quantum numbers  $n_j$  in (2.3) would be

$$n_j \in \{1, \dots, N-R-1\}, \quad (2.15)$$

which means in particular that we could have at most  $N-R-1$  real Bethe roots in a sector with  $R$  Bethe roots.

The question is whether the counting function is indeed an increasing function. This should be true on any compact interval of the real axis and for  $N$  large enough due to (2.11). However, it cannot be assured that it is true on the whole real axis, which is non-compact. To clarify this point, let us evaluate the derivative of the counting function at large values of  $\pm\lambda$ :

$$\begin{aligned} \widehat{\xi}'(\lambda) &= \frac{1}{1+1/4} + \frac{1}{N} \sum_{k=1}^R \frac{1}{(\lambda - \lambda_k)^2 + 1} \\ &= \frac{N-2R}{N\lambda^2} - \frac{4}{N\lambda^3} \sum_{k=1}^R \lambda_k + O(1/\lambda^4). \end{aligned} \quad (2.16)$$

Hence, if  $N-2R > 0$ , the counting function is indeed strictly increasing at large  $\lambda$ . This does not prove that it is increasing on the whole real axis but at least it does not contradict this hypothesis.

On the contrary, if  $N-2R < 0$ , the counting function is strictly decreasing at large  $\lambda$ . This means that the restriction (2.15) is certainly not valid in that case, since both limiting values in (2.14) can be reached for finite values of  $\lambda$  and therefore should be included in the set of allowed integers. Hence, we have (at least)  $N-R+1$  possible vacancies on the real axis in that case.

In the particular case  $N=2R$  for  $N$  even, the sign of  $\widehat{\xi}'(\lambda)$  is given by the sign of the sum of the Bethe roots:

$$\widehat{\xi}'(\lambda) \begin{cases} < 0 & \text{if } \sum \lambda_k > 0 \\ > 0 & \text{if } \sum \lambda_k < 0 \end{cases} \quad \text{when } \lambda \rightarrow +\infty, \quad (2.17)$$

$$\widehat{\xi}'(\lambda) \begin{cases} > 0 & \text{if } \sum \lambda_k > 0 \\ < 0 & \text{if } \sum \lambda_k < 0 \end{cases} \quad \text{when } \lambda \rightarrow -\infty. \quad (2.18)$$

Hence, in that case (provided that  $\sum \lambda_k \neq 0$ ), one of the limiting values in (2.14) can be reached for finite  $\lambda$ . It means that we have (at least)  $N/2$  possible vacancies on the real axis.

It is therefore natural to expect that, for  $N$  even, the ground state of the model is given by a state with exactly  $R = N/2$  real roots, as in the periodic and the diagonal twist cases<sup>2</sup>. Note that, from Remark 1.6, the ground state is doubly degenerated. We have indeed two such states related to  $Q$  and  $\widehat{Q}$  with the same numbers of roots  $\lambda_1, \dots, \lambda_{N/2}$  and  $\widehat{\lambda}_1, \dots, \widehat{\lambda}_{N/2}$ , and the sum rule (1.97) imposes moreover that

$$\sum_{k=1}^{N/2} \lambda_k = - \sum_{k=1}^{N/2} \widehat{\lambda}_k \quad (2.19)$$

in the homogeneous limit. Hence we expect these two states to have adjacent sets of quantum numbers shifted by one to each other.

For  $N$  odd, instead, we expect that the two degenerate ground states are in the two different sectors  $R = \frac{N-1}{2}$  and  $R = \frac{N+1}{2}$ . In the sector  $R = \frac{N-1}{2}$ , there are indeed from our previous study (at least)  $\frac{N-1}{2}$  possible vacancies on the real axis. Hence, there exists a solution in that sector with only real roots  $\lambda_1, \dots, \lambda_{\frac{N-1}{2}}$  which should be the ground state. In the sector  $R = \frac{N+1}{2}$ , we have a state with the same energy, which corresponds to a polynomial  $\widehat{Q}$  with  $N - R = \frac{N-1}{2}$  real roots  $\widehat{\lambda}_1, \dots, \widehat{\lambda}_{\frac{N-1}{2}}$  which solve exactly the same set of equations as  $\lambda_1, \dots, \lambda_{\frac{N-1}{2}}$ .

**Remark 2.2.** *It is natural to expect that the ground states in the sector  $\frac{N}{2}$  (for  $N$  even) or  $\frac{N-1}{2}$  (for  $N$  odd) have no holes in their distribution of the Bethe roots. However, this hypothesis is not essential for our purpose (computation of the correlation functions in the thermodynamic limit): we essentially build our study on the replacement of sums by integrals as in (2.8), and the holes contribute only to sub-leading orders to (2.8). It is neither essential for our purpose to know the precise sector  $R$  of the ground state since the replacement (2.8) remains valid for all states given by  $R$  real roots with  $R$  of order  $N/2$  in the thermodynamic limit. Hence we do not have to distinguish further between even and odd  $N$ .*

As in the periodic case [80], it is also convenient to consider the inhomogeneous deformation of the ground state when we introduce inhomogeneity parameters  $\xi_1, \dots, \xi_N$  in the model. For the previous analysis to remain valid, we may for instance restrict ourselves to the consideration of inhomogeneity parameters  $\xi_1, \dots, \xi_N$  such that  $\Im(\xi_n) = \eta/2 = -i/2$ ,  $1 \leq n \leq N$ . In that case, we can define

$$p_{\text{tot}}(\lambda) = \frac{1}{N} \sum_{n=1}^N p(\lambda - \xi_n + \eta/2), \quad (2.20)$$

and it leads to the inhomogeneous density

$$\rho_{\text{tot}}(\lambda) = \frac{1}{N} \sum_{n=1}^N \rho(\lambda - \xi_n + \eta/2), \quad (2.21)$$

and the solution to the integral equation

$$2\pi \rho_{\text{tot}}(\lambda) - \int_{-\infty}^{\infty} \theta'(\lambda - \mu) \rho_{\text{tot}}(\mu) d\mu = p'_{\text{tot}}(\lambda). \quad (2.22)$$

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<sup>2</sup>This hypothesis is supported by the fact that the Bethe equations (2.1) coincide with the Bethe equations of the  $\sigma^z$ -twisted case [114], a case that can be obtained by a continuous variation of the twist from the periodic case.

## 2.2 The XXZ case

Let us now discuss the description of the ground state of the anti-periodic XXZ chain in terms of the solution of the Bethe equations:

$$\mathbf{a}_Q(\lambda_j) = 1. \quad (2.23)$$

We recall the sum rule satisfied by the Bethe roots [115]:

$$\sum_{j=1}^N \lambda_j = \sum_{n=1}^N \left( \xi_n - \frac{\eta}{2} \right) + ik\pi, \quad k \in \mathbb{Z}. \quad (2.24)$$

In the homogeneous limit  $\xi_n = \eta/2$ ,  $1 \leq n \leq N$ , the energy of the Hamiltonian associated with an eigenstate of parameters  $\{\lambda\}$  is

$$E(\{\lambda\}) = -2 \sum_{k=1}^N \frac{\sinh \eta \sinh \frac{\eta}{2}}{\cosh \frac{\eta}{2} - \cosh \lambda_k} + \text{constant}. \quad (2.25)$$

### 2.2.1 In the antiferromagnetic regime

To study the low-energy states in the antiferromagnetic regime  $\Delta > 1$ , it is more convenient to make the following change of variables:

$$u_j = i\lambda_j, \quad \zeta_j = i\xi_j, \quad \zeta = -\eta > 0, \quad (2.26)$$

and the homogeneous limit corresponds to the limit  $\zeta_n = -i\zeta/2$ ,  $1 \leq n \leq N$ . With this change of variables, the Bethe equations can be rewritten as

$$\prod_{n=1}^N \frac{\sin(u_j - \zeta_n - i\zeta)}{\sin(u_j - \zeta_n)} \prod_{k=1}^N \frac{\sin(\frac{u_j - u_k + i\zeta}{2})}{\sin(\frac{u_j - u_k - i\zeta}{2})} = 1, \quad j = 1, \dots, N, \quad (2.27)$$

i.e.

$$\prod_{n=1}^N \frac{\sin(i\zeta + \zeta_n - u_j)}{\sin(-\zeta_n + u_j)} \prod_{k=1}^N \frac{\sin(\frac{i\zeta}{2} + \frac{u_j - u_k}{2})}{\sin(\frac{i\zeta}{2} - \frac{u_j - u_k}{2})} = 1, \quad j = 1, \dots, N. \quad (2.28)$$

These Bethe equations are invariant under a shift of  $2\pi$  of any of the Bethe roots, so we can restrict ourselves to the consideration of the Bethe roots  $u_k$  such that  $-\pi < \Re(u_k) \leq \pi$ .

We consider only solutions with a finite number of complex roots in the homogeneous limit  $\zeta_n = -i\zeta/2$ ,  $1 \leq n \leq N$ , and in the  $N \rightarrow \infty$  limit. Using the same argument as in [138], we can show that, if a set of such solutions  $\{u\} \equiv \{u_1, \dots, u_N\}$  of (2.27) contains a complex root  $u_\ell$ , it also contains the conjugate root  $\bar{u}_\ell$ . Hence complex roots appear by pairs  $u_\ell, \bar{u}_\ell$ .

**Bethe equations for real roots and counting function**

Let us define, for  $u, x, y \in \mathbb{R}$ ,

$$p(u) = \frac{i}{N} \log \prod_{n=1}^N \frac{\sin(-\zeta_n + u)}{\sin(i\zeta + \zeta_n - u)} \xrightarrow{\zeta_n \rightarrow -i\frac{\zeta}{2}} i \log \frac{\sin(i\frac{\zeta}{2} + u)}{\sin(i\frac{\zeta}{2} - u)} = \varphi(u, \zeta/2), \quad (2.29)$$

$$\theta(u) = i \log \frac{\sin(i\frac{\zeta}{2} - \frac{u}{2})}{\sin(i\frac{\zeta}{2} + \frac{u}{2})} = -\varphi(u/2, \zeta/2), \quad (2.30)$$

$$\begin{aligned} \Theta(u, x + iy) &= \frac{i}{2} \log \frac{\sin(i\frac{\zeta}{2} - \frac{u-x-iy}{2}) \sin(i\frac{\zeta}{2} - \frac{u-x+iy}{2})}{\sin(i\frac{\zeta}{2} + \frac{u-x-iy}{2}) \sin(i\frac{\zeta}{2} + \frac{u-x+iy}{2})} \\ &= \frac{i}{2} \log \frac{\sin(i\frac{\zeta+y}{2} - \frac{u-x}{2}) \sin(i\frac{\zeta-y}{2} - \frac{u-x}{2})}{\sin(i\frac{\zeta+y}{2} + \frac{u-x}{2}) \sin(i\frac{\zeta-y}{2} + \frac{u-x}{2})} \\ &= -\frac{1}{2} \left[ \varphi\left(\frac{u-x}{2}, \frac{\zeta+y}{2}\right) + \varphi\left(\frac{u-x}{2}, \frac{\zeta-y}{2}\right) \right], \end{aligned} \quad (2.31)$$

in which we have set, for  $u, \gamma \in \mathbb{R}$ ,

$$\varphi(u, \gamma) = \int_0^u \frac{\sinh(2\gamma)}{\sin(\alpha + i\gamma) \sin(\alpha - i\gamma)} d\alpha = \int_0^u \frac{2 \sinh(2\gamma)}{\cosh(2\gamma) - \cos(2\alpha)} d\alpha. \quad (2.32)$$

Note that  $\varphi$  satisfies the properties,

$$\varphi'(u, \gamma) > 0 \quad \text{if } \gamma > 0, \quad (2.33)$$

$$\varphi(-u, \gamma) = -\varphi(u, \gamma) \quad (2.34)$$

$$\varphi(u + \pi, \gamma) = \varphi(u, \gamma) + \varphi(\pi, \gamma) = \varphi(u, \gamma) + 2\pi \operatorname{sgn}(\gamma), \quad (2.35)$$

$$\varphi(u, \gamma) \underset{\gamma \rightarrow \pm\infty}{\sim} \pm 2u, \quad (2.36)$$

and that, for  $\gamma > 0$  and  $x, y \in \mathbb{R}$ ,  $\varphi'(\alpha, \gamma)$  can be represented as the following Fourier series:

$$\varphi'(x + iy, \gamma) = \sum_{k=-\infty}^{+\infty} \varphi'_k(y, \gamma) e^{2ikx} = \sum_{k=-\infty}^{+\infty} \tilde{\varphi}'_k(y, \gamma) e^{2ik(x+iy)}, \quad (2.37)$$

with

$$\begin{aligned} \varphi'_k(y, \gamma) &= \frac{1}{\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{\sinh(2\gamma)}{\sin(x + i(\gamma + y)) \sin(x - i(\gamma - y))} e^{-2ikx} dx \\ &= \begin{cases} 2 e^{-2ky} e^{-2|k|\gamma} & \text{if } |y| < \gamma \\ -4 H(k) e^{-2ky} \sinh(2k\gamma) & \text{if } y > \gamma > 0 \\ 4 H(-k) e^{-2ky} \sinh(2k\gamma) & \text{if } y < -\gamma < 0 \end{cases} \\ &= \sum_{\sigma=\pm} 2 \operatorname{sgn}(\gamma + \sigma y) H(k(y + \sigma\gamma)) e^{-2k(y+\sigma\gamma)}, \end{aligned} \quad (2.38)$$

i.e.

$$\begin{aligned}\tilde{\varphi}'_k(y, \gamma) &= \begin{cases} 2e^{-2|k|\gamma} & \text{if } |y| < \gamma, \\ -4H(k) \sinh(2k\gamma) & \text{if } y > \gamma > 0, \\ 4H(-k) \sinh(2k\gamma) & \text{if } y < -\gamma < 0, \end{cases} \\ &= \begin{cases} 2e^{-2|k|\gamma} & \text{if } |y| < \gamma, \\ -4H(ky) \sinh(2|k|\gamma) & \text{if } |y| > \gamma, \end{cases}\end{aligned}\quad (2.39)$$

where  $H$  denotes the Heaviside function and  $\text{sgn}$  the sign function.

Note also that,

$$\Theta(u, x) = \theta(u - x), \quad x \in \mathbb{R} \quad (2.40)$$

$$\Theta'(u, x + iy) = \frac{1}{2} [\theta'(u - z) + \theta'(u - \bar{z})], \quad z = x + iy, \quad (2.41)$$

where

$$\theta'(u) = -\frac{\sinh \zeta}{\cosh \zeta - \cos u}. \quad (2.42)$$

The Bethe equation (2.27) for a real root  $u_j$  can be conveniently rewritten in logarithmic form as

$$\widehat{\xi}(u_j | \{u\}) = \frac{2\pi n_j}{N}, \quad (2.43)$$

where  $n_j$  is an integer and  $\widehat{\xi}(\alpha | \{u\})$  is the counting function. The latter is defined, for the given set of Bethe roots  $\{u\}$ , as

$$\widehat{\xi}(\alpha | \{u\}) = p(\alpha) + \frac{1}{N} \sum_{k=1}^N \Theta(\alpha, u_k), \quad (2.44)$$

where we have used the fact that the complex roots  $u_k$  always appear in pairs  $u_k, \bar{u}_k$ .

From (2.35), we have

$$p(u + 2\pi) = p(u) + 4\pi, \quad (2.45)$$

$$\Theta(u + 2\pi, u_k) = \begin{cases} \Theta(u, u_k) - 2\pi & \text{if } |\Im(u_k)| < \zeta, \\ \Theta(u, u_k) & \text{if } \zeta < |\Im(u_k)| \end{cases} \quad (2.46)$$

so that

$$\widehat{\xi}(\alpha + 2\pi | \{u\}) = \widehat{\xi}(\alpha | \{u\}) + 2\pi \left(1 + \frac{n_w}{N}\right). \quad (2.47)$$

Here and in the following, we define

$$\mathcal{Z}_w = \{u_k \in \{u\}, |\Im(u_k)| > \zeta\}, \quad n_w = \#\mathcal{Z}_w, \quad (2.48)$$

i.e.  $\mathcal{Z}_w$  is the set of indices corresponding to the wide roots (in the terminology of [138]), and  $n_w$  is the number of wide roots (which should be even since the latter appear in pairs).

### The Ising limit

Let us consider the Ising limit  $\zeta \rightarrow +\infty$ . For large but finite  $\zeta$ , we obtain for  $\alpha \in \mathbb{R}$  at the leading order in  $\zeta$ ,

$$p(\alpha) \xrightarrow[\zeta \rightarrow +\infty]{} 2\alpha, \quad (2.49)$$

$$\theta(\alpha) \xrightarrow[\zeta \rightarrow +\infty]{} -\alpha, \quad (2.50)$$

$$\Theta(\alpha, u_k) \xrightarrow[\zeta \rightarrow +\infty]{} \begin{cases} -(\alpha - \Re(u_k)) & \text{if } |\Im(u_k)| = o(\zeta), \\ 0 & \text{if } \zeta = o(|\Im(u_k)|), \end{cases} \quad (2.51)$$

so that, in the homogeneous limit ( $\zeta_n = -i\zeta/2$ ),

$$\widehat{\xi}(\alpha|\{u\}) \xrightarrow[\zeta \rightarrow +\infty]{} 2\alpha - \frac{1}{N} \sum_{\substack{k=1 \\ k \notin \mathcal{Z}_w}} (\alpha - \Re(u_k)) = \frac{N + n_w}{N} \alpha + \frac{1}{N} \sum_{\substack{k=1 \\ k \notin \mathcal{Z}_w}} \Re(u_k). \quad (2.52)$$

Hence the logarithmic Bethe equations (2.43) for the real roots linearise in this limit:

$$\frac{N + n_w}{N} u_j + \frac{1}{N} \sum_{\substack{k=1 \\ k \notin \mathcal{Z}_w}} \Re(u_k) = \frac{2\pi n_j}{N}, \quad (2.53)$$

i.e.

$$u_j = \frac{1}{N + n_w} \left( 2\pi n_j - \sum_{\substack{k=1 \\ k \notin \mathcal{Z}_w}} \Re(u_k) \right). \quad (2.54)$$

Hence, for the Bethe roots to be contained in an interval of length  $2\pi$ , the integers  $n_j$  should be contained in an interval of length  $N + n_w$ , i.e. there exists  $n_0 \in \mathbb{Z}$  such that

$$n_j \in \{n_0 + 1, n_0 + 2, \dots, n_0 + N + n_w\}. \quad (2.55)$$

This gives us the allowed set of integers for the real roots of a given Bethe state. By continuity in  $\zeta$  of the functions of the model (and notably of the counting function), we expect this to be valid also at finite  $\zeta$ .

In particular, if we suppose that the set  $\{u\}$  is only composed of distinct real roots, we would have

$$u_j + \frac{1}{N} \sum_{k=1}^N u_k = \frac{2\pi n_j}{N}, \quad (2.56)$$

which implies that the  $n_j$  should be adjacent numbers:  $n_j = n_0 + j$ ,  $1 \leq j \leq N$ . This implies notably the following sum rule:

$$\sum_{j=1}^N u_j = \frac{\pi}{N} \sum_{j=1}^N n_j = \pi n_0 + \frac{\pi}{N} \sum_{j=1}^N j = \pi \left( n_0 + \frac{N+1}{2} \right). \quad (2.57)$$

This is consistent with the sum rule (2.24) only if  $n_0 + \frac{N+1}{2}$  is an integer, i.e. only if  $N$  is odd.

### The large $N$ limit

Let  $\{u\} \equiv \{u_1, \dots, u_N\}$  be a solution to the Bethe equations given by an infinite number of real roots (i.e. of order  $N$ ), with a finite number of complex roots and a finite number of holes in the thermodynamic limit. Let us now suppose that, in the large  $N$  limit, the real roots  $u_j$  of the Bethe equations tend to have a continuous distribution given by some density function  $\rho$  in the interval  $(-\pi, \pi]$ :

$$\frac{1}{N(u_{j+1} - u_j)} \underset{N \rightarrow \infty}{\sim} \rho(u_j). \quad (2.58)$$

In other words, we make the usual assumption that, for any  $2\pi$ -periodic and sufficiently regular function  $f$ , the sum over real Bethe roots tends to integrals with some measure given by the density function  $\rho$ , i.e. that

$$\frac{1}{N} \sum_{\substack{j=1 \\ j \in \mathcal{R}}}^N f(u_j) \underset{N \rightarrow \infty}{\longrightarrow} \int_{-\pi}^{\pi} f(\alpha) \rho(\alpha) d\alpha. \quad (2.59)$$

Then, by the usual argument which consists of taking the difference between (2.43) for  $u_{j+1}$  and  $u_j$ , we obtain that  $\rho$  is the solution to the following integral equation:

$$p'(u) + \int_{-\pi}^{\pi} \theta'(u-v) \rho(v) dv = 2\pi \rho(u), \quad (2.60)$$

or, in terms of the function  $\varphi$ :

$$\varphi'\left(u, \frac{\zeta}{2}\right) - \frac{1}{2} \int_{-\pi}^{\pi} \varphi'\left(\frac{u-v}{2}, \frac{\zeta}{2}\right) \rho(v) dv = 2\pi \rho(u). \quad (2.61)$$

This equation can easily be solved by Fourier series by using (2.37) and (2.38), and we obtain that

$$\rho(u) = \frac{1}{2\pi} \sum_{n=-\infty}^{+\infty} \frac{e^{2inu}}{\cosh(n\zeta)} = \frac{1}{2\pi} \frac{\vartheta'_1 \vartheta_3(u, q)}{\vartheta_2 \vartheta_4(u, q)}, \quad q = e^{-\zeta}, \quad (2.62)$$

where  $\vartheta_i(u, q)$ ,  $i \in \{1, 2, 3, 4\}$  are the Theta functions of nome  $q$  defined as in [139], with  $\vartheta'_1 \equiv \vartheta'_1(0, q)$ ,  $\vartheta_2 \equiv \vartheta_2(0, q)$ . Note that the function (2.62) coincides (as expected) with the density of the periodic case.

The leading finite-size corrections will of course be different. It is possible to control them precisely by computing the corrections to the sum-integral transformation.

### Corrections to the leading order

Let  $\{u\} \equiv \{u_1, \dots, u_N\}$  be a solution to the Bethe equations, and let  $\widehat{\xi}(\alpha) \equiv \widehat{\xi}(\alpha|\{u\})$  be the corresponding counting function. We suppose that this solution corresponds to an infinite number of real roots (i.e. of order  $N$ ), with a finite number of complex roots and a finite number of holes in the thermodynamic limit. The logarithmic equation for the real roots can be written as in (2.43), in terms of the positions  $h_1, \dots, h_n$  of the holes in the adjacent set of quantum numbers for the real roots. Moreover,

$$\widehat{\xi}'(\alpha) = p'(\alpha) + \frac{1}{N} \sum_{k=1}^N \theta'(\alpha - u_k) \underset{N \rightarrow \infty}{\longrightarrow} 2\pi \rho(\alpha) > 0, \quad (2.63)$$



so that  $\widehat{\xi}$  is an increasing, and hence invertible function for  $N$  large enough (see the argument in the footnote of [147]). We can therefore introduce the inverse images  $\check{u}_j$  of  $\frac{\pi(n_0+j)}{N}$  for  $j \in \{1, \dots, M\}$  with  $M = N + n_w$ :

$$\widehat{\xi}(\check{u}_j|\{u\}) = \frac{2\pi(n_0+j)}{N}, \quad j \in \{1, \dots, M\}, \quad (2.64)$$

which defines in particular the hole rapidities  $\check{u}_{h_k}$  for  $k \in \{1, \dots, n\}$  (recall that  $\check{u}_j$  coincides with the real root  $u_j$  if  $j \neq h_1, \dots, h_n$ ).

Let  $f$  be a  $\mathcal{C}^\infty$   $2\pi$ -periodic function. Then, for any  $n_0$  and in the large  $M$  limit,

$$\frac{1}{M} \sum_{k=1}^M f\left(\frac{2\pi(n_0+k)}{M}\right) = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) dx + O(M^{-\infty}). \quad (2.65)$$

We make a change of variables in (2.65) using the function  $\widetilde{\xi}$  defined from the counting function  $\widehat{\xi}$  as

$$\widetilde{\xi}(\alpha) = \frac{N}{M} \widehat{\xi}(\alpha), \quad (2.66)$$

which is still invertible and satisfies the properties:

$$\widetilde{\xi}(\alpha + 2\pi) = \widetilde{\xi}(\alpha) + 2\pi, \quad \text{and} \quad \widetilde{\xi}(\check{u}_j) = \frac{2\pi(n_0+j)}{M}, \quad j \in \{1, \dots, M\}. \quad (2.67)$$

Hence, the function  $f \circ \widetilde{\xi}^{-1}$  is also  $2\pi$ -periodic, so that we have

$$\begin{aligned} \frac{1}{M} \sum_{k=1}^M f(\check{u}_k) &= \frac{1}{M} \sum_{k=1}^M f \circ \widetilde{\xi}^{-1}\left(\frac{2\pi(n_0+k)}{M}\right) \\ &= \frac{1}{2\pi} \int_{-\pi}^{\pi} f \circ \widetilde{\xi}^{-1}(x) dx + O(M^{-\infty}) \\ &= \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\mu) \widetilde{\xi}'(\mu) d\mu + O(M^{-\infty}). \end{aligned} \quad (2.68)$$

Multiplying by  $M/N$  and setting apart the contributions of the holes from the ones of the real roots we obtain that

$$\frac{1}{N} \sum_{\substack{j=1 \\ j \neq h_1, \dots, h_n}}^M f(u_j) = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) \widehat{\xi}'(x) dx - \frac{1}{N} \sum_{j=1}^n f(\check{u}_{h_j}) + O(N^{-\infty}). \quad (2.69)$$

We can notably apply this relation to the sum over real roots in (2.63), which gives

$$\begin{aligned} \widehat{\xi}'(\alpha) &= p'(\alpha) + \frac{1}{2\pi} \int_{-\pi}^{\pi} \theta'(\alpha - x) \widehat{\xi}'(x) dx \\ &\quad - \frac{1}{N} \sum_{k=1}^n \theta'(\alpha - \check{u}_{h_k}) + \frac{1}{N} \sum_{k \in \mathcal{Z}} \theta'(\alpha - u_k) + O(N^{-\infty}) \\ &= 2\pi\rho(\alpha) - \frac{1}{N} \sum_{k=1}^n \widehat{\xi}'_{\check{u}_{h_k}}(\alpha) + \frac{1}{N} \sum_{k \in \mathcal{Z}} \widehat{\xi}'_{u_k}(\alpha) + O(N^{-\infty}), \end{aligned} \quad (2.70)$$

in which the function  $\widehat{\xi}'_v$  is defined to be the solution of the integral equation

$$\widehat{\xi}'_v(\alpha) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \theta'(\alpha - x) \widehat{\xi}'_v(x) dx + \theta'(\alpha - v), \quad (2.71)$$

or, in terms of the function  $\varphi'$ :

$$\widehat{\xi}'_v(\alpha) + \frac{1}{4\pi} \int_{-\pi}^{\pi} \varphi' \left( \frac{\alpha - x}{2}, \frac{\zeta}{2} \right) \widehat{\xi}'_v(x) dx = -\frac{1}{2} \varphi' \left( \frac{\alpha - v}{2}, \frac{\zeta}{2} \right), \quad (2.72)$$

which can also be rewritten as

$$\widehat{\xi}'_v(2u) + \frac{1}{2\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \varphi' \left( u - y, \frac{\zeta}{2} \right) \widehat{\xi}'_v(2y) dy = -\frac{1}{2} \varphi' \left( 2u - \frac{v}{2}, \frac{\zeta}{2} \right). \quad (2.73)$$

The solution to this equation can easily be computed in Fourier modes by means of (2.37)-(2.38). We obtain that

$$\widehat{\xi}'_v(\alpha) = \begin{cases} -\frac{1}{2} \sum_{k=-\infty}^{+\infty} \frac{e^{-|k|\frac{\zeta}{2}}}{\cosh(k\frac{\zeta}{2})} e^{ik(\alpha-v)} & \text{if } |\Im(v)| < \zeta, \\ 2 \sum_{\substack{k=-\infty \\ \Im(v)k < 0}}^{\infty} e^{|k|\frac{\zeta}{2}} \sinh(|k|\zeta/2) e^{ik(\alpha-v)} & \text{if } |\Im(v)| > \zeta. \end{cases} \quad (2.74)$$

**Remark 2.3.** We can generalise formula (2.69) to functions which are not  $2\pi$ -periodic but whose derivative is  $2\pi$ -periodic. Indeed, let  $g$  be a  $C^\infty$ -function such that  $g'(x)$  is  $2\pi$ -periodic. Then  $g(x) - c_g x$  is also  $2\pi$ -periodic, where

$$c_g = \frac{1}{2\pi} \int_{-\pi}^{\pi} g'(x) dx = \frac{g(\pi) - g(-\pi)}{2\pi} = \frac{g(y + 2\pi) - g(y)}{2\pi}, \quad \forall y, \quad (2.75)$$

so that

$$\frac{1}{N} \sum_{\substack{j=1 \\ j \neq h_1, \dots, h_n}}^M [g(u_j) - c_g u_j] = \frac{1}{2\pi} \int_{-\pi}^{\pi} [g(x) - c_g x] \widehat{\xi}'(x) dx - \frac{1}{N} \sum_{j=1}^n [g(\check{u}_{h_j}) - c_g \check{u}_{h_j}] + O(N^{-\infty}), \quad (2.76)$$

i.e.

$$\begin{aligned} \frac{1}{N} \sum_{\substack{j=1 \\ j \neq h_1, \dots, h_n}}^M g(u_j) &= \frac{1}{2\pi} \int_{-\pi}^{\pi} g(x) \widehat{\xi}'(x) dx - \frac{1}{N} \sum_{j=1}^n g(\check{u}_{h_j}) + \frac{c_g}{N} \sum_{j=1}^M \check{u}_j \\ &\quad - \frac{c_g}{2\pi} \int_{-\pi}^{\pi} x \left[ 2\pi \rho(x) - \frac{1}{N} \sum_{k=1}^n \widehat{\xi}'_{\check{u}_{h_k}}(x) + \frac{1}{N} \sum_{k \in \mathcal{Z}} \widehat{\xi}'_{u_k}(x) \right] dx + O(N^{-\infty}) \\ &= \frac{1}{2\pi} \int_{-\pi}^{\pi} g(x) \widehat{\xi}'(x) dx - \frac{1}{N} \sum_{j=1}^n g(\check{u}_{h_j}) + c_g \frac{C(\{u\})}{N} + O(N^{-\infty}), \end{aligned} \quad (2.77)$$

where

$$C(\{u\}) = \sum_{j=1}^M \check{u}_j + \frac{1}{2\pi} \int_{-\pi}^{\pi} x \left[ \sum_{k=1}^n \widehat{\xi}'_{\check{u}_{h_k}}(x) - \sum_{k \in \mathcal{Z}} \widehat{\xi}'_{u_k}(x) \right] dx. \quad (2.78)$$

### Bethe equations for complex roots

We now investigate the large  $N$  behaviour of the complex solutions of the Bethe equations. Hence, let us now suppose that  $u_j \in \{u\}$  is a complex root. One can use (2.77) to rewrite the sum over real Bethe roots as integrals in the corresponding Bethe equation for large  $N$ , which gives

$$\exp \left\{ N F(u_j) + \frac{i}{2\pi} \int_{-\pi}^{\pi} \theta(u_j - x) \left[ \sum_{\ell \in \mathcal{Z}} \widehat{\xi}_{u_\ell}(x) - \sum_{\ell=1}^n \widehat{\xi}_{\check{u}_{h_\ell}}(x) \right] dx + ic_\theta C(\{u\}) - i \sum_{\ell=1}^n \theta(u_j - \check{u}_{h_\ell}) + O(L^{-\infty}) \right\} \prod_{\substack{k \in \mathcal{Z} \\ k \neq j}} \frac{\sin(i\frac{\zeta}{2} + \frac{u_j - u_k}{2})}{\sin(i\frac{\zeta}{2} - \frac{u_j - u_k}{2})} = 1. \quad (2.79)$$

In (2.79) we have set

$$F(u) = ip(u) + i \int_{-\pi}^{\pi} \theta(u - x) \rho(x) dx, \quad (2.80)$$

and the functions  $p$  and  $\theta$  are defined such that

$$e^{ip(\alpha)} = \frac{\sin(i\zeta/2 - \alpha)}{\sin(i\zeta/2 + \alpha)}, \quad e^{i\theta(\alpha)} = \frac{\sin(i\frac{\zeta}{2} + \frac{\alpha}{2})}{\sin(i\frac{\zeta}{2} - \frac{\alpha}{2})}, \quad (2.81)$$

and such that they coincide with the definitions (2.29) and (2.30) for  $\alpha$  real.

