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学士学位论文

大规模并行的计算代数几何方法在可积自旋链模型中的应用

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Application of Massively Parallel Computational Algebraic Geometry Methods to Integrable Spin Chain Models

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摘　要

量子可积系统模型具有优美的数学结构和丰富的物理学内涵，近些年来在物理学和数学的多个领域，例如场论、弦理论、统计物理、凝聚态物理、量子群中起着非常重要的作用。而计算代数几何方法可以为研究可积自旋链模型提供强有力的工具。其中，Groebner bases 的求解是最为重要的部分。

本文旨在比较多种传统的计算 Groebner bases 的方法的优劣，并从中提出一种新的方法，即利用并行应用程序工作流管理系统 GPI-space 等工具，实现有限域上 Groebner bases 计算的大规模并行，从而最大限度地提高计算速度。在 XXX 型与 XXZ 型可积自旋链模型的各种分析中，用以完成高效检查 Bethe ansatz 完整性，计算配分函数等任务，进而实现研究更加复杂的可积自旋链模型的目的。本文中方法的优点在于 Buchberger 算法非常成熟，在进行全新的程序移植后，并行计算可以大大提高其计算的效率。

关键词：量子可积系统，计算代数几何，并行计算

ABSTRACT

Quantum integrable system has beautiful mathematical structure with rich contents of physics, which has been playing an important role in many fields in physics and mathematics, such as field theory, string theory, statistic physics, condensed matter physics, quantum group, etc. When studying integrable systems, computational algebraic method can be a powerful tool, in which the computation of Groebner basis is the most important part.

In this thesis, one tries to compare multiple traditional methods for computing Groebner basis. And we put forward a new technique to realize the massively parallel computation of Buchberger algorithm over finite field via GPI-space framework, a workflow managing system, which will largely increase the speed of computation. For analysis of XXX and XXZ model of integrable spin chain, it can be used in checking the completeness of Bethe ansatz, calculating partition functions, etc. And then realize the goal to analyze more sophisticated model of integrable spin chain. The advantage of this method is that parallelization of the well-implemented Buchberger algorithm can promote the computation efficiency at a large scale.

Key Words: Quantum Integrable System, Computational Algebraic Geometry, Parallel Computation

Contents

Chapter 1 Introduction

1.1 Integrable systems in high energy physics

Integrable systems play a significant role in the field of high energy physics, offering powerful mathematical tools to study and understand the dynamics of physical systems. These systems exhibit remarkable properties that allow for exact solutions, making them valuable in both theoretical investigations and practical applications.

In high energy physics, integrable systems refer to physical models that possess an extensive number of conserved quantities. These quantities are quantities that remain constant over time, providing valuable insights into the underlying dynamics. Integrability implies the existence of a sufficient number of conserved quantities to fully determine the system's evolution.

One of the fundamental concepts in integrable systems is that of a soliton. Solitons are stable, localized wave-like entities that can propagate through a medium without dispersing or changing their shape. They behave as "particles" within the system, and their interactions can be described exactly through mathematical equations. Solitons have been observed experimentally in various physical systems, such as water waves, optical fibers, and even in certain field theories in high energy physics.

Integrable systems are typically associated with nonlinear partial differential equations (PDEs) that govern the dynamics of the system. These equations are often derived from specific physical models, such as classical field theories or quantum mechanical systems. The equations shed lights on a range of mathematical structures, including symmetries and some algebraic properties. And such properties enable their integrability.

The study of integrable systems involves a combination of mathematical techniques, such as algebraic geometry, complex analysis, and the theory of special functions. These tools allow researchers to obtain exact solutions, analyze the system's symmetries, and explore its behavior in various regimes.

Integrable systems find applications in several areas of high energy physics. For

example, they have been used to study the dynamics of gauge theories, which are fundamental in understanding the strong force interactions between elementary particles. Integrable models have also shed light on the behavior of string theories and their connections to gravity through the AdS/CFT correspondence.

Moreover, integrable systems have been employed in condensed matter physics to describe phenomena like quantum spin chains and low-dimensional magnets. They have provided valuable insights into the behavior of these complex systems, allowing for a deeper understanding of their properties.

In summary, integrable systems offer a powerful framework for studying the dynamics of physical systems in high energy physics. Their exact solvability and rich mathematical structures make them indispensable tools for theoretical investigations, and their applications extend to various areas of physics, including gauge theories, string theory, and condensed matter physics.

1.2 Spin chain model and computational algebraic geometry

Integrable spin chain models serve as valuable tools in high energy physics for studying the behavior of quantum systems with many interacting spins. These models capture the collective behavior of spins and provide insights into various phenomena, such as quantum phase transitions and the emergence of exotic states of matter.

A spin chain consists of a linear array of spins, where each spin can be in a particular quantum state. The interaction between neighboring spins gives rise to the collective dynamics of the system. Integrability in spin chain models implies the existence of an extensive number of conserved quantities, which determine the system's behavior.

The most well-known example of an integrable spin chain model is the Heisenberg spin chain, which describes the interactions between quantum spins governed by the famous Heisenberg exchange interaction. The model's Hamiltonian, which represents the total energy of the system, exhibits an underlying symmetry algebra and possesses a rich mathematical structure.

The integrability of spin chain models makes it possible to calculate of various

physical objects exactly, including correlation functions and so on. The Bethe ansatz technique, a powerful mathematical method, plays a crucial role in solving these models. The Bethe ansatz provides a systematic way of finding the exact eigenstates of the Hamiltonian by exploiting the integrability of the system. This allows for a detailed understanding of the system's properties, including its ground state, excited states, and their dynamics.

Computational algebraic geometry provides a powerful approach to studying integrable spin chain models. Algebraic geometry deals with the study of geometric objects defined by polynomial equations. In the context of integrable systems, computational algebraic geometry provides numerical and symbolic methods for solving the underlying equations and analyzing their solutions.

By formulating the problem in the language of algebraic geometry, researchers can exploit powerful algorithms and techniques to study the properties of integrable spin chain models. Computational methods such as Gröbner basis computations, numerical algebraic geometry, and geometric algorithms enable the analysis of the model's symmetries, computation of conserved quantities, and determination of the system's integrability conditions.

Furthermore, computational algebraic geometry facilitates the exploration of the phase diagram and the identification of critical points, which are crucial for understanding the system's phase transitions. It also enables the investigation of entanglement properties, quantum correlations, and the behavior of the system under various perturbations.

In summary, integrable spin chain models provide a framework for studying the collective behavior of quantum systems with many interacting spins. Computational algebraic geometry offers powerful tools and techniques to analyze and solve these models, allowing for a deeper understanding of their properties, symmetries, and dynamics. The combination of integrable spin chain models and computational algebraic geometry contributes to advancing our knowledge of high energy physics and the behavior of quantum systems.

1.3 Arrangement of this thesis

The thesis will be written in 5 parts.

In chapter 2, one will have a brief introduction to integrable spin chain model, which is the main physical object in this thesis. The Heisenberg XXX and XXZ spin chain model will be described in detail, together with the Bethe ansatz equation method (BAEs) for both models.

In chapter 3, computational algebraic geometry (CAG) method will be introduced. Firstly some basic facts including most of the definitions and theorems needed will be stated. Then one can have a look at the Gröbner basis computation. At the end there will be some introduction to the relations between spin chain and CAG.

In chapter 4, one will get to know the algorithms to calculate Gröbner basis , mainly, Buchberger and F4 algorithms. Their current implementation will also be introduced.

In chapter 5, there will be 2 certain applications of CAG to spin chain model: counting solutions of BAEs in XXX spin chain model and finding the sum of solutions for Loschmidt problem in XXZ spin chain model. For the 2 problems, the choice of Buchberger algorithm and the reason will be presented.

In chapter 6, one will be introduced to the idea of massive parallelization. Modern tools as SINGULAR/GPI-SPACE will be presented. And the creative work of parallel Buchberger algorithm will be introduced with certain applications to the 2 problems above.

Chapter 2 Introduction to Integrable Spin Chain Model

2.1 Overiview of one-dimensional quantum integrable systems

One-dimensional quantum integrable systems are highly interesting and important in the field of theoretical physics. They represent quantum mechanical models that exhibit remarkable properties, such as exact solvability and an extensive number of conserved quantities. These systems provide valuable insights into the behavior of quantum particles and have connections to various areas of physics, including condensed matter physics, quantum field theory, and statistical mechanics.

A one-dimensional quantum integrable system typically consists of a chain or lattice of quantum particles, such as spins or interacting fermions, arranged along a line. The interactions between the particles are usually described by specific mathematical models, often involving pairwise interactions or long-range forces. These models can be derived from realistic physical systems or proposed as simplified theoretical constructs to study fundamental aspects of quantum mechanics.

The main characteristic of integrable systems is the presence of a sufficiently large number of conserved quantities. These quantities are operators that commute with the Hamiltonian of the system and therefore remain constant during its time evolution. The existence of these conserved quantities allows for the system's exact solvability and provides a deeper understanding of its dynamics.

One of the prominent examples of one-dimensional quantum integrable systems is the Heisenberg spin chain, which describes the behavior of interacting quantum spins. This model has a rich mathematical structure and can be solved exactly using techniques like the Bethe ansatz, enabling the calculation of various physical quantities and the exploration of the system's properties.

Another essential class of one-dimensional quantum integrable systems is the Luttinger liquid model, which describes interacting fermions in one dimension. Luttinger

liquids exhibit unique features, such as fractionalized excitations and nontrivial correlations, and have connections to the physics of one-dimensional conductors and quantum wires.

The study of one-dimensional quantum integrable systems involves the application of powerful mathematical techniques, such as the Bethe ansatz, algebraic methods, and the theory of special functions. These methods allow researchers to obtain exact solutions for the wave functions, energy spectra, and correlation functions of the systems.