It is interesting to investigate the behaviour of (2.80) so as to see how the first line of (2.79) behaves with  $L$ . Using the terminology of [138], we find that

$$F(u_j) = 2\pi i \int_0^{u_j} \rho(x) dx \quad (2.82)$$

if  $u_j$  is a close root, i.e. if  $|\Im(u_j)| < \zeta$ . The real part of (2.82) is moreover positive if  $-\zeta < \Im(u_j) < 0$ , which means that, in that case, the first factor in (2.79) is exponentially diverging in  $N$ . Hence, for (2.79) to be satisfied,  $u_j$  has to approach a zero of the expression with exponentially small corrections in  $N$ , so that there exists  $u_k \in \{u\}$  such that  $u_j - u_k = -i\zeta + O(N^{-\infty})$ . If we suppose moreover there exists only two complex roots  $u_j$  and  $\bar{u}_j$  in the set  $\{u\}$  (so as to minimise the number of holes with positive energy, cf. below), i.e. that all other roots are real, this means that  $\{u_j, \bar{u}_j\}$  approaches, with exponentially small corrections in  $N$ , a two-string of the form  $\{u_s - i\zeta/2, u_s + i\zeta/2\}$  with centre  $u_s \in \mathbb{R}$ .

If instead  $u_j$  is a wide root, i.e. if  $|\Im(u_j)| > \zeta$ , then, using similar arguments as in [138], we find that

$$\Re(F(u_j)) = 0, \quad (2.83)$$

so that the first factor in (2.79) remains finite.

### Energy of a configuration of the Bethe roots

We now apply this result so as to compute the sub-leading contributions to the energy of the corresponding Bethe state:

$$E(\{u\}) = \sum_{k=1}^N \varepsilon_0(u_k) + \text{constant}, \quad \text{with} \quad \varepsilon_0(u) = -2 \frac{\sinh \zeta \sinh \frac{\zeta}{2}}{\cosh \frac{\zeta}{2} - \cos u}. \quad (2.84)$$

Note that

$$\begin{aligned} \varepsilon_0(u) &= -\sinh \zeta \varphi' \left( \frac{u}{2}, \frac{\zeta}{4} \right) \\ &= -\sinh \zeta \begin{cases} 2 \sum_{k=-\infty}^{+\infty} e^{-|k|\frac{\zeta}{2}} e^{iku} & \text{if } |\Im(u)| < \frac{\zeta}{2}, \\ -4 \sum_{\substack{k=-\infty \\ \Im(u)k > 0}}^{\infty} \sinh(|k|\zeta/2) e^{iku} & \text{if } |\Im(u)| > \frac{\zeta}{2}. \end{cases} \end{aligned} \quad (2.85)$$

For large  $N$ , it is given as

$$E(\{u\}) = E_0 + \sum_{k \in \mathcal{Z}} \varepsilon(u_k) - \sum_{j=1}^n \varepsilon(\check{u}_{h_j}) + O(N^{-\infty}), \quad (2.86)$$

where

$$E_0 = \text{constant} + N \int_{-\pi}^{\pi} \varepsilon_0(u) \rho(u) du \quad (2.87)$$

is the contribution of the real roots which is common to all low-energy states, whereas  $\varepsilon(v)$  is the dressed energy of an excitation with rapidity  $v$ , defined as

$$\varepsilon(v) = \varepsilon_0(v) + \frac{1}{2\pi} \int_{-\pi}^{\pi} \varepsilon_0(x) \widehat{\xi}'_v(x) dx. \quad (2.88)$$

Using the series representation of (2.85) and (2.74), we find that

$$\begin{aligned} \varepsilon(v) &= -\sinh \zeta \begin{cases} \sum_{k \in \mathbb{Z}} \frac{e^{ikv}}{\cosh(k\frac{\zeta}{2})} & \text{if } |\Im(v)| < \frac{\zeta}{2}, \\ -\sum_{k \in \mathbb{Z}} \frac{e^{ik(v-i \operatorname{sgn}(\Im v)\zeta)}}{\cosh(k\frac{\zeta}{2})} & \text{if } \frac{\zeta}{2} < |\Im(v)| < \zeta, \\ 0 & \text{if } |\Im(v)| > \zeta, \end{cases} \\ &= \begin{cases} -\sinh \zeta \frac{\vartheta'_1(0, q^{1/2})}{\vartheta_2(0, q^{1/2})} \frac{\vartheta_3(\frac{v}{2}, q^{1/2})}{\vartheta_4(\frac{v}{2}, q^{1/2})} & \text{if } |\Im(v)| < \zeta, \\ 0 & \text{if } |\Im(v)| > \zeta, \end{cases} \end{aligned} \quad (2.89)$$

in which we have used the quasi-periodicity property

$$\frac{\vartheta_3(u \pm i\frac{\zeta}{2}, q^{1/2})}{\vartheta_4(u \pm i\frac{\zeta}{2}, q^{1/2})} = -\frac{\vartheta_3(u, q^{1/2})}{\vartheta_4(u, q^{1/2})}, \quad q^{1/2} = e^{-\frac{\zeta}{2}}, \quad (2.90)$$

so that, in the strip delimited by the lines  $\mathbb{R} \pm i\zeta$ , the function  $\varepsilon$  satisfies the properties:

$$\varepsilon(-v) = \varepsilon(v), \quad \varepsilon(v + 2\pi) = \varepsilon(v), \quad \varepsilon(v \pm i\zeta) = -\varepsilon(v), \quad (2.91)$$

and

$$\varepsilon(u) < 0 \quad \text{if } u \in \mathbb{R}, \quad (2.92)$$

$$-\varepsilon(u) \text{ is a decreasing function on } (0, \pi), \quad (2.93)$$

so that the energy of a hole  $\varepsilon_h(\check{u}_h) = -\varepsilon(\check{u}_h)$  is always positive and reaches its minimum at  $\pm\pi$ . From (2.91), the energy of a two-string or a quartet vanishes (up to exponentially small corrections in  $N$ ). Moreover, from (2.89), the energy of wide roots also vanishes. Hence, the only contribution to the energy comes from the holes which have positive energy.

### Configuration of the Bethe roots describing the ground state

The ground state corresponds to the state of minimal energy. From the previous study, it is given by the state with a minimal number of holes, and therefore with a maximal number of real Bethe roots.

**The case  $N$  odd** If  $N$  is odd, it should correspond to the state with  $N$  real roots and  $N$  adjacent quantum numbers (given by the choice  $n_0 = \frac{N+1}{2}$ ):

$$n_j = -\frac{N-1}{2}, -\frac{N-3}{2}, \dots, \frac{N-3}{2}, \frac{N-1}{2}, \quad (2.94)$$

and the Bethe roots  $u_j$ ,  $j = 1, \dots, N$ , should satisfy the equation

$$\widehat{\xi}_{\text{odd}}(u_j) = \frac{2\pi}{N} \left( -\frac{N+1}{2} + j \right), \quad j = 1, \dots, N. \quad (2.95)$$

where  $\widehat{\xi}_{\text{odd}}$  is the corresponding counting function. The latter should be such that

$$\widehat{\xi}'_{\text{odd}}(\alpha) = 2\pi\rho(\alpha) + O(N^{-\infty}), \quad (2.96)$$

so that  $\widehat{\xi}'_{\text{odd}}$  is a  $\pi$ -periodic function up to exponentially small corrections in  $N$ . Integrating this relation and using (2.47), we therefore obtain that

$$\widehat{\xi}_{\text{odd}}(\alpha + \pi) = \widehat{\xi}_{\text{odd}}(\alpha) + \pi + O(N^{-\infty}). \quad (2.97)$$

Hence

$$\begin{aligned} \widehat{\xi}_{\text{odd}}(u_j + \pi) &= \left( -\frac{N+1}{2} + j + \frac{N}{2} \right) \frac{2\pi}{N} + O(N^{-\infty}) \\ &= \widehat{\xi}_{\text{odd}}(u_{j+\frac{N-1}{2}}) + \frac{\pi}{N} + O(N^{-\infty}), \end{aligned} \quad (2.98)$$

so that

$$\begin{aligned} u_j + \pi &= \widehat{\xi}_{\text{odd}}^{-1} \left( \widehat{\xi}_{\text{odd}}(u_{j+\frac{N-1}{2}}) + \frac{\pi}{N} + O(N^{-\infty}) \right) \\ &= u_{j+\frac{N-1}{2}} + \frac{\pi}{N} \left( \widehat{\xi}_{\text{odd}}^{-1} \right)' \left( \widehat{\xi}_{\text{odd}}(u_{j+\frac{N-1}{2}}) \right) + O(N^{-2}) \\ &= u_{j+\frac{N-1}{2}} + \frac{\pi}{N} \frac{1}{\widehat{\xi}'_{\text{odd}} \circ \widehat{\xi}_{\text{odd}}^{-1} \left( \widehat{\xi}_{\text{odd}}(u_{j+\frac{N-1}{2}}) \right)} + O(N^{-2}) \\ &= u_{j+\frac{N-1}{2}} + \frac{1}{2N\rho(u_{j+\frac{N-1}{2}})} + O(N^{-2}). \end{aligned} \quad (2.99)$$

**The case  $N$  even** Instead, if  $N$  is even, it follows from the study of the Ising limit that a state with  $N$  real Bethe roots is incompatible with the sum rule. Hence our candidate (which also corresponds to the state found in [117]) is a state with two holes and a two-string (which corresponds to a state with the minimal number of holes). Moreover, the holes should be at a

position which minimises their energy, i.e. with rapidity close to  $\pm\pi$ . The  $N - 2$  real Bethe roots should therefore correspond to  $N - 2$  of the  $N$  following quantum numbers:

$$n_j = -\frac{N}{2} + 1, -\frac{N}{2} + 2, \dots, \frac{N}{2} - 1, \frac{N}{2}, \quad (2.100)$$

and the rapidities of the real Bethe roots and the holes  $\check{u}_j$ ,  $j = 1, \dots, N$ , should satisfy the equation

$$\widehat{\xi}_{\text{even}}(\check{u}_j) = \frac{2\pi}{N} \left( -\frac{N}{2} + j \right) = -\pi + \frac{2\pi j}{N}, \quad j = 1, \dots, N. \quad (2.101)$$

where  $\widehat{\xi}_{\text{even}}$  is the corresponding counting function. From (2.70), the latter should be of the form

$$\widehat{\xi}'_{\text{even}}(\alpha) = 2\pi\rho(\alpha) + \frac{1}{N}\widehat{\xi}'_1(\alpha) + O(N^{-\infty}), \quad (2.102)$$

where  $\widehat{\xi}'_1(\alpha)$  is the correction due to the presence of the two holes and the two-string:

$$\widehat{\xi}'_1(\alpha) = -\sum_{k=1}^2 \widehat{\xi}'_{\check{u}_{h_k}}(\alpha) + \widehat{\xi}'_{u_s+i\zeta/2}(\alpha) + \widehat{\xi}'_{u_s-i\zeta/2}(\alpha). \quad (2.103)$$

Hence

$$\widehat{\xi}'_{\text{even}}(\alpha + \pi) = \widehat{\xi}'_{\text{even}}(\alpha) + \frac{1}{N} \left[ \widehat{\xi}'_1(\alpha + \pi) - \widehat{\xi}'_1(\alpha) \right] + O(N^{-\infty}), \quad (2.104)$$

so that, by integrating this relation and using (2.47), we obtain that

$$\widehat{\xi}_{\text{even}}(\alpha + \pi) = \widehat{\xi}_{\text{even}}(\alpha) + \pi + \frac{1}{N} \left[ \widehat{\xi}_1(\alpha + \pi) - \widehat{\xi}_1(\alpha) \right] + O(N^{-\infty}), \quad (2.105)$$

where  $\widehat{\xi}_1(\alpha)$  is the  $2\pi$ -periodic primitive of  $\widehat{\xi}'_1(\alpha)$ . Hence

$$\begin{aligned} \widehat{\xi}_{\text{even}}(\check{u}_j + \pi) &= \left( -\frac{N}{2} + j + \frac{N}{2} \right) \frac{2\pi}{N} + \frac{1}{N} \left[ \widehat{\xi}_1(\check{u}_j + \pi) - \widehat{\xi}_1(\check{u}_j) \right] + O(N^{-\infty}) \\ &= \widehat{\xi}_{\text{even}}(\check{u}_{j+\frac{N}{2}}) + \frac{1}{N} \left[ \widehat{\xi}_1(\check{u}_j + \pi) - \widehat{\xi}_1(\check{u}_j) \right] + O(N^{-\infty}), \end{aligned} \quad (2.106)$$

so that

$$\begin{aligned} \check{u}_j + \pi &= \widehat{\xi}_{\text{even}}^{-1} \left( \widehat{\xi}_{\text{even}}(\check{u}_{j+\frac{N}{2}}) + \frac{1}{N} \left[ \widehat{\xi}_1(\check{u}_j + \pi) - \widehat{\xi}_1(\check{u}_j) \right] + O(N^{-\infty}) \right) \\ &= \check{u}_{j+\frac{N}{2}} + \frac{1}{N} \left[ \widehat{\xi}_1(\check{u}_j + \pi) - \widehat{\xi}_1(\check{u}_j) \right] \left( \widehat{\xi}_{\text{even}}^{-1} \right)' \left( \widehat{\xi}_{\text{even}}(\check{u}_{j+\frac{N}{2}}) \right) + O(N^{-2}) \\ &= \check{u}_{j+\frac{N}{2}} + \frac{1}{N} \left[ \widehat{\xi}_1(\check{u}_j + \pi) - \widehat{\xi}_1(\check{u}_j) \right] \frac{1}{\widehat{\xi}'_{\text{even}} \circ \widehat{\xi}_{\text{even}}^{-1} \left( \widehat{\xi}_{\text{even}}(\check{u}_{j+\frac{N}{2}}) \right)} + O(N^{-2}) \\ &= \check{u}_{j+\frac{N}{2}} + \frac{\widehat{\xi}_1(\check{u}_j + \pi) - \widehat{\xi}_1(\check{u}_j)}{2\pi N \rho(\check{u}_{j+\frac{N}{2}})} + O(N^{-2}). \end{aligned} \quad (2.107)$$

### 2.2.2 In the disordered regime

In the disordered regime  $-1 < \Delta < 1$ , we set

$$\eta = -i\zeta, \quad 0 < \zeta < \pi, \quad (2.108)$$

and the homogeneous limit corresponds to the limit  $\xi_n = -i\zeta/2$ ,  $1 \leq n \leq N$ . then, the Bethe equations can be rewritten as

$$\prod_{n=1}^N \frac{\sinh(i\zeta + \xi_n - \lambda_j)}{\sinh(-\xi_n + \lambda_j)} \prod_{k=1}^N \frac{\sinh(\frac{i\zeta}{2} + \frac{\lambda_j - \lambda_k}{2})}{\sinh(\frac{i\zeta}{2} - \frac{\lambda_j - \lambda_k}{2})} = 1, \quad j = 1, \dots, N. \quad (2.109)$$

These Bethe equations are invariant under a shift of  $2i\pi$  of any of the Bethe roots, so we can restrict ourselves to the consideration of Bethe roots  $\lambda_k$  such that  $-\frac{\pi}{2} < \Im(\lambda_k) \leq \frac{3\pi}{2}$ .

We consider only solutions with a finite number of roots  $\lambda_k$  such that  $\Im(\lambda_k) \notin \{0, \pi\}$  in the homogeneous limit  $\xi_n = -i\zeta/2$ ,  $1 \leq n \leq N$ , and in the  $N \rightarrow \infty$  limit. Using again the same argument as in [138], we can show that, *for generic*  $\zeta$  (i.e. not in the root of unity case for which we can also have exact strings), if a set of such solutions  $\{\lambda\} \equiv \{\lambda_1, \dots, \lambda_N\}$  of (2.27) contains a complex root  $\lambda_\ell$ , then it also contains the conjugate root  $\bar{\lambda}_\ell \pmod{2i\pi}$ . Hence, *for generic*  $\zeta$ , complex roots appear by pairs  $\lambda_\ell, \bar{\lambda}_\ell \pmod{2i\pi}$ .

#### Bethe equations for real roots and counting function

Similarly in the homogeneous limit  $\xi_n \rightarrow -i\zeta/2$  we define, for  $u, x, y \in \mathbb{R}$ ,

$$p(u) = i \log \frac{\sinh(i\frac{\zeta}{2} + u)}{\sinh(i\frac{\zeta}{2} - u)} = \phi(u), \quad (2.110)$$

$$\theta(u) = i \log \frac{\sinh(i\frac{\zeta}{2} - \frac{u}{2})}{\sinh(i\frac{\zeta}{2} + \frac{u}{2})} = -\phi(u/2), \quad (2.111)$$

in which we have set

$$\phi(\lambda) = i \log \frac{\sinh(i\frac{\zeta}{2} + \lambda)}{\sinh(i\frac{\zeta}{2} - \lambda)}. \quad (2.112)$$

The function (2.112) is odd, and holomorphic in a band of width  $i\zeta$  around the real axis, i.e. for  $|\Im(\lambda)| < \zeta/2$ . In this band, one uses the principal determination of the logarithm ( $\arg \in ]-\pi, \pi[$ ). Outside of this band, i.e. for  $|\Im(\lambda)| > \zeta/2$ , one should use another determination of the logarithmic ( $\arg \in ]0, 2\pi[$ ). Hence

$$\phi(\lambda) \xrightarrow{\Re\lambda \rightarrow +\infty} i \log(-e^{i\zeta}) = \begin{cases} \pi - \zeta & \text{if } |\Im(\lambda)| < \zeta/2, \\ -\pi - \zeta & \text{if } |\Im(\lambda)| > \zeta/2, \end{cases} \quad (2.113)$$

$$\phi(\lambda) \xrightarrow{\Re\lambda \rightarrow -\infty} i \log(-e^{-i\zeta}) = \zeta - \pi. \quad (2.114)$$

The Bethe equation (2.109) for a root  $u_j \in \mathbb{R}$  or  $u_j \in \mathbb{R} + i\pi$  can be conveniently rewritten in logarithmic form as

$$\widehat{\xi}(u_j | \{u\}) = \frac{2\pi n_j}{N}, \quad (2.115)$$

where  $n_j$  is an integer and  $\widehat{\xi}(\alpha|\{u\})$  is the counting function. The latter is defined, for the given set of Bethe roots  $\{u\} \equiv \{u_1, \dots, u_N\}$ , as

$$\widehat{\xi}(\alpha|\{u\}) = p(\alpha) + \frac{1}{N} \sum_{k=1}^N \theta(\alpha - u_k) \xrightarrow{\xi_n \rightarrow -i\frac{\zeta}{2}} \phi(\alpha) - \frac{1}{N} \sum_{k=1}^N \phi\left(\frac{\alpha - u_k}{2}\right). \quad (2.116)$$

Let us define

$$\mathcal{Z}_w = \{u_k \in \{u\}, |\Im(u_k)| > \zeta\}, \quad n_w = \#\mathcal{Z}_w, \quad (2.117)$$

$$\widetilde{\mathcal{Z}}_w = \{u_k \in \{u\}, |\Im(u_k - i\pi)| > \zeta\}, \quad \widetilde{n}_w = \#\widetilde{\mathcal{Z}}_w, \quad (2.118)$$

i.e  $\mathcal{Z}_w$  is the set of indices corresponding to the wide roots with respect to the real axis, whereas  $\widetilde{\mathcal{Z}}_w$  is the set of indices corresponding to the wide roots with respect to the axis  $\mathbb{R} + i\pi$ . From (2.113)-(2.114), we have

$$\lim_{\alpha \rightarrow +\infty} \widehat{\xi}(\alpha|\{u\}) - \lim_{\alpha \rightarrow -\infty} \widehat{\xi}(\alpha|\{u\}) = \frac{2\pi n_w}{N}, \quad \text{if } \alpha \in \mathbb{R}, \quad (2.119)$$

$$\lim_{\Re\alpha \rightarrow +\infty} \widehat{\xi}(\alpha|\{u\}) - \lim_{\Re\alpha \rightarrow -\infty} \widehat{\xi}(\alpha|\{u\}) = \frac{2\pi \widetilde{n}_w}{N}, \quad \text{if } \alpha \in \mathbb{R} + i\pi, \quad (2.120)$$

which gives us the allowed range of integers in (2.115). Namely, the number of allowed roots in real line  $\mathbb{R}$  (resp.  $\mathbb{R} + i\pi$ ) equals the number of wide roots respectively. And it is compatible with our setting (2.117)-(2.118), note that  $u_j \in \mathbb{R} + i\pi$  is a wide root with respect to the real axis, whereas  $u_k \in \mathbb{R}$  is a wide root with respect to the axis  $\mathbb{R} + i\pi$ .

More precisely, let  $M$  be the number of real Bethe roots, let  $\widetilde{M}$  be the number of roots on the axis  $\mathbb{R} + i\pi$ , let  $n_c$  and  $\widetilde{n}_c$  be the number of close Bethe roots with respect to the real axis and the axis  $\mathbb{R} + i\pi$  respectively, and let  $\bar{n}_w$  be the number of complex roots which are wide roots with respect to *both* the real axis and to the axis  $\mathbb{R} + i\pi$ . Then

$$N = M + \widetilde{M} + n_c + \widetilde{n}_c + \bar{n}_w, \quad (2.121)$$

and

$$n_w = \widetilde{M} + \widetilde{n}_c + \bar{n}_w, \quad \widetilde{n}_w = M + n_c + \bar{n}_w. \quad (2.122)$$

We expect that, in the large  $N$  limit, the low-energy states will be given by solutions  $\{u\} \equiv \{u_1, \dots, u_N\}$  of the Bethe equations with  $M \sim \frac{N}{2}$  real Bethe roots,  $\widetilde{M} \sim \frac{N}{2}$  Bethe roots on the axis  $\mathbb{R} + i\pi$ , and a finite number  $N - M - \widetilde{M}$  of other complex Bethe roots. we suppose that (as proved in periodic case [137]), for such states, the real Bethe roots and the Bethe roots on the axis  $\mathbb{R} + i\pi$  have some continuous distribution in the thermodynamic limit:

$$\frac{1}{N(u_{j+1} - u_j)} \underset{N \rightarrow \infty}{\sim} \rho(u_j), \quad \text{if } u_j, u_{j+1} \in \mathbb{R} \quad (2.123)$$

$$\frac{1}{N(u_{j+1} - u_j)} \underset{N \rightarrow \infty}{\sim} \widetilde{\rho}(u_j), \quad \text{if } u_j, u_{j+1} \in \mathbb{R} + i\pi \quad (2.124)$$

so that we suppose we can, in the leading order in the thermodynamic limit, replace the sums by integrals:

$$\begin{aligned} \frac{1}{N} \sum_{k=1}^M f(u_k) &= \int_{\mathbb{R}} f(\alpha) \rho(\alpha) d\alpha \\ \frac{1}{N} \sum_{k=1}^{\widetilde{M}} f(u_k) &= \int_{\mathbb{R} + i\pi} f(\alpha) \widetilde{\rho}(\alpha) d\alpha. \end{aligned} \quad (2.125)$$



Then the difference of the Bethe equations gives us two copies of the integral equations:

$$\begin{aligned}\phi'(\alpha) - \frac{1}{2} \int_{\mathbb{R}} \phi' \left( \frac{\alpha - \nu}{2} \right) \rho(\nu) d\nu - \frac{1}{2} \int_{\mathbb{R} + i\pi} \phi' \left( \frac{\alpha - \mu}{2} \right) \tilde{\rho}(\mu) d\mu &= \rho(\alpha) \\ \phi'(\beta) - \frac{1}{2} \int_{\mathbb{R}} \phi' \left( \frac{\beta - \nu}{2} \right) \rho(\nu) d\nu - \frac{1}{2} \int_{\mathbb{R} + i\pi} \phi' \left( \frac{\beta - \mu}{2} \right) \tilde{\rho}(\mu) d\mu &= \tilde{\rho}(\beta)\end{aligned}\quad (2.126)$$

with  $\alpha \in \mathbb{R}$  and  $\beta \in \mathbb{R} + i\pi$ . We used the Fourier modes to solve the integral equation and obtained the densities:

$$\rho(\alpha) = \tilde{\rho}(\beta) = \frac{1}{2\zeta \cosh\left(\frac{\pi\alpha}{\zeta}\right)}.\quad (2.127)$$

Note this result coincides with that in the periodic case [138], the only difference is that we obtained two copies of the roots shifted by  $i\pi$ .

## Chapter 3

# Scalar products of separate states and form factors

Recall that the quantum SoV approach imposes to introduce a set of inhomogeneous parameters  $\{\xi_1, \dots, \xi_N\}$  subject to the conditions 1.1 or 1.2, which modifies the physical model with Hamiltonian (1.5) to the inhomogeneous chain defined by the monodromy matrix (1.18). Thus one must be able to take the homogeneous limit to recover the physical model in the computation of the scalar product and the form factors [94] if one wants to develop an approach towards the computation correlation function as in the periodic case solvable by ABA.

The explicit construction of the SoV basis leads to a natural determinant representation for the scalar product between two general separate states of the form (1.66) and (1.67). It is in the form of a sum of two dressed generalised Vandermonde matrix [114]:

$$\langle \alpha | \beta \rangle = \frac{1}{V(\{\xi\})} \det_N \left[ \alpha(\xi_a) \beta(\xi_a) \left( v_{a,b}(\xi) - \frac{a(\xi_a) \alpha(\xi_a - \eta) \beta(\xi_a - \eta)}{d(\xi_a - \eta) \alpha(\xi_a) \beta(\xi_a)} v_{a,b}(\xi - \eta) \right) \right], \quad (3.1)$$

where  $V(\{\xi\})$  is defined same as in (1.65) and  $v_{a,b}(\lambda)$  denotes the Vandermonde matrix element. For the  $XXX$  case,  $v_{a,b}(\lambda) = \lambda_a^{b-1}$  and for the  $XXZ$  case  $v_{a,b}(\lambda) = \frac{e^{(2j-N-1)\lambda_a}}{2^{b-1}}$ .

It is worth mentioning that such a determinant representation is quite common for a class of models in the SoV framework. In principle, this is a good sign for the computation of correlation functions since the determinant representations appearing for the scalar products of Bethe states in the ABA framework [84] led to convenient representations for the correlation functions and the form factors [81]. However, the representation (3.1) is not a convenient one. The problem is that its rows are labelled by the set of inhomogeneous parameters  $\{\xi_1, \dots, \xi_N\}$ , and this will lead to an indefinite (or at least complicated) result when we take the homogeneous limit  $\xi_1, \dots, \xi_N \rightarrow \eta/2$ .

The idea is therefore to transform the representation (3.1) to get a more convenient one for the consideration of the homogeneous limit and thermodynamic limit. It has been done for the  $XXX_{1/2}$  anti-periodic spin chain in [114]. Roughly speaking, the idea is to transform the determinant in equation (3.1) by noticing the possibility to find some other matrix whose elements are labelled by the set of spectral parameters  $\{\alpha\}$ ,  $\{\beta\}$  and the set of inhomogeneous parameters  $\{\xi\}$  on an equal footing. The resulting determinant is the so-called *generalised Izergin determinant*<sup>1</sup>, which is symmetric between the set of spectral parameters and inhomogeneous

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<sup>1</sup>First introduced as a representation for the partition function of the six-vertex model with domain-wall boundary conditions [148].

geneous parameters. Such a determinant can be further transformed into a determinant in which rows and columns are respectively labelled by the two sets of Bethe roots  $\{\alpha\}$  and  $\{\beta\}$ . In the antiperiodic XXX case [114], the resulting determinant is very similar, in its form, to the determinant obtained by N. Slavnov in the periodic case for the scalar products of Bethe states [84] (in the following, determinants of such type will be called *Slavnov determinants*). The same strategy can be directly applied to the computation of the scalar product for the  $XXZ_{1/2}$  open spin chain with boundary fields [144]. The reason why the same procedure can be applied is that the functional form of the  $Q$  functions appearing in the determinant is usual polynomials.

But unfortunately, this procedure cannot be repeated for the anti-periodic  $XXZ_{1/2}$  model. The scalar product between two arbitrary separate states (1.111)-(1.112) can still be initially written as the determinant of the sum of two dressed generalised Vandermonde matrices. However, the functions involved there are not usual trigonometric polynomials, thus the solution to this problem is different.

It is still possible to transform such a determinant into some generalized version of the Izergin determinant but, unlike in the paper [114], the *generalised Izergin determinant* that we obtained in the  $XXZ$  case is not symmetric into the two sets of parameters. The function involved in it has different periodicity from the initial functions of the polynomial, i.e. is not a polynomial in the Vandermonde variables. Therefore, we proposed an alternative way of transforming the determinant [118].

### 3.1 A short review on the anti-periodic XXX chain

This section aims at giving a short review and at showing explicitly some important intermediate steps on how the convenient determinant representation, namely, the Slavnov determinant was obtained from the expression (3.1) in the paper [114] for the anti-periodic XXX chain .

#### 3.1.1 Scalar products and form factors for the anti-periodic XXX chain

It is convenient to introduce a set of notions and definitions to show how the transformation of the determinant in (3.1) was done. For any set of complex parameters  $\{x_1, \dots, x_L\}$  and an arbitrary function  $f$ , define:

$$E_{\{x\}}^{\pm}(y) = \prod_{n=1}^N \frac{y - x_n \pm \eta}{y - x_n} \quad (3.2)$$

$$\mathcal{A}_{\{x\}}^{\pm}[f] = \frac{\det_L [x_a^{b-1} - f(x_a)(x_a \pm \eta)^{b-1}]}{V(\{x\})}. \quad (3.3)$$

Then the scalar product (3.1) can be written as:

$$\langle \alpha | \beta \rangle = \prod_{n=1}^N (\alpha(\xi_n) \beta(\xi_n)) \mathcal{A}_{\{\xi\}}^+ \left[ \mu E_{\{\alpha_1, \dots, \alpha_R\} \cup \{\beta_1, \dots, \beta_S\}}^- \right]. \quad (3.4)$$

For  $\mu \in \mathbb{C}$  and two sets of parameters  $\{x_1, \dots, x_N\}$  and  $\{y_1, \dots, y_N\}$  with  $t_\mu(x) = \frac{\mu}{x} - \frac{1}{x+\eta}$ , the generalised Izergin determinant was defined as follows:

$$\mathcal{I}_N^\mu(\{x\}, \{y\}) = \frac{\prod_{a,b=1}^N (x_a - y_b + \eta)}{V(x_1, \dots, x_N)V(y_N, \dots, y_1)} \det_N [t_\mu(x_a - y_b)]. \quad (3.5)$$

One can see a crucial feature of the generalised Izergin determinant (3.5) that it depends on the two sets of parameters  $\{x\}$  and  $\{y\}$  symmetrically. It was shown in [114] as a generalisation of the result of Kostov [149, 150, 151, 152] that:

$$\mathcal{I}_N^\mu(\{x\}, \{y\}) = (-1)^N \mathcal{A}_{\{x\}}^- [\mu E_{\{y\}}^+] = (-1)^N \mathcal{A}_{\{y\}}^+ [\mu E_{\{x\}}^+] \quad (3.6)$$

which allows writing the scalar product (3.4) in terms of the Izergin determinant. What's more, it serves as a bridge allowing us to exchange the two set of parameters<sup>2</sup>:

$$\{\alpha_1, \dots, \alpha_R\} \cup \{\beta_1, \dots, \beta_S\} \leftrightarrow \{\xi_1, \dots, \xi_N\}. \quad (3.8)$$

Thus the scalar product (3.4) can be written in terms of:

$$\mathcal{A}_{\{\alpha_1, \dots, \alpha_R\} \cup \{\beta_1, \dots, \beta_S\}}^- [\mu E_{\{\xi\}}^+]. \quad (3.9)$$

Then the last step is to transform it into the so-called Slavnov determinant:

$$\mathcal{S}_M^{(\mu)}(\{x\}, \{y\}|\{\xi\}) = \frac{\prod_{j,k=1}^M (x_j - y_k + \eta)}{V(x_1, \dots, x_M)V(y_M, \dots, y_1)} \det_M \mathcal{H}^{(\mu)}(\{x\}, \{y\}|\{\xi\}) \quad (3.10)$$

with the matrix elements of  $\mathcal{H}^{(\mu)}(\{x\}, \{y\}|\{\xi\})$  defined as:

$$[\mathcal{H}^{(\mu)}(\{x\}, \{y\}|\{\xi\})]_{j,k} = \mu E_{\{\xi\}}^+(y_k) t_1(x_j - y_k) - \frac{E_{\{x\}}^+(y_k)}{E_{\{x\}}^-(y_k)} t_1(y_k - x_j). \quad (3.11)$$

With the set of parameters  $\{x_1, \dots, x_M\}$  as the solution to the Bethe equations,  $\{y_1, \dots, y_{M+S}\}$  as a set of arbitrary parameters and  $\{\xi_1, \dots, \xi_N\}$  as the inhomogeneous parameters, the following relation holds:

$$\mathcal{S}_{M, M+S}^{(\mu)}(\{x\}, \{y\}|\{\xi\}) = \mathcal{A}_{\{x\} \cup \{y\}}^- [\mu E_{\{\xi\}}^+] \quad (3.12)$$

**Remark 3.1.** *In the paper [114], in the last transformation to the Slavnov determinant, it was supposed that one of the separate states was an eigenstate of the twisted transfer matrix (by requiring  $\{x_1, \dots, x_M\}$  to be a solution to the Bethe equations). But it also works for two general separate states.*

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<sup>2</sup>The identity (3.6) can only be applied when the two sets of parameters share the same cardinality. It can be generalised to the case when the cardinalities of the two sets  $\{x\}$  and  $\{y\}$  are not equal. In fact, the exchange of the two sets relies on the generalised version of (3.6):

$$\mathcal{A}_{\{\xi\}}^+ [\mu E_{\{\alpha_1, \dots, \alpha_R\} \cup \{\beta_1, \dots, \beta_S\}}^+] = (1 - \mu)^{N - (R+S)} \mathcal{A}_{\{\alpha_1, \dots, \alpha_R\} \cup \{\beta_1, \dots, \beta_S\}}^- [\mu E_{\{\xi\}}^+] \quad (3.7)$$

Finally, the scalar product can be indeed written in the form of a Slavnov determinant as in Theorem 3.3 of [114] which remains finite and manageable in the homogeneous limit.

After the convenient determinant representation of the scalar product was obtained, together with the solution to the quantum inverse scattering method, the matrix elements of  $\sigma_n^-$  between two eigenstate  $\langle Q_\tau | \sigma_n^- | Q_{\tau'} \rangle$  were computed in section 4 of [114]. And the matrix elements of  $\sigma_n^+$  and  $\sigma_n^z$  between two eigenstates can be obtained from  $\langle Q_\tau | \sigma_n^- | Q_{\tau'} \rangle$  by using the symmetries:

$$[S^x, \mathcal{T}_K(\lambda)] = 0, \quad [\Gamma^x, \mathcal{T}_K(\lambda)] = 0. \quad (3.13)$$

**Remark 3.2.** *The case of the anti-periodic XXX chain treated in [114] and that we have just summarized here or for more general twists in [153, 154, 155] is quite particular. Indeed, the  $SU(2)$  symmetry of the monodromy matrix provides a correspondence between the chain with the anti-periodic boundary condition (a twist by  $\sigma^x$ ) and the chain with a diagonal twist (a twist of the form  $\sigma^z$  or for the most general case any two by two diagonal matrix) which can be solved within the ABA framework. It is therefore not surprising that the form factors have the same form in the anti-periodic case as in the diagonal case, since these two cases can be explicitly related by the above transformation.*

## 3.2 Scalar products and form factors for the anti-periodic XXZ chain

In this section, we would like to present the results from our paper [118] concerning scalar products of separate states and form factors of local operators in the anti-periodic XXZ case by SoV. We obtained some determinant representations in which, as in the Slavnov determinant [84] for the scalar products of Bethe states, or as in the determinant representations for the ABA forms factors [80], the rows and columns are labelled by the roots of the  $Q$ -function (or in other words the Bethe roots). I would like to point out that these computations in the XXZ case are not simply a replica of the work reviewed in the last section [114]. In short, the difficulties come from the fact that the solution to the functional Baxter equation (1.102) is not a usual trigonometric polynomial. Instead, it has a *double period* with respect to the  $Q$ -function form in the periodic case:

$$Q(\lambda) = \prod_{n=1}^N \sinh\left(\frac{\lambda - q_n}{2}\right). \quad (3.14)$$

Due to this discrepancy of periods, the transformations involved, as well as the final formulas, are quite different from what we had in the XXX case.

### 3.2.1 The scalar product of two separate states

So as to simplify the global normalization factor in the final formulas for the scalar products and form factors, let us introduce the following normalisation of the separate states (1.111)-(1.112):

$$\langle P, \epsilon | = \sum_{\mathbf{h} \in \{0,1\}^N} \prod_{n=1}^N \{ \epsilon^{h_n} P(\xi_n^{(h_n)}) \} V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle \mathbf{h} |, \quad (3.15)$$

$$= \prod_{n=1}^N [\epsilon P(\xi_n - \eta)]_{\mathbf{n}} \langle P, \epsilon |, \quad (3.16)$$

$$\begin{aligned}
 |P, \epsilon\rangle &= \sum_{\mathbf{h} \in \{0,1\}^N} \prod_{n=1}^N \left\{ (-\epsilon)^{-h_n} \left( \frac{a(\xi_n)}{d(\xi_n - \eta)} \right)^{h_n} P(\xi_n^{(h_n)}) \right\} V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) |\mathbf{h}\rangle \\
 &= \sum_{\mathbf{h} \in \{0,1\}^N} \prod_{n=1}^N \left\{ \epsilon^{-h_n} P(\xi_n^{(h_n)}) \right\} V(\xi_1^{(1-h_1)}, \dots, \xi_N^{(1-h_N)}) |\mathbf{h}\rangle
 \end{aligned} \tag{3.17}$$

$$= V(\xi_1, \dots, \xi_N) \prod_{n=1}^N [\epsilon P(\xi_n - \eta)] |P, \epsilon\rangle_{\mathbf{n}}, \tag{3.18}$$

where

$${}_{\mathbf{n}}\langle P, \epsilon| = \sum_{\mathbf{h} \in \{0,1\}^N} \prod_{n=1}^N \left( \epsilon \frac{P(\xi_n)}{P(\xi_n - \eta)} \right)^{1-h_n} V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle \mathbf{h}|, \tag{3.19}$$

$$|P, \epsilon\rangle_{\mathbf{n}} = \sum_{\mathbf{h} \in \{0,1\}^N} \prod_{n=1}^N \left( \epsilon \frac{P(\xi_n)}{P(\xi_n - \eta)} \right)^{1-h_n} \frac{V(\xi_1^{(1-h_1)}, \dots, \xi_N^{(1-h_N)})}{V(\xi_1, \dots, \xi_N)} |\mathbf{h}\rangle. \tag{3.20}$$

Then the scalar product of the states (3.19) and (3.20) built from  $P$  and  $Q$  can be written as:

$$\begin{aligned}
 \mathbf{S}(PQ, \epsilon\epsilon') &= {}_{\mathbf{n}}\langle P, \epsilon| Q, \epsilon'\rangle_{\mathbf{n}} \\
 &= \sum_{\mathbf{h}} \prod_{n=1}^N \left[ \epsilon\epsilon' \frac{(PQ)(\xi_n)}{(PQ)(\xi_n - \eta)} \right]^{1-h_n} \frac{V(\xi_1^{(1-h_1)}, \dots, \xi_N^{(1-h_N)})}{V(\xi_1, \dots, \xi_N)} \\
 &= \frac{\det_{1 \leq i, j \leq N} \left[ e^{(2j-N-1)\xi_i} + \epsilon\epsilon' \frac{(PQ)(\xi_i)}{(PQ)(\xi_i - \eta)} e^{(2j-N-1)(\xi_i - \eta)} \right]}{\det_{1 \leq i, j \leq N} \left[ e^{(2j-N-1)\xi_i} \right]}
 \end{aligned} \tag{3.21}$$

Note that it depends only on the product function  $(PQ)$  and the global sign  $\epsilon\epsilon'$ . As usual for the separate states constructed within the SoV approach, this scalar product can be written as a single determinant of the sum of two dressed generalised Vandermonde matrices. This determinant representation depends intricately on the inhomogeneity parameters and is therefore not convenient for the consideration of the physical model.

From now on, we will also suppose that the functions  $P$  and  $Q$  are trigonometric polynomials of the form

$$P(\lambda) = \prod_{j=1}^N \sinh\left(\frac{\lambda - p_j}{2}\right), \quad Q(\lambda) = \prod_{j=1}^N \sinh\left(\frac{\lambda - q_j}{2}\right), \tag{3.22}$$

$$\text{with } p_1, \dots, p_N, q_1, \dots, q_N \in \mathbb{C} \setminus \bigcup_{i=1}^N \Xi_i. \tag{3.23}$$

Let us introduce some similar notations as in the  $XXX$  case. For any set of complex numbers  $\{x\} \equiv \{x_1, \dots, x_M\}$ , and a function  $f$ , we define

$$\mathcal{A}_{\{x\}}[f] = \frac{\det_{1 \leq i, j \leq M} \left[ \frac{e^{(2j-M-1)x_i}}{2^{j-1}} - f(x_i) \frac{e^{(2j-M-1)(x_i - \eta)}}{2^{j-1}} \right]}{V(x_1, \dots, x_M)}. \tag{3.24}$$

Then the scalar product (3.21) can be rewritten as:

$$\mathbf{S}(PQ, \alpha) = \mathcal{A}_{\{\xi_1, \dots, \xi_N\}} [-\alpha f_{PQ}] \quad (3.25)$$

with

$$f_{PQ}(\lambda) = \frac{(PQ)(\lambda)}{(PQ)(\lambda - \eta)}, \quad \alpha = \epsilon \epsilon'. \quad (3.26)$$

In the same spirit as in the XXX case [114], expressions of the form (3.24) can be transformed into some generalised Izergin determinant by means of the following identity:

**Identity 1.** (*Transformation into a generalised Izergin determinant*)

For any two sets of arbitrary complex numbers  $\{x\} \equiv \{x_1, \dots, x_L\}$  and  $\{y\} = \{y_1, \dots, y_L\}$  and any function  $f$ , we have

$$\mathcal{A}_{\{x\}}[f] = \mathcal{I}_{\{x\}, \{y\}} [f \cdot E_{\{y\}}] \quad (3.27)$$

where

$$E_{\{y\}}(u) = \prod_{\ell=1}^L \frac{\sinh(u - y_\ell - \eta)}{\sinh(u - y_\ell)}, \quad (3.28)$$

and

$$\begin{aligned} \mathcal{I}_{\{x\}, \{y\}}[f] &= \frac{\prod_{i, \ell=1}^L \sinh(x_i - y_\ell)}{\prod_{i < j} \sinh(x_j - x_i) \sinh(y_i - y_j)} \det_L \left[ \frac{1}{\sinh(x_i - y_k)} - \frac{f(x_i)}{\sinh(x_i - y_k - \eta)} \right] \\ &= \frac{\det_L \left[ \frac{1}{\sinh(x_i - y_k)} - \frac{f(x_i)}{\sinh(x_i - y_k - \eta)} \right]}{\det_L \left[ \frac{1}{\sinh(x_i - y_k)} \right]}. \end{aligned} \quad (3.29)$$

*Proof.* We multiply and divide  $\mathcal{A}_{\{x\}}[f]$  with the determinant of the  $L \times L$  matrix  $\mathcal{C}_{\{z\}}$  with elements  $(\mathcal{C}_{\{z\}})_{j,k}$ ,  $1 \leq j, k \leq L$ , defined as

$$\prod_{\substack{\ell=1 \\ \ell \neq k}}^L \sinh(\lambda - z_\ell) = e^{-(L-1)\lambda} \sum_{j=1}^L (\mathcal{C}_{\{z\}})_{j,k} \left( \frac{e^{2\lambda}}{2} \right)^{j-1} = \sum_{j=1}^L (\mathcal{C}_{\{z\}})_{j,k} \frac{e^{(2j-L-1)\lambda}}{2^{j-1}}, \quad (3.30)$$

and with determinant:  $\det_L \mathcal{C}_{\{z\}} = V(z_L, \dots, z_1) = \prod_{j < k} \sinh(z_j - z_k)$ .  $\square$

**Remark 3.3.** Unlike in the XXX case (3.5), the generalized Izergin determinant (3.29) that we obtain from this transformation is a priori not symmetric between the two sets of parameters  $\{x\}$ ,  $\{y\}$ . It depends on the function  $f$  appearing inside the determinant. And from equation (3.25)-(3.26) it is obvious that the function  $f$  has different periodicities from the functions appearing in the denominators in (3.29).

Therefore, from now on, we can no longer apply the same strategy as in [114]. It is necessary to propose some other type of transformation. Roughly speaking, our idea is that since the expression (3.29) is a ratio of two determinants, it will remain unchanged if we multiply both the numerator and denominator in (3.29) by the determinant of a properly chosen (invertible) matrix  $\mathcal{X}$  :

$$\frac{\det[\mathcal{M}]}{\det[\mathcal{N}]} = \frac{\det[\mathcal{X}] \det[\mathcal{M}]}{\det[\mathcal{X}] \det[\mathcal{N}]} = \frac{\det[\mathcal{X} \cdot \mathcal{M}]}{\det[\mathcal{X} \cdot \mathcal{N}]} \quad (3.31)$$

The last equality holds because the determinant operation is a homomorphism. Note that the rows of  $\mathcal{M}$  and  $\mathcal{N}$  are labelled by  $\{x\}$  (which when considering the scalar products will become the inhomogeneity parameters  $\{\xi\}$ ):

$$\mathcal{M}_{j,k} = \mathcal{M}_k(x_j). \quad (3.32)$$

Thus our idea is to find such  $\mathcal{X}$  whose columns are labelled by the same set  $\{x\}$ :

$$\mathcal{X}_{i,j} = \mathcal{X}_i(x_j). \quad (3.33)$$

Such a matrix has to be well chosen such that the matrix multiplication can be written as a sum of residues of a certain function  $\mathcal{J}(\zeta)$  at  $\{x\}$  inside some well-chosen contour  $\Gamma$ . This contour must include the other set of parameters  $\{y\}$  as the rest of the residues. And we must be able to compute the integral along this contour, namely, we want the following:

$$\sum_{j=1}^L \mathcal{X}_{i,j} \mathcal{M}_{j,k} = \sum_{\{x\}} \text{Res} [\mathcal{J}(\zeta)] = \oint_{\Gamma} \mathcal{J}(\zeta) d\zeta - \sum_{\{y\}} \text{Res} [\mathcal{J}(\zeta)]. \quad (3.34)$$

The last equality is a consequence of the Cauchy theorem. Applying this to the scalar product, the set  $\{x\}$  corresponds to the inhomogeneous parameters  $\{\xi_1, \dots, \xi_N\}$  and  $\{y\}$  corresponds to the set of spectral parameters  $\{p_1, \dots, p_N\}$  and  $\{q_1, \dots, q_N\}$ . All of these depend on the matrix  $\mathcal{X}$ , and it is not a trivial task to find one. For the scalar product we proposed the following:

$$\begin{aligned} \mathcal{X}_{i,j} &\equiv \mathcal{X}(q_i, \xi_j) \\ &= \frac{1}{\prod_{\substack{\ell=1 \\ \ell \neq j}}^N \sinh(\xi_j - \xi_\ell)} \left[ Q(\xi_j - \eta) P(\xi_j + i\pi) \coth\left(\frac{\xi_j - q_i - \eta}{2}\right) \right. \\ &\quad \left. - Q(\xi_j - \eta + i\pi) P(\xi_j) \coth\left(\frac{\xi_j - q_i - \eta + i\pi}{2}\right) \right], \end{aligned} \quad (3.35)$$

for  $1 \leq i, j \leq N$ .

Use Identity 1 and the formula (3.25) becomes:

$$\mathbf{S}(PQ, \alpha) = \mathcal{I}_{\{\xi_1, \dots, \xi_N\}, \{p_1, \dots, p_N\}} \left[ -\alpha \tilde{f}_{P,Q} \right] = \frac{\det_N \mathcal{M}^{(\alpha)}}{\det_N \mathcal{M}^{(0)}}, \quad (3.36)$$

in terms of the function

$$\tilde{f}_{P,Q}(u) = \frac{P(u - \eta + i\pi) Q(u)}{P(u + i\pi) Q(u - \eta)}, \quad (3.37)$$

where we have set

$$\mathcal{M}_{i,k}^{(\beta)} = \mathcal{M}^{(\beta)}(\xi_i, p_k) = \frac{1}{\sinh(\xi_i - p_k)} + \frac{\beta \tilde{f}_{P,Q}(\xi_i)}{\sinh(\xi_i - p_k - \eta)}, \quad (3.38)$$

for  $\beta = \alpha$  or  $\beta = 0$ . And with the matrix  $\mathcal{X}$  and the method above, it leads to the following identity.



**Identity 2.** Let  $\{\xi_1, \dots, \xi_N\}$  be a set of arbitrary parameters and let  $P$  and  $Q$  be trigonometric polynomials of the form (3.22)-(3.23), satisfying moreover the condition

$$\frac{(PQ)(\xi_n - \eta)}{(PQ)(\xi_n)} = \frac{(PQ)(\xi_n - \eta + i\pi)}{(PQ)(\xi_n + i\pi)}, \quad \forall n \in \{1, \dots, N\}. \quad (3.39)$$

Let  $\{p_1, \dots, p_N\}$  and  $\{q_1, \dots, q_N\}$  denote their respective sets of roots, and let  $\tilde{f}_{P,Q}$  be the function defined in terms of  $P$  and  $Q$  as in (3.37). Then, for any arbitrary parameter  $\alpha$ ,

$$\mathcal{I}_{\{\xi_1, \dots, \xi_N\}, \{p_1, \dots, p_N\}}[-\alpha \tilde{f}_{P,Q}] = \frac{\det_{1 \leq i, k \leq N} \left[ S_{Q,P}^{(\alpha)}(q_j, p_k) \right]}{\det_{1 \leq j, k \leq N} \left[ \coth\left(\frac{p_k - q_j - \eta}{2}\right) \right]}, \quad (3.40)$$

where  $S_{Q,P}^{(\alpha)}(q_j, p_k)$  is defined as:

$$\begin{aligned} S_{Q,P}^{(\alpha)}(q_j, p_k) &= \coth\left(\frac{p_k - q_j - \eta}{2}\right) + \alpha \mathbf{a}_Q(p_k) \coth\left(\frac{p_k - q_j}{2}\right) \\ &\quad - 2\alpha \frac{d(p_k)}{a(q_j)} \frac{Q(q_j + \eta)}{Q(p_k - \eta)} \frac{P(q_j + i\pi)}{P(p_k + i\pi)} \frac{1}{\sinh(p_k - q_j)}, \end{aligned} \quad (3.41)$$

in terms of the function:

$$\mathbf{a}_Q(u) \equiv \mathbf{a}_Q(u|\{\xi_1, \dots, \xi_N\}) = \prod_{\ell=1}^N \frac{\sinh(u - \xi_\ell)}{\sinh(u - \xi_\ell + \eta)} \frac{Q(u + \eta)}{Q(u - \eta)}. \quad (3.42)$$

**Remark 3.4.** The condition (3.39) is obviously satisfied if, for all  $n \in \{1, \dots, N\}$ ,

$$\frac{P(\xi_n - \eta)}{P(\xi_n)} = -\frac{P(\xi_n - \eta + i\pi)}{P(\xi_n + i\pi)}, \quad \frac{Q(\xi_n - \eta)}{Q(\xi_n)} = -\frac{Q(\xi_n - \eta + i\pi)}{Q(\xi_n + i\pi)}. \quad (3.43)$$

Therefore, it is obviously satisfied in the case of transfer matrix eigenstates due to (1.113). Hence, the class of states built from trigonometric polynomials of the form (3.22)-(3.23) satisfying (3.43) contains in particular the class of all transfer matrix eigenstates. It is however much wider.

**Remark 3.5.** The quantity (3.42) turns out to coincide with the function appearing in the left hand side of the Bethe equations (1.104) if  $Q$  is the solution to the functional Baxter equation (1.102) with the roots  $\{q_1, \dots, q_N\}$ .

Apply Identity 1 and Identity 2 to the scalar product formula (3.25), we straightforwardly obtain the following Proposition:

**Proposition 3.2.1.** The scalar product (3.21) of two separate states (3.19) and (3.20) built from  $P$  and  $Q$  of the form (3.22)-(3.23) can be expressed as

$$\mathbf{S}(PQ, \alpha) = \frac{\det_N \left[ \frac{1}{\sinh(\xi_i - p_k)} + \frac{\alpha \tilde{f}_{P,Q}(\xi_i)}{\sinh(\xi_i - p_k - \eta)} \right]}{\det_N \left[ \frac{1}{\sinh(\xi_i - p_k)} \right]} \quad (3.44)$$

in which we have set  $\alpha = \epsilon\epsilon'$  and

$$\tilde{f}_{P,Q}(u) = \frac{P(u - \eta + i\pi)}{P(u + i\pi)} \frac{Q(u)}{Q(u - \eta)}. \quad (3.45)$$

If moreover  $P$  and  $Q$  are such that the following condition is satisfied:

$$\frac{(PQ)(\xi_n - \eta)}{(PQ)(\xi_n)} = \frac{(PQ)(\xi_n - \eta + i\pi)}{(PQ)(\xi_n + i\pi)}, \quad \forall n \in \{1, \dots, N\}, \quad (3.46)$$

then (3.44) can be rewritten as

$$\mathbf{S}(PQ, \alpha) = \frac{\det_N [\mathcal{S}^{(\alpha)}(\mathbf{q}|\mathbf{p})]}{\det_{1 \leq j, k \leq N} [\coth(\frac{p_k - q_j - \eta}{2})]} \quad (3.47)$$

$$= \frac{\prod_{i,j=1}^N \sinh(\frac{p_i - q_j - \eta}{2}) \det_N [\mathcal{S}^{(\alpha)}(\mathbf{q}|\mathbf{p})]}{\cosh(\frac{\sum_{\ell} (p_{\ell} - q_{\ell} - N\eta)}{2}) \prod_{i < j} [\sinh(\frac{p_i - p_j}{2}) \sinh(\frac{q_j - q_i}{2})]}, \quad (3.48)$$

in which we have defined, for any parameter  $\alpha$ ,

$$\begin{aligned} [\mathcal{S}^{(\alpha)}(\mathbf{q}|\mathbf{p})]_{j,k} &\equiv \mathbf{S}_{Q,P}^{(\alpha)}(q_j, p_k) \\ &= \coth\left(\frac{p_k - q_j - \eta}{2}\right) + \alpha \mathbf{a}_Q(p_k) \coth\left(\frac{p_k - q_j}{2}\right) \\ &\quad - 2\alpha \frac{d(p_k)}{a(q_j)} \frac{Q(q_j + \eta)}{Q(p_k - \eta)} \frac{P(q_j + i\pi)}{P(p_k + i\pi)} \frac{1}{\sinh(p_k - q_j)}, \end{aligned} \quad (3.49)$$

with  $\mathbf{a}_Q$  defined as in (3.42).

The representation (3.44) is a generalization of the formula obtained in [148] for the partition function of the six-vertex model with domain-wall boundary conditions, but with in addition the presence of a non-trivial function  $\tilde{f}_{P,Q}$  (3.45). In its turn, the determinant in (3.47), with rows and columns labelled by the roots of  $Q$  and  $P$ , is reminiscent in its form from its analog in the periodic case obtained by Bethe Ansatz [84], but its matrix elements (3.49) are less symmetric as those of [84]: they seem to contain only parts of the terms that one could expect from a direct generalization of the determinant of [84]. In fact, (3.47) appears closer to the "square root" of some analog of the determinant of [84]. More precisely, one can show the following property:

**Proposition 3.2.2.** *The scalar products (3.21) of two separate states (3.19) and (3.20) built from  $P$  and  $Q$  of the form (3.22) - (3.23) satisfying (3.43) verify the following property for any parameters  $\alpha$  and  $\beta$ :*

$$\mathbf{S}(PQ, \alpha) \mathbf{S}(PQ, \beta) = (-1)^N \frac{e^{\sum_i (\xi_i - p_i)}}{2^{N(N-1)}} \prod_{i=1}^N \frac{Q(\xi_i)}{Q(\xi_i - \eta)} \frac{\det_N [\bar{\mathcal{S}}^{(\alpha, \beta)}(\mathbf{q}|\mathbf{p})]}{\det_{1 \leq i, k \leq N} \left[ \frac{1}{\sinh(\frac{p_k - q_i - \eta}{2})} \right]} \quad (3.50)$$

with

$$[\bar{\mathcal{S}}^{(\alpha,\beta)}(\mathbf{q}|\mathbf{p})]_{j,k} = \bar{\mathcal{S}}_{P,Q}^{(\alpha,\beta)}(q_j, p_k) \quad (3.51)$$

$$= \left[ \frac{\alpha e^{-\frac{\eta}{2}}}{\sinh(\frac{p_k - q_j - \eta}{2})} - \frac{1}{\sinh(\frac{p_k - q_j}{2})} \right] + \beta e^{-\frac{\eta}{2}} \mathbf{a}_Q(p_k) \left[ \frac{\alpha e^{-\frac{\eta}{2}}}{\sinh(\frac{p_k - q_j}{2})} - \frac{1}{\sinh(\frac{p_k - q_j + \eta}{2})} \right] \quad (3.52)$$

$$+ 2 \frac{d(p_k)}{d(q_j)} \frac{Q(q_j - \eta)P(q_j + i\pi)}{Q(p_k - \eta)P(p_k + i\pi)} (1 - \alpha\beta e^{-\eta} \mathbf{a}_Q(q_j)) \frac{e^{\frac{p_k - q_j}{2}}}{\sinh(p_k - q_j)}. \quad (3.53)$$

In particular, when  $\alpha\beta e^{-\eta} = 1$  and when the roots of  $Q$  satisfy in addition the system of Bethe equation (3.42), the last line of cancels, and appears as quite similar, in its form, of the determinant of [84].