The field of one-dimensional quantum integrable systems has far-reaching implications in various branches of physics. In condensed matter physics, these systems provide insights into the behavior of low-dimensional materials, such as one-dimensional conductors, quantum magnets, and interacting electron systems. They also play a role in the study of quantum entanglement, topological phases, and quantum information processing.

Furthermore, one-dimensional quantum integrable systems have connections to quantum field theory through the AdS/CFT correspondence, where they are related to certain string theories in higher-dimensional spaces. This connection offers a unique perspective on the interplay between quantum mechanics and gravity, as well as the study of strong interactions.

In summary, one-dimensional quantum integrable systems are intriguing models that possess exact solvability and an extensive number of conserved quantities. They serve as valuable tools for understanding quantum mechanics, condensed matter physics, and quantum field theory. The study of these systems involves the application of sophisticated mathematical methods and contributes to advancing our knowledge of fundamental physical phenomena.

2.2 Heisenberg XXX and XXZ spin chain model

2.2.1 Heisenberg XXX model

The Heisenberg XXX spin chain model is a paradigmatic example of a one-dimensional quantum integrable system. It describes the behavior of interacting quantum spins arranged in a linear chain and is named after Werner Heisenberg, one of the pioneers of quantum mechanics.

In the Heisenberg XXX spin chain model, each site of the chain is associated with a spin-1/2 particle, which can be in either an "up" or "down" state. The interaction between neighboring spins is governed by the Heisenberg exchange interaction, which is characterized by a coupling constant usually denoted as J.

Here we consider $SU(2)$ invariant XXX spin chain, so the coupling constant $J = \frac{1}{4}$

The Hamiltonian of the Heisenberg XXX spin chain model is given by:

$$H_{\mathrm{XXX}} = \frac{1}{4}\sum_{j=1}^{L}(\vec{\sigma}_j \cdot \vec{\sigma}_{j+1} - 1), \qquad \vec{\sigma}_{L+1} = \vec{\sigma}_1 \tag{2.2.1}$$

Here L is the length of the spin chain and periodic boundary condition is applied. Note that $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the 2×2 Pauli matrices and $\vec{\sigma}_k$ denotes the spin operator at position k. At each site, the spin can have 2 orientations. So the Hilbert space spanned by them has dimension of 2^L.

The Heisenberg XXX spin chain model exhibits several intriguing properties. One of its most significant features is its integrability, which means that it possesses an extensive number of conserved quantities. These conserved quantities are operators that commute with the Hamiltonian, and they can be used to fully determine the system's dynamics.

The exact solvability of the Heisenberg XXX spin chain model is achieved through the Bethe ansatz technique. The Bethe ansatz provides a systematic way of finding the exact eigenstates of the Hamiltonian and obtaining the corresponding energy spectra. This technique has been instrumental in understanding the properties of the model, including its ground state, excited states, and their dynamics.

The Heisenberg XXX spin chain model has connections to various areas of physics. In condensed matter physics, it serves as a model for describing the behavior of one-dimensional magnetic systems, such as chains of interacting spins in magnetic materials. The model captures important phenomena, such as magnetic ordering, quantum phase transitions, and the emergence of exotic states of matter.

Furthermore, the Heisenberg XXX spin chain model has connections to quantum field theory through the AdS/CFT correspondence. This correspondence relates certain string theories in higher-dimensional spaces to conformal field theories in lower dimensions. The study of the Heisenberg XXX spin chain and its generalizations has provided insights into the behavior of quantum field theories and their dual gravitational descriptions.

In summary, the Heisenberg XXX spin chain model is a fundamental example of a one-dimensional quantum integrable system. It describes the interactions between quantum spins in a linear chain and possesses remarkable properties, including integrability and exact solvability. The model finds applications in condensed matter physics and quantum field theory, contributing to our understanding of magnetic systems, quantum phase transitions, and the interplay between quantum mechanics and gravity.

2.2.2 Heisenberg XXZ model

The Heisenberg XXZ spin chain model is another important example of a one-dimensional quantum integrable system. It shares similarities with the Heisenberg XXX spin chain model but includes an anisotropic term that distinguishes it.

In the Heisenberg XXZ spin chain model, like in the XXX model, quantum spins are arranged in a linear chain, and each site is associated with a spin-1/2 particle. However, the interaction between neighboring spins in the XXZ model includes an anisotropic term that differentiates it from the isotropic XXX model.

The Hamiltonian of the Heisenberg XXZ spin chain model is given by:

$$H_{\mathrm{XXX}} = -\frac{1}{2}\sum_{j=1}^{L}(\sigma_j^1\sigma_{j+1}^1 + \sigma_j^2\sigma_{j+1}^2 + \Delta\sigma_j^3\sigma_{j+1}^3), \qquad \vec{\sigma}_{L+1} = \vec{\sigma}_1 \tag{2.2.2}$$

where $\vec{\sigma} = (\sigma_j^1, \sigma_j^2, \sigma_j^3)$ are the Pauli matrices corresponding to the x, y, z components of the spin at site j, respectively. The sum runs over all pairs of neighboring spins in the chain. The parameter $\Delta = -cos\gamma$ represents the anisotropy of the model, which determines the strength of the interaction along the z-direction relative to the x-y plane.

The Heisenberg XXZ spin chain model exhibits rich physics, and its behavior depends on the value of the anisotropy parameter Δ. For $\Delta = 1$, the model is isotropic and reduces to the Heisenberg XXX spin chain model. When $\Delta > 1$, the system favors alignment along the z-direction, leading to ferromagnetic behavior. Conversely, for $\Delta < 1$, the system prefers alignment in the x-y plane, resulting in antiferromagnetic behavior.

Similar to the Heisenberg XXX spin chain model, the Heisenberg XXZ spin chain model is integrable, meaning it possesses an extensive number of conserved quantities. The Bethe ansatz technique can be applied to obtain exact solutions for the eigenstates and energy spectra of the model, providing valuable insights into its properties and dynamics.

The Heisenberg XXZ spin chain model finds applications in various areas of physics. In condensed matter physics, it serves as a model for studying magnetic systems with anisotropic interactions, such as spin chains in materials exhibiting spin-orbit coupling. The model helps to understand the emergence of magnetic ordering, quantum phase transitions, and the interplay between different types of interactions.

Furthermore, the Heisenberg XXZ spin chain model has connections to quantum field theory, statistical mechanics, and quantum information theory. It provides insights into the behavior of interacting quantum systems, entanglement properties, and the emergence of critical phenomena.

In summary, the Heisenberg XXZ spin chain model is a one-dimensional quantum integrable system that includes anisotropic interactions between quantum spins. It

exhibits rich physics, ranging from ferromagnetic to antiferromagnetic behavior, depending on the value of the anisotropy parameter Δ. The model's integrability and exact solvability, along with its connections to various fields, make it a valuable tool for understanding magnetic systems, quantum phase transitions, and the behavior of interacting quantum systems.

2.3 Bethe ansatz method for solving integrable spin chain model

The Bethe ansatz method is a powerful mathematical technique used to solve integrable models, particularly spin chain models, in theoretical physics. It was initially developed by Hans Bethe in the 1930s to solve the Heisenberg spin chain model and has since become a cornerstone of integrable systems theory.

The Bethe ansatz method provides a systematic approach to finding the exact eigenstates and energy spectra of a spin chain model. It exploits the integrability of the system, which implies the existence of an extensive number of conserved quantities that commute with the Hamiltonian.

The basic idea behind the Bethe ansatz method is to construct a set of "Bethe ansatz" or "quasi-particle" states that diagonalize the Hamiltonian. These states are composed of individual excitations, often referred to as "quasi-particles," that propagate through the spin chain and interact with each other.

To find the eigenstates of the Hamiltonian, one starts by assuming a particular form for the Bethe ansatz wave function. This form incorporates the quasi-particle excitations and their properties, such as their momenta and polarization. The ansatz is typically chosen based on the symmetries and physical properties of the system.

Next, one imposes certain conditions, known as the Bethe equations, on the parameters of the wave function. These equations encode the requirement that the wave function must satisfy the Schrödinger equation and the boundary conditions of the spin chain. Solving the Bethe equations determines the allowed momenta of the quasi-particles and the corresponding eigenstates of the Hamiltonian.

The Bethe ansatz method enables the calculation of various physical quantities of

the spin chain model, including the energy spectrum, correlation functions, and scattering properties of the quasi-particles. It provides exact solutions for these quantities, allowing for a detailed understanding of the system's behavior and dynamics.

The method has found applications in diverse areas of theoretical physics, ranging from condensed matter physics and statistical mechanics to quantum field theory and string theory. It has been used to study a wide range of spin chain models, including the Heisenberg XXX spin chain, the Heisenberg XXZ spin chain, and many others.

In summary, the Bethe ansatz method is a powerful mathematical technique used to solve integrable spin chain models. It provides a systematic approach to finding the exact eigenstates and energy spectra of the models by constructing quasi-particle excitations and imposing Bethe equations. The method has had significant impact in various fields of theoretical physics, enabling precise calculations and deeper insights into the behavior of quantum systems.

Here we give the Bethe ansatz equation formalism of Heisenberg XXX and XXZ spin chain model.

2.3.1 Bethe ansatz for Heisenberg XXX spin chain

One can solve the Heisenberg XXX spin chain via constructing the following Bethe ansatz equation:

$$\left(\frac{u_j + i/2}{u_j - i/2}\right)^L = \prod_{k\neq j}^{N} \frac{u_j - u_k + i}{u_j - u_k - i}, \qquad j = 1, \cdots, N. \tag{2.3.3}$$

Here each eigenstate is labeled by a set of variables $\{u_1, \cdots, u_N\}$ called the rapidities where N is the number of flipped spins. And the corresponding eigenvalue is denoted by

$$E_N = -\frac{1}{2}\sum_{k=1}^{N} \frac{1}{u_k^2 + 1/4} \tag{2.3.4}$$

According to the definition of the Bethe ansatz, one may suppose that there's a 1-1 onto morphism between the solution set and the eigenstate set of the spin chain system. But unfortunately, this is a false assumption. There are certain kind of solutions that one

should get rid of. Here one can mainly consider four specific kind of solutions of the interest[3].