The proof of this result rely on the following Identity:

**Identity 3.** Under the hypothesis of Identity 2 and supposing in addition that  $P$  and  $Q$  satisfy (3.43), the expression (3.36) can be rewritten as:

$$\mathbf{S}(PQ, \alpha) = \frac{e^{\sum_i \frac{\xi_i - p_i}{2}} \det_{1 \leq i, k \leq N} \mathbf{M}_{P,Q}^{(\alpha)}(\xi_i, p_k)}{2^N \det_{1 \leq i, k \leq N} \left[ \frac{1}{\sinh(\xi_i - p_k)} \right]} \quad (3.54)$$

$$= \frac{e^{\sum_i \frac{\xi_i - p_i}{2}}}{2^N} \prod_{i=1}^N \frac{Q(\xi_i)}{P(\xi_i)} \prod_{i < j} \frac{\sinh(\frac{p_i - p_j}{2})}{\sinh(\frac{q_j - q_i}{2})} \frac{\det_{1 \leq i, k \leq N} \widehat{\mathbf{M}}_{P,Q}^{(\alpha)}(\xi_i, q_k)}{\det_{1 \leq i, k \leq N} \left[ \frac{1}{\sinh(\xi_i - p_k)} \right]}, \quad (3.55)$$

with

$$\mathbf{M}_{P,Q}^{(\alpha)}(\xi_i, p_k) = \frac{1}{\sinh(\frac{\xi_i - p_k}{2})} - \frac{i}{\sinh(\frac{\xi_i - p_k + i\pi}{2})} \quad (3.56)$$

$$+ \alpha e^{-\frac{\eta}{2}} \left( \frac{\tilde{f}_{P,Q}(\xi_i)}{\sinh(\frac{\xi_i - p_k - \eta}{2})} - \frac{i \tilde{f}_{P,Q}(\xi_i + i\pi)}{\sinh(\frac{\xi_i - p_k - \eta + i\pi}{2})} \right), \quad (3.57)$$

and

$$\begin{aligned} \widehat{\mathbf{M}}_{P,Q}^{(\alpha)}(\xi_i, q_k) &= \frac{1}{\sinh(\frac{\xi_i - q_k}{2})} - \frac{\alpha e^{-\frac{\eta}{2}}}{\sinh(\frac{\xi_i - q_k - \eta}{2})} \\ &\quad - i \frac{P(\xi_i)Q(\xi_i + i\pi)}{P(\xi_i + i\pi)Q(\xi_i)} \left( \frac{1}{\sinh(\frac{\xi_i - q_k + i\pi}{2})} - \frac{\alpha e^{-\frac{\eta}{2}}}{\sinh(\frac{\xi_i - q_k - \eta + i\pi}{2})} \right) \\ &= \frac{1}{\sinh(\frac{\xi_i - q_k}{2})} - \frac{\alpha e^{-\frac{\eta}{2}}}{\sinh(\frac{\xi_i - q_k - \eta}{2})} \\ &\quad + i \frac{P(\xi_i)Q(\xi_i + i\pi - \eta)}{P(\xi_i + i\pi)Q(\xi_i - \eta)} \left( \frac{1}{\sinh(\frac{\xi_i - q_k + i\pi}{2})} - \frac{\alpha e^{-\frac{\eta}{2}}}{\sinh(\frac{\xi_i - q_k - \eta + i\pi}{2})} \right) \end{aligned} \quad (3.58)$$

*Proof.* The idea is to make explicit the fact that the expression is in fact  $i\pi$ -quasi-periodic in  $\xi_i$ . Using for instance the identity

$$\frac{1}{\sinh u} = \frac{e^{\frac{u}{2}}}{2} \left( \frac{1}{\sinh \frac{u}{2}} - \frac{i}{\sinh \frac{u + i\pi}{2}} \right), \quad (3.59)$$

we obtain (3.54). Then multiplying each row by  $P(\xi_i)$ , we obtain

$$\mathbf{S}(PQ, \alpha) = \frac{e^{\sum_i \frac{\xi_i - p_i}{2}} \det_N \widetilde{\mathcal{M}}^{(\alpha)}}{2^N \prod_{i=1}^N P(\xi_i) \det_N \mathcal{M}^{(0)}} \quad (3.60)$$

with

$$\begin{aligned} \widetilde{\mathcal{M}}_{j,k}^{(\alpha)} &= P^{(k)}(\xi_i) - \alpha e^{-\frac{\eta}{2}} \frac{Q(\xi_i)}{Q(\xi_i - \eta)} P^{(k)}(\xi_i - \eta) \\ &\quad - i \frac{Q(\xi_i)}{P(\xi_i + i\pi)} \left( P^{(k)}(\xi_i + i\pi) - \alpha e^{-\frac{\eta}{2}} \frac{Q(\xi_i + i\pi)}{Q(\xi_i + i\pi - \eta)} P^{(k)}(\xi_i + i\pi - \eta) \right), \end{aligned} \quad (3.61)$$

$$P^{(k)}(u) = \frac{P(u)}{\sinh\left(\frac{u - p_k}{2}\right)}. \quad (3.62)$$

Factorizing out the matrix  $\widetilde{\mathcal{C}}_{\{p\},\{q\}}$  with elements defined as

$$P^{(k)}(u) = \sum_{j=1}^N \left( \widetilde{\mathcal{C}}_{\{p\},\{q\}} \right)_{j,k} Q^{(j)}(u), \quad \text{with } Q^{(j)}(u) = \frac{Q(u)}{\sinh\left(\frac{u - q_j}{2}\right)}, \quad (3.63)$$

of determinant  $\det_N \widetilde{\mathcal{C}}_{\{p\},\{q\}} = \prod_{i < j} \frac{\sinh\left(\frac{p_j - p_i}{2}\right)}{\sinh\left(\frac{q_j - q_i}{2}\right)}$ , and factorizing  $Q(\xi_i)$  out of each row, we obtain the second identity (3.55).  $\square$

Proposition 3.2.2 then follows by using both representations (3.54) and (3.55) to compute the product.

Finally, let us make some brief comments about the case  $P = Q$ . The quantity  $\mathbf{S}(Q^2, \alpha)$  can of course be obtained from taking the appropriate limit in the above results. It can also be noticed that, in this case, the function  $\widetilde{f}_{Q,Q}$  (3.45) is the constant function equal to  $-1$  if  $Q$  satisfies (3.43). Hence (3.44) reduces to a usual ( $\alpha$ -twisted) Izergin determinant:

$$\mathbf{S}(Q^2, \alpha) = \frac{\det_N \left[ \frac{1}{\sinh(\xi_i - q_k)} - \frac{\alpha}{\sinh(\xi_i - q_k - \eta)} \right]}{\det_N \left[ \frac{1}{\sinh(\xi_i - q_k)} \right]}. \quad (3.64)$$

For this particular case, the same type of transformations as in [114, 144, 156] can be applied, leading to some kind "Slavnov type" determinant. However, the rows of this resulting determinant are labelled by only half (or a subset) of the roots of  $Q$ , whereas the columns are labelled by the other half (or the complementary subset). Moreover, such a determinant is in that case not expressed in terms of the quantity  $\mathbf{a}_Q$  involved in the Bethe equations, contrary to (3.49). Nevertheless, it should be noticed that (3.64) also allows for alternative types of compact determinant representations. For instance, one can easily transform (3.64) as

$$\mathbf{S}(Q^2, \alpha) = \det_{1 \leq i, k \leq N} \left[ \delta_{j,k} - \frac{d(q_k) \prod_{\ell=1}^N \sinh(q_k - q_\ell + \eta)}{a(q_k) \prod_{\ell \neq k} \sinh(q_k - q_\ell)} \frac{\alpha}{\sinh(q_k - q_j + \eta)} \right]. \quad (3.65)$$

*Proof.* The representation (3.65) can be obtained from (3.64) along the same lines as above, by multiplying both determinant in (3.64) by the determinant of the same matrix  $\tilde{\mathcal{X}}$  of elements

$$\tilde{\mathcal{X}}_{a,b} = \frac{\prod_{\ell=1}^N \sinh(\xi_b - q_\ell)}{\prod_{\ell \neq b} \sinh(\xi_b - \xi_\ell)} \frac{1}{\sinh(\xi_b - q_a)}, \quad 1 \leq a, b \leq N. \quad (3.66)$$

□

### 3.2.2 The form factors of local spin operators

In this section, we formulate the results that we obtained in [118] for the form factors of local spin operators, i.e. the matrix elements of the spin operators acting on a given site  $n$  of the chain between two eigenstates of the transfer matrix. We do not present the proofs here, they can be found in [118].

Therefore, we consider the matrix elements of the form

$$\langle P, \epsilon | \sigma_n^\alpha | Q, \epsilon' \rangle, \quad \alpha \in \{+, -, z\}, \quad \epsilon, \epsilon' \in \{+, -\}, \quad (3.67)$$

where  $\langle P, \epsilon |$  and  $|Q, \epsilon'\rangle$  are the eigenstates of the anti-periodic transfer matrix (1.47) with respective eigenvalues  $\epsilon\tau_P$  and  $\epsilon'\tau_Q$ . Due to the proportionality relation (1.114), we can without loss of generality restrict our study to the case  $\epsilon' = \epsilon$ .

**Proposition 3.2.3.** *The form factor of the local operator  $\sigma_n^z$  in two eigenstates  $\langle P, \epsilon |$  and  $|Q, \epsilon\rangle$  of the anti-periodic transfer matrix (1.47) with respective eigenvalues  $\epsilon\tau_P$  and  $\epsilon\tau_Q$  is given by the following ratio of determinants:*

$$\langle P, \epsilon | \sigma_n^z | Q, \epsilon \rangle = - \prod_{k=1}^n \frac{\tau_P(\xi_k)}{\tau_Q(\xi_k)} \frac{\det_N [\mathcal{S}(\mathbf{q}|\mathbf{p}) - \mathcal{P}^{(z)}(\mathbf{q}|\mathbf{p}, \xi_n)]}{\det_{1 \leq j, k \leq N} [\coth(\frac{p_k - q_j - \eta}{2})]}, \quad (3.68)$$

in which  $\mathcal{S}(\mathbf{q}|\mathbf{p}) \equiv \mathcal{S}^{(1)}(\mathbf{q}|\mathbf{p})$  is the matrix of the scalar product with elements  $\mathcal{S}_{Q,P}^{(1)}(q_j, p_k)$  (3.49) with  $\alpha = 1$ , and  $\mathcal{P}^{(z)}(\mathbf{q}|\mathbf{p}, \xi_n)$  is a matrix of rank one with elements

$$[\mathcal{P}^{(-)}(\mathbf{q}|\mathbf{p}, \xi_n)]_{j,k} = \frac{P(p_k - \eta)}{Q(p_k - \eta)} \left[ \frac{Q(\xi_n - \eta)}{P(\xi_n - \eta)} \coth\left(\frac{\xi_n - q_j - \eta}{2}\right) + \frac{Q(\xi_n - \eta + i\pi)}{P(\xi_n - \eta + i\pi)} \coth\left(\frac{\xi_n + i\pi - q_j - \eta}{2}\right) \right], \quad (3.69)$$

for  $1 \leq j, k \leq N$ .

**Proposition 3.2.4.** *The form factors of the local operators  $\sigma_n^+$  and  $\sigma_n^-$  in two eigenstates  $\langle P, \epsilon |$  and  $|Q, \epsilon\rangle$  of the  $K$ -twisted transfer matrix (1.47) with respective eigenvalues  $\epsilon\tau_P$  and  $\epsilon\tau_Q$  coincide and are given by :*

$$\begin{aligned} \langle P, \epsilon | \sigma_n^- | Q, \epsilon \rangle &= \langle P, \epsilon | \sigma_n^+ | Q, \epsilon \rangle \\ &= \epsilon e^{-\sum_j (p_j - \xi_j)} \frac{\prod_{k=1}^{n-1} \tau_P(\xi_k)}{\prod_{k=1}^n \tau_Q(\xi_k)} \\ &\quad \times \frac{\det_N [\mathcal{S}^{(e^{-\eta})}(\mathbf{q}|\mathbf{p}) - \mathcal{P}^{(-)}(\mathbf{q}|\mathbf{p}, \xi_n)] - \det_N [\mathcal{S}^{(e^{-\eta})}(\mathbf{q}|\mathbf{p})]}{\det_{1 \leq i, k \leq N} [\coth(\frac{p_k - q_j - \eta}{2})]}, \end{aligned} \quad (3.70)$$

in which  $\mathcal{S}^{(e^{-\eta})}(\mathbf{q}|\mathbf{p})$  is the matrix of the product (3.49), and  $\mathcal{P}^{(-)}(\mathbf{q}|\mathbf{p}, \xi_n)$  is a matrix of rank one with elements

$$[\mathcal{P}^{(-)}(\mathbf{q}|\mathbf{p}, \xi_n)]_{j,k} = \frac{e^{-\xi_n + p_k} a(\xi_n) d(p_k)}{(-2i)^N Q(p_k - \eta) P(p_k + i\pi)} \left[ \frac{Q(\xi_n - \eta)}{P(\xi_n)} \coth \left( \frac{\xi_n - q_j - \eta}{2} \right) - \frac{Q(\xi_n - \eta + i\pi)}{P(\xi_n + i\pi)} \coth \left( \frac{\xi_n - q_j - \eta + i\pi}{2} \right) \right], \quad (3.71)$$

for  $1 \leq j, k \leq N$ .



# Chapter 4

## Finite-size correlation functions

In this chapter we first present our results on the computation of correlation functions of the anti-periodic  $XXX$  and  $XXZ$  chains at zero temperature:

$$F_m = \frac{\langle \psi_g | \prod_{j=1}^m \sigma_j^{\alpha_j} | \psi_g \rangle}{\langle \psi_g | \psi_g \rangle}. \quad (4.1)$$

And the generalisation to the non-diagonal twist  $K$  for the  $XXX$  case can be found in our paper [116].

After the separate state and the determinant representations for the scalar product have been obtained, the next step is to determine the multiple actions of local spin operators on a separate state, which is equivalent to determine the multiple actions of generators of the Yang-Baxter algebra on a separate state with the solution to the quantum inverse scattering problem. The multiple actions on a separate state are naturally expressed in terms of multiple sums over the inhomogeneous parameters in both cases. Here we transform it into multiple contour integrals and re-evaluate it by summing the set of residues outside the contours. In the  $XXX$  model, the set of "other" residues consists of the roots of Baxter polynomial and infinities. While in the  $XXZ$  model, it consists of the roots of Baxter polynomial plus some extra residues forming a "string" depending on the order of the evaluation of the function. Roughly speaking, every residue of this type  $p_i$  in the  $i$ th integral is a function of the integrand variable  $z_{i-1}$  in the previous i.e.  $(i-1)$ th integral.

### 4.1 The finite-size correlation functions

In this section, we explain how to compute the elementary building blocks of these correlation functions<sup>1</sup> in the model in the finite volume starting from the SoV solution presented in chapter 2. In particular, given  $|Q_\tau\rangle$  an eigenstate of the anti-periodic transfer matrix, we consider matrix elements of the form

$$F_{n,n+m-1}(\tau, \epsilon) = \frac{\langle Q_\tau | \prod_{j=1}^m E_{n+j-1}^{\epsilon_{2j-1}, \epsilon_{2j}} | Q_\tau \rangle}{\langle Q_\tau | Q_\tau \rangle}, \quad (4.2)$$

for any  $\epsilon \equiv (\epsilon_1, \epsilon_2, \dots, \epsilon_{2m}) \in \{1, 2\}^{2m}$ . Here  $E^{\epsilon_1, \epsilon_2}$   $\epsilon_1, \epsilon_2 \in \{1, 2\}$ , stands for the  $2 \times 2$  elementary matrix with the matrix elements  $(E^{\epsilon_1, \epsilon_2})_{i,j} = \delta_{i, \epsilon_1} \delta_{j, \epsilon_2}$ . At this stage we use the notation  $|Q_\tau\rangle$  for both the  $XXX$  and  $XXZ$  chains (we fix  $|Q_\tau\rangle = |Q_\tau, +\rangle$ ) as the discussion is general for

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<sup>1</sup>These are also called the matrix elements of the density matrix of a chain segment of length  $m$ .



both cases. We explain how to compute the matrix elements (4.2) in a convenient form for the consideration of the homogeneous limit and the thermodynamic limit which will be taken in the next section.

As in the periodic case [80], we use the solution of the quantum inverse problem [81, 82, 83] to reconstruct the elementary matrices acting on the  $n$ -th site of the chain to some elements of the monodromy matrix dressed by a product of the anti-periodic transfer matrices evaluated at the inhomogeneity parameters. It is indeed easy to show that [143, 146]:

**Proposition 4.1.1.** *Let  $E_n^{\epsilon_1, \epsilon_2} \in \text{End } V_n$ ,  $(\epsilon_1, \epsilon_2) \in \{1, 2\}^2$ , be an elementary matrix acting on the  $n$ -th site of the chain. Then*

$$\begin{aligned} E_n^{\epsilon_1, \epsilon_2} &= \prod_{k=1}^{n-1} \mathcal{T}(\xi_k) \cdot [\sigma^x T(\xi_n)]_{\epsilon_2, \epsilon_1} \cdot \prod_{k=1}^n [\mathcal{T}(\xi_k)]^{-1} \\ &= \prod_{k=1}^{n-1} \mathcal{T}(\xi_k) \cdot [T(\xi_n)]_{3-\epsilon_2, \epsilon_1} \cdot \prod_{k=1}^n [\mathcal{T}(\xi_k)]^{-1}, \end{aligned} \quad (4.3)$$

where  $\mathcal{T}(\lambda)$  and  $T(\lambda)$  denote the twisted transfer matrix and the monodromy matrix respectively for both  $XXX$  and  $XXZ$  chain.

Hence, the mean value on an eigenstate  $|Q_\tau\rangle$  of a product of such elementary operators at the adjacent sites is given by

$$\begin{aligned} \langle Q_\tau | \prod_{j=1}^m E_{n+j-1}^{\epsilon_{2j-1}, \epsilon_{2j}} | Q_\tau \rangle &= \frac{\prod_{k=1}^{n-1} \tau(\xi_k)}{\prod_{k=1}^{n+m-1} \tau(\xi_k)} \\ &\quad \times \langle Q_\tau | T_{3-\epsilon_{2n}, \epsilon_{2n-1}}(\xi_n) \cdots T_{3-\epsilon_{2(n+m-1)}, \epsilon_{2(n+m-1)-1}}(\xi_{n+m}) | Q_\tau \rangle. \end{aligned} \quad (4.4)$$

Therefore, to have access to the correlation functions, it is sufficient to compute the generic action of a product of elements of the monodromy matrix on an eigenstate and take the consequent scalar product.

Note that, as in the periodic case [80], the only effect of a translation on the chain is a numerical factor given by a product of the corresponding transfer matrix eigenvalues. For simplicity, we shall from now on restrict our study to the matrix elements of the form:

$$F_m(\tau, \epsilon) \equiv F_{1,m}(\tau, \epsilon) = \frac{\langle Q_\tau | \prod_{j=1}^m E_j^{\epsilon_{2j-1}, \epsilon_{2j}} | Q_\tau \rangle}{\langle Q_\tau | Q_\tau \rangle} \quad (4.5)$$

$$= \frac{\langle Q_\tau | T_{3-\epsilon_2, \epsilon_1}(\xi_1) \cdots T_{3-\epsilon_{2m}, \epsilon_{2m-1}}(\xi_m) | Q_\tau \rangle}{\prod_{k=1}^m \tau(\xi_k) \langle Q_\tau | Q_\tau \rangle}. \quad (4.6)$$

Let us also remark that since each eigenstate  $|Q_\tau\rangle$  of the anti-periodic transfer matrix is also an eigenstate of the operator  $\Gamma^x = \otimes_{n=1}^N \sigma_n^x$  (see (1.98)), one has the following relation among the elementary building blocks:

$$\begin{aligned} F_m(\tau, \epsilon) &= \frac{\langle Q_\tau | \Gamma^x \prod_{j=1}^m E_j^{\epsilon_{2j-1}, \epsilon_{2j}} \Gamma^x | Q_\tau \rangle}{\langle Q_\tau | Q_\tau \rangle} = \frac{\langle Q_\tau | \prod_{j=1}^m E_j^{3-\epsilon_{2j-1}, 3-\epsilon_{2j}} | Q_\tau \rangle}{\langle Q_\tau | Q_\tau \rangle} \\ &= F_m(\tau, 3 - \epsilon), \end{aligned} \quad (4.7)$$

in which the  $2m$ -tuple  $3 - \epsilon$  is defined in terms of the  $2m$ -tuple  $\epsilon \equiv (\epsilon_1, \dots, \epsilon_{2m})$  as  $3 - \epsilon \equiv (3 - \epsilon_1, \dots, 3 - \epsilon_{2m})$ .

### 4.1.1 The left action on separate states

In this section, we compute the generic action of a product of matrix elements of the monodromy matrix on a left separate state  $\langle Q|$  of the form

$$\langle Q| = \sum_{\mathbf{h} \in \{0,1\}^N} \prod_{n=1}^N Q(\xi_n^{(h_n)}) V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) |\mathbf{h}\rangle, \quad (4.8)$$

where in the  $XXZ$  case  $Q(\lambda) = \prod_{k=1}^R (\lambda - q_k)$  is a polynomial of degree  $R \leq N$ , and while in the  $XXX$  case  $Q(\lambda) = \prod_{k=1}^N \sinh(\frac{\lambda - q_k}{2})$  is a trigonometric polynomial of double periodicity satisfying  $Q(\xi_n - \eta)/Q(\xi_n) = Q(\xi_n - \eta + i\pi)/Q(\xi_n + i\pi)$  for  $\forall n \in \{1, \dots, N\}$  (in both cases we do not require  $Q(\lambda)$  to be a solution to the TQ-equation (1.75)). Our starting point is the action of the monodromy matrix elements  $D(\lambda), C(\lambda), B(\lambda)$  (1.56)-(1.58) and  $A(\lambda)$  (1.63) on the left SoV basis.

**Remark 4.1.** *In the  $XXX$  chain, instead of computing the action on a state of the form (4.8) using (1.56)-(1.58) and (1.63), we could alternatively compute the multiple actions of a product of transfer matrix elements directly on a Bethe-type state of the form (1.86) using the Yang-Baxter commutation relations, in the spirit of what is done for the model solved by the Bethe Ansatz [80]. However, the fact that the transfer matrix eigenstates can be re-expressed as Bethe-type states involving the multiple actions of an element of the monodromy matrix as in (1.86)-(1.87) is not completely general in the SoV approach, but rather a specificity of models for which the  $Q$ -functions have the same functional form as the transfer matrix eigenfunctions of the model. For instance, it is not true in the anti-periodic  $XXZ$  model, for which the  $Q$ -functions have a double periodicity with respect to the transfer matrix eigenfunctions of the model [115]. Therefore, to remain as general as possible, it is better to start directly from (4.8) and (1.56)-(1.58), (1.63).*

Since we need ultimately to evaluate this action only at the inhomogeneity parameters (see (4.3)), it is more convenient to consider the operators  $\bar{T}_{\epsilon, \epsilon'}(\lambda)$  defined as

$$\bar{T}_{\epsilon, \epsilon'}(\lambda) = \begin{cases} D^{-1}(\lambda + \eta) C(\lambda + \eta) B(\lambda) & \text{if } (\epsilon, \epsilon') = (1, 1), \\ T_{\epsilon, \epsilon'}(\lambda) & \text{otherwise.} \end{cases} \quad (4.9)$$

instead of  $T_{\epsilon, \epsilon'}(\lambda)$ . Indeed, since  $\det_q T(\xi_i + \eta) = 0$ , it follows from (1.24) that

$$\bar{T}_{\epsilon, \epsilon'}(\xi_i) = T_{\epsilon, \epsilon'}(\xi_i) \quad \forall i \in \{1, \dots, N\}, \quad \forall \epsilon, \epsilon' \in \{1, 2\}. \quad (4.10)$$

Thus the formula (4.3) can be written in terms of the matrix elements  $\bar{T}_{\epsilon, \epsilon'}$  instead of  $T_{\epsilon, \epsilon'}$ . Note that (4.9) is well defined as soon as  $\lambda \notin \{\xi_i - \eta, \xi_i - 2\eta \mid i = 1, \dots, N\}$  since  $D(\lambda)$  is invertible for any  $\lambda \neq \xi_i, \xi_i - \eta, i = 1, \dots, N$ . The action of  $\bar{A}(\lambda) \equiv \bar{T}_{1,1}(\lambda)$  on a SoV state  $\langle \mathbf{h}|$  is then slightly simpler than the action of  $A(\lambda)$  (1.63).

It is easy to compute the action of the operators  $\bar{T}_{\epsilon, \epsilon'}(\lambda)$  on the separate state (4.8). We obtain

$$\langle Q| D(\lambda) = \sum_{\mathbf{h}} d_{\mathbf{h}}(\lambda) \prod_{n=1}^N Q(\xi_n^{(h_n)}) V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) |\mathbf{h}\rangle, \quad (4.11)$$

$$\begin{aligned}
\langle Q| B(\lambda) &= - \sum_{b=1}^N a(\xi_b) \sum_{\mathbf{h}} \delta_{h_b,1} \prod_{n=1}^N Q(\xi_n^{(h_n)}) \prod_{\substack{n=1 \\ n \neq b}}^N \frac{\varphi(\lambda - \xi_n^{(h_n)})}{\varphi(\xi_b^{(1)} - \xi_n^{(h_n)})} V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle T_b^- \mathbf{h} | \\
&= - \sum_{b=1}^N \frac{a(\xi_b)}{\varphi(\lambda - \xi_b)} \frac{Q(\xi_b - \eta)}{Q(\xi_b)} \sum_{\mathbf{h}} \delta_{h_b,0} \frac{d_{\mathbf{h}}(\lambda) \prod_{n=1}^N Q(\xi_n^{(h_n)})}{\prod_{n \neq b} \varphi(\xi_b - \xi_n^{(h_n)})} \\
&\quad \times V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle \mathbf{h} |, \tag{4.12}
\end{aligned}$$

$$\begin{aligned}
\langle Q| C(\lambda) &= \sum_{b=1}^N d(\xi_b^{(1)}) \sum_{\mathbf{h}} \delta_{h_b,0} \prod_{n=1}^N Q(\xi_n^{(h_n)}) \prod_{\substack{n=1 \\ n \neq b}}^N \frac{\varphi(\lambda - \xi_n^{(h_n)})}{\varphi(\xi_b - \xi_n^{(h_n)})} V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle T_b^+ \mathbf{h} | \\
&= \sum_{b=1}^N \frac{d(\xi_b^{(1)})}{\varphi(\lambda - \xi_b^{(1)})} \frac{Q(\xi_b)}{Q(\xi_b - \eta)} \sum_{\mathbf{h}} \delta_{h_b,1} \frac{d_{\mathbf{h}}(\lambda) \prod_{n=1}^N Q(\xi_n^{(h_n)})}{\prod_{n \neq b} \varphi(\xi_b - \xi_n^{(h_n)})} \\
&\quad \times V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle \mathbf{h} |. \tag{4.13}
\end{aligned}$$

And a similar (though more involved) expression can be obtained for the action of  $\bar{A}(\lambda)$  on  $\langle Q|$ .

It is obviously possible, from these formulas, to compute the multiple actions of any string of the operators  $\bar{T}_{\epsilon_2, \epsilon_1}(\lambda_1) \bar{T}_{\epsilon_4, \epsilon_3}(\lambda_2) \dots \bar{T}_{\epsilon_{2m}, \epsilon_{2m-1}}(\lambda_m)$  on the state  $\langle Q|$  as a multiple sum over choices of the inhomogeneity parameters along the chain, but such an expression would not be convenient for the consideration of the homogeneous limit. Therefore, we now explain how to write this action in terms of a multiple contour integral that we can transform into a more convenient form for the consideration of the homogeneous limit. The process and result are explained as follows:

**Proposition 4.1.1.** *Let  $\lambda$  be a generic parameter. The left action of the operator  $\bar{T}_{\epsilon_2, \epsilon_1}(\lambda)$ ,  $\epsilon_1, \epsilon_2 \in \{1, 2\}$ , on a generic separate state  $\langle Q|$  of the form (4.8) can be written as the following sum of contour integrals:*

$$\begin{aligned}
\langle Q| \bar{T}_{\epsilon_2, \epsilon_1}(\lambda) &= \sum_{\mathbf{h}} d_{\mathbf{h}}(\lambda) \prod_{n=1}^N Q(\xi_n^{(h_n)}) \left( - \oint_{\Gamma_2} \frac{dz_2}{2\pi i} \frac{a(z_2)}{\varphi(\lambda - z_2)} \frac{Q(z_2 - \eta)}{d_{\mathbf{h}}(z_2)} \frac{Q(z_2)}{Q(z_2)} \right)^{2-\epsilon_2} \\
&\quad \times \left( \oint_{\Gamma_1} \frac{dz_1}{2\pi i} \frac{d(z_1)}{\varphi(\lambda - z_1)} \frac{Q(z_1 + \eta)}{d_{\mathbf{h}}(z_1)} \frac{Q(z_1)}{Q(z_1)} \right)^{2-\epsilon_1} \left( \frac{\varphi(z_1 - z_2)}{\varphi(z_1 - z_2 + \eta)} \right)^{(2-\epsilon_1)(2-\epsilon_2)} \\
&\quad \times V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle \mathbf{h} |, \tag{4.14}
\end{aligned}$$

in which the contour  $\Gamma_2$  surrounds counter-clockwise the points  $\xi_n$ ,  $1 \leq n \leq N$ , and with no other poles in the integrand, whereas the contour  $\Gamma_1$  surrounds counter-clockwise the points  $\xi_n - \eta$ ,  $1 \leq n \leq N$ , the point  $z_2 - \eta$  if  $\epsilon_2 = 1$ , and with no other poles in the integrand.