（1） Coinciding rapidities

As is known, one can always solve Bethe ansatz equations without constraints, with the solutions in the form of $\{u, u, u_1, \cdots, u_N\}$. They are correct solutions of BAEs mathematically. When considering coinciding solutions, the BAEs are different from the form derived below. Recall the RTT relation for $\mathrm{XXX}_{1/2}$ spin chain

$$\begin{aligned} A(\lambda)B(\mu) &= f(\lambda,\mu)B(\mu)A(\lambda) + g(\lambda,\mu)B(\lambda)A(\mu), \\ D(\lambda)B(\mu) &= f(\mu,\lambda)B(\mu)D(\lambda) + g(\mu,\lambda)B(\lambda)D(\mu), \\ B(\lambda)B(\mu) &= B(\mu)B(\lambda). \end{aligned} \tag{2.3.5}$$

Using the relations above, one can derive the following results[35,66]

$$\begin{aligned} A(\lambda)B(\mu)^2 =& a_1(\lambda,\mu)B(\mu)^2A(\lambda) + a_2(\lambda,\mu)B(\lambda)B'(\mu)A(\mu) \\ &+ a_3(\lambda,\mu)B(\lambda)B(\mu)A(\mu) + a_4(\lambda,\mu)B(\lambda)B(\mu)A'(\mu) \\ D(\lambda)B(\mu)^2 =& b_1(\lambda,\mu)B(\mu)^2D(\lambda) + b_2(\lambda,\mu)B(\lambda)B'(\mu)D(\mu) \\ &+ b_3(\lambda,\mu)B(\lambda)B(\mu)A(\mu) + b_4(\lambda,\mu)B(\lambda)B(\mu)D'(\mu) \end{aligned} \tag{2.3.6}$$

here $a_i(\lambda,\mu)$ and $b_i(\lambda,\mu)$ $(i = 1, 2, 3, 4)$ are functions with respect to $f(\mu,\lambda)$ and $g(\mu,\lambda)$. Since the occurrence of coinciding rapidities, one have the following relations $B'(u) = \partial_u B(u)$ together with $A'(u) = \partial_u A(u)$ and $D'(u) = \partial_u D(u)$.

To make sure that the off-shell Bethe state

$$|\Psi\rangle = B(u)^2 \prod_{i=1}^{N} B(u_i)|\uparrow^L\rangle \tag{2.3.7}$$

is an eigenstate of the transfer matrix, one can compute

$$T(v)|\Psi\rangle = (A(v) + D(v))|\Psi\rangle \tag{2.3.8}$$

by moving $A(u)$ and $D(u)$, which are diagonal elements of the matrix, to the right hand side and acting on the pseudovacuum state using the known commutation relations (2.3.6). By demanding the so-called "unwanted terms" to be 0, one finally has

the usual BAEs. There are two major modifications for current case. Firstly, $A'(v)$ and $D'(v)$ together with the resuting $a'(u)$ and $d'(u)$ could change the form of the cancellation conditions. Secondly, $B'(u)$ existence means that one need to apply cancelation conditions to the states with $B'(u)$ involving. If more coinciding rapidities appears, one can always obtain more additional cancellation conditions via similar analysis.

One can actually obtain the cancellation conditions by demanding the eigenvalue of transfer matrix to be regular at the Bethe roots. Considering the solution of BAEs for a spin chain of length L in the spin-s representation with $K+N$ magnons $\{u,u,\cdots,u,u_1,\cdots,u_N\}$. The eigenvalue of the transfer matrix is as following

$$T(\lambda)=a(\lambda)\left(\frac{\lambda-u-i}{\lambda-u}\right)^K\prod_{j=1}^{N}\frac{\lambda-u_j-i}{\lambda-u_j}+d(\lambda)\left(\frac{\lambda-u+i}{\lambda-u}\right)^K\prod_{j=1}^{N}\frac{\lambda-u_j+i}{\lambda-u_j} \tag{2.3.9}$$

here

$$a(\lambda)=(\lambda+is)^L,\qquad d(\lambda)=(\lambda-is)^L. \tag{2.3.10}$$

Then, as one can see, $T(\lambda)$ is a polynomial with respect to λ with poles at $\lambda=u,u_1,\cdots,u_N$. By requiring the residues of these 'poles' to vanish, one obtains the BAEs. For $\mu=u_j$, $(j=1,\cdots,N)$ one has

$$\mathrm{B}_j=a(u_j)(u_j-u-i)^K Q_{\mathbf{u}}(u_j-i)+d(u_j)(u_j-u+i)^K Q_{\mathbf{u}}(u_j+i)=0 \tag{2.3.11}$$

As done above, let $\lambda=u$ be regular, one gets the following conditions

$$\mathrm{R}_l=\frac{\partial^l}{\partial\lambda^l}\left(T(\lambda)(\lambda-u)^K\right)\Big|_{\lambda=u}=0,\qquad l=0,\cdots,K-1. \tag{2.3.12}$$

For the Heisenberg spin chain, it was found in[35] that there are no solutions with $K\geq 3$ and the ones with more than one group of repeated roots such as $\{u,u,v,v,u_1,\cdots,u_N\}$. However, one can find many solutions of the form $\{u,u,u_1,\cdots,u_N\}$. So, alongside the general believe that these are not physical solutions, currently there lacks a rigorous proof of this assertion for spin chain model.

(2) Solutions beyond the equator

one always use the constraint that the magnons falls in the region $N \leq L/2$ when searching for physical solutions. And one usually choose to ignore the solutions when $N > L/2$ since the solutions are included in the previous situation. To understand the inclusion, one can consider the $N < L/2$ number of magnons' Bethe state of a spin chain with length L. The Bethe vector is generated by acting N operators $B(u)$ on the pseudovacuum states

$$|\Psi\rangle = B(u_1)\cdots B(u_N)|\uparrow^L\rangle \tag{2.3.13}$$

Here the rapidities satisfies the BAEs of N position particles. N down spins and $L-N$ up spins are included in this state. One can generate the eigenstates with the same amount of up spins and down spins by acting $L-N$ operators $C(v)$ on the flipped pseudovacuum states

$$|\tilde{\Psi}\rangle = C(v_1)\cdots C(v_{L-N})|\downarrow^L\rangle \tag{2.3.14}$$

Here the rapidities $v_1,\cdots,v_{L-N}$ satisfies the BAEs of $L-N$ position particles. Then one have $|\Psi\rangle = |\tilde{\Psi}\rangle$. By this, (2.3.13) and (2.3.13) are only two ways of constructing the same eigenstates. One should know that $\mathbf{u} = \{u_1,\cdots,u_N\}$ and $\mathbf{v} = \{v_1,\cdots,v_{L-N}\}$ should be related.

To get this result, one can define the Baxter polynomials

$$Q_{\mathbf{u}}(u) = \prod_{k=1}^{N}(u-u_k), \qquad Q_{\mathbf{v}}(u) = \prod_{k=1}^{L-N}(u-v_k). \tag{2.3.15}$$

One can show that the two polynomials satisfy the Wronskian relation. Then actually one can always know a polynomial on the condition of given the other one. They are actually two solutions of Baxter's TQ-relation. The above analysis shows that one can restrict the solution to one side of the equator, say $N \leq L/2$, safely. Rest of the solutions on the other side correspond to the same physical states, as we say, included.

(3) Solutions at infinity

The Bethe states corresponding to rapidities $\{u_1, u_2, \cdots, u_N\}$ with none of the elements at infinity is highest weight state, as we say. This means

$$S^+ B(u_1)B(u_2)\cdots B(u_N)|\Omega\rangle = 0, \qquad S^+ = \sum_{i=1}^{L} S_i^+. \tag{2.3.16}$$

One can prove the relation above straightforwardly. At this highest weight state, the spin reads $J = \frac{L}{2} - N$. With the normal notation of quantum mechanics, one can use S^- to decrease the spins. For a spin-J representation, the dimension reads $2J + 1$. Then for a highest weight state $|u_1, \cdots, u_N\rangle$, the following states

$$(S^-)^n |u_1, \cdots, u_N\rangle, \qquad n = 0, \cdots, L - 2N \tag{2.3.17}$$

spans a space of $\mathfrak{su}(2)$ algebra for representation. For the completeness of Bethe ansatz, the number of physical solutions of N-particle BAEs is expected to be

$$Z_{L,N} = \binom{L}{N} - \binom{L}{N-1} \tag{2.3.18}$$

And the number of Bethe states is

$$\sum_{N=0}^{L/2} Z_{L,N}(L - 2N + 1) = 2^L \tag{2.3.19}$$

which reads the dimension of the corresponding Hilbert space. The solution of BAEs allows putting one or more excitations to the infinity. Each rapidity at the infinity corresponds to the action of an S^- since the following fact holds

$$\lim_{u\to\infty} B(u) \propto S^-. \tag{2.3.20}$$

Then the solutions at the infinity are physical. To show the completeness of Bethe ansatz, one only need to count the number of solutions that correspond to primary states. And one can easily work out the descendants of a primary state. Thus one only need to count the solutions corresponding to primary states.

(4) Singular solutions

The solutions of BAE with two of the rapidities being $\pm i/2$, say

$$\{i/2, -i/2, u_3, \cdots, u_N\} \tag{2.3.21}$$

are singular. To find out the problem at $u = \pm i/2$, the simplest way is to consider the eigenvalues with respect to the rapidities

$$E_N = -\frac{1}{2}\sum_{k=1}^{N}\frac{1}{u_k^2 + 1/4}. \tag{2.3.22}$$

Obviously, the function $(u^2 + 1/4)^{-1}$ has two poles at $u = \pm i/2$. Then the solutions including $u = \pm i/2$ are kind of special. They are much more subtle than those above. That's because sometimes these solutions are physical but sometimes not. To judge whether a solution is physical or not, one needs to do a regularization. Such analysis has been worked out in detail in the work of Nepomechie and Wang[44]. The conclusion is that the solutions are physical as long as the remaining rapidities $u_3, \cdots, u_N$ satisfy

$$\left(\frac{u_k + i/2}{u_k - i/2}\right)^{L-1}\left(\frac{u_k - 3i/2}{u_k + 3i/2}\right) = \prod_{\substack{j\neq k\\ j=3}}^{M}\frac{u_k - u_j + i}{u_k - u_j - i}, \qquad k = 3, \cdots, N. \tag{2.3.23}$$

$$\prod_{k=3}^{N}\left(\frac{u_k + i/2}{u_k - i/2}\right)^{L} = (-1)^L.$$

The first equation is the usual BAE and the second one is an additional rule for selection.

2.3.2 Bethe ansatz for Heisenberg XXX spin chain

Basically emerging from the Hamiltonian of the spin chain, the Bethe ansatz equations of XXZ model can be derived with the following analysis

The R-matrix is given by

$$R_{an}(u) \propto \begin{pmatrix} \sinh(u + \frac{i\gamma}{2}) & 0 & 0 & 0 \\ 0 & \sinh(u - \frac{\eta}{2}) & \sinh(i\gamma) & 0 \\ 0 & \sinh(i\gamma) & \sinh(u - \frac{i\gamma}{2}) & 0 \\ 0 & 0 & 0 & \sinh(u + \frac{i\gamma}{2}) \end{pmatrix}. \tag{2.3.24}$$

One can consider diagonal twisted boundary condition. Here it can be used in the algebraic Bethe ansatz by a constant matrix

$$K_a = \begin{pmatrix} \kappa^+ & 0 \\ 0 & \kappa^- \end{pmatrix} \tag{2.3.25}$$

in the auxiliary space. The monodromy matrix and the transfer matrix are then defined as

$$\widetilde{\mathbb{M}}_a(u) = K_a\, R_{a1}(u) R_{a2}(u) \dots R_{aL}(u)\,, \qquad \widetilde{\mathbb{T}}(u) = \mathrm{tr}_a \widetilde{\mathbb{M}}_a(u)\,, \tag{2.3.26}$$

One can have the following results after regarding the former one as matrix of operators acting on L space

$$\widetilde{\mathbb{M}}_a(u) = \begin{bmatrix} \tilde{A}(u) & \tilde{B}(u) \\ \tilde{C}(u) & \tilde{D}(u) \end{bmatrix}, \qquad \widetilde{\mathbb{T}}(u) = \tilde{A}(u) + \tilde{D}(u)\,. \tag{2.3.27}$$

One can start doing diagonalization with the pseudovacuum state $|\Omega\rangle = |\uparrow^L\rangle$

$$\tilde{A}(u)|\Omega\rangle = a(u)|\Omega\rangle\,, \qquad \tilde{D}(u)|\Omega\rangle = d(u)|\Omega\rangle\,, \tag{2.3.28}$$

here

$$a(u) = \kappa^+ \left(\sinh(u + \tfrac{i\gamma}{2})\right)^L, \qquad d(u) = \kappa^- \left(\sinh(u - \tfrac{i\gamma}{2})\right)^L. \tag{2.3.29}$$

Bethe states $|\mathbf{u}\rangle$ are constructed by acting on $|\Omega\rangle$ by the $\tilde{B}(u)$ operators,

$$|\mathbf{u}\rangle = \tilde{B}(u_1) \dots \tilde{B}(u_M)|\Omega\rangle\,. \tag{2.3.30}$$

If the Bethe roots $\mathbf{u} = \{u_1, \dots, u_M\}$ satisfy the Bethe ansatz equations

$$\left(\frac{\sinh(u_j + \frac{i\gamma}{2})}{\sinh(u_j - \frac{i\gamma}{2})}\right)^L = -\frac{\kappa^-}{\kappa^+} \prod_{k=1}^{M} \frac{\sinh(u_j - u_k + i\gamma)}{\sinh(u_j - u_k - i\gamma)}\,, \tag{2.3.31}$$

the state $|\mathbf{u}\rangle$ diagonalizes the transfer matrix

$$\widetilde{\mathbb{T}}(u)|\mathbf{u}\rangle = \tilde{\tau}(u)|\mathbf{u}\rangle\,. \tag{2.3.32}$$

The corresponding eigenvalue,

$$\tilde{\tau}(u) \propto a(u)\frac{\tilde{Q}(u - i\gamma)}{\tilde{Q}(u)} + d(u)\frac{\tilde{Q}(u + i\gamma)}{\tilde{Q}(u)}\,, \tag{2.3.33}$$

can be expressed in terms of the Q-function defined by

$$\tilde{Q}(u) = \prod_{j=1}^{M} \sinh(u - u_j)\,. \tag{2.3.34}$$

. And the analysis of the Bethe roots can be an analogy to what one has done for XXX model.

2.3.3 Analysis of the completeness of the solutions to BAEs

Here we take the XXX model for example, one can have similar analysis for XXZ model. One can always solve BAEs for several simple cases by hand, with or without any constraints, to get all mathematical solutions of them. It is noticed that the multiple solutions are singular solutions, containing $u_j = \pm i/2$. To get the correct counting of the solutions, the basic strategy is to consider the singular solutions and the rest ones separately. Without loss of generosity, one can introduce an variable w and add the constraint following

$$w\prod_{j=1}^{N}(u_j^2+1/4)-1=0 \tag{2.3.35}$$

to the original set of BAE.

To obtain the singular solutions, let $u_1 = i/2$ and $u_2 = -i/2$ and solve for the rest of the variables.

Finally, the completeness of Bethe ansatz can be formulated as a statement of the numbers of solutions of BAEs with various constraints. Denote the number of pairwise distinct finite solutions for $N \leq L/2$ by $\mathcal{N}_{L,N}$. Denote the number of singular solutions by $\mathcal{N}^{\mathrm{s}}_{L,N}$ and the singular physical solutions by $\mathcal{N}^{\mathrm{sphy}}_{L,N}$. The number of solutions are counted *without multiplicities*. The statement of completeness of Bethe ansatz is[11]

$$\mathcal{N}_{L,N}-\mathcal{N}^{\mathrm{s}}_{L,N}+\mathcal{N}^{\mathrm{sphys}}_{L,N}=\binom{L}{N}-\binom{L}{N-1}. \tag{2.3.36}$$

Chapter 3 Introduction to Computational Algebraic Geometry

3.1 Some facts of affine algebraic geometry

Consider a polynomial ring $R = \mathbb{F}[z_1, \dots z_n]$ as is the collection of all polynomials in n variables $z_1, \dots z_n$ with coefficients in the *field* $\mathbb{F}$. Here, $\mathbb{F}$ can be $\mathbb{Q}$, the rational numbers, $\mathbb{C}$, the complex numbers, $\mathbb{Z}/p\mathbb{Z}$, the *finite field* of integers modulo a prime number p, or $\mathbb{C}(c_1, c_2, \dots c_k)$, the complex rational functions of parameters $c_1, \dots, c_k$, and so on. The selection of $\mathbb{F}$ can largely affect the calculation within this polynomial ring.

To define the sum in general sense, one need *ideal* first.

Definition 3.1 An ideal I in the polynomial ring $R = \mathbb{F}[z_1, \dots z_n]$ is a subset of R such that,

- $0 \in I$. For any two $f_1, f_2 \in I$, $f_1 + f_2 \in I$. For any $f \in I$, $-f \in I$.
- For $\forall f \in I$ and $\forall h \in R$, $hf \in I$.

The ideal in the polynomial ring $R = \mathbb{F}[z_1, \dots z_n]$ generated by a subset S of R is the collection of all such polynomials,

$$\sum_i h_i f_i, \quad h_i \in R, \quad f_i \in S. \tag{3.1.1}$$

This ideal is denoted as $\langle S \rangle$. In particular, $\langle 1 \rangle = R$, which is an ideal which contains all polynomials. Note that even if S is an infinite set, the sum in (3.1.1) is always restricted to a sum of a finite number of terms. S is called the generating set of this ideal.

And then, one can have the following properties of ideals.

Theorem 3.1 (Noether) The generating set of an ideal I of $R = \mathbb{F}[z_1, \dots z_n]$ can always be chosen to be finite.

This theorem implies that one only needs to consider ideals generated by finite sets in the polynomial ring R.

Definition 3.2 Let I be an ideal of R, one can define an equivalence relation,

$$f \sim g, \quad \text{if and only if } f - g \in I\,. \tag{3.1.2}$$

Here one define an equivalence class, $[f]$ as the set of all $g \in R$ such that $g \sim f$. The *quotient ring* R/I is set of equivalence classes,

$$R/I = \{[f] | f \in R\}\,. \tag{3.1.3}$$

with multiplication $[f_1][f_2] \equiv [f_1 f_2]$. (Check this multiplication is well-defined.)

To study the structure of an ideal, it is very useful to consider the algebra-geometry relation.

Definition 3.3 Let $\mathbb{K}$ be a field, $\mathbb{F} \subset \mathbb{K}$. The n-dimensional $\mathbb{K}$-affine space $\mathbf{A}^n_{\mathbb{K}}$ is the set of all n-tuple of $\mathbb{K}$. Given a subset S of the polynomial ring $\mathbb{F}[z_1, \ldots, z_n]$, its *algebraic set* over $\mathbb{K}$ is,

$$\mathcal{Z}_{\mathbb{K}}(S) = \{p \in \mathbf{A}^n_{\mathbb{K}} | f(p) = 0, \text{ for every } f \in S\}. \tag{3.1.4}$$

If $\mathbb{K} = \mathbb{F}$, one can drop the subscript $\mathbb{K}$ in $\mathbf{A}^n_{\mathbb{K}}$ and $\mathcal{Z}_{\mathbb{K}}(S)$.