Similarly, for generic parameters  $\lambda_1, \dots, \lambda_m$ , the multiple actions of a product of operators  $\bar{T}_{\epsilon_2, \epsilon_1}(\lambda_1) \bar{T}_{\epsilon_4, \epsilon_3}(\lambda_2) \dots \bar{T}_{\epsilon_{2m}, \epsilon_{2m-1}}(\lambda_m)$ ,  $\epsilon_i \in \{1, 2\}$ ,  $1 \leq i \leq 2m$ , on a generic separate state  $\langle Q|$

of the form (4.8) can be written as the following sum of contour integrals:

$$\begin{aligned}
\langle Q | \bar{T}_{\epsilon_2, \epsilon_1}(\lambda_1) \bar{T}_{\epsilon_4, \epsilon_3}(\lambda_2) \dots \bar{T}_{\epsilon_{2m}, \epsilon_{2m-1}}(\lambda_m) &= \sum_{\mathbf{h}} \prod_{j=1}^m d_{\mathbf{h}}(\lambda_j) \prod_{n=1}^N Q(\xi_n^{(h_n)}) \\
&\times \prod_{j=m}^1 \left[ \left( - \oint_{\Gamma_{2j}} \frac{dz_{2j}}{2\pi i \varphi(\lambda_j - z_{2j})} \frac{a(z_{2j})}{d_{\mathbf{h}}(z_{2j})} \frac{Q(z_{2j} - \eta)}{Q(z_{2j})} \prod_{k=1}^{j-1} \frac{\varphi(z_{2j} - \lambda_k - \eta)}{\varphi(z_{2j} - \lambda_k)} \right)^{2-\epsilon_{2j}} \right. \\
&\times \left. \left( \oint_{\Gamma_{2j-1}} \frac{dz_{2j-1}}{2\pi i \varphi(\lambda_j - z_{2j-1})} \frac{d(z_{2j-1})}{d_{\mathbf{h}}(z_{2j-1})} \frac{Q(z_{2j-1} + \eta)}{Q(z_{2j-1})} \prod_{k=1}^{j-1} \frac{\varphi(z_{2j-1} - \lambda_k + \eta)}{\varphi(z_{2j-1} - \lambda_k)} \right)^{2-\epsilon_{2j-1}} \right] \\
&\times \prod_{1 \leq j < k \leq 2m} \left( \frac{\varphi(z_j - z_k)}{\varphi(z_j - z_k + (-1)^k \eta)} \right)^{(2-\epsilon_j)(2-\epsilon_k)} V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle \mathbf{h} |, \quad (4.15)
\end{aligned}$$

in which the contours  $\Gamma_{2j}$  surround counter-clockwise the points  $\xi_n$ ,  $1 \leq n \leq N$ , the points  $z_{2k-1} + \eta$ ,  $k > j$ , and with no other poles in the integrand, whereas the contours  $\Gamma_{2j-1}$  surround counter-clockwise the points  $\xi_n - \eta$ ,  $1 \leq n \leq N$ , the points  $z_{2k} - \eta$ ,  $k \geq j$ , and with no other poles in the integrand.

*Proof.* The expression (4.14) clearly coincides with (4.11) in the case  $(\epsilon_2, \epsilon_1) = (2, 2)$ .

Let us now consider the action (4.12) of  $\bar{T}_{1,2}(\lambda) = B(\lambda)$  on  $\langle Q |$ . The idea is to see the sum as the development of an integral around a contour by the residue theorem, which leads to the identity:

$$\begin{aligned}
\langle Q | B(\lambda) &= - \oint_{\Gamma(\{\xi_n\}_{n=1 \rightarrow N})} \frac{dz}{2\pi i} \frac{a(z)}{\varphi(\lambda - z)} \frac{Q(z - \eta)}{Q(z)} \\
&\times \sum_{\mathbf{h}} \frac{d_{\mathbf{h}}(\lambda)}{d_{\mathbf{h}}(z)} \prod_{n=1}^N Q(\xi_n^{(h_n)}) V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle \mathbf{h} |, \quad (4.16)
\end{aligned}$$

where the contour  $\Gamma(\{\xi_n\}_{n=1 \rightarrow N})$  surrounds counter-clockwise the points  $\xi_n$ ,  $1 \leq n \leq N$ , with no other pole of the integrand. This result coincides with (4.14) for  $(\epsilon_2, \epsilon_1) = (1, 2)$ .

We can proceed similarly for the action of  $\bar{T}_{2,1}(\lambda) = C(\lambda)$ , rewriting (4.13) as an integral around a contour by the residue theorem, which leads to the identity:

$$\begin{aligned}
\langle Q | C(\lambda) &= \oint_{\Gamma(\{\xi_n - \eta\}_{n=1 \rightarrow N})} \frac{dz}{2\pi i} \frac{d(z)}{\varphi(\lambda - z)} \frac{Q(z + \eta)}{Q(z)} \\
&\times \sum_{\mathbf{h}} \frac{d_{\mathbf{h}}(\lambda)}{d_{\mathbf{h}}(z)} \prod_{n=1}^N Q(\xi_n^{(h_n)}) V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle \mathbf{h} |, \quad (4.17)
\end{aligned}$$

with  $\Gamma(\{\xi_n - \eta\}_{n=1 \rightarrow N})$  surrounding counter-clockwise the points  $\xi_n - \eta$ ,  $1 \leq n \leq N$ , with no other pole of the integrand. This result coincides with (4.14) for  $(\epsilon_2, \epsilon_1) = (2, 1)$ .

Finally, let us consider the action of  $\bar{T}_{1,1}(\lambda) = \bar{A}(\lambda)$  on  $\langle Q |$ , which is the most involved one, as it requires to compute the successive action of  $D^{-1}(\lambda + \eta)$ ,  $C(\lambda + \eta)$ , and  $B(\lambda)$  on the state

$\langle Q |$ . Using (1.56) and (1.57), one can write:

$$\langle Q | \bar{A}(\lambda) = \sum_{b=1}^N \frac{d(\xi_b - \eta)}{\varphi(\lambda - \xi_b + \eta)} \frac{Q(\xi_b)}{Q(\xi_b - \eta)} \sum_{\mathbf{h}} \delta_{h_b, 1} \prod_{n=1}^N Q(\xi_n^{(h_n)}) \times \frac{V(\xi_1^{(h_1)}, \dots, \xi_n^{(h_N)})}{\prod_{\ell \neq b} \varphi(\xi_b^{(1)} - \xi_\ell^{(h_\ell)})} \langle \mathbf{h} | B(\lambda), \quad (4.18)$$

which corresponds to the evaluation by the sum over the residues of the following contour integral:

$$\langle Q | \bar{A}(\lambda) = \oint_{\Gamma(\{\xi_n - \eta\}_{n=1 \rightarrow N})} \frac{dz}{2\pi i} \frac{d(z)}{\varphi(\lambda - z)} \frac{Q(z + \eta)}{Q(z)} \times \sum_{\mathbf{h}} \frac{V(\xi_1^{(h_1)}, \dots, \xi_n^{(h_N)})}{d_{\mathbf{h}}(z)} \prod_{n=1}^N Q(\xi_n^{(h_n)}) \langle \mathbf{h} | B(\lambda) \quad (4.19)$$

Using (1.58), now we obtain:

$$\begin{aligned} \langle Q | \bar{A}(\lambda) &= - \sum_{b=1}^N a(\xi_b) \oint_{\Gamma(\{\xi_n - \eta\}_{n=1 \rightarrow N})} \frac{dz}{2\pi i} \frac{d(z)}{\varphi(\lambda - z)} \frac{Q(z + \eta)}{Q(z)} \frac{\varphi(z - \xi_b)}{\varphi(z - \xi_b + \eta)} \frac{Q(\xi_b - \eta)}{Q(\xi_b)} \\ &\times \sum_{\mathbf{h}} \delta_{h_b, 0} \prod_{\ell \neq b} \frac{\varphi(\lambda - \xi_\ell^{(h_\ell)})}{\varphi(\xi_b - \xi_\ell^{(h_\ell)})} \frac{V(\xi_1^{(h_1)}, \dots, \xi_n^{(h_N)})}{d_{\mathbf{h}}(z)} \prod_{n=1}^N Q(\xi_n^{(h_n)}) \langle \mathbf{h} | \\ &= - \oint_{\Gamma(\{\xi_n\}_{n=1 \rightarrow N})} \frac{dz'}{2\pi i} \frac{a(z')}{\varphi(\lambda - z')} \frac{Q(z' - \eta)}{Q(z')} \oint_{\Gamma(\{\xi_n - \eta\}_{n=1 \rightarrow N} \cup \{z' - \eta\})} \frac{dz}{2\pi i} \frac{d(z)}{\varphi(\lambda - z)} \\ &\times \frac{Q(z + \eta)}{Q(z)} \frac{\varphi(z - z')}{\varphi(z - z' + \eta)} \sum_{\mathbf{h}} \frac{d_{\mathbf{h}}(\lambda)}{d_{\mathbf{h}}(z) d_{\mathbf{h}}(z')} \prod_{n=1}^N Q(\xi_n^{(h_n)}) V(\xi_1^{(h_1)}, \dots, \xi_n^{(h_N)}) \langle \mathbf{h} |, \quad (4.20) \end{aligned}$$

in which we have again used the residue theorem to recast the sum as a contour integral over  $z'$ . Note that by doing this the pole at  $\xi_b - \eta$  becomes a pole at  $z' - \eta$ . Hence we have to deform the contour of the integral over  $z$  to take into account the residue at this pole. The expression (4.20) coincides with (4.14) in the case  $(\epsilon_2, \epsilon_1) = (1, 1)$ .

The general result is then obtained by induction along the same lines.  $\square$

The multiple integral representation (4.15) of Proposition 4.1.1 can easily be recast into a more convenient form for the further consideration of the homogeneous limit.

Note that we can successively move the integration contours to encircle the poles at  $q_j$ ,  $1 \leq j \leq N$ , and  $\lambda_k$ ,  $1 \leq k \leq m$  instead of the poles at  $\xi_n, \xi_n - \eta$ ,  $1 \leq n \leq N$ . Due to the different quasi-periodicities of the functions involved, in particular of the  $Q$  function (1.103) for the  $XXZ$  chain, the result of this procedure slightly differs from those for the  $XXX$  chain. In the  $XXX$  case, there will be extra poles at infinities while in the  $XXZ$  case the extra poles come from the previously evaluated residues at the spectral parameters.

## 4.2 Multiple sum representation in the $XXX$ case

For the anti-periodic  $XXX$  chain, we have the following proposition:

**Proposition 4.2.1.** *For the generic parameters  $\lambda_1, \dots, \lambda_m$ , the multiple actions of a product of the operators  $\bar{T}_{\epsilon_2, \epsilon_1}(\lambda_1) \bar{T}_{\epsilon_4, \epsilon_3}(\lambda_2) \dots \bar{T}_{\epsilon_{2m}, \epsilon_{2m-1}}(\lambda_m)$ ,  $\epsilon_i \in \{1, 2\}$ ,  $1 \leq i \leq 2m$ , on a generic separate state  $\langle Q |$  of the form (4.8) can be written as the following sum of contour integrals:*

$$\begin{aligned}
\langle Q | \bar{T}_{\epsilon_2, \epsilon_1}(\lambda_1) \bar{T}_{\epsilon_4, \epsilon_3}(\lambda_2) \dots \bar{T}_{\epsilon_{2m}, \epsilon_{2m-1}}(\lambda_m) &= \sum_{\mathbf{h}} \prod_{j=1}^m d_{\mathbf{h}}(\lambda_j) \prod_{n=1}^N Q(\xi_n^{(h_n)}) \\
&\times \prod_{j=m}^1 \left[ \left( - \oint_{\mathcal{C}_j^\infty} \frac{dz_{2j}}{2\pi i (z_{2j} - \lambda_j)} \frac{a(z_{2j})}{d_{\mathbf{h}}(z_{2j})} \frac{Q(z_{2j} - \eta)}{Q(z_{2j})} \prod_{k=1}^{j-1} \frac{z_{2j} - \lambda_k - \eta}{z_{2j} - \lambda_k} \right)^{2-\epsilon_{2j}} \right. \\
&\times \left. \left( \oint_{\mathcal{C}_j^\infty} \frac{dz_{2j-1}}{2\pi i (z_{2j-1} - \lambda_j)} \frac{d(z_{2j-1})}{d_{\mathbf{h}}(z_{2j-1})} \frac{Q(z_{2j-1} + \eta)}{Q(z_{2j-1})} \prod_{k=1}^{j-1} \frac{z_{2j-1} - \lambda_k + \eta}{z_{2j-1} - \lambda_k} \right)^{2-\epsilon_{2j-1}} \right] \\
&\times \prod_{1 \leq j < k \leq 2m} \left( \frac{z_j - z_k}{z_j - z_k + (-1)^k \eta} \right)^{(2-\epsilon_j)(2-\epsilon_k)} V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle \mathbf{h} |, \quad (4.21)
\end{aligned}$$

where the contours  $\mathcal{C}_j^\infty$   $1 \leq j \leq 2m$ , surround counter-clockwise the points  $q_n$ ,  $1 \leq n \leq R$ ,  $\lambda_\ell$ ,  $1 \leq \ell \leq j$ , the pole at infinity, with no other pole of the integrand.

*Proof.* Let us prove the formula by recursion on  $\ell$ :

$$\begin{aligned}
\langle Q | \bar{T}_{\epsilon_2, \epsilon_1}(\lambda_1) \bar{T}_{\epsilon_4, \epsilon_3}(\lambda_2) \dots \bar{T}_{\epsilon_{2m}, \epsilon_{2m-1}}(\lambda_m) &= \sum_{\mathbf{h}} \prod_{j=1}^m d_{\mathbf{h}}(\lambda_j) \prod_{n=1}^N Q(\xi_n^{(h_n)}) \\
&\times \prod_{j=m}^{\ell} \left[ \left( - \oint_{\Gamma_{2j}} \frac{dz_{2j}}{2\pi i (\lambda_j - z_{2j})} \frac{a(z_{2j})}{d_{\mathbf{h}}(z_{2j})} \frac{Q(z_{2j} - \eta)}{Q(z_{2j})} \prod_{k=1}^{j-1} \frac{z_{2j} - \lambda_k - \eta}{z_{2j} - \lambda_k} \right)^{2-\epsilon_{2j}} \right. \\
&\times \left. \left( \oint_{\Gamma_{2j-1}} \frac{dz_{2j-1}}{2\pi i (\lambda_j - z_{2j-1})} \frac{d(z_{2j-1})}{d_{\mathbf{h}}(z_{2j-1})} \frac{Q(z_{2j-1} + \eta)}{Q(z_{2j-1})} \prod_{k=1}^{j-1} \frac{z_{2j-1} - \lambda_k + \eta}{z_{2j-1} - \lambda_k} \right)^{2-\epsilon_{2j-1}} \right] \\
&\times \prod_{j=\ell-1}^1 \left[ \left( \oint_{\mathcal{C}_j^\infty} \frac{dz_{2j}}{2\pi i (\lambda_j - z_{2j})} \frac{a(z_{2j})}{d_{\mathbf{h}}(z_{2j})} \frac{Q(z_{2j} - \eta)}{Q(z_{2j})} \prod_{k=1}^{j-1} \frac{z_{2j} - \lambda_k - \eta}{z_{2j} - \lambda_k} \right)^{2-\epsilon_{2j}} \right. \\
&\times \left. \left( - \oint_{\mathcal{C}_j^\infty} \frac{dz_{2j-1}}{2\pi i (\lambda_j - z_{2j-1})} \frac{d(z_{2j-1})}{d_{\mathbf{h}}(z_{2j-1})} \frac{Q(z_{2j-1} + \eta)}{Q(z_{2j-1})} \prod_{k=1}^{j-1} \frac{z_{2j-1} - \lambda_k + \eta}{z_{2j-1} - \lambda_k} \right)^{2-\epsilon_{2j-1}} \right] \\
&\times \prod_{1 \leq j < k \leq 2m} \left( \frac{z_j - z_k}{z_j - z_k + (-1)^k \eta} \right)^{(2-\epsilon_j)(2-\epsilon_k)} V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle \mathbf{h} |, \quad (4.22)
\end{aligned}$$

which coincides with (4.15) for  $\ell = 1$  and with (4.21) for  $\ell = m$  with taking into account that for the XXX case  $\varphi(\lambda) = \lambda$ .

Let us suppose that (4.22) holds for a given  $\ell$ ,  $1 \leq \ell < m$ , and let us rewrite the integral over  $z_{2\ell-1}$  using the poles outside of the integration contour  $\Gamma_{2\ell-1}$ . These poles are at the zeroes  $q_1, \dots, q_R$  of  $Q$ , at  $\lambda_j$  for  $j < \ell$  and at infinity. Note that the apparent poles at  $\xi_j$ ,  $1 \leq j \leq N$ , are regular points due to the factor  $d(z_{2\ell-1})$  in the numerator. Similarly, the poles at  $z_{2k-1} + \eta$

for  $k > \ell$  are also regular points since the integral over  $z_{2k-1}$  has to be finally evaluated by its residue at  $z_{2k-1} = \xi_\alpha - \eta$  for some  $\alpha \in \{1, \dots, N\}$ . Finally, the apparent poles at  $z_j - \eta$  for  $j < 2\ell - 1$  are also regular points since the integral over  $z_j$  is first evaluated by its residues at  $\infty$  (and the corresponding factor disappears), at a roots  $q_k$  of  $Q$  (and the factor  $Q(z_{2\ell-1} + \eta)$  in the numerator vanishes) or at  $\lambda_j$  for  $j < \ell$  (and the factor  $z_{2j-1} - \lambda_j + \eta$  in the numerator vanishes). Hence the integral over  $z_{2\ell-1}$  can be rewritten as a contour integral surrounding the points  $q_1, \dots, q_R, \lambda_j$  for  $j < \ell$ , and  $\infty$  with index  $-1$ . One then considers the integral over  $z_{2\ell}$  and shows similarly that the points  $\xi_j - \eta$ ,  $1 \leq j \leq N$ ,  $z_{2k} - \eta$ ,  $k > \ell$ , and  $z_\alpha + \eta$ ,  $\alpha < 2\ell$ , are regular points so that the integral can be written as a contour integral around the poles at  $q_1, \dots, q_R, \lambda_j$  for  $j < \ell$ , and  $\infty$  with index  $-1$ . Hence the representation (4.22) holds also for  $\ell + 1$ .  $\square$

The integral representation (4.21) can be evaluated as a sum over its residues, which leads to:

**Corollary 4.2.1.** *The multiple actions of a product of the operators  $\bar{T}_{\epsilon_2, \epsilon_1}(\lambda_1) \bar{T}_{\epsilon_4, \epsilon_3}(\lambda_2) \dots \bar{T}_{\epsilon_{2m}, \epsilon_{2m-1}}(\lambda_m)$ ,  $\epsilon_i \in \{1, 2\}$ ,  $1 \leq i \leq 2m$ , on a generic separate state  $\langle Q |$  of the form (4.8) can be written as a sum over separate states of the form (4.8) as*

$$\begin{aligned} \langle Q | \bar{T}_{\epsilon_2, \epsilon_1}(\lambda_1) \bar{T}_{\epsilon_4, \epsilon_3}(\lambda_2) \dots \bar{T}_{\epsilon_{2m}, \epsilon_{2m-1}}(\lambda_m) &= \sum_{n_\infty=0}^{m_\epsilon} (-1)^{(m-m_\epsilon+n_\infty)N} \\ &\times [\langle Q | \bar{T}_{\epsilon_2, \epsilon_1}(\lambda_1) \bar{T}_{\epsilon_4, \epsilon_3}(\lambda_2) \dots \bar{T}_{\epsilon_{2m}, \epsilon_{2m-1}}(\lambda_m)]_{n_\infty}, \end{aligned} \quad (4.23)$$

where

$$\begin{aligned} &[\langle Q | \bar{T}_{\epsilon_2, \epsilon_1}(\lambda_1) \bar{T}_{\epsilon_4, \epsilon_3}(\lambda_2) \dots \bar{T}_{\epsilon_{2m}, \epsilon_{2m-1}}(\lambda_m)]_{n_\infty} \\ &= \sum_{(\bar{\epsilon}_1, \dots, \bar{\epsilon}_{2m}) \in \mathcal{E}_{\epsilon, n_\infty}} \sum_{a_1=1}^{(R+1)\bar{\epsilon}_1} \sum_{\substack{a_2=1 \\ a_2 \neq a_1}}^{(R+1)\bar{\epsilon}_2} \dots \sum_{\substack{a_{2m-1}=1 \\ a_{2m-1} \notin \{a_1, \dots, a_{2m-2}\}}}^{(R+m)\bar{\epsilon}_{2m-1}} \sum_{\substack{a_{2m}=1 \\ a_{2m} \notin \{a_1, \dots, a_{2m-1}\}}}^{(R+m)\bar{\epsilon}_{2m}} \\ &\times \prod_{j=1}^m \left( \frac{d(q_{a_{2j-1}}) \prod_{k=1}^{R+j-1} (q_{a_{2j-1}} - q_k + \eta)}{\prod_{\substack{k=1 \\ k \neq a_{2j-1}}}^{R+j} (q_{a_{2j-1}} - q_k)} \right)^{\bar{\epsilon}_{2j-1}} \left( \frac{a(q_{a_{2j}}) \prod_{k=1}^{R+j-1} (q_{a_{2j}} - q_k - \eta)}{\prod_{\substack{k=1 \\ k \neq a_{2j}}}^{R+j} (q_{a_{2j}} - q_k)} \right)^{\bar{\epsilon}_{2j}} \\ &\times \prod_{1 \leq j < k \leq 2m} \left( \frac{q_{a_j} - q_{a_k}}{q_{a_j} - q_{a_k} + (-1)^k \eta} \right)^{\bar{\epsilon}_j \bar{\epsilon}_k} \langle \bar{Q}_{\mathbf{a}, \bar{\epsilon}}^\lambda |. \end{aligned} \quad (4.24)$$

Here we have defined, for a given  $2m$ -tuple  $\epsilon \equiv (\epsilon_1, \dots, \epsilon_{2m})$ ,

$$m_\epsilon = \sum_{j=1}^{2m} (2 - \epsilon_j), \quad (4.25)$$

$$\mathcal{E}_{\epsilon, n_\infty} = \left\{ (\bar{\epsilon}_1, \dots, \bar{\epsilon}_{2m}) \in \{0, 1\}^N \mid \bar{\epsilon}_j \leq 2 - \epsilon_j \text{ and } \sum_{j=1}^{2m} \bar{\epsilon}_j = m_\epsilon - n_\infty \right\}. \quad (4.26)$$

Moreover, we have used the shortcut notation:

$$q_{R+j} = \lambda_j, \quad 1 \leq j \leq m, \quad (4.27)$$

and  $\bar{Q}_{\mathbf{a}, \bar{\epsilon}}^\lambda$  is a polynomial of degree  $R+m-m_\epsilon+n_\infty$  defined in terms of  $Q$ , of the  $\lambda_k$ ,  $1 \leq k \leq m$ , and of the  $a_j$  and the  $\bar{\epsilon}_j$  ( $1 \leq j \leq 2m$ ) as

$$\bar{Q}_{\mathbf{a}, \bar{\epsilon}}^\lambda(\lambda) = Q(\lambda) \frac{\prod_{j=1}^m (\lambda - \lambda_j)}{\prod_{j=1}^{2m} (\lambda - q_{a_j})^{\bar{\epsilon}_j}} = \frac{\prod_{j=1}^{R+m} (\lambda - q_j)}{\prod_{j=1}^{2m} (\lambda - q_{a_j})^{\bar{\epsilon}_j}}. \quad (4.28)$$

*Proof.* We just write the development of the multiple contour integrals (4.21) in terms of the sum on the residues. Here  $0 \leq n_\infty \leq m_\epsilon$  corresponds to the number of residues at infinity that we take so that we organise these sums w.r.t.  $n_\infty$ .  $\square$

Note that, in the expression (4.23)-(4.24), we can now particularise the parameters  $\lambda_i$ ,  $1 \leq i \leq m$ , to be equal to some inhomogeneity parameters. We can therefore directly use (4.23)-(4.24) to express the matrix elements of the form (4.5).

Based on the results of the previous subsection, we can now write any matrix elements of the form (4.5) as a sum over the scalar products of separate states:

$$\begin{aligned} F_m(\tau, \epsilon) &= \prod_{k=1}^m \frac{1}{\tau(\xi_k)} \sum_{n_\infty=0}^{m'_\epsilon} (-1)^{(m-m_{\epsilon'}+n_\infty)N} \\ &\quad \times \sum_{(\bar{\epsilon}_1, \dots, \bar{\epsilon}_{2m}) \in \mathcal{E}_{\epsilon', n_\infty}} \sum_{a_1=1}^{(R+1)\bar{\epsilon}_1} \sum_{\substack{a_2=1 \\ a_2 \neq a_1}}^{(R+1)\bar{\epsilon}_2} \dots \sum_{\substack{a_{2m-1}=1 \\ a_{2m-1} \notin \{a_1, \dots, a_{2m-2}\}}}^{(R+m)\bar{\epsilon}_{2m-1}} \sum_{\substack{a_{2m}=1 \\ a_{2m} \notin \{a_1, \dots, a_{2m-1}\}}}^{(R+m)\bar{\epsilon}_{2m}} \\ &\quad \times \prod_{j=1}^m \left( \frac{d(q_{a_{2j-1}}) \prod_{k=1}^{R+j-1} (q_{a_{2j-1}} - q_k + \eta)}{\prod_{\substack{k=1 \\ k \neq a_{2j-1}}}^{R+j} (q_{a_{2j-1}} - q_k)} \right)^{\bar{\epsilon}_{2j-1}} \left( \frac{a(q_{a_{2j}}) \prod_{k=1}^{R+j-1} (q_{a_{2j}} - q_k - \eta)}{\prod_{\substack{k=1 \\ k \neq a_{2j}}}^{R+j} (q_{a_{2j}} - q_k)} \right)^{\bar{\epsilon}_{2j}} \\ &\quad \times \prod_{1 \leq j < k \leq 2m} \left( \frac{q_{a_j} - q_{a_k}}{q_{a_j} - q_{a_k} + (-1)^k \eta} \right)^{\bar{\epsilon}_j \bar{\epsilon}_k} \frac{\langle \bar{Q}_{\mathbf{a}, \bar{\epsilon}}^\xi | Q_\tau \rangle}{\langle Q_\tau | Q_\tau \rangle}, \quad (4.29) \end{aligned}$$

in which we have defined the  $2m$ -tuple  $\epsilon' \equiv (\epsilon'_1, \dots, \epsilon'_{2m})$  in terms of the  $2m$ -tuple  $\epsilon \equiv (\epsilon_1, \dots, \epsilon_{2m})$  by

$$\epsilon'_{2j-1} = \epsilon_{2j-1}, \quad \epsilon'_{2j} = 3 - \epsilon_{2j}, \quad 1 \leq j \leq m, \quad (4.30)$$

and defined  $m_{\epsilon'}$ ,  $\mathcal{E}_{\epsilon', n_\infty}$  as in (4.25)-(4.26) but in terms of  $\epsilon'$  rather than  $\epsilon$ . Similarly as in (4.31)-(4.32), we have used the shortcut notations:

$$q_{R+j} = \xi_j, \quad 1 \leq j \leq m, \quad (4.31)$$

and  $\bar{Q}_{\mathbf{a}, \bar{\epsilon}}^\xi$  is a polynomial of degree  $R+m-m_{\epsilon'}+n_\infty$  defined in terms of  $Q \equiv Q_\tau$ , of the  $\xi_k$ ,  $1 \leq k \leq m$ , and of the  $a_j$  and the  $\bar{\epsilon}_j$  ( $1 \leq j \leq 2m$ ) as

$$\bar{Q}_{\mathbf{a}, \bar{\epsilon}}^\xi(\lambda) = Q(\lambda) \frac{\prod_{j=1}^m (\lambda - \xi_j)}{\prod_{j=1}^{2m} (\lambda - q_{a_j})^{\bar{\epsilon}_j}} = \frac{\prod_{j=1}^{R+m} (\lambda - q_j)}{\prod_{j=1}^{2m} (\lambda - q_{a_j})^{\bar{\epsilon}_j}}. \quad (4.32)$$

We also recall that  $R$  is the degree of the polynomial  $Q_\tau$ .

This expression (4.29) can be rewritten with similar notations to those used in the periodic case [80].



**Proposition 4.2.1.** For a given  $2m$ -tuple  $\epsilon \equiv (\epsilon_1, \dots, \epsilon_{2m}) \in \{1, 2\}^{2m}$ , let us define the sets  $\alpha_\epsilon^-$  and  $\alpha_\epsilon^+$  as

$$\alpha_\epsilon^- = \{j : 1 \leq j \leq m, \epsilon_{2j-1} = 1\}, \quad \#\alpha_\epsilon^- = s_\epsilon \quad (4.33)$$

$$\alpha_\epsilon^+ = \{j : 1 \leq j \leq m, \epsilon_{2j} = 2\}, \quad \#\alpha_\epsilon^+ = s'_\epsilon. \quad (4.34)$$

Then,

$$\begin{aligned} F_m(\tau, \epsilon) &= \prod_{k=1}^m \frac{1}{\tau(\xi_k)} \sum_{\substack{\bar{\alpha}_\epsilon^- \subset \alpha_\epsilon^- \\ \bar{\alpha}_\epsilon^+ \subset \alpha_\epsilon^+}} (-1)^{(m - \#\bar{\alpha}_\epsilon^- + \#\bar{\alpha}_\epsilon^+)N} \sum_{\{a_j, a'_j\}} \\ &\times \prod_{j \in \bar{\alpha}_\epsilon^-} \left( \frac{d(q_{a_j}) \prod_{\substack{k=1 \\ k \in \mathbf{A}_j}}^{R+j-1} (q_{a_j} - q_k + \eta)}{\prod_{\substack{k=1 \\ k \in \mathbf{A}'_j}}^{R+j} (q_{a_j} - q_k)} \right) \prod_{j \in \bar{\alpha}_\epsilon^+} \left( - \frac{a(q_{a'_j}) \prod_{\substack{k=1 \\ k \in \mathbf{A}'_j}}^{R+j-1} (q_k - q_{a'_j} + \eta)}{\prod_{\substack{k=1 \\ k \in \mathbf{A}_{j+1}}}^{R+j} (q_k - q_{a'_j})} \right) \\ &\times \frac{\langle \bar{Q}_{\mathbf{A}_{m+1}} | Q_\tau \rangle}{\langle Q_\tau | Q_\tau \rangle}. \quad (4.35) \end{aligned}$$

In (4.35), the first summation is taken over all subsets  $\bar{\alpha}_\epsilon^-$  of  $\alpha_\epsilon^-$  and  $\bar{\alpha}_\epsilon^+$  of  $\alpha_\epsilon^+$ , whereas the second summation is taken over the indices  $a_j$  for  $j \in \bar{\alpha}_\epsilon^-$  and  $a'_j$  for  $j \in \bar{\alpha}_\epsilon^+$  such that

$$1 \leq a_j \leq R + j, \quad a_j \in \mathbf{A}_j, \quad 1 \leq a'_j \leq R + j, \quad a'_j \in \mathbf{A}'_j, \quad (4.36)$$

where

$$\mathbf{A}_j = \{b : 1 \leq b \leq R + m, b \neq a_k, a'_k, k < j\}, \quad (4.37)$$

$$\mathbf{A}'_j = \{b : 1 \leq b \leq R + m, b \neq a'_k, k < j \text{ and } b \neq a_k, k \leq j\}. \quad (4.38)$$

Moreover,  $\bar{Q}_{\mathbf{A}_{m+1}}$  is the polynomial of degree  $\#\mathbf{A}_{m+1} = R + m - \#\bar{\alpha}_\epsilon^- - \#\bar{\alpha}_\epsilon^+$  defined in terms of the roots  $q_1, \dots, q_R$  of  $Q_\tau$  and of  $q_{R+j} \equiv \xi_j$ ,  $1 \leq j \leq m$ , as

$$\bar{Q}_{\mathbf{A}_{m+1}}(\lambda) = \prod_{j \in \mathbf{A}_{m+1}} (\lambda - q_j). \quad (4.39)$$

**Remark 4.2.** The set (4.34) and (4.33) are complementary to the set  $\alpha_\epsilon^+$  and  $\alpha_\epsilon^-$  defined in [80] in the periodic case. One recovers the same sets by considering the sets for  $F_m(\tau, 3 - \epsilon)$  using the fact that  $F_m(\tau, \epsilon) = F_m(\tau, 3 - \epsilon)$  (4.7) due to the  $\Gamma^x$  symmetry.

**Remark 4.3.** The sum over the subsets  $\bar{\alpha}_\epsilon^-$  and  $\bar{\alpha}_\epsilon^+$  of  $\alpha_\epsilon^-$  and  $\alpha_\epsilon^+$  can be organised as in (4.29) in terms of the number  $n_\infty$  of residues taken at infinity by writing

$$\sum_{\substack{\bar{\alpha}_\epsilon^- \subset \alpha_\epsilon^- \\ \bar{\alpha}_\epsilon^+ \subset \alpha_\epsilon^+}} = \sum_{n_\infty=0}^{s_\epsilon + s'_\epsilon} \sum_{\substack{\bar{\alpha}_\epsilon^- \subset \alpha_\epsilon^- \\ \bar{\alpha}_\epsilon^+ \subset \alpha_\epsilon^+ \\ \#\bar{\alpha}_\epsilon^- + \#\bar{\alpha}_\epsilon^+ = s_\epsilon + s'_\epsilon - n_\infty}}. \quad (4.40)$$

Each scalar product of separate states appearing in (4.29) or (4.35) can now be expressed in terms of the generalised Slavnov's determinants using the results of [114]. Using Theorem 3.3 of [114], we can write

$$\begin{aligned} \frac{\langle \bar{Q}_{\mathbf{A}_{m+1}} | Q_\tau \rangle}{\langle Q_\tau | Q_\tau \rangle} &= 0 \quad \text{if } m < \#\bar{\alpha}_\epsilon^- + \#\bar{\alpha}_\epsilon^+, \\ &= (-1)^{N(R-\bar{R})} 2^{R-\bar{R}} \frac{\prod_{j=1}^{\bar{R}} \left[ -a(\bar{q}_j) \prod_{k=1}^R (q_k - \bar{q}_j + \eta) \right]}{\prod_{j=1}^R \left[ -a(q_j) \prod_{k=1}^R (q_k - q_j + \eta) \right]} \frac{V(q_R, \dots, q_1)}{V(\bar{q}_{\bar{R}}, \dots, \bar{q}_1)} \\ &\quad \times \frac{\det_{\bar{R}} \mathcal{M}^{(-)}(\mathbf{q} | \bar{\mathbf{q}})}{\det_R \mathcal{N}^{(-)}(\mathbf{q})} \quad \text{if } m \geq \#\bar{\alpha}_\epsilon^- + \#\bar{\alpha}_\epsilon^+. \end{aligned} \quad (4.41)$$

Here we have set

$$\bar{R} = \#\mathbf{A}_{m+1} = R + m - \#\bar{\alpha}_- - \#\bar{\alpha}_+, \quad (4.43)$$

$$\{q_j\}_{j \in \mathbf{A}_{m+1}} = \{\bar{q}_1, \dots, \bar{q}_{\bar{R}}\}. \quad (4.44)$$

Moreover, for  $\bar{R} \geq R$ , the matrix  $\mathcal{M}^{(-)}(\mathbf{q} | \bar{\mathbf{q}})$  is defined in terms of the  $R$ -tuple  $\mathbf{q} = (q_1, \dots, q_R)$  and of the  $\bar{R}$ -tuple  $\bar{\mathbf{q}} = (\bar{q}_1, \dots, \bar{q}_{\bar{R}})$  as

$$[\mathcal{M}^{(-)}(\mathbf{q} | \bar{\mathbf{q}})]_{j,k} = \begin{cases} t(q_j - \bar{q}_k) + \mathbf{a}_Q(\bar{q}_k) t(\bar{q}_k - q_j) & \text{if } j \leq R, \\ (\bar{q}_k)^{j-R-1} + \mathbf{a}_Q(\bar{q}_k) (\bar{q}_k + \eta)^{j-R-1} & \text{if } j > R, \end{cases} \quad (4.45)$$

whereas the matrix  $\mathcal{N}^{(-)}(\mathbf{q})$  is given by

$$[\mathcal{N}^{(-)}(\mathbf{q})]_{j,k} = \frac{\mathbf{a}'_Q(q_j)}{\mathbf{a}_Q(q_j)} \delta_{j,k} + K(q_j - q_k), \quad (4.46)$$

with  $\mathbf{a}_Q$  given in terms of the roots  $\{q_1, \dots, q_R\}$  of  $Q \equiv Q_\tau$  as in (1.80) and

$$t(\lambda) = \frac{\eta}{\lambda(\lambda + \eta)}, \quad K(\lambda) = t(\lambda) + t(-\lambda) = \frac{2\eta}{(\lambda + \eta)(\lambda - \eta)}. \quad (4.47)$$

Note that, for  $\{q_1, \dots, q_R\}$  solution of the anti-periodic Bethe equations  $\mathbf{a}_Q(q_j) = 1$ ,  $j = 1, \dots, R$ , one has

$$\mathcal{M}^{(-)}(\mathbf{q} | \mathbf{q}) = \mathcal{N}^{(-)}(\mathbf{q}). \quad (4.48)$$

### 4.3 Multiple sum representation in the $XXZ$ case

For the anti-periodic  $XXZ$  chain we have the following proposition:

**Proposition 4.3.1.** *For the generic parameters  $\lambda_1, \dots, \lambda_m$ , the multiple actions of a product of the operators  $\bar{T}_{\epsilon_2, \epsilon_1}(\lambda_1) \bar{T}_{\epsilon_4, \epsilon_3}(\lambda_2) \dots \bar{T}_{\epsilon_{2m}, \epsilon_{2m-1}}(\lambda_m)$ ,  $\epsilon_i \in \{1, 2\}$ ,  $1 \leq i \leq 2m$ , on a generic separate state  $\langle Q |$  of the form (4.8) can be written as the following contour integral:*

$$\begin{aligned}
\langle Q | \bar{T}_{\epsilon_2, \epsilon_1}(\lambda_1) \bar{T}_{\epsilon_4, \epsilon_3}(\lambda_2) \dots \bar{T}_{\epsilon_{2m}, \epsilon_{2m-1}}(\lambda_m) &= \sum_{\mathbf{h}} \prod_{j=1}^m d_{\mathbf{h}}(\lambda_j) \prod_{n=1}^N Q(\xi_n^{(h_n)}) \\
&\times \prod_{j=1}^m \left[ \left( \oint_{\mathcal{C}_{2j-1}} \frac{dz_{2j-1}}{4\pi i \sinh(z_{2j-1} - \lambda_j)} \frac{d(z_{2j-1})}{d_{\mathbf{h}}(z_{2j-1})} \frac{Q(z_{2j-1} + \eta)}{Q(z_{2j-1})} \prod_{k=1}^{j-1} \frac{\sinh(z_{2j-1} - \lambda_k + \eta)}{\sinh(z_{2j-1} - \lambda_k)} \right)^{2-\epsilon_{2j-1}} \right. \\
&\times \left. \left( - \oint_{\mathcal{C}_{2j}} \frac{dz_{2j}}{4\pi i \sinh(z_{2j} - \lambda_j)} \frac{a(z_{2j})}{d_{\mathbf{h}}(z_{2j})} \frac{Q(z_{2j} - \eta)}{Q(z_{2j})} \prod_{k=1}^{j-1} \frac{\sinh(z_{2j} - \lambda_k - \eta)}{\sinh(z_{2j} - \lambda_k)} \right)^{2-\epsilon_{2j}} \right] \\
&\times \prod_{1 \leq j < k \leq 2m} \left( \frac{\sinh(z_j - z_k)}{\sinh(z_j - z_k + (-1)^k \eta)} \right)^{(2-\epsilon_j)(2-\epsilon_k)} V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle \mathbf{h} |, \quad (4.49)
\end{aligned}$$

which can be rewritten as

$$\begin{aligned}
\langle Q | \bar{T}_{\epsilon_2, \epsilon_1}(\lambda_1) \bar{T}_{\epsilon_4, \epsilon_3}(\lambda_2) \dots \bar{T}_{\epsilon_{2m}, \epsilon_{2m-1}}(\lambda_m) &= (-1)^N [m - \sum_{j=1}^{2m} (2-\epsilon_j)] \\
&\times \prod_{j=1}^m \left\{ \left[ \oint_{\mathcal{C}_{2j-1}} \frac{dz_{2j-1}}{4\pi i} \frac{d(z_{2j-1})}{\sinh(z_{2j-1} - \lambda_j)} \frac{Q(z_{2j-1} + \eta)}{Q(z_{2j-1})} \prod_{k=1}^{j-1} \frac{\sinh(z_{2j-1} - \lambda_k + \eta)}{\sinh(z_{2j-1} - \lambda_k)} \right. \right. \\
&\times \left. \left. \prod_{k < 2j-1} \left( \frac{\sinh(z_{2j-1} - z_k)}{\sinh(z_{2j-1} - z_k + \eta)} \right)^{2-\epsilon_k} \right]^{2-\epsilon_{2j-1}} \right. \\
&\times \left. \left[ - \oint_{\mathcal{C}_{2j}} \frac{dz_{2j}}{4\pi i} \frac{a(z_{2j})}{\sinh(z_{2j} - \lambda_j)} \frac{Q(z_{2j} - \eta)}{Q(z_{2j})} \prod_{k=1}^{j-1} \frac{\sinh(z_{2j} - \lambda_k - \eta)}{\sinh(z_{2j} - \lambda_k)} \right. \right. \\
&\times \left. \left. \prod_{k < 2j} \left( \frac{\sinh(z_{2j} - z_k)}{\sinh(z_{2j} - z_k - \eta)} \right)^{2-\epsilon_k} \right]^{2-\epsilon_{2j}} \right\} \langle Q_{\mathbf{z}, \epsilon}^\lambda |, \quad (4.50)
\end{aligned}$$

in which  $\langle Q_{\mathbf{z}, \epsilon}^\lambda |$  is the separate state of the form

$$\langle Q_{\mathbf{z}, \epsilon}^\lambda | = \sum_{\mathbf{h} \in \{0,1\}^N} \prod_{n=1}^N Q_{\mathbf{z}, \epsilon}^\lambda(\xi_n^{(h_n)}) V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle \mathbf{h} |, \quad (4.51)$$

defined in terms of the function

$$Q_{\mathbf{z}, \epsilon}^\lambda(\lambda) = Q(\lambda) \frac{\prod_{j=1}^m \sinh(\lambda - \lambda_j)}{\prod_{j=1}^{2m} \sinh(\lambda - z_j)^{2-\epsilon_j}}. \quad (4.52)$$

Here the contours  $\mathcal{C}_{2j}$ ,  $1 \leq j \leq m$ , surround counter-clockwise the points  $q_n$  for  $1 \leq n \leq N$ ,  $\lambda_k$  and  $\lambda_k + i\pi$  for  $1 \leq k \leq j$ ,  $z_\ell + \eta$  and  $z_\ell + \eta + i\pi$  for  $\ell < 2j$ , with no other pole of the integrand. The contours  $\mathcal{C}_{2j-1}$ ,  $1 \leq j \leq m$ , surround counter-clockwise the points  $q_n$  for  $1 \leq n \leq N$ ,  $\lambda_k$  and  $\lambda_k + i\pi$  for  $1 \leq k \leq j$ ,  $z_\ell - \eta$  and  $z_\ell - \eta + i\pi$  for  $\ell < 2j - 1$ , with no other pole of the integrand.

**Remark 4.4.** Note that  $Q_{z,\epsilon}^\lambda$  (4.52) is not a trigonometric polynomial but a ratio of trigonometric polynomials.

*Proof.* Let us first remark that, due to the property (1.101), the integral representation (4.49) can be rewritten as

$$\begin{aligned} \langle Q | \bar{T}_{\epsilon_2, \epsilon_1}(\lambda_1) \bar{T}_{\epsilon_4, \epsilon_3}(\lambda_2) \dots \bar{T}_{\epsilon_{2m}, \epsilon_{2m-1}}(\lambda_m) &= \sum_{\mathbf{h}} \prod_{j=1}^m d_{\mathbf{h}}(\lambda_j) \prod_{n=1}^N Q(\xi_n^{(h_n)}) \\ &\times \prod_{j=m}^1 \left[ \left( - \oint_{\tilde{\Gamma}_{2j}} \frac{dz_{2j}}{4\pi i \sinh(\lambda_j - z_{2j})} \frac{a(z_{2j})}{d_{\mathbf{h}}(z_{2j})} \frac{Q(z_{2j} - \eta)}{Q(z_{2j})} \prod_{k=1}^{j-1} \frac{\sinh(z_{2j} - \lambda_k - \eta)}{\sinh(z_{2j} - \lambda_k)} \right)^{2-\epsilon_{2j}} \right. \\ &\times \left. \left( \oint_{\tilde{\Gamma}_{2j-1}} \frac{dz_{2j-1}}{4\pi i \sinh(\lambda_j - z_{2j-1})} \frac{d(z_{2j-1})}{d_{\mathbf{h}}(z_{2j-1})} \frac{Q(z_{2j-1} + \eta)}{Q(z_{2j-1})} \prod_{k=1}^{j-1} \frac{\sinh(z_{2j-1} - \lambda_k + \eta)}{\sinh(z_{2j-1} - \lambda_k)} \right)^{2-\epsilon_{2j-1}} \right] \\ &\times \prod_{1 \leq j < k \leq 2m} \left( \frac{\sinh(z_j - z_k)}{\sinh(z_j - z_k + (-1)^k \eta)} \right)^{(2-\epsilon_j)(2-\epsilon_k)} V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle \mathbf{h} |, \end{aligned} \quad (4.53)$$

in which the contours  $\tilde{\Gamma}_{2j}$  surround counter-clockwise the points  $\xi_n$  and  $\xi_n + i\pi$ ,  $1 \leq n \leq N$ , the points  $z_{2k-1} + \eta$  and  $z_{2k-1} + \eta + i\pi$ ,  $k > j$ , with no other poles in the integrand, whereas the contours  $\tilde{\Gamma}_{2j-1}$  surround counter-clockwise the points  $\xi_n - \eta$  and  $\xi_n - \eta + i\pi$ ,  $1 \leq n \leq N$ , the points  $z_{2k} - \eta$  and  $z_{2k} - \eta + i\pi$ ,  $k \geq j$ , with no other poles in the integrand.

Let us now prove the formula by recursion on  $\ell$ :

$$\begin{aligned} \langle Q | \bar{T}_{\epsilon_2, \epsilon_1}(\lambda_1) \bar{T}_{\epsilon_4, \epsilon_3}(\lambda_2) \dots \bar{T}_{\epsilon_{2m}, \epsilon_{2m-1}}(\lambda_m) &= \sum_{\mathbf{h}} \prod_{j=1}^m d_{\mathbf{h}}(\lambda_j) \prod_{n=1}^N Q(\xi_n^{(h_n)}) \\ &\times \prod_{j=m}^{\ell} \left[ \left( - \oint_{\tilde{\Gamma}_{2j}} \frac{dz_{2j}}{4\pi i \sinh(\lambda_j - z_{2j})} \frac{a(z_{2j})}{d_{\mathbf{h}}(z_{2j})} \frac{Q(z_{2j} - \eta)}{Q(z_{2j})} \prod_{k=1}^{j-1} \frac{\sinh(z_{2j} - \lambda_k - \eta)}{\sinh(z_{2j} - \lambda_k)} \right)^{2-\epsilon_{2j}} \right. \\ &\times \left. \left( \oint_{\tilde{\Gamma}_{2j-1}} \frac{dz_{2j-1}}{4\pi i \sinh(\lambda_j - z_{2j-1})} \frac{d(z_{2j-1})}{d_{\mathbf{h}}(z_{2j-1})} \frac{Q(z_{2j-1} + \eta)}{Q(z_{2j-1})} \prod_{k=1}^{j-1} \frac{\sinh(z_{2j-1} - \lambda_k + \eta)}{\sinh(z_{2j-1} - \lambda_k)} \right)^{2-\epsilon_{2j-1}} \right] \\ &\times \prod_{j=1}^{\ell-1} \left[ \left( - \oint_{\mathcal{C}_{2j-1}} \frac{dz_{2j-1}}{4\pi i \sinh(\lambda_j - z_{2j-1})} \frac{d(z_{2j-1})}{d_{\mathbf{h}}(z_{2j-1})} \frac{Q(z_{2j-1} + \eta)}{Q(z_{2j-1})} \prod_{k=1}^{j-1} \frac{\sinh(z_{2j-1} - \lambda_k + \eta)}{\sinh(z_{2j-1} - \lambda_k)} \right)^{2-\epsilon_{2j-1}} \right. \\ &\times \left. \left( \oint_{\mathcal{C}_{2j}} \frac{dz_{2j}}{4\pi i \sinh(\lambda_j - z_{2j})} \frac{a(z_{2j})}{d_{\mathbf{h}}(z_{2j})} \frac{Q(z_{2j} - \eta)}{Q(z_{2j})} \prod_{k=1}^{j-1} \frac{\sinh(z_{2j} - \lambda_k - \eta)}{\sinh(z_{2j} - \lambda_k)} \right)^{2-\epsilon_{2j}} \right] \\ &\times \prod_{1 \leq j < k \leq 2m} \left( \frac{\sinh(z_j - z_k)}{\sinh(z_j - z_k + (-1)^k \eta)} \right)^{(2-\epsilon_j)(2-\epsilon_k)} V(\xi_1^{(h_1)}, \dots, \xi_N^{(h_N)}) \langle \mathbf{h} |, \end{aligned} \quad (4.54)$$

which coincides with (4.53) for  $\ell = 1$  and with (4.49) for  $\ell = m$  noticing that  $\varphi(\lambda) = \sinh(\lambda)$  for the  $XXZ$  case.

Let us suppose that (4.54) holds for a given  $n$ ,  $1 \leq \ell < m$ , and let us first consider the integral over the contour  $\tilde{\Gamma}_{2\ell-1}$ . Note that the integrand over  $z_{2\ell-1}$  is a  $2\pi i$ -periodic function of  $z_{2\ell-1}$ , which vanishes when  $\Re(z_{2\ell-1}) \rightarrow \pm\infty$  as  $O(e^{-|\Re(z_{2\ell-1})|})$ . Hence, its integral around a strip of width  $2\pi i$  vanishes. We can therefore rewrite the integral over  $\tilde{\Gamma}_{2\ell-1}$  using the poles outside of this integration contour within this strip of width  $2\pi i$ . These poles are at the zeroes  $q_1, \dots, q_N$  of  $Q$ , at  $\lambda_j$  and  $\lambda_j + i\pi$  for  $j < \ell$ , and at  $z_j - \eta$  and  $z_j - \eta + i\pi$  for  $j < 2\ell - 1 \pmod{2\pi i}$ . Note that the apparent poles at  $\xi_j(+i\pi)$ ,  $1 \leq j \leq N$ , are in fact regular points due to the factor  $d(z_{2\ell-1})$  in the numerator. Similarly, the poles at  $z_{2k-1} + \eta(+i\pi)$  for  $k > \ell$  are also regular points since the integral over  $z_{2k-1}$  has to be finally evaluated by its residue at  $z_{2k-1} = \xi_\alpha - \eta(+i\pi)$  for some  $\alpha \in \{1, \dots, N\}$ . Hence the integral over  $z_{2\alpha-1}$  can be rewritten as a contour integral surrounding, with index  $-1$ , the points  $q_1, \dots, q_N$ ,  $\lambda_j$  and  $\lambda_j + i\pi$  for  $j < n$ , and  $z_\alpha - \eta$  and  $z_\alpha - \eta + i\pi$  for  $\alpha < 2\ell - 1$ .

One then considers the integral over  $z_{2\ell}$  and shows similarly that the points  $\xi_j - \eta(+i\pi)$ ,  $1 \leq j \leq N$ ,  $z_{2k} - \eta(+i\pi)$ ,  $k > \ell$ , are regular points, so that the integral can be written as a contour integral with index  $-1$  around the poles at  $q_1, \dots, q_N$ ,  $\lambda_j$  and  $\lambda_j + i\pi$  for  $j < \ell$ , and  $z_\alpha + \eta$ ,  $z_\alpha + \eta + i\pi$ , for  $\alpha < 2\ell$ .

Hence the representation (4.54) holds also for  $\ell + 1$ .  $\square$

The integral representation (4.50) can now be evaluated as a sum over its residues.

**Corollary 4.3.1.** *The multiple actions of a product of the operators  $\bar{T}_{\epsilon_2, \epsilon_1}(\lambda_1) \bar{T}_{\epsilon_4, \epsilon_3}(\lambda_2) \dots \bar{T}_{\epsilon_{2m}, \epsilon_{2m-1}}(\lambda_m)$ ,  $\epsilon_i \in \{1, 2\}$ ,  $1 \leq i \leq 2m$ , on a generic separate state  $\langle Q |$  of the form (4.8) can be written as a sum over separate states as*

$$\begin{aligned} \langle Q | \bar{T}_{\epsilon_2, \epsilon_1}(\lambda_1) \bar{T}_{\epsilon_4, \epsilon_3}(\lambda_2) \dots \bar{T}_{\epsilon_{2m}, \epsilon_{2m-1}}(\lambda_m) &= (-1)^{(m-m_\epsilon)N} \prod_{j=1}^{2m} \left( \sum_{\bar{q}_j \in \mathcal{Q}_j} + \frac{1}{2} \sum_{\bar{q}_j \in \mathcal{Q}_{\epsilon, j}} \right) \\ &\times \prod_{j=1}^m \left( \frac{d(\bar{q}_{2j-1}) Q(\bar{q}_{2j-1} + \eta) \prod_{k=1}^{j-1} \sinh(\bar{q}_{2j-1} - \lambda_k + \eta) \prod_{k < 2j-1} \sinh(\bar{q}_{2j-1} - \bar{q}_k)}{\prod_{\substack{n=1 \\ q_n \neq \bar{q}_{2j-1}}}^N \sinh\left(\frac{\bar{q}_{2j-1} - q_n}{2}\right) \prod_{\substack{k=1 \\ \lambda_k \neq \bar{q}_{2j-1} \pmod{i\pi}}^j \sinh(\bar{q}_{2j-1} - \lambda_k) \prod_{\substack{k < 2j-1 \\ \bar{q}_k - \eta \neq \bar{q}_{2j-1} \pmod{i\pi}}} \sinh(\bar{q}_{2j-1} - \bar{q}_k + \eta)} \right)^{2-\epsilon_{2j-1}} \\ &\times \left( \frac{-a(\bar{q}_{2j}) Q(\bar{q}_{2j} - \eta) \prod_{k=1}^{j-1} \sinh(\bar{q}_{2j} - \lambda_k - \eta) \prod_{k < 2j} \sinh(\bar{q}_{2j} - \bar{q}_k)}{\prod_{\substack{n=1 \\ q_n \neq \bar{q}_{2j}}}^N \sinh\left(\frac{\bar{q}_{2j} - q_n}{2}\right) \prod_{\substack{k=1 \\ \lambda_k \neq \bar{q}_{2j} \pmod{i\pi}}^j \sinh(\bar{q}_{2j} - \lambda_k) \prod_{\substack{k < 2j \\ \bar{q}_k + \eta \neq \bar{q}_{2j} \pmod{i\pi}}} \sinh(\bar{q}_{2j} - \bar{q}_k - \eta)} \right)^{2-\epsilon_{2j}} \langle Q_{\bar{q}, \epsilon}^\lambda |. \end{aligned} \quad (4.55)$$

Here we have defined, for a given  $2m$ -tuple  $\epsilon \equiv (\epsilon_1, \dots, \epsilon_{2m})$ ,

$$m_\epsilon = \sum_{j=1}^{2m} (2 - \epsilon_j). \quad (4.56)$$

Moreover, the sets  $\mathcal{Q}_j$  and  $\mathcal{Q}_{\epsilon,j}$  are empty if  $\epsilon_j = 2$ , and are defined otherwise as

$$\mathcal{Q}_j = \{q_1, \dots, q_N\} \setminus \{\bar{q}_\ell \bmod i\pi\}_{\ell < j}, \quad (4.57)$$

$$\mathcal{Q}_{\epsilon,2j-1} = \{\lambda_k, \lambda_k + i\pi\}_{1 \leq k \leq j} \cup \{\bar{q}_\ell - \eta, \bar{q}_\ell - \eta + i\pi\}_{\ell < 2j-1} \setminus \{\bar{q}_\ell \bmod i\pi\}_{\ell < 2j-1}, \quad (4.58)$$

$$\mathcal{Q}_{\epsilon,2j} = \{\lambda_k, \lambda_k + i\pi\}_{1 \leq k \leq j} \cup \{\bar{q}_\ell + \eta, \bar{q}_\ell + \eta + i\pi\}_{\ell < 2j} \setminus \{\bar{q}_\ell \bmod i\pi\}_{\ell < 2j}. \quad (4.59)$$

Finally,  $Q_{\bar{q},\epsilon}^\lambda$  is a function which is defined in terms of  $Q$  as

$$Q_{\bar{q},\epsilon}^\lambda(\lambda) = Q(\lambda) \frac{\prod_{j=1}^m \sinh(\lambda - \lambda_j)}{\prod_{j=1}^{2m} \sinh(\lambda - \bar{q}_j)^{2-\epsilon_j}}. \quad (4.60)$$

**Remark 4.5.** The number of non-empty sums in (4.23) is  $m_\epsilon$ .

**Remark 4.6.** The state  $\langle Q_{\bar{q},\epsilon}^\lambda |$  is a separate state in the sense that it can still be written in the form (4.8). But  $Q_{\bar{q},\epsilon}^\lambda$  is a priori no longer a trigonometric polynomial. In general, it is only a ratio of such trigonometric polynomial due to the possible contribution of the extra poles at  $\bar{q}_\ell \pm \eta$ ,  $\bar{q}_\ell \pm \eta + i\pi$  (see (4.58)-(4.59)). Note however that,  $\langle Q_{\bar{q},\epsilon}^\lambda |$  being built from  $Q$  as in (4.60), it still satisfies the property (3.39).