The algebraic set $\mathcal{Z}(S)$ consists of all *common solutions* of polynomials in S. Note that to solve polynomials in S is equivalent to solve all polynomials simultaneously in the ideal generated by S,

$$\mathcal{Z}(S) = \mathcal{Z}(\langle S \rangle), \tag{3.1.5}$$

since if $p \in \mathcal{Z}(S)$, then $f(p) = 0, \forall f \in S$. Hence,

$$h_1(p) f_1(p) + \ldots + h_k(p) f_k(p) = 0, \quad \forall h_i \in R,\ \forall f_i \in S. \tag{3.1.6}$$

To learn the structure of an ideal from its algebraic set, one can firstly consider the empty algebraic set.

The following theorem holds

Theorem 3.2 (Hilbert's weak Nullstellensatz) Let I be an ideal of $\mathbb{F}[z_1, \ldots z_n]$ and $\mathbb{K}$ be an algebraically closed field, $\mathbb{F} \subset \mathbb{K}$. If $\mathcal{Z}_{\mathbb{K}}(I) = \emptyset$, then $I = \langle 1 \rangle$.

Remark The field extension $\mathbb{K}$ must be algebraically closed. Otherwise, say, $\mathbb{K} = \mathbb{F} = \mathbb{Q}$, the ideal $\langle x^2 - 2 \rangle$ has empty algebraic set in $\mathbb{Q}$. (The solutions are not

rational). However, $\langle x^2 - 2\rangle \neq \langle 1\rangle$. On the other hand, $\mathbb{F}$ need not be algebraically closed. $I = \langle 1\rangle$ means,

$$1 = h_1 f_1 + \ldots + h_k f_k, \quad f_i \in I,\ h_i \in \mathbb{F}[z_1, \ldots z_n]\,. \tag{3.1.7}$$

where h_i's coefficients are in $\mathbb{F}$, instead of an algebraic extension of $\mathbb{F}$.

For a general algebraic set, one has the important theorem:

Theorem 3.3 (Hilbert's Nullstellensatz) Let $\mathbb{F}$ be an algebraically closed field and $R = \mathbb{F}[z_1, \ldots z_n]$. Let I be an ideal of R. If $f \in R$ and,

$$f(p) = 0, \quad \forall p \in \mathcal{Z}(I), \tag{3.1.8}$$

then there exists a positive integer k such that $f^k \in I$.

Hilbert's Nullstellensatz characterizes all polynomials vanishing on $\mathcal{Z}(I)$, they are "not far away" from elements in I.

Definition 3.4 Let I be an ideal in R, define the *radical ideal* of I as,

$$\sqrt{I} = \{f \in R | \exists k \in \mathbb{Z}^+, f^k \in I\}\,. \tag{3.1.9}$$

For any subset V of $\mathbf{A}^n$, define the ideal of V as

$$\mathcal{I}(V) = \{f \in R | f(p) = 0,\ \forall p \in V\}\,. \tag{3.1.10}$$

Then Hilbert's Nullstellensatz reads, over an algebraically closed field,

$$\mathcal{I}(\mathcal{Z}(I)) = \sqrt{I}\,. \tag{3.1.11}$$

An ideal I is called *radical*, if $\sqrt{I} = I$.

If two ideals I_1 and I_2 have the same algebraic set $\mathcal{Z}(I_1) = \mathcal{Z}(I_2)$, then they have the same radical ideals $\sqrt{I}_1 = \sqrt{I}_2$. On the other hand, if two sets in $\mathbb{A}^n$ have the same ideal, what could one say about them? To answer this question, the topology of $\mathbb{A}^n$ needs to be defined as:

Definition 3.5 (Zariski topology) Define Zariski topology of $\mathbf{A}^n_{\mathbb{F}}$ by setting all algebraic set to be topologically closed. (Here $\mathbb{F}$ need not be algebraic closed.)

Remark The intersection of any number of Zariski closed sets is closed since,

$$\bigcap_i \mathcal{Z}(I_i) = \mathcal{Z}(\bigcup_i I_i). \tag{3.1.12}$$

The union of two closed sets is closed since,

$$\mathcal{Z}(I_1) \bigcup \mathcal{Z}(I_2) = \mathcal{Z}(I_1 I_2) = \mathcal{Z}(I_1 \cap I_2). \tag{3.1.13}$$

$\mathbf{A}^n_{\mathbb{F}}$ and $\varnothing$ are both closed because $\mathbf{A}^n_{\mathbb{F}} = \mathcal{Z}(\{0\})$, $\varnothing = \mathcal{Z}(\langle 1 \rangle)$. That means Zariski topology is well-defined.

Zariski topology is the foundation of affine algebraic geometry. With this topology, one can establish the dictionary between algebra and geometry.

Proposition 3.1 (Here $\mathbb{F}$ need not be algebraic closed.)

1. If $I_1 \subset I_2$ are ideals of $\mathbb{F}[z_1, \ldots z_n]$, $\mathcal{Z}(I_1) \supset \mathcal{Z}(I_2)$
2. If $V_1 \subset V_2$ are subsets of $\mathbf{A}^n_{\mathbb{F}}$, $\mathcal{I}(V_1) \supset \mathcal{I}(V_2)$
3. For any subset V in $\mathbf{A}^n_{\mathbb{F}}$, $\mathcal{Z}(\mathcal{I}(V)) = \overline{V}$, the Zariski closure of V.

Proof The first two statements follow directly from the definitions. For the third one, $V \subset \mathcal{Z}(\mathcal{I}(V))$. Since the latter is Zariski closed, $\overline{V} \subset \mathcal{Z}(\mathcal{I}(V))$. On the other hand, for any Zariski closed set X containing V, $X = \mathcal{Z}(I)$. $I \subset \mathcal{I}(V)$. From statement 1, $X = \mathcal{Z}(I) \supset \mathcal{Z}(\mathcal{I}(V))$. As a closed set, $\mathcal{Z}(\mathcal{I}(V))$ is contained in any closed set which contains V, hence $\mathcal{Z}(\mathcal{I}(V)) = \overline{V}$. ∎

In the case $\mathbb{F}$ is algebraic closed, the above proposition and Hilbert's Nullstellensatz established the one-to-one correspondence between radical ideals in $\mathbb{F}[z_1, \ldots z_n]$ and closed sets in $\mathbf{A}^n_{\mathbb{F}}$.

In the following part, the computational aspect of affine algebraic geometry is introduced, to see how to compute objects like $I_1 \cap I_2$ and $\mathcal{Z}(I)$.

3.2 Gröbner basis

3.2.1 One-variable case as an invitation

One may have noticed that *ideal* is the central concept for the algebraic side of affine algebraic geometry. An ideal can be generated by different generating sets, some

may be redundant or complicated. For ideals, choosing a "good basis" can dramatically simplify algebraic geometry computation just like what one can do in linear algebra.

For the univariate case, there is a natural monomial order $\prec$ from the degree, for example, take $I = \langle x^3 - x - 1 \rangle$, the following ordering holds

$$1 \prec x \prec x^2 \prec x^3 \prec x^4 \prec \dots , \tag{3.2.14}$$

and all monomials are sorted. For any polynomial F, define the *leading term*, $\mathrm{LT}(F)$ to be the highest monomial in F by this order (with the coefficient). For multivariate cases, the degree criterion is not fine enough to sort all monomials, so one needs more general monomial orders.

Definition 3.6 Let M be the set of all monomials with coefficients 1, in the ring $R = \mathbb{F}[z_1, \dots z_n]$. A monomial order $\prec$ of R is an ordering on M such that,

1. $\prec$ is a total ordering, which means any two different monomials are sorted by $\prec$.
2. $\prec$ respects monomial products, i.e., if $u \prec v$ then for any $w \in M$, $uw \prec vw$.
3. $1 \prec u$, if $u \in M$ and u is not constant.

There are several important monomial orders. For the ring $\mathbb{F}[z_1, \dots z_n]$, one can use the convention $1 \prec z_n \prec z_{n-1} \prec \dots \prec z_1$ for all monomial orders. Given two monomials, $g_1 = z_1^{\alpha_1} \dots z_n^{\alpha_n}$ and $g_2 = z_1^{\beta_1} \dots z_n^{\beta_n}$, consider the following orders:

- Lexicographic order (*lex*). First compare α_1 and β_1. If $\alpha_1 < \beta_1$, then $g_1 \prec g_2$. If $\alpha_1 = \alpha_2$, compare α_2 and β_2. Repeat this process until for certain α_i and β_i the tie is broken.
- Degree lexicographic order (*grlex*). First compare the total degrees. If $\sum_{i=1}^n \alpha_i < \sum_{i=1}^n \beta_i$, then $g_1 \prec g_2$. If total degrees are equal, compare (α_1, β_1), (α_2, β_2) ... until the tie is broken, like *lex*.
- Degree reversed lexicographic order (*grevlex*). First compare the total degrees. If $\sum_{i=1}^n \alpha_i < \sum_{i=1}^n \beta_i$, then $g_1 \prec g_2$. If total degrees are equal, compare α_n and β_n. If $\alpha_n < \beta_n$, then $g_1 \succ g_2$ (reversed!). If $\alpha_n = \beta_n$, then one may further compare $(\alpha_{n-1}, \beta_{n-1})$, $(\alpha_{n-2}, \beta_{n-2})$ ... until the tie is broken, and use the reversed result.
- Block order. This is the combination of *lex* and other orders. Here one can sepa-

rate the variables into k blocks, say,

$$\{z_1, z_2, \dots z_n\} = \{z_1, \dots z_{s_1}\} \cup \{z_{s_1+1}, \dots z_{s_2}\} \dots \cup \{z_{s_{k-1}+1}, \dots z_n\}\,. \quad (3.2.15)$$

Furthermore, define the monomial order for variables in each block. To compare g_1 and g_2, firstly compare the first block by the given monomial order. If it is a tie, it is useful to compare the second block... until the tie is broken.

With a monomial order, one can define the leading term as the highest monomial (with coefficient) of a polynomial in this order. To find a stable basis for computation, one may lead to the concept of Gröbner basis.

3.2.2 Gröbner basis

Definition 3.7 For an ideal I in $\mathbb{F}[z_1, \dots z_n]$ with a monomial order, a Gröbner basis $G(I) = \{g_1, \dots g_m\}$ is a generating set for I such that for each $f \in I$, there always exists $g_i \in G(I)$ such that,

$$\mathrm{LT}(g_i) | \mathrm{LT}(f)\,. \quad (3.2.16)$$

Beyond the definition, here are have some comments on Gröbner basis:

1. For $\mathbb{F}[z_1, \dots z_n]$, the computation of polynomial division and Buchberger's Algorithm only used addition, multiplication and division in $\mathbb{F}$. No algebraic extension is needed. Let $\mathbb{F} \subset \mathbb{K}$ be a field extension. If $\boldsymbol{B} = \{f_1, \dots, f_k\} \subset \mathbb{F}[z_1, \dots z_n]$, then the Gröbner basis computation of $\boldsymbol{B}$ in $\mathbb{K}[x_1, \dots, x_n]$ produces a Gröbner basis which is still in $\mathbb{F}[z_1, \dots z_n]$, irrelevant of the algebraic extension.
2. The form of a Gröbner basis and computation time dramatically depend on the monomial order. Usually, *grevlex* is the fastest choice while *lex* is the slowest. However, in some cases, Gröbner basis with *lex* is preferred. In these cases, we may instead consider some "midway" monomial order the like block order, or convert a known *grevlex* basis to *lex* basis[29].
3. If all input polynomials are linear, then the reduced Gröbner basis is the *echelon form* in linear algebra.

The computation of Gröbner basis will be introduced in the next section together with the applications.

3.2.3 Zero dimensional ideal

A zero dimensional ideal is a special case of ideals such that its algebraic set in an *algebraic closed field* is a finite set, i.e., $|\mathcal{Z}_{\bar{K}}(I)| < \infty$. The study of zero dimensional ideals are crucial for our Bethe Ansatz computations.

One of the important properties of a zero dimensional ideal I define over K is that the number of solutions (in an algebraically closed field) equals the linear dimension of the quotient ring

$$|\mathcal{Z}_{\bar{K}}(I)| = \dim_K(A_K/I) \tag{3.2.17}$$

Note that the field K need not be algebraically closed, but the field extension $\bar{K}$ must be algebraically closed for this formula. Let $G(I)$ be the Gröbner basis of I in any monomial ordering. Since (A_K/I) is linearly spanned by monomials which are not divisible by any elements in $\mathrm{LT}(G(I))$, the number of solutions, $|\mathcal{Z}_{\bar{K}}(I)|$ equals the number of monomials which are not divisible by $\mathrm{LT}(G(I))$. This statement provides a valuable method of determining the number of solutions. In practice, we can use the lattice algorithm[24] to list these monomials.

Let $(m_1, \ldots, m_k)$ be the monomial basis of A_K/I determined from the above Gröbner basis $G(I)$. We can reformulate the algebraic structure of (A_K/I) as matrix operations. For any $f \in A_k$,

$$[f][m_i] = \sum_{j=1}^{k} [m_j] c_{ji}, \quad c_j \in K, \quad i = 1, \ldots, k \tag{3.2.18}$$

The $k \times k$ matrix c_{ji} is called the *companion matrix*. We denote the companion matrix of the polynomial f by M_f. It is clear that M_f=M_g if and only if $[f] = [g]$ in A/I and

$$M_{f+g} = M_f + M_g, \quad M_{fg} = M_f M_g = M_g M_f, . \tag{3.2.19}$$

Furthermore, if a polynomial f is in the ideal $\langle g \rangle + I$, we say the fraction f/g is a "polynomial" in the quotient ring A/I by the abuse of terminologies. The reason is that, in this case,

$$f = gq + s, \quad s \in I\,. \tag{3.2.20}$$

Hence in the quotient ring A/I, $[f] = [g][q]$. For a point $\xi \in \mathcal{Z}(I)$, if $g(\xi) \neq 0$, then $f(\xi)/g(\xi) = q(\xi)$. In this sense, the computation of a fraction over the solution set is converted to the computation of a polynomial over the solutions.

Furthermore, we define $M_{f/g} \equiv M_q$. It is clear that when M_g is an invertible matrix,

$$M_{f/g} = M_f M_g^{-1} . \tag{3.2.21}$$

Companion matrix is a powerful tool for computing the sum of values of f evaluated at the algebraic set (solutions) of I over the algebraically closed field extension $\bar{K}$. Let $(\xi_1, \ldots, \xi_k)$ be the elements of $|\mathcal{Z}_{\bar{K}}(I)|$,

$$\sum_{i=1}^{k} f(\xi_i) = \operatorname{tr} M_f \tag{3.2.22}$$

Hence this sum over solutions over $\bar{K}$ can be evaluated directly from the Gröbner basis over the field K. It also proves that this sum must be inside K, even though individual terms may not be.

3.3 Connections between spin chain model and computational algebraic geometry

Computational algebraic geometry plays a crucial role in the study of spin chain models, particularly in understanding their properties, symmetries, and exact solvability. Here are some key aspects of the relationship between computational algebraic geometry and spin chain models:

1. Solving Bethe Equations: Spin chain models, including the Heisenberg XXX and XXZ spin chain models, often involve solving a set of nonlinear equations called Bethe equations. These equations arise from the Bethe ansatz method, which is used to find the eigenstates of the system. Computational algebraic geometry provides powerful numerical and symbolic methods to solve these equations, often involving techniques like Gröbner basis computations and numerical algebraic geometry. These methods enable the determination of the allowed momenta of

the quasi-particles and the identification of the exact eigenstates of the spin chain model.

2. Symmetry Analysis: Spin chain models possess various symmetries, such as translational symmetry, rotational symmetry, and permutation symmetry. Computational algebraic geometry techniques, such as the theory of group representations and symbolic computations, can be employed to analyze and exploit these symmetries. By studying the symmetry properties of the spin chain model using algebraic methods, researchers can simplify the analysis and gain deeper insights into the system's behavior.
3. Integrability Conditions: Integrable spin chain models have an extensive number of conserved quantities, which are crucial for their exact solvability. Computational algebraic geometry provides tools to study the integrability conditions of these models. By formulating the problem in the language of algebraic geometry, researchers can analyze the algebraic properties of the conserved quantities and investigate the conditions under which they commute with the Hamiltonian. This analysis contributes to understanding the underlying mathematical structure of the integrable spin chain models.
4. Phase Diagram Analysis: Computational algebraic geometry techniques are valuable in studying the phase diagrams of spin chain models. By analyzing the algebraic equations that describe the model and their solutions, researchers can explore the different phases of the system, identify phase transitions, and determine critical points. Numerical methods in algebraic geometry, such as numerical continuation and bifurcation analysis, aid in tracing the phase boundaries and characterizing the critical behavior of the spin chain model.
5. Entanglement and Correlation Analysis: Computational algebraic geometry also facilitates the study of entanglement properties and correlation functions in spin chain models. By using algebraic methods and symbolic computations, researchers can calculate entanglement measures, such as entanglement entropy, and analyze correlation functions to understand the quantum correlations and sta-

tistical properties of the system.

In summary, computational algebraic geometry provides powerful tools and techniques to analyze and solve spin chain models. It aids in solving Bethe equations, studying symmetry properties, analyzing integrability conditions, exploring phase diagrams, and investigating entanglement and correlation properties. The combination of computational algebraic geometry with spin chain models contributes to a deeper understanding of these quantum systems and advances our knowledge in the field of theoretical physics.

Chapter 4 Algorithms to calculate Gröbner basis

4.1 Multivariate polynomial division

To calculate and use Gröbner basis firstly one need the multivariate division algorithm, which is a generalization of univariate Euclidean algorithm (Algorithm 4.1). The basic procedure is that: given a polynomial F and a list of k polynomials f_i's, if $\mathrm{LT}(F)$ is divisible by some $\mathrm{LT}(f_i)$, then remove $\mathrm{LT}(F)$ by subtracting a multiplier of f_i. Otherwise move $\mathrm{LT}(F)$ to the remainder r. The output will be

$$F = q_1 f_1 + \dots q_k f_k + r\,, \tag{4.1.1}$$

where r consists of monomials cannot be divided by any $LT(f_i)$. Let $B = \{f_1, \dots f_k\}$, and denote $\overline{F}^B$ as the remainder r. Recall that the one-loop OPP integrand reduction

Algorithm 4.1 Multivariate division algorithm

Input: $F, f_1 \dots f_k, \succ$
$q_1 := \dots := q_k = 0, r := 0$
while $F \neq 0$ **do**
    $reductionstatus := 0$
    for $i = 1$ to k **do**
        if $\mathrm{LT}(f_i) | \mathrm{LT}(F)$ **then**
            $q_i := q_i + \frac{\mathrm{LT}(F)}{\mathrm{LT}(f_i)}$
            $F := F - \frac{\mathrm{LT}(F)}{\mathrm{LT}(f_i)} f_i$
            $reductionstatus := 1$
            break
        end if
    end for
    if $reductionstatus = 0$ **then**
        $r := r + \mathrm{LT}(F)$
        $F := F - \mathrm{LT}(F)$
    end if
end while
return $q_1 \dots q_k, r$

and the naive trial of two-loop integrand reduction are very similar to this algorithm.