It follows from the previous action that the matrix elements (4.5) can be evaluated as the following multiple sums over ratios of the scalar products:

$$\begin{aligned} F_m(\tau, \epsilon) &= \prod_{k=1}^m \frac{1}{\tau(\xi_k)} (-1)^{(m-\bar{m}_\epsilon)N} \prod_{j=1}^{2m} \left( \sum_{\bar{q}_j \in \bar{\mathcal{Q}}_j} + \frac{1}{2} \sum_{\bar{q}_j \in \bar{\mathcal{Q}}_{\epsilon,j}} \right) \\ &\times \prod_{j=1}^m \left( \frac{d(\bar{q}_{2j-1}) Q(\bar{q}_{2j-1} + \eta) \prod_{k=1}^{j-1} \sinh(\bar{q}_{2j-1} - \lambda_k + \eta) \prod_{k < 2j-1} \sinh(\bar{q}_{2j-1} - \bar{q}_k)}{\prod_{\substack{n=1 \\ q_n \neq \bar{q}_{2j-1}}}^N \sinh\left(\frac{\bar{q}_{2j-1} - q_n}{2}\right) \prod_{\substack{k=1 \\ \lambda_k \neq \bar{q}_{2j-1} \bmod i\pi}}^j \sinh(\bar{q}_{2j-1} - \lambda_k) \prod_{\substack{k < 2j-1 \\ \bar{q}_k - \eta \neq \bar{q}_{2j-1} \bmod i\pi}} \sinh(\bar{q}_{2j-1} - \bar{q}_k + \eta)} \right)^{2-\epsilon_{2j-1}} \\ &\times \left( \frac{-a(\bar{q}_{2j}) Q(\bar{q}_{2j} - \eta) \prod_{k=1}^{j-1} \sinh(\bar{q}_{2j} - \lambda_k - \eta) \prod_{k < 2j} \sinh(\bar{q}_{2j} - \bar{q}_k)}{\prod_{\substack{n=1 \\ q_n \neq \bar{q}_{2j}}}^N \sinh\left(\frac{\bar{q}_{2j} - q_n}{2}\right) \prod_{\substack{k=1 \\ \lambda_k \neq \bar{q}_{2j} \bmod i\pi}}^j \sinh(\bar{q}_{2j} - \lambda_k) \prod_{\substack{k < 2j \\ \bar{q}_k + \eta \neq \bar{q}_{2j} \bmod i\pi}} \sinh(\bar{q}_{2j} - \bar{q}_k - \eta)} \right)^{\epsilon_{2j}-1} \frac{\langle \bar{Q}_{\bar{q},\epsilon}^\xi | Q_\tau \rangle}{\langle Q_\tau | Q_\tau \rangle}. \quad (4.61) \end{aligned}$$

Here we have defined, for a given  $2m$ -tuple  $\epsilon \equiv (\epsilon_1, \dots, \epsilon_{2m})$ ,

$$\bar{m}_\epsilon = \sum_{j=1}^m (2 - \epsilon_{2j-1}) + \sum_{j=1}^m (\epsilon_{2j} - 1) = \sum_{j=1}^m (1 + \epsilon_{2j} - \epsilon_{2j-1}). \quad (4.62)$$

Moreover, the sets  $\bar{\mathcal{Q}}_{2j-1}$  and  $\bar{\mathcal{Q}}_{\epsilon,2j-1}$  are empty if  $\epsilon_{2j-1} = 2$ , and are defined otherwise as

$$\bar{\mathcal{Q}}_{2j-1} = \{q_1, \dots, q_N\} \setminus \{\bar{q}_\ell \bmod i\pi\}_{\ell < 2j-1}, \quad (4.63)$$

$$\bar{\mathcal{Q}}_{\epsilon,2j-1} = \{\lambda_k, \lambda_k + i\pi\}_{1 \leq k \leq j} \cup \{\bar{q}_\ell - \eta, \bar{q}_\ell - \eta + i\pi\}_{\ell < 2j-1} \setminus \{\bar{q}_\ell \bmod i\pi\}_{\ell < 2j-1}, \quad (4.64)$$

whereas the sets  $\bar{Q}_{2j}$  and  $\bar{Q}_{\epsilon,2j}$  are empty if  $\epsilon_{2j} = 1$ , and are defined otherwise as

$$\bar{Q}_{2j} = \{q_1, \dots, q_N\} \setminus \{\bar{q}_\ell \bmod i\pi\}_{\ell < 2j}, \quad (4.65)$$

$$\bar{Q}_{\epsilon,2j} = \{\lambda_k, \lambda_k + i\pi\}_{1 \leq k \leq j} \cup \{\bar{q}_\ell + \eta, \bar{q}_\ell + \eta + i\pi\}_{\ell < 2j} \setminus \{\bar{q}_\ell \bmod i\pi\}_{\ell < 2j}. \quad (4.66)$$

Finally,  $\bar{Q}_{\bar{q},\epsilon}^\xi$  is a function which is defined in terms of  $Q$  as

$$\bar{Q}_{\bar{q},\epsilon}^\xi(\lambda) = Q(\lambda) \prod_{j=1}^m \frac{\sinh(\lambda - \xi_j)}{\sinh(\lambda - \bar{q}_{2j-1})^{2-\epsilon_{2j-1}} \sinh(\lambda - \bar{q}_{2j})^{\epsilon_{2j-1}}}. \quad (4.67)$$

**Remark 4.7.** Here again, as in Corollary 4.3.1, the notation means that there are only  $\bar{m}_\epsilon$  non-empty sums. Moreover, the function  $\bar{Q}_{\bar{q},\epsilon}^\xi$  is in general not a trigonometric polynomial, but a ratio of trigonometric polynomials.

# Chapter 5

## The correlation functions in the thermodynamic limit

In this chapter we will show explicitly that for the  $XXX$  case the contribution of the poles at infinity vanishes in the thermodynamic limit. In this limit for the zero-temperature correlation functions, we recover the multiple integral representation that were previously obtained through the study of the periodic case by the Bethe Ansatz [80] and the study of the infinite volume model by the  $q$ -vertex operator approach [79]. We will explain our method using the anti-periodic boundary condition. Moreover, in our paper [116], we show that this method can easily be generalised to the case of a more general non-diagonal twist. There we recover in the thermodynamic limit the same multiple integral representation as in the periodic or the anti-periodic case. Hence we have proved the independence of the thermodynamic limit of the correlation functions with respect to the particular form of the boundary twist.

As for the  $XXZ$  case, the task to show the vanishing and non-vanishing contributions in the thermodynamic limit from the summand in (4.61) is more complicated and it is still in progress. We will show some important intermediate results concerning terms that give back the multiple integral representation of [80].

### 5.1 The $XXX$ case

We now explain how to take the thermodynamic limit of the result obtained in the previous section for  $|Q_\tau\rangle$  being one of the ground state of (1.5) in the homogeneous limit. This will lead to the multiple integral representations for the zero-temperature correlation functions of the anti-periodic  $XXX$  chain in the thermodynamic limit which coincide in this limit with the results obtained in the periodic case in [80] and directly with the infinite size model in [79].

#### 5.1.1 The vanishing and non-vanishing terms in the thermodynamic limit

In this subsection, we find the conditions under which the terms of the expansion (4.35) are non-zero in the thermodynamic limit for  $|Q_\tau\rangle$  being the ground state of the  $XXX$  chain (1.5).

We first compute the ratio of the scalar products appearing in the last line of (4.35) in the thermodynamic limit.



**Proposition 5.1.1.** *Let  $Q$  be a polynomial of the form*

$$Q(\lambda) = \prod_{j=1}^R (\lambda - q_j) \quad (5.1)$$

with the roots  $q_1, \dots, q_R$  solving the system of the anti-periodic Bethe equations  $\mathbf{a}_Q(q_j) = 1$ ,  $j = 1, \dots, R$ , where  $\mathbf{a}_Q$  is defined as in (1.80). We further suppose that  $R$  should scale as  $N$  in the thermodynamic limit and that the roots  $q_1, \dots, q_R$  become in these limits distributed on the real axis according to the density  $\rho_{\text{tot}}$  (2.21), (2.10).

Let  $\bar{Q}$  be a polynomial built from  $Q$  in the form:

$$\bar{Q}(\lambda) = \prod_{j=1}^{R'} (\lambda - q_{\sigma_j}) \prod_{k=1}^{m'} (\lambda - \xi_{\pi_k}) \quad (5.2)$$

where  $\sigma$  and  $\pi$  are permutations of  $\{1, \dots, R\}$  and of  $\{1, \dots, N\}$  respectively, and where  $R - R'$  and  $m'$  remain finite in the thermodynamic limit.

Then,

$$\frac{\langle Q | \bar{Q} \rangle}{\langle Q | Q \rangle} = \frac{\langle \bar{Q} | Q \rangle}{\langle Q | Q \rangle} = \begin{cases} 0 & \text{if } R' + m' < R, \\ o\left(\frac{1}{N^{R-R'}}\right) & \text{if } R' + m' > R, \end{cases} \quad (5.3)$$

whereas, if  $R' + m' = R$ ,

$$\begin{aligned} \frac{\langle Q | \bar{Q} \rangle}{\langle Q | Q \rangle} &= \frac{\langle \bar{Q} | Q \rangle}{\langle Q | Q \rangle} \underset{N \rightarrow \infty}{\sim} \prod_{j=1}^{m'} \left\{ \frac{a(\xi_{\pi_j}) \prod_{k=1}^R (q_k - \xi_{\pi_j} + \eta)}{a(q_{\sigma_{R'+j}}) \prod_{k=1}^R (q_k - q_{\sigma_{R'+j}} + \eta)} \prod_{i=1}^{R'} \frac{q_{\sigma_i} - q_{\sigma_{R'+j}}}{q_{\sigma_i} - \xi_{\pi_j}} \right\} \\ &\quad \times \prod_{1 \leq i < j \leq m'} \frac{q_{\sigma_{R'+i}} - q_{\sigma_{R'+j}}}{\xi_{\pi_i} - \xi_{\pi_j}} \det_{1 \leq j, k \leq m'} \frac{\rho(q_{\sigma_{R'+j}} - \xi_{\pi_k} + \eta/2)}{N \rho_{\text{tot}}(q_{\sigma_{R'+j}})}. \end{aligned} \quad (5.4)$$

*Proof.* In the case  $R' + m' < R$ , it was shown in [114] that the ratio of scalar products vanishes (see (4.41)).

In the case  $R' + m' \geq R$ , the ratio of scalar products can be expressed from [114] as a ratio of determinants as in (4.42):

$$\begin{aligned} \frac{\langle Q | \bar{Q} \rangle}{\langle Q | Q \rangle} &= \frac{\langle \bar{Q} | Q \rangle}{\langle Q | Q \rangle} \\ &= (-1)^{N(R'+m'-R)} 2^{R-R'-m'} \frac{\prod_{j=1}^{m'} \left[ -a(\xi_{\pi_j}) \prod_{k=1}^R (q_k - \xi_{\pi_j} + \eta) \right]}{\prod_{j=R'+1}^R \left[ -a(q_{\sigma_j}) \prod_{k=1}^R (q_k - q_{\sigma_j} + \eta) \right]} \\ &\quad \times \prod_{i=1}^{R'} \frac{\prod_{j=R'+1}^R (q_{\sigma_i} - q_{\sigma_j})}{\prod_{j=1}^{m'} (q_{\sigma_i} - \xi_{\pi_j})} \frac{\prod_{R' < i < j \leq R} (q_{\sigma_i} - q_{\sigma_j})}{\prod_{1 \leq i < j \leq m'} (\xi_{\pi_i} - \xi_{\pi_j})} \frac{\det_{R'+m'} \mathcal{M}^{(-)}(\mathbf{q}_\sigma | \bar{\mathbf{q}})}{\det_R \mathcal{N}^{(-)}(\mathbf{q}_\sigma)}, \end{aligned} \quad (5.5)$$

in which we have used the notations of (4.45)-(4.46) and the shortcut notations  $\mathbf{q}_\sigma = (q_{\sigma_1}, \dots, q_{\sigma_R})$  and  $\bar{\mathbf{q}} = (q_{\sigma_1}, \dots, q_{\sigma_{R'}}, \xi_{\pi_1}, \dots, \xi_{\pi_{m'}})$ . More explicitly,  $\mathcal{M}^{(-)}(\mathbf{q}_\sigma | \bar{\mathbf{q}})$  can be written as the following block matrix:

$$\mathcal{M}^{(-)}(\mathbf{q}_\sigma | \bar{\mathbf{q}}) = \begin{pmatrix} \mathcal{M}^{(1,1)} & \mathcal{M}^{(1,2)} \\ \mathcal{M}^{(2,1)} & \mathcal{M}^{(2,2)} \end{pmatrix} \quad (5.6)$$

where  $\mathcal{M}^{(1,1)}$ ,  $\mathcal{M}^{(1,2)}$ ,  $\mathcal{M}^{(2,1)}$  and  $\mathcal{M}^{(2,2)}$  are respectively of size  $R \times R'$ ,  $R \times m'$ ,  $\bar{n} \times R'$  and  $\bar{n} \times m'$ , with  $\bar{n} = R' + m' - R$ , and with elements

$$\mathcal{M}_{j,k}^{(1,1)} = \mathcal{N}_{j,k}, \quad j \leq R, \quad k \leq R', \quad (5.7)$$

$$\mathcal{M}_{j,k}^{(1,2)} = t(q_{\sigma_j} - \xi_{\pi_k}), \quad j \leq R, \quad k \leq m', \quad (5.8)$$

$$\mathcal{M}_{j,k}^{(2,1)} = (q_{\sigma_k})^{j-1} + (q_{\sigma_k} + \eta)^{j-1}, \quad j \leq \bar{n}, \quad k \leq R', \quad (5.9)$$

$$\mathcal{M}_{j,k}^{(2,2)} = \xi_{\pi_k}^{j-1}, \quad j \leq \bar{n}, \quad k \leq m', \quad (5.10)$$

in which we have used the shortcut notation  $\mathcal{N} = \mathcal{N}^{(-)}(\mathbf{q}_\sigma)$ . Hence, the ratio of determinants in (5.5) can be written as

$$\frac{\det_{R'+m'} \mathcal{M}^{(-)}(\mathbf{q}_\sigma | \bar{\mathbf{q}})}{\det_R \mathcal{N}^{(-)}(\mathbf{q}_\sigma)} = \det_{R'+m'} \mathcal{S}, \quad (5.11)$$

where

$$\mathcal{S} = \begin{pmatrix} \mathcal{N}^{-1} \mathcal{M}^{(1,1)} & \mathcal{N}^{-1} \mathcal{M}^{(1,2)} \\ \mathcal{M}^{(2,1)} & \mathcal{M}^{(2,2)} \end{pmatrix}, \quad (5.12)$$

with in particular  $[\mathcal{N}^{-1} \mathcal{M}^{(1,1)}]_{j,k} = \delta_{j,k}$  for  $j \leq R, k \leq R'$ . The thermodynamic limit  $N \rightarrow \infty$  of the matrix elements of  $\mathcal{N}^{-1} \mathcal{M}^{(1,2)}$  can be computed similarly as in the periodic case [80] using the integral equation (2.9):

$$[\mathcal{N}^{-1} \mathcal{M}^{(1,2)}]_{j,k} = \frac{\rho(q_{\sigma_j} - \xi_{\pi_k} + \eta/2)}{N \rho_{\text{tot}}(q_{\sigma_j})} + o\left(\frac{1}{N}\right), \quad (5.13)$$

in which  $\rho$  is given by (2.10) and  $\rho_{\text{tot}}$  by (2.21). In particular, when  $\bar{n} = R' + m' - R = 0$ , we recover the result (5.4).

In the case  $R' + m' > R$ , it is convenient to rewrite  $\mathcal{S}$  (5.12) in terms of blocks of slightly different sizes:

$$\mathcal{S} = \begin{pmatrix} \mathbb{I}_{R'} & \mathcal{S}^{(1,2)} \\ \mathcal{S}^{(2,1)} & \mathcal{S}^{(2,2)} \end{pmatrix}, \quad (5.14)$$

where  $\mathbb{I}_{R'}$  is the identity square matrix of size  $R'$ , and where  $\mathcal{S}^{(1,2)}$ ,  $\mathcal{S}^{(2,1)}$ , and  $\mathcal{S}^{(2,2)}$  are respectively of size  $R' \times m'$ ,  $m' \times R'$  and  $m' \times m'$ , with elements

$$\mathcal{S}_{j,k}^{(1,2)} = [\mathcal{N}^{-1} \mathcal{M}^{(1,2)}]_{j,k} \quad (5.15)$$

$$\mathcal{S}_{j,k}^{(2,1)} = \begin{cases} 0 & \text{if } j \leq R - R', \\ \mathcal{M}_{j-(R-R'),k}^{(2,1)} & \text{if } R - R' < j \leq m', \end{cases} \quad (5.16)$$

$$\mathcal{S}_{j,k}^{(2,2)} = \begin{cases} [\mathcal{N}^{-1} \mathcal{M}^{(1,2)}]_{j+R',k} & \text{if } j \leq R - R', \\ \mathcal{M}_{j-(R-R'),k}^{(2,2)} = \xi_{\pi_k}^{j-1-R+R'} & \text{if } R - R' < j \leq m'. \end{cases} \quad (5.17)$$

Hence,

$$\det_{R'+m'} \mathcal{S} = \det_{m'} \mathcal{S}' \quad (5.18)$$

with  $\mathcal{S}' = \mathcal{S}^{(2,2)} - \mathcal{S}^{(2,1)} \mathcal{S}^{(1,2)}$ , i.e.

$$\mathcal{S}'_{j,k} = [\mathcal{N}^{-1} \mathcal{M}^{(1,2)}]_{j+R',k} = \frac{\rho(q_{\sigma_{j+R'}} - \xi_{\pi_k} + \eta/2)}{N \rho_{\text{tot}}(q_{\sigma_{j+R'}})} + o\left(\frac{1}{N}\right) \quad \text{if } j \leq R - R', \quad (5.19)$$

whereas, for  $1 \leq j \leq m' + R' - R$ ,

$$\mathcal{S}'_{R-R'+j,k} = \mathcal{M}_{j,k}^{(2,2)} - \sum_{\ell=1}^{R'} \mathcal{M}_{j,\ell}^{(2,1)} [\mathcal{N}^{-1} \mathcal{M}^{(1,2)}]_{\ell,k}. \quad (5.20)$$

In particular, the  $(R - R' + 1)$ -th line of  $\mathcal{S}'$  is

$$\begin{aligned} \mathcal{S}'_{R-R'+1,k} &= 1 - 2 \sum_{\ell=1}^{R'} [\mathcal{N}^{-1} \mathcal{M}^{(1,2)}]_{\ell,k} \\ &\xrightarrow{N \rightarrow \infty} 1 - 2 \int_{-\infty}^{\infty} \rho(\lambda - \xi_{\pi_k} + \eta/2) d\lambda = 0, \end{aligned} \quad (5.21)$$

which proves (5.3).  $\square$

**Remark 5.1.** *If we suppose further that the sums in (5.20) can be transformed into integrals  $\forall j$ , we obtain that all the lines of (5.20) vanish in the thermodynamic limit:*

$$\mathcal{S}'_{R-R'+j,k} \xrightarrow{N \rightarrow \infty} \xi_{\pi_k}^{j-1} - \int_{-\infty}^{\infty} [\lambda^{j-1} + (\lambda + \eta)^{j-1}] \rho(\lambda - \xi_{\pi_k} + \eta/2) d\lambda = 0. \quad (5.22)$$

Indeed, setting  $\eta = -i$  and supposing  $|\Im(\xi_{\pi_k} + i/2)| < 1/2$ , we have:

$$\begin{aligned} \int_{-\infty}^{\infty} \lambda^{j-1} \rho(\lambda - \xi_{\pi_k} - i/2) d\lambda - \int_{-\infty}^{\infty} (\lambda - i)^{j-1} \rho(\lambda - \xi_{\pi_k} - i/2 - i) d\lambda \\ = -2\pi i \operatorname{Res}_{\lambda=\xi_{\pi_k}} [\lambda^{j-1} \rho(\lambda - \xi_{\pi_k} - i/2)] = \xi_{\pi_k}^{j-1}, \end{aligned} \quad (5.23)$$

and we can conclude by using the quasi-periodicity property  $\rho(\lambda - i) = -\rho(\lambda)$ . Note however that we do not need (5.22) for  $j > 1$  for the proof of Proposition 5.1.1. It is enough that these lines remain finite in the thermodynamic limit.

As a consequence of this proposition, we can formulate the following corollary:

**Corollary 5.1.1.** *For a given  $2m$ -tuple  $\epsilon \equiv (\epsilon_1, \dots, \epsilon_{2m}) \in \{1, 2\}^{2m}$ , let us define the sets  $\alpha_{\epsilon}^{-}$  and  $\alpha_{\epsilon}^{+}$  of respective cardinality  $s_{\epsilon}$  and  $s'_{\epsilon}$  as in (4.34)- (4.33), and let us consider the matrix element  $F_m(\tau, \epsilon)$  in a state  $|Q_{\tau}\rangle$  with  $Q_{\tau} \equiv Q$  satisfying the same hypothesis as in Proposition 5.1.1. Then*

$$\lim_{N \rightarrow \infty} F_m(\tau, \epsilon) = 0 \quad \text{if } s_{\epsilon} + s'_{\epsilon} \neq m. \quad (5.24)$$

Moreover, if  $s_{\epsilon} + s'_{\epsilon} = m$ , the non-vanishing contribution of  $F_m(\tau, \epsilon)$  in the thermodynamic limit is given by

$$\begin{aligned} \lim_{N \rightarrow \infty} F_m(\tau, \epsilon) &= \lim_{N \rightarrow \infty} \prod_{k=1}^m \frac{1}{\tau(\xi_k)} \sum_{\{a_j, a'_j\}} \prod_{j \in \alpha_{\epsilon}^{-}} \left( \frac{d(q_{a_j}) \prod_{\substack{k=1 \\ k \in \mathbf{A}_j}}^{R+j-1} (q_{a_j} - q_k + \eta)}{\prod_{\substack{k=1 \\ k \in \mathbf{A}'_j}}^{R+j} (q_{a_j} - q_k)} \right) \\ &\quad \times \prod_{j \in \alpha_{\epsilon}^{+}} \left( \frac{a(q_{a'_j}) \prod_{\substack{k=1 \\ k \in \mathbf{A}'_j}}^{R+j-1} (q_k - q_{a'_j} + \eta)}{\prod_{\substack{k=1 \\ k \in \mathbf{A}_{j+1}}^{R+j} (q_k - q_{a'_j})} \right) \frac{\langle \bar{Q}_{\mathbf{A}_{m+1}} | Q_{\tau} \rangle}{\langle Q_{\tau} | Q_{\tau} \rangle}, \end{aligned} \quad (5.25)$$

in which the summation is taken over the indices  $a_j$  for  $j \in \alpha_{\epsilon}^{-}$  and  $a'_j$  for  $j \in \alpha_{\epsilon}^{+}$  satisfying (4.36)-(4.38), and we have used the notation (4.39).

In other words, it means that in the thermodynamic limit we recover the same selection rules (5.24) for the elementary blocks as in the periodic case. Moreover, the only non-vanishing terms in the series (4.35) corresponds to  $\bar{\alpha}_\epsilon^+ = \alpha_\epsilon^+$  and  $\bar{\alpha}_\epsilon^- = \alpha_\epsilon^-$ , i.e. to  $n_\infty = 0$ . This means that the residues of the poles at infinity that appeared when moving the integration contours in the computation of the action of Section 4.1.1 (see Proposition 4.2.1 and Corollary 4.2.1) do not contribute to the thermodynamic limit of the correlation functions.

*Proof.* Let us consider the expansion (4.35) for  $F_m(\tau, \epsilon)$ , which involves multiple sums over the indices  $\{a_j, a'_j\}$ .

For a given term of the sum, the polynomial  $\bar{Q}_{\mathbf{A}_{m+1}}$  is of the form (5.2) with  $R - R'$  equal to the number of indices  $a_j$  or  $a'_j$  in the multiple sums which are taken between 1 and  $R$ . On the other hand, each of the sums over an index  $a_j$  or  $a'_j$  from 1 to  $R$  leads to an integral in the thermodynamic limit provided that it is balanced by a factor  $1/N$ , the other terms of the sums (for  $a_j$  or  $a'_j$  from  $R + 1$  to  $R + m$ ) contributing to order 1 to the thermodynamic limit. Hence, the non-vanishing contributions in the thermodynamic limits correspond to the configurations in the expansion (4.35) for which the ratio of determinants is exactly of order  $O(1/N^{R-R'})$ . This, from Proposition 5.1.1, happens only when the two polynomials  $\bar{Q}_{\mathbf{A}_{m+1}}$  and  $Q_\tau$  are of the same degree  $R$ , i.e. when  $\#\bar{\alpha}_\epsilon^- + \#\bar{\alpha}_\epsilon^+ = m$ .

Since  $\#\bar{\alpha}_\epsilon^- + \#\bar{\alpha}_\epsilon^+ \leq \#\alpha_\epsilon^- + \#\alpha_\epsilon^+ = s_\epsilon + s'_\epsilon$ , the whole sum (4.35) is vanishing in the thermodynamic limit if  $s_\epsilon + s'_\epsilon < m$ , so that

$$\lim_{N \rightarrow \infty} F_m(\tau, \epsilon) = 0 \quad \text{if } s_\epsilon + s'_\epsilon < m. \quad (5.26)$$

If  $s_\epsilon + s'_\epsilon > m$  we use the symmetry (4.7) and the fact that  $s_{3-\epsilon} + s'_{3-\epsilon} < m$  to conclude that

$$\lim_{N \rightarrow \infty} F_m(\tau, \epsilon) = \lim_{N \rightarrow \infty} F_m(\tau, 3 - \epsilon) = 0 \quad \text{if } s_\epsilon + s'_\epsilon > m. \quad (5.27)$$

This proves (5.24).

If now  $s_\epsilon + s'_\epsilon = m$ , the only terms contributing to the thermodynamic limit of  $F_m(\tau, \epsilon)$  in the sum (4.35) are those for which  $\#\bar{\alpha}_\epsilon^- + \#\bar{\alpha}_\epsilon^+ = \#\alpha_\epsilon^- + \#\alpha_\epsilon^+$ , i.e.  $\bar{\alpha}_\epsilon^\pm = \alpha_\epsilon^\pm$ . This also proves (5.25).  $\square$

Note that by using the explicit expression for the transfer matrix eigenvalue evaluated at  $\xi_k$ ,  $k = 1, \dots, m$ ,

$$\tau(\xi_k) = -a(\xi_k) \frac{Q_\tau(\xi_k - \eta)}{Q_\tau(\xi_k)}, \quad (5.28)$$

together with the Bethe equations

$$d(q_{a_j}) = a(q_{a_j}) \frac{Q_\tau(q_{a_j} - \eta)}{Q_\tau(q_{a_j} + \eta)}, \quad \forall a_j \leq R, \quad (5.29)$$

and the observation that  $d(q_{a_j}) = 0$  for any  $a_j > R$ , one can rewrite (5.25) in the following way:

$$\begin{aligned} \lim_{N \rightarrow \infty} F_m(\tau, \epsilon) &= \lim_{N \rightarrow \infty} \prod_{k=1}^m \frac{Q_\tau(\xi_k)}{a(\xi_k) Q_\tau(\xi_k - \eta)} \\ &\times \sum_{\{a_j, a'_j\}} \prod_{j \in \alpha_\epsilon^-} \left( -a(q_{a_j}) \frac{Q_\tau(q_{a_j} - \eta)}{Q_\tau(q_{a_j} + \eta)} \frac{\prod_{k \in \mathbf{A}_j}^{R+j-1} (q_{a_j} - q_k + \eta)}{\prod_{k \in \mathbf{A}'_j}^{R+j} (q_{a_j} - q_k)} \right) \\ &\times \prod_{j \in \alpha_\epsilon^+} \left( a(q_{a'_j}) \frac{\prod_{k \in \mathbf{A}'_j}^{R+j-1} (q_k - q_{a'_j} + \eta)}{\prod_{k \in \mathbf{A}_{j+1}}^{R+j} (q_k - q_{a'_j})} \right) \frac{\langle \bar{Q}_{\mathbf{A}_{m+1}} | Q_\tau \rangle}{\langle Q_\tau | Q_\tau \rangle}, \quad (5.30) \end{aligned}$$

where the summation is taken here over the indices  $a_j$  for  $j \in \alpha_\epsilon^-$  and  $a'_j$  for  $j \in \alpha_\epsilon^+$  such that

$$1 \leq a_j \leq R, \quad a_j \in \mathbf{A}_j, \quad 1 \leq a'_j \leq R + j, \quad a'_j \in \mathbf{A}'_j. \quad (5.31)$$

### 5.1.2 Multiple integral representation for the correlation functions in the thermodynamic limit

Let us now consider, for any  $2m$ -tuple  $\epsilon \equiv (\epsilon_1, \dots, \epsilon_{2m})$ , the matrix elements

$$\mathcal{F}_m(\epsilon) = \lim_{N \rightarrow \infty} \frac{\langle Q_\tau | \prod_{j=1}^m E_j^{\epsilon_{2j-1}, \epsilon_{2j}} | Q_\tau \rangle}{\langle Q_\tau | Q_\tau \rangle}, \quad (5.32)$$

for  $|Q_\tau\rangle$  as an eigenstate of the transfer matrix (1.47) described in the thermodynamic limit by the density of roots  $\rho_{\text{tot}}$ , and which tends to one of the ground states of the anti-periodic XXX chain (1.5) in the homogeneous limit. It follows from Corollary 5.1.1, (5.4) and (5.30) that the terms contributing to the thermodynamic limit in the anti-periodic model are exactly of the same form as the terms contributing to the thermodynamic limit in the periodic case, see formulas (4.6)-(4.7) and (5.3)-(5.4) (in which we use the periodic analogue of (5.28) and (5.29)) of [80]. Hence their thermodynamic limits coincide.