Note that for a general list of polynomials, the algorithm has two drawbacks: (1) the remainder r depends on the order of the list, $\{f_1, \dots f_n\}$ (2) if $F \in \langle f_1 \dots f_n \rangle$, the algorithm may not give a zero remainder r. These made the previous two-loop integrand

reduction unsuccessful. Gröbner basis eliminates these problems.

Proposition 4.1 Let $G = \{g_1, \dots g_m\}$ be a Gröbner basis in $\mathbb{F}[z_1, \dots z_n]$ with the monomial order $\succ$. Let r be the remainder of the division of F by G, from Algorithm 4.1.

1. r does not depend on the order of $g_1, \dots g_m$.
2. If $F \in I = \langle g_1, \dots g_m \rangle$, then $r = 0$.

Proof If the division with different orders of $g_1, \dots g_n$ provides two remainder r_1 and r_2. If $r_1 \neq r_2$, then $r_1 - r_2$ contains monomials which are not divisible by any $\mathrm{LT}(g_i)$. But $r_1 - r_2 \in I$, this is a contradiction to the definition of Gröbner basis.

If $F \in I$, then $r \in I$. Again by the definition of Gröbner basis, if $r \neq 0$, $\mathrm{LT}(r)$ is divisible by some $\mathrm{LT}(g_i)$. This is a contradiction to multivariate division algorithm. ∎

Then the question is: given an ideal $I = \langle f_1 \dots f_k \rangle$ in $\mathbb{F}[z_1, \dots z_n]$ and a monomial order $\succ$, does the Gröbner basis exist and how does one find it? This is answered by Buchberger's Algorithm, which was presented in 1970s and marked the beginning of computational algebraic geometry.

4.2 Buchberger's Algorithm

Recall that Euclidean algorithm computes the gcd of two polynomials hence the Gröbner basis is given. The key step is to cancel leading terms of two polynomials. That inspires the concept of S-polynomial in multivariate cases.

Definition 4.1 Given a monomial order $\succ$ in $R = \mathbb{F}[z_1, \dots z_n]$, the S-polynomial of two polynomials f_i and f_j in R is,

$$S(f_i, f_j) = \frac{\mathrm{LT}(f_j)}{\gcd\big(\mathrm{LT}(f_i), \mathrm{LT}(f_j)\big)} f_i - \frac{\mathrm{LT}(f_i)}{\gcd\big(\mathrm{LT}(f_i), \mathrm{LT}(f_j)\big)} f_j. \tag{4.2.2}$$

Note that the leading terms of the two terms on the r.h.s cancel.

Theorem 4.1 (Buchberger) Given a monomial order $\succ$ in $R = \mathbb{F}[z_1, \dots z_n]$, Gröbner basis with respect to $\succ$ exists and can be found by Buchberger's Algorithm (Algorithm 4.2).

Proof See Cox, Little, O'Shea[24]. ∎

Algorithm 4.2 Buchberger algorithm

```
1: Input: B = {f_1 ... f_n} and a monomial order ≻
2: queue := all subsets of B with exactly two elements
3: while queue! = ∅ do
4:         {f, g} := head of queue
5:         r := S(f, g) mod B
6:         if r ≠ 0 then
7:                 B := B ∪ r
8:                 queue << {{B_1, r}, ... {last of B, r}}
9:         end if
10:        delete head of queue
11: end while
12: return B (Gröbner basis)
```

The uniqueness of Gröbner basis is given via *reduced Gröbner basis*.

Definition 4.2 For $R = \mathbb{F}[z_1, \dots z_n]$ with a monomial order $\succ$, a reduced Gröbner basis is a Gröbner basis $G = \{g_1, \dots g_k\}$ with respect to $\succ$, such that

1. Every $\mathrm{LT}(g_i)$ has the coefficient 1, $i = 1, \dots, k$.
2. Every monomial in g_i is not divisible by $\mathrm{LT}(g_j)$, if $j \neq i$.

Proposition 4.2 For $R = \mathbb{F}[z_1, \dots z_n]$ with a monomial order $\succ$, I is an ideal. The reduced Gröbner basis of I with respect to $\succ$, $G = \{g_1, \dots g_m\}$, is unique up to the order of the list $\{g_1, \dots g_m\}$. It is independent of the choice of the generating set of I.

Proof See Cox, Little, O'Shea[24]Chapter 2. Note that given a Gröbner basis $B = \{h_1 \dots h_m\}$, the reduced Gröbner basis G can be obtained as follows,

1. For any $h_i \in B$, if $\mathrm{LT}(h_j) | \mathrm{LT}(h_i)$, $j \neq i$, then remove h_i. Repeat this process, and finally we get the *minimal basis* $G' \subset B$.
2. For every $f \in G'$, divide f towards $G' - \{f\}$. Then replace f by the remainder of the division. Finally, normalize the resulting set such that every polynomial has leading coefficient 1, and one can get the reduced Gröbner basis G.

∎

Note that Buchberger's Algorithm reduces only one polynomial pair every time, more recent algorithms attempt to

1. reduce many polynomial pairs at once

2. identify the “unless” polynomial pairs *a priori*.

Here, Faugere's F4 algorithm will be introduced as the representative of the rest[29].

4.2.1 Faugere's F4 algorithm

Faugère's F4 algorithm is a powerful algorithm in the field of computational algebraic geometry, specifically in the area of polynomial system solving. It was developed by Jean-Charles Faugère and provides an efficient method for computing Gröbner bases, which are fundamental objects in algebraic geometry and polynomial algebra.

The F4 algorithm utilizes the concept of ”F4 reduction,” which involves reducing a given polynomial system to a smaller and simpler system while preserving its Gröbner basis. This reduction process exploits various algebraic properties and relations among the polynomials in the system to eliminate unnecessary computations and reduce memory requirements.

The key idea behind the F4 algorithm is to construct a so-called ”S-pair matrix” that represents the reductions and relations between the polynomials. By carefully organizing and manipulating this matrix, the algorithm reduces the problem of computing a Gröbner basis to a series of linear algebra operations, such as matrix reduction and Gaussian elimination.

Here is the basic idea of ”F4 reduction”.

Algorithm 4.3 Faugere's F4 reduction

Input: P_d *a finite subset of selected critical pairs*
G *a finite subset of* $R[x]$
$\mathbb{F} = (F_k)_{k=1,\dots,d}$, F_k *a finite subset of* $R[x]$
$F := SymbolicProcess(P_d, G, \mathbb{F})$
$\tilde{F} := RREF(F) w.r.t <$
$\tilde{F}^+ := \{f \in \tilde{F} | HT(f) \notin HT(F)\}$
return $(\tilde{F}^+, F)$

Here $RREF$ and $SymbolicProcess$ algorithms are algorithms for Gauss reduction to row echelon form and some matrix construction process. One may find detailed information in the reference[29]

And the F4 algorithm is as below:

Notice that the efficiency of the F4 algorithm largely depends on the selection strat-

Algorithm 4.4 Faugere's F4 algorithm

Input: $F = \{f_1 \dots f_n\}$
$G := \emptyset$
$P := \emptyset$
$d := 0$
while $F! = \emptyset$ **do**
    $f := first(F)$
    $F := F \backslash \{f\}$
    $(G, P) := Update(G, P, f)$
end while
while $P! = \emptyset$ **do**
    $d := d + 1$
    $P_d = Select(P)$
    $P = P \backslash P_d$
    $(\tilde{F}_d^+, F_d) := Reduction(P_d, G, (F_i)_{d=1,\dots,(d-1)})$
    for $h \in \tilde{F}_d^+$ **do**
        $(G, P) := Update(G, P, h)$
    end for
end while
return G (Gröbner basis)

egy and $RREF$ function. One may need a lot of work to choose the right function for the computation.

However, it's important to note that while the F4 algorithm provides significant advancements in Gröbner basis computations, it is not a universally superior algorithm for all scenarios. The choice of algorithm depends on the specific characteristics of the problem at hand, and other algorithms, such as F5 or tailored variants, may be more efficient in certain cases.

4.3 Current Implementations of the algorithms

There are already some implementations of Buchberger algorithm and F4 algorithm in computer algebra systems.

Usually one can compute Gröbner basis by programs, for example,

- in MATHEMATICA The embedded function **GroebnerBasis** computes Gröbner basis by Buchberger's Algorithm. The relation between Gröbner basis and the original generating set is not given. Usually, Gröbner basis computation in MATHEMATICA is not very fast.

- in MAPLE Maple computes Gröbner basis by either Buchberger's Algorithm or highly efficient F4 algorithm.
- SINGULAR is a powerful computer algebraic system[31] developed in Technische Universität Kaiserslautern. SINGULAR uses Buchberger's Algorithm to compute Gröbner basis
- MACAULAY2 is a sophisticated algebraic geometry program, which orients to research mathematical problems in algebraic geometry. It contains Buchberger's Algorithm and experimental codes of F4 algorithm.
- Fgb package[48]. This is a highly efficient package of F4 and F5 algorithms by Jean-Charles Faugére. It has both MAPLE and C++ interfaces. Usually, it is faster than the F4 implement in MAPLE. Currently, coefficients of polynomials are restricted to $\mathbb{Q}$ or $\mathbb{Z}/p$, in this package.

Chapter 5 Application of CAG methods in spin chain model

5.1 Application I: counting the number of BAEs' solution

In this section, one is introduced to apply the method of Gröbner basis to compute the numbers $\mathcal{N}_{L,N}$, $\mathcal{N}^{\mathrm{s}}_{L,N}$ and $\mathcal{N}^{\mathrm{sphys}}_{L,N}$ for given L and N. The notations are from 2.3.36. The basic idea is that the number of solutions for a given set of polynomial equations is the dimension of the corresponding quotient ring. Instead of solving equations, one can construct the quotient rings and compute their dimensions.