Therefore we obtain the following multiple integral representation for the correlation functions (5.32) in the thermodynamic limit, which coincides with the results of [80, 79]:

$$\begin{aligned} \mathcal{F}_m(\epsilon) &= \delta_{s_\epsilon + s'_\epsilon, m} \prod_{k < l} \frac{\sinh \pi(\xi_k - \xi_l)}{\xi_k - \xi_l} \prod_{j=1}^{s'_\epsilon} \int_{-\infty-i}^{\infty-i} \frac{d\lambda_j}{2i} \prod_{j=s'_\epsilon+1}^m \int_{-\infty}^{\infty} i \frac{d\lambda_j}{2} \prod_{a > b} \frac{\sinh \pi(\lambda_a - \lambda_b)}{\lambda_a - \lambda_b - i} \\ &\times \prod_{a=1}^m \prod_{k=1}^m \frac{1}{\sinh \pi(\lambda_a - \xi_k)} \prod_{j \in \alpha_\epsilon^-} \left[ \prod_{k=1}^{j-1} (\mu_j - \xi_k - i) \prod_{k=j+1}^m (\mu_j - \xi_k) \right] \\ &\times \prod_{j \in \alpha_\epsilon^+} \left[ \prod_{k=1}^{j-1} (\mu'_j - \xi_k + i) \prod_{k=j+1}^m (\mu'_j - \xi_k) \right], \quad (5.33) \end{aligned}$$

in which the sets  $\alpha_\epsilon^-$  and  $\alpha_\epsilon^+$  are defined as in (4.33)-(4.34), and the integration parameters are ordered as

$$(\lambda_1, \dots, \lambda_m) = (\mu'_{j_{\max}}, \dots, \mu'_{j_{\min}}, \mu_{j_{\min}}, \dots, \mu_{j_{\max}}), \quad (5.34)$$

with

$$j'_{\min} = \min\{j \mid j \in \alpha_{\epsilon}^+\}, \quad j'_{\max} = \max\{j \mid j \in \alpha_{\epsilon}^+\}, \quad (5.35)$$

$$j_{\min} = \min\{j \mid j \in \alpha_{\epsilon}^-\}, \quad j_{\max} = \max\{j \mid j \in \alpha_{\epsilon}^-\}. \quad (5.36)$$

In the homogeneous limit ( $\xi_j = -i/2, \forall j$ ) the correlation function  $\mathcal{F}_m(\epsilon)$  has the following form:

$$\begin{aligned} \mathcal{F}_m(\epsilon) &= \delta_{s_{\epsilon}+s'_{\epsilon},m} (-1)^{s_{\epsilon}} (-\pi)^{\frac{m(m+1)}{2}} \prod_{j=1}^{s'_{\epsilon}} \int_{-\infty-i}^{\infty-i} \frac{d\lambda_j}{2\pi} \prod_{j=s'_{\epsilon}+1}^m \int_{-\infty}^{\infty} \frac{d\lambda_j}{2\pi} \prod_{a>b} \frac{\sinh \pi(\lambda_a - \lambda_b)}{\lambda_a - \lambda_b - i} \\ &\times \prod_{j \in \alpha_{\epsilon}^-} \frac{(\mu_j - \frac{i}{2})^{j-1} (\mu_j + \frac{i}{2})^{m-j}}{\cosh^m(\pi\mu_j)} \prod_{j \in \alpha_{\epsilon}^+} \frac{(\mu'_j + \frac{3i}{2})^{j-1} (\mu'_j + \frac{i}{2})^{m-j}}{\cosh^m(\pi\mu'_j)}. \end{aligned} \quad (5.37)$$

So far, we have shown how to compute the (elementary building blocks of the) correlation functions in the XXX chain with anti-periodic boundary conditions. We have obtained similar results for the general non-diagonal twist case in [116]. We have there explicitly shown that, as expected from physical arguments, the ground state correlation functions of the XXX spin 1/2 chain with quasi-periodic boundary conditions do not depend, in the thermodynamic limit, on the particular boundary condition that we consider, i.e. on the particular form of the twist matrix  $K$ . And they coincide with the correlation functions of the periodic chain in the thermodynamic limit, at least for non-diagonal twists. Of course, the same statement can be proven for a diagonal twist by developing the same computations in the Algebraic Bethe Ansatz framework as done in the periodic case in [80].

## 5.2 The XXZ case

Since the representation (4.61) is given as multiple sums over ratios of scalar products, the question is now to compute and evaluate the corresponding scalar products. Due to the different analyticity properties of the involved  $Q$ -functions (which is in general no longer an entire function) and the new form of the scalar products formulas that were obtained in Chapter 3 and in our paper [118], this question is more complicated than in the XXX case and requires a priori the development of new techniques. For the moment, we have not been able to solve entirely this problem. However, for a whole class of terms in the sum (4.61) – the terms that we expect to be the non-vanishing terms in the thermodynamic limit – we can explicitly compute the scalar products and perform the limit  $N \rightarrow \infty$ , hence recovering the multiple integral representation of [80].

To evaluate the sum (4.61), we therefore need to compute the following ratios of scalar products:

$$\frac{\langle \bar{Q}_{\bar{q},\epsilon}^{\xi} | Q \rangle}{\langle Q | Q \rangle} = \lim_{P \rightarrow Q} \frac{\langle \bar{P}_{\bar{p},\epsilon}^{\xi} | Q \rangle}{\langle P | Q \rangle} \quad (5.38)$$

where  $|Q\rangle$  is an eigenstate (the ground state), with  $Q(\lambda) = \prod_{j=1}^N \sinh\left(\frac{\lambda - q_j}{2}\right)$  having roots  $\mathbf{q} \equiv \{q_1, \dots, q_N\}$ , and where  $\langle P|$ ,  $\langle \bar{P}_{\bar{\mathbf{p}}}|$  are separate states built respectively from  $P(\lambda) = \prod_{j=1}^N \sinh\left(\frac{\lambda - p_j}{2}\right)$  and from  $\bar{P}_{\bar{\mathbf{p}},\epsilon}^\xi(\lambda)$  defined from  $P$  as in (4.67). Here the limit has to be understood as  $p_j \rightarrow q_j$ ,  $j = 1 \dots N$ .

Hence we have, with the notations of Chapter 3,

$$\frac{\langle \bar{P}_{\bar{\mathbf{p}},\epsilon}^\xi | Q \rangle}{\langle P | Q \rangle} = \prod_{i=1}^N \frac{\bar{P}_{\bar{\mathbf{p}},\epsilon}^\xi(\xi_i - \eta)}{Q(\xi_i - \eta)} \frac{\mathcal{A}_{\{\xi_1, \dots, \xi_N\}}[-f_{\bar{P}_{\bar{\mathbf{p}},\epsilon}^\xi Q}]}{\mathcal{A}_{\{\xi_1, \dots, \xi_N\}}[-f_{PQ}]} \quad (5.39)$$

with  $f_{PQ}$  given by (3.26) and

$$f_{\bar{P}_{\bar{\mathbf{p}},\epsilon}^\xi Q}(\lambda) = f_{PQ}(\lambda) \prod_{j=m'+1}^m \frac{\sinh(\lambda - \xi_{\pi_j})}{\sinh(\lambda - \eta - \xi_{\pi_j})} \prod_{j=R+1}^N \frac{\sinh(\lambda - \eta - p_{\sigma_j})}{\sinh(\lambda - p_{\sigma_j})} \prod_{\ell=1}^s \frac{\sinh(\lambda - \eta - z_\ell)}{\sinh(\lambda - z_\ell)} \quad (5.40)$$

where  $\sigma$  is a permutation of  $\{1, \dots, N\}$ ,  $\pi$  is a permutation of  $\{1, \dots, m\}$ , the set of  $s$  parameters  $\{z_1, \dots, z_s\}$  are made of "strings" of the form

$$p_k + \eta + i\pi, p_k + 2\eta \pmod{i\pi}, \dots, p_k + n_k\eta \pmod{i\pi}, \quad (5.41)$$

or

$$p_k - \eta + i\pi, p_k - 2\eta \pmod{i\pi}, \dots, p_k - \bar{n}_k\eta \pmod{i\pi}, \quad (5.42)$$

for some  $p_k \in \{p_{\sigma_{R+1}}, \dots, p_{\sigma_N}\}$ , with  $n_k, \bar{n}_k \in \mathbb{N} \setminus \{0\}$ . And with this notation we have  $\bar{m}_\epsilon = N - R + m - m' + s$ .

The problem of analyzing the representation (5.38) in the thermodynamic limit is still not completely solved. However, in the particular case  $s = 0$  and  $\bar{m}_\epsilon = m$ , i.e when  $N = R + m'$ , the situation becomes much simpler. We can in that case adapt the results of Chapter 3 to study the corresponding determinants. We can for instance, to mimic the XXX solution, use the connexion with a generalized Slavnov determinant that we have brought out in Proposition 3.2.2, or some slight modification of it.

In that case, we can first transform the ratio (5.39) using Identity 1, which gives

$$\begin{aligned} \frac{\mathcal{A}_{\{\xi_1, \dots, \xi_N\}}[-f_{\bar{P}_{\bar{\mathbf{p}},\epsilon}^\xi Q}]}{\mathcal{A}_{\{\xi_1, \dots, \xi_N\}}[-f_{PQ}]} &= \frac{\mathcal{I}_{\{\xi_1, \dots, \xi_N\}, \{\bar{p}_1, \dots, \bar{p}_N\}}[-\tilde{f}_{P,Q}]}{\mathcal{I}_{\{\xi_1, \dots, \xi_N\}, \{p_1, \dots, p_N\}}[-\tilde{f}_{P,Q}]} \\ &= \prod_{i=1}^N \prod_{j=1}^{m'} \frac{\sinh(\xi_i - \lambda_{\pi_j})}{\sinh(\xi_i - p_{\sigma_{R+j}})} \prod_{i=1}^R \prod_{j=1}^{m'} \frac{\sinh(p_{\sigma_{R+j}} - p_{\sigma_i})}{\sinh(\lambda_{\pi_j} - p_{\sigma_i})} \\ &\quad \times \prod_{i < j} \frac{\sinh(p_{\sigma_{R+j}} - p_{\sigma_{R+i}})}{\sinh(\lambda_{\pi_j} - \lambda_{\pi_i})} \frac{\det_{1 \leq i, k \leq N} \mathcal{M}(\xi_i, \bar{p}_k)}{\det_{1 \leq i, k \leq N} \mathcal{M}(\xi_i, p_k)} \end{aligned} \quad (5.43)$$

where

$$\mathcal{M}(\xi, p) = \frac{1}{\sinh(\xi - p)} + \frac{\tilde{f}_{P,Q}(\xi)}{\sinh(\xi - p + \eta)}. \quad (5.44)$$

Here  $\{\bar{p}_1, \dots, \bar{p}_N\} = \{p_{\sigma_1}, \dots, p_{\sigma_R}\} \cup \{\lambda_{\pi_1}, \dots, \lambda_{\pi_R}\}$ .

Multiplying both determinants in (5.43) with the determinant of the same matrix  $\tilde{\mathcal{X}}$  of elements

$$\begin{aligned} \tilde{\mathcal{X}}_{a,b} = & \frac{1}{\prod_{\ell \neq b} \sinh(\xi_b - \xi_\ell)} \left\{ \left[ \coth\left(\frac{\xi_b - q_j - \eta}{2}\right) - \coth\left(\frac{\xi_b - q_j}{2}\right) \right] Q(\xi_b - \eta) P(\xi_b + i\pi) \right. \\ & \left. - \left[ \coth\left(\frac{\xi_b - q_j - \eta + i\pi}{2}\right) - \coth\left(\frac{\xi_b - q_j + i\pi}{2}\right) \right] Q(\xi_b - \eta + i\pi) P(\xi_b) \right\} \end{aligned} \quad (5.45)$$

we obtain

$$\frac{\det_{1 \leq i, k \leq N} \mathcal{M}(\xi_i, \bar{p}_k)}{\det_{1 \leq i, k \leq N} \mathcal{M}(\xi_i, p_k)} = \prod_{k=1}^N \frac{d(p_k) Q(\bar{p}_k - \eta) P(\bar{p}_k + i\pi)}{d(\bar{p}_k) Q(p_k - \eta) P(p_k + i\pi)} \frac{\det_{1 \leq i, j \leq N} \bar{\mathcal{S}}_{Q,P}(q_j, \bar{p}_k)}{\det_{1 \leq i, j \leq N} \bar{\mathcal{S}}_{Q,P}(q_j, p_k)} \quad (5.46)$$

where

$$\bar{\mathcal{S}}_{Q,P}(q, \bar{p}) = \mathcal{S}_Q(q, p) - \frac{Q(p - \eta + i\pi) P(p)}{Q(p - \eta) P(p + i\pi)} \mathcal{S}_Q(q, p + i\pi), \quad (5.47)$$

$$\begin{aligned} \mathcal{S}_Q(q, p) = & \left[ \coth\left(\frac{p - q - \eta}{2}\right) - \coth\left(\frac{p - q}{2}\right) \right] \\ & + \mathfrak{a}_Q(p) \left[ \coth\left(\frac{p - q}{2}\right) - \coth\left(\frac{p - q + \eta}{2}\right) \right]. \end{aligned} \quad (5.48)$$

Here we have used that the roots of  $Q$  satisfy the Bethe equations. We have also supposed that  $P$  satisfy the quasi-periodicity properties (3.43).

We can now take the limit  $P \rightarrow Q$  and  $\lambda_{\pi_i} \rightarrow \xi_{\pi_i}$ ,  $1 \leq i \leq m'$ , in these formulas. We obtain, still in the case  $s = 0$  and  $R + m' = N$ ,

$$\begin{aligned} \frac{\langle \bar{Q}_{\bar{\mathbf{q}}, \epsilon}^\xi | Q \rangle}{\langle Q | Q \rangle} = & \prod_{\ell=1}^{m'} \left[ \frac{a(\xi_{\pi_\ell})}{a(q_{\sigma_{R+\ell}})} \frac{Q(\xi_{\pi_\ell} + i\pi) Q(\xi_{\pi_\ell} - \eta)}{Q(q_{\sigma_{R+\ell}} + i\pi) Q(q_{\sigma_{R+\ell}} - \eta)} \prod_{i=1}^R \frac{\sinh(q_{\sigma_i} - q_{\sigma_{R+\ell}})}{\sinh(q_{\sigma_i} - \xi_{\pi_\ell})} \right] \\ & \times \prod_{i < j}^{m'} \frac{\sinh(q_{\sigma_{R+i}} - q_{\sigma_{R+j}})}{\sinh(\xi_{\pi_i} - \xi_{\pi_j})} \frac{\det_N \bar{\mathcal{S}}_{\bar{Q}, Q}(\mathbf{q} | \bar{\mathbf{q}}_{\sigma\pi})}{\det_N \mathcal{S}_Q(q_j, q_k)}, \end{aligned} \quad (5.49)$$

with

$$[\mathcal{S}_{\bar{Q}, Q}(\mathbf{q} | \bar{\mathbf{q}}_{\sigma\pi})]_{j, \ell} = \begin{cases} \mathcal{S}_Q(q_j, q_{\sigma_\ell}), & \text{for } 1 \leq \ell \leq R, \\ 2 [\coth(\xi_{\pi_k} - q_{\sigma_j} - \eta) - \coth(\xi_{\pi_k} - q_{\sigma_j})] & \text{for } R + 1 \leq \ell \leq R + m', \end{cases} \quad (5.50)$$

$$\mathcal{S}_Q(q_j, q_k) = 2\delta_{j,k} \frac{\mathfrak{a}'_Q(q_j)}{\mathfrak{a}_Q(q_j)} + \coth\left(\frac{q_k - q_j - \eta}{2}\right) - \coth\left(\frac{q_k - q_j + \eta}{2}\right). \quad (5.51)$$

Similarly as in the XXX case, we can therefore extract the leading contributions of this ratio in the thermodynamic limit:

$$\begin{aligned} \frac{\langle \bar{Q}_{\bar{\mathbf{q}}, \epsilon}^\xi | Q \rangle}{\langle Q | Q \rangle} \underset{N \rightarrow \infty}{\sim} & \prod_{\ell=1}^{m'} \left[ \frac{a(\xi_{\pi_\ell})}{a(q_{\sigma_{R+\ell}})} \frac{Q(\xi_{\pi_\ell} + i\pi) Q(\xi_{\pi_\ell} - \eta)}{Q(q_{\sigma_{R+\ell}} + i\pi) Q(q_{\sigma_{R+\ell}} - \eta)} \prod_{i=1}^R \frac{\sinh(q_{\sigma_i} - q_{\sigma_{R+\ell}})}{\sinh(q_{\sigma_i} - \xi_{\pi_\ell})} \right] \\ & \times \prod_{i < j}^{m'} \frac{\sinh(q_{\sigma_{R+i}} - q_{\sigma_{R+j}})}{\sinh(\xi_{\pi_i} - \xi_{\pi_j})} \frac{\det_{1 \leq j, k \leq m'} \tilde{\rho}(q_{\sigma_{R+j}} - \xi_{\pi_k} + \eta/2)}{N \tilde{\rho}_{\text{tot}}(q_{\sigma_{R+j}})}. \end{aligned} \quad (5.52)$$



If we adapt the same notations as in Proposition (4.2.1), the part  $F_m(\tau, \epsilon)_{\text{restr}}$  of the multiple sum representation (4.61) which corresponds to these terms can be rewritten in a similar form as in (5.30). Indeed if we define:

$$\alpha_\epsilon^- = \{j : 1 \leq j \leq m, \epsilon_{2j-1} = 1\}, \quad \#\alpha_\epsilon^- = s_\epsilon \quad (5.53)$$

$$\alpha_\epsilon^+ = \{j : 1 \leq j \leq m, \epsilon_{2j} = 2\}, \quad \#\alpha_\epsilon^+ = s'_\epsilon \quad (5.54)$$

then

$$\lim_{N \rightarrow \infty} F_m(\tau, \epsilon)_{\text{restr}} = \delta_{s_\epsilon + s'_\epsilon, m} \lim_{N \rightarrow \infty} \prod_{k=1}^m \frac{1}{\tau(\xi_k)} \quad (5.55)$$

$$\times \sum_{\{a_j, a'_j\}} \prod_{j \in \alpha_\epsilon^-} \left( \frac{d(q_{a_j}) Q(q_{a_j} + i\pi) \prod_{k \in \mathbf{A}_j}^{N+j-1} \sinh(q_{a_j} - q_k + \eta)}{Q(q_{a_j} + \eta + i\pi) \prod_{k \in \mathbf{A}'_j}^{N+j} \sinh(q_{a_j} - q_k)} \right) \quad (5.56)$$

$$\times \prod_{j \in \alpha_\epsilon^+} \left( \frac{-a(q_{a'_j}) Q(q_{a'_j} + i\pi) \prod_{k \in \mathbf{A}'_j}^{N+j-1} \sinh(q_k - q_{a'_j} + \eta)}{Q(q_{a'_j} - \eta + i\pi) \prod_{k \in \mathbf{A}_j}^{N+j} \sinh(q_k - q_{a'_j})} \right) \frac{\langle \bar{Q}_{\mathbf{A}_{m+1}} | Q \rangle}{\langle Q | Q \rangle}, \quad (5.57)$$

where we have set  $q_{N+j} \equiv \xi_j$ ,  $1 \leq j \leq m$ , and there the summation is taken over the indices  $a_j$  for  $j \in \alpha_\epsilon^-$  and  $a'_j$  for  $j \in \alpha_\epsilon^+$  such that:

$$1 \leq a_j \leq N + j, \quad a_j \in \mathbf{A}_j, \quad 1 \leq a'_j \leq N + j, \quad a'_j \in \mathbf{A}'_j, \quad (5.58)$$

with

$$\mathbf{A}_j = \{b : 1 \leq b \leq N + m, b \neq a_k, a'_k, k < j\}, \quad (5.59)$$

$$\mathbf{A}'_j = \{b : 1 \leq b \leq N + m, b \neq a'_k, k < j \text{ and } b \neq a_k, k \leq j\}. \quad (5.60)$$

The function  $\bar{Q}_{\mathbf{A}_{m+1}}$  is defined as:

$$\bar{Q}_{\mathbf{A}_{m+1}} = Q(\lambda) \frac{\prod_{j=1}^m \sinh(\lambda - \xi_j)}{\prod_{j \in \alpha_\epsilon^-} \sinh(\lambda - q_{a_j}) \prod_{j \in \alpha_\epsilon^+} \sinh(\lambda - q_{a'_j})}. \quad (5.61)$$

Note that, by using the explicit expression for the transfer matrix eigenvalue evaluated at  $\xi_k$ ,  $k = 1, \dots, m$ ,

$$\tau(\xi_k) = -a(\xi_k) \frac{Q_\tau(\xi_k - \eta)}{Q_\tau(\xi_k)}, \quad (5.62)$$

together with the Bethe equations

$$d(q_{a_j}) = a(q_{a_j}) \frac{Q_\tau(q_{a_j} - \eta)}{Q_\tau(q_{a_j} + \eta)}, \quad \forall a_j \leq N, \quad (5.63)$$

and the observation that  $d(q_{a_j}) = 0$  for any  $a_j > N$ , one can rewrite (5.25) in the following

way:

$$\begin{aligned}
\lim_{N \rightarrow \infty} F_m(\tau, \epsilon)_{\text{restr}} &= \lim_{N \rightarrow \infty} \prod_{k=1}^m \frac{Q_\tau(\xi_k)}{a(\xi_k)Q_\tau(\xi_k - \eta)} \\
&\times \sum_{\{a_j, a'_j\}} \prod_{j \in \alpha_\epsilon^-} \left( -a(q_{a_j}) \frac{Q_\tau(q_{a_j} - \eta)}{Q_\tau(q_{a_j} + \eta)} \frac{Q_\tau(q_{a_j} + i\pi)}{Q_\tau(q_{a_j} + \eta + i\pi)} \frac{\prod_{k=1}^{R+j-1} \sinh(q_{a_j} - q_k + \eta)}{\prod_{k=1}^{R+j} \sinh(q_{a_j} - q_k)} \right) \\
&\times \prod_{j \in \alpha_\epsilon^+} \left( a(q_{a'_j}) \frac{Q_\tau(q_{a'_j} + i\pi)}{Q_\tau(q_{a'_j} - \eta + i\pi)} \frac{\prod_{k=1}^{R+j-1} \sinh(q_k - q_{a'_j} + \eta)}{\prod_{k=1}^{R+j} \sinh(q_k - q_{a'_j})} \right) \frac{\langle \bar{Q}_{\mathbf{A}_{m+1}} | Q_\tau \rangle}{\langle Q_\tau | Q_\tau \rangle}, \quad (5.64)
\end{aligned}$$

where the summation is taken here over the indices  $a_j$  for  $j \in \alpha_\epsilon^-$  and  $a'_j$  for  $j \in \alpha_\epsilon^+$  such that

$$1 \leq a_j \leq N, \quad a_j \in \mathbf{A}_j, \quad 1 \leq a'_j \leq N + j, \quad a'_j \in \mathbf{A}'_j. \quad (5.65)$$

Further based on the fact that

$$\prod_{n=1}^N \sinh(\lambda - q_n) = (-2i)^N Q(\lambda)Q(\lambda + i\pi) \quad (5.66)$$

the expression (5.64) coincides with (4.6),(5.2)-(5.4) of [80]. Thus it will give the same expression for  $F_m(\tau, \epsilon)_{\text{restr}}$  as in (5.5)-(5.6) of [80].

One may expect that the remaining terms vanish in the thermodynamic limit, similarly as what happens in the XXX case. A proper analysis of these remaining terms is however still to be done to confirm such a conjecture.



# Conclusion

There are in general two methods to compute the correlation functions for quantum integrable lattice models. One is to compute the form factors and sum them over to get the correlation functions. The other is to compute the elementary building blocks and take linear combinations of them to obtain the correlation functions. In the Algebraic Bethe Ansatz approach, as for the simple model of the  $XXZ$  periodic chain, both methods have been used to obtain analytical results [81, 80] and are analytically linked by a single integral representation called the *master equation* [94].

In this thesis, our goal is to develop an approach towards the computation of the form factors and the correlation functions within the quantum separation of variables (SoV) method. To achieve this goal and be able to compare the results with the ones obtained by Algebraic Bethe Ansatz, we consider two simple models: the anti-periodic  $XXX$  and  $XXZ$  Heisenberg spin chains.

One of the difficulties of the SoV approach in terms of its applications to physical systems is that all results are a priori obtained in terms of the non-physical inhomogeneity parameters that have to be introduced for the method to work. Getting rid of these inhomogeneity parameters, i.e. taking the homogeneous limit, might be a very non-trivial task.

At the level of the spectrum, one naturally obtains a description in terms of a set of discrete Baxter TQ-equations that need to be reformulated into a more conventional form [157]. As for the  $XXX$  case, one can find the Baxter's  $Q$ -function that takes the form of a polynomial [114]. As for the  $XXZ$  case, the Baxter's  $Q$ -function can no longer take the same function form as the eigenvalue function. In fact, in the  $XXZ$  case, the Baxter's  $Q$ -function is a trigonometric polynomial with a double period [117, 115].

The SoV method naturally provides a determinant representation for the scalar products for a large class of models. This is a priori an advantage of the method. However, this determinant representation for the scalar products that one naturally obtains is highly dependent on the inhomogeneous parameters in an explicit way. Thus one also needs to transform it into a more tractable form to take the homogeneous limit. In the  $XXX$  case, this problem was solved by noticing the existence of a set of algebraic identities which lead to the wanted transformation [114]. With this transformation and the solution to the so-called quantum inverse problem [82, 83, 143], the form factors for the anti-periodic  $XXX$  chain was obtained in [114].

Due to the inconsistency of periods, these identities cannot be applied directly to the  $XXZ$  case. In this thesis, we have solved the problem by providing an alternative transformation. This transformation leads to a suitable determinant representation that enables us to take the homogeneous limit. By employing this determinant representation we have obtained in this thesis (result in [118]) a determinant representation for the form factors in the anti-periodic  $XXZ$  chain.

As for the correlation functions, we have shown that in the SoV framework it is possible to

obtain the same kind of results for the  $XXX$  case as in the algebraic Bethe Ansatz framework [80] or in the  $q$ -vertex operator approach [79]. And we have given some hint for the  $XXZ$  case. After a suitable determinant representation for separate states has been obtained, the difficulty for computing the elementary building blocks is that the action of local operators on separate states involves the inhomogeneity parameters in a very intricate way and needs reformulation. This point is crucial if we want to use this approach to directly compute the correlation functions and bring the SoV approach to the same level of achievement as the algebraic Bethe Ansatz [80] or the  $q$ -vertex operator approach [79]. In this thesis, we have therefore explained how to transform the SoV action into a more conventional one, involving the roots of the Baxter  $Q$ -function (the "Bethe roots") rather than the inhomogeneity parameters. More precisely, we have expressed these actions using multiple contour integrals. By taking the residues inside the contours, we have recovered the SoV action in terms of the inhomogeneity parameters; and by taking the residues outside the contours, we obtain an ABA-type action in terms of "Bethe roots".

As a result, in the  $XXX$  case, we have also obtained some extra contributions from the poles at infinity. Since the spin  $S_z$  is no longer conserved, the correlation functions of the (non-diagonally) twisted  $XXX$  chain in finite volume involve many additional contributions with respect to the periodic or diagonally-twisted chain. We have explicitly shown here that all these extra contributions vanish in the thermodynamic limit, and thus have the same result as in the periodic case. In the  $XXZ$  case, the extra contributions from "strings" of poles lead to more complicated scalar products, which makes the identification of their contributions in the thermodynamic limit more difficult than in the  $XXX$  case. The detailed analysis is still under investigation. However under the assumption that the extra terms do not contribute in the thermodynamic limit as in the  $XXX$  case, we are able to recover the multiple integral representation for the elementary building blocks.

We expect our approach to correlation functions in SoV to be applicable to more complicated models. The following research work may start from the correlation functions of open chains ( $XXX$  or  $XXZ$ ) with non-diagonal boundaries, for which preliminary results have been obtained concerning the scalar products of separate states [144, 156].

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**Titre:** Séparation des variables et fonctions de corrélation des systèmes intégrables quantiques

**Mots clés:** Séparation des variables, Fonctions de corrélation, Systèmes Intégrables Quantiques

**Résumé:** Le but de cette thèse est de développer une approche au calcul des fonctions de corrélation des modèles intégrables quantiques sur réseau dans le cadre de la version quantique de la méthode de séparation des variables (SoV). SoV est une méthode puissante applicable à une large classe de modèles quantiques intégrables avec des conditions aux limites variées. Cependant, le calcul des fonctions de corrélation reste dans ce cadre un problème encore largement ouvert. Nous considérons ici plus précisément deux modèles simples solubles par SoV: les chaînes de Heisenberg XXX et XXZ de spins  $1/2$ , avec des conditions aux limites anti-périodiques, ou plus généralement des conditions aux limites quasi-périodiques avec un twist non diagonal. Nous rappelons leurs solutions par SoV, qui présentent des similitudes mais aussi des différences cruciales. Puis nous étudions les produits scalaires d'états séparés, une

classe d'états qui contient notamment tous les états propres du modèle. Nous expliquons comment obtenir, pour ces produits scalaires, des représentations sous forme de déterminant utilisables pour l'étude du modèle. Nous expliquons également comment généraliser ces représentations dans le cas des facteurs de forme, c'est-à-dire des éléments matriciels des opérateurs locaux dans la base des états propres. Ces facteurs de forme sont d'un intérêt particulier pour le calcul des corrélations puisque toutes les fonctions de corrélation peuvent être obtenues sous forme de somme sur des facteurs de forme. Enfin, nous considérons des blocs élémentaires plus généraux pour les fonctions de corrélation, et expliquons comment retrouver, dans la limite thermodynamique du modèle, les représentations sous forme d'intégrales multiples précédemment obtenues à partir de l'étude des modèles périodiques par Ansatz de Bethe algébrique.

**Title:** Separation of Variables and Correlation Functions of Quantum Integrable Systems

**Keywords:** Separation of Variables, Correlation Functions, Quantum Integrable Systems

**Abstract:** The aim of this thesis is to develop an approach to the computation of the correlation functions of quantum integrable lattice models within the quantum version of the Separation of Variables (SoV) method. SoV is a powerful method which applies to a wide range of quantum integrable models with various boundary conditions. Yet, the problem of computing correlation functions within this framework is still widely open. Here, we more precisely consider two simple models solvable by SoV: the XXX and XXZ Heisenberg chains of spins  $1/2$ , with anti-periodic boundary conditions, or more generally quasi-periodic boundary conditions with a non-diagonal twist. We first review their solution by SoV, which presents some similarities but also crucial differences. Then

we study the scalar products of separate states, a class of states that notably contains all the eigenstates of the model. We explain how to obtain convenient determinant representations for these scalar products. We also explain how to generalise these determinant representations in the case of form factors, i.e. of matrix elements of the local operators in the basis of eigenstates. These form factors are of particular interest for the computation of correlation since all correlation functions can be obtained as a sum over form factors. Finally, we consider more general elementary building blocks for the correlation functions, and explain how to recover, in the thermodynamic limit of the model, the multiple integral representations that were previously obtained from the consideration of the periodic models by algebraic Bethe Ansatz.