For a given L and N, define the following polynomials.

$$\mathrm{B}_j = (u_j + i/2)^L Q_{\mathbf{u}}(u_j - i) + (u_j - i/2)^L Q_{\mathbf{u}}(u_j + i), \qquad j = 1, \cdots, N \tag{5.1.1}$$

$$\mathrm{B} = w\,(u_1^2 + 1/4) \cdots (u_N^2 + 1/4) - 1 \tag{5.1.2}$$

$$\mathrm{B}' = w\,(u_3^2 + 1/4) \cdots (u_N^2 + 1/4) - 1 \tag{5.1.3}$$

where $Q_{\mathbf{u}}(u)$ is the Baxter polynomial defined by

$$Q_{\mathbf{u}}(u) = \prod_{k=1}^{N} (u - u_k). \tag{5.1.4}$$

To have pairwise distinct roots, one may define the polynomials

$$\mathrm{A}_{ij} = \frac{\mathrm{B}_i - \mathrm{B}_j}{u_i - u_j}, \qquad i = 1, \cdots, N-1;\ j = i+1, \cdots, N. \tag{5.1.5}$$

This is a classical trick of getting distinct roots in algebraic geometry. For singular and singular physical solutions, define the following polynomials

$$\begin{aligned} \mathrm{S}_k = \ & (u_k + i/2)^{L-1}(u_k - 3i/2) \prod_{j=3}^{N} (u_k - u_j - i) \\ & + (u_k - i/2)^{L-1}(u_k + 3i/2) \prod_{j=3}^{N} (u_k - u_j + i), \qquad k = 3, \cdots, N, \end{aligned} \tag{5.1.6}$$

$$\mathrm{S} = \prod_{k=3}^{N} (u_k + i/2)^L + (-1)^{L+1} \prod_{k=3}^{N} (u_k - i/2)^L.$$

Using these polynomials, one can define the following ideals

$$\begin{aligned} I_{\mathrm{NS}} &= \langle \mathrm{B}_1, \cdots, \mathrm{B}_N, \mathrm{B}, \mathrm{A}_{12}, \cdots, \mathrm{A}_{N-1,N} \rangle, \\ I_{\mathrm{S}} &= \langle \mathrm{S}_3, \cdots, \mathrm{S}_N, \mathrm{B}', A_{34}, \cdots, \mathrm{A}_{N-1,N} \rangle, \\ I_{\mathrm{SP}} &= \langle \mathrm{S}_3, \cdots, \mathrm{S}_N, \mathrm{B}', \mathrm{S}, A_{34}, \cdots, \mathrm{A}_{N-1,N} \rangle \end{aligned} \tag{5.1.7}$$

where the subscribes denote 'Non-Singular', 'Singular' and 'Singular Physical'. The corresponding quotient rings are defined as

$$\begin{aligned} Q_{\mathrm{NS}} &= \mathbb{C}[u_1, \cdots, u_N]/I_{\mathrm{NS}}, \\ Q_{\mathrm{S}} &= \mathbb{C}[u_3, \cdots, u_N]/I_{\mathrm{S}}, \\ Q_{\mathrm{SP}} &= \mathbb{C}[u_3, \cdots, u_N]/I_{\mathrm{SP}}. \end{aligned} \tag{5.1.8}$$

All the three quotient rings are finite dimensional linear spaces. The numbers $\mathcal{N}_{L,N}$, $\mathcal{N}^{\mathrm{s}}_{L,N}$ and $\mathcal{N}^{\mathrm{sphys}}_{L,N}$ are given in terms of the dimensions of the quotient rings as

$$\mathcal{N}_{L,N} = \frac{\dim Q_{\mathrm{NS}}}{N!} + \frac{\dim Q_{\mathrm{S}}}{(N-2)!}, \qquad \mathcal{N}^{\mathrm{s}}_{L,N} = \frac{\dim Q_{\mathrm{S}}}{(N-2)!}, \qquad \mathcal{N}^{\mathrm{sphys}}_{L,N} = \frac{\dim Q_{\mathrm{SP}}}{(N-2)!} \tag{5.1.9}$$

One may divide the dimensions by factorials to get rid of the permutation redundancy. Any permutation of the set of Bethe roots is considered to be the same solution, yet they correspond to different points in the affine variety. From the definitions of the ideals (5.1.7), it is straightforward to compute the corresponding Gröbner basis. Then one can construct the standard basis for the quotient rings and the dimensions of the quotient rings follows.

Note that BAE (for non-singular and singular solutions) is totally symmetric in $u_1, \ldots u_n$, i.e., the ideal for BAE is symmetric under the full permutation group of u_i's. One can take advantage of this feature to speed up the Gröbner basis computation. One immediate choice is to apply the symmetric ideal Gröbner algorithm, "symodstd.lib" in SINGULAR. However, this approach is still not fast enough for our propose. Instead, the following trick is developed:

For a totally symmetric ideal I in variables $u_1, \ldots u_n$, add n auxiliary variables

$s_1, \dots s_n$ and n auxiliary equations to make a new ideal $\tilde{I}$,

$$s_k - \sum_{j_1 < \dots j_k} u_{j_1} \dots u_{j_k} = 0, \quad k = 1, \dots, n\,. \tag{5.1.10}$$

Therefore one may define s_k as the k-th elementary polynomials in $u_1, \dots u_n$. It is found find that with auxiliary variables and equations, and a block order $[u_1, \dots u_n] \succ [s_n, \dots s_1]$, the Gröbner basis computation is much faster. Furthermore the resulting Gröbner basis for $\tilde{I}$ is much shorter comparing with that for I. It's believed that the improvement comes from the fact that BAE is much simpler in terms of the symmetric variables $s_1, \dots, s_n$. The solutions of $\tilde{I}$' are in one-to-one correspondence to the solution of I, so this method is sufficient.

As a very interesting byproduct, this trick provides a new representation of BAE: The Gröbner basis $G(\tilde{I})$, in the block order mentioned above, eliminates the original variables $u_1, \dots u_n$ and gives a set of equations only in $s_1, \dots, s_n$.

$$\langle G(\tilde{I}) \cap \mathbb{K}[s_1, \dots s_n] \rangle = \tilde{I} \cap \mathbb{K}[s_1, \dots s_n]\,. \tag{5.1.11}$$

(On the left hand side of the equation, $\langle \dots \rangle$ means the ideal inside $K[s_1, \dots s_n]$.) Usually the symmetrized BAE in $s_1, \dots, s_n$ is simpler than the original one since the permutation symmetry group S_n is removed.

5.1.1 Comparison of 2 algorithms

So the basic idea is to compute the Gröbner basis of (5.1.7). Then, as is talked above, one has 2 choices on the algorithm to compute it: Buchberger or F4? Here's the comparison of them in the problem mentioned above.

During the comparison, the implementations chosen are:

1. Buchberger algorithm: "std" function implemented in Singular, which returns a standard basis.
2. F4 algorithm: **Fgb** package on Maple, which is a direct implementation, returns a reduced Gröbner basis

Here the examples used are the ideals generated by variables $\{s_1, \dots, s_n\}$ with respect to the XXX spin chain of length $10 \leq L \leq 20$ and magnons $5 \leq M \leq 9$, and one

computes the Gröbner basis of them with the implementations above. Notice that for the idea of efficiency, the finite field technique is introduced in the calculation of Gröbner basisOne calculates over $\mathbb{Z}/p_1, \ldots, \mathbb{Z}/p_k$, where p_i is prime. Then it is easy to calculate the lift result in $\mathbb{Q}$ by Chinese Remainder Theorem and Farey sequences. One may use package "modstd.lib" in SINGULAR to do this. It is also applied on the MAPLE process.

Here are the results:

Length or magnons	5	6	7	8	9
10	0.2	N/A	N/A	N/A	N/A
11	N/A	N/A	N/A	N/A	N/A
12	0.3	0.6	N/A	N/A	N/A
13	0.3	0.7	N/A	N/A	N/A
14	0.7	1.2	N/A	N/A	N/A
15	1.1	2.7	9.9	N/A	N/A
16	9.3	13.3	30.5	N/A	N/A
17	107.1	297.6	403.7	904.1	N/A
18	1000.3	1300.2	3700.9	4991.4	6103.2
19	3547.9	8427.1	17853.2	21821.7	37090.4
20	12070.8	19587.9	26439.0	N/A	N/A

Table 5.1 Result of Buchberger calculation (s)

Length or magnons	5	6	7	8	9
10	0.2	N/A	N/A	N/A	N/A
11	0.2	N/A	N/A	N/A	N/A
12	0.3	1.0	N/A	N/A	N/A
13	0.6	1.1	N/A	N/A	N/A
14	1.4	5.0	N/A	N/A	N/A
15	3.0	5.2	12.9	N/A	N/A
16	15.1	23.7	33.9	N/A	N/A
17	118.1	347.9	461.2	1193.1	N/A
18	1276.6	1892.2	7946.3	10892.0	21487.3
19	4303.1	27790.6	34751.2	N/A	N/A
20	17450.2	N/A	N/A	N/A	N/A

Table 5.2 Result of F4 calculation (s)

During the test, the CPU being used is Intel(R) Core(TM) i7-10750H CPU @ 2.60GHz 2.59 GHz with 32GB RAM. Both programs are running with single core.

Here "N/A" for $19 \leq L \leq 20$ reads that the results cannot be calculated within the acceptable time. (Other "N/A" means that no such examples given)

One can easily find out that Buchberger algorithm is much better than the F4 al-

gorithm for the same Gröbner basis calculation task since the time consumption is far less. So we choose Buchberger algorithm for further test.

5.2 Application II: calculation of companion matrix in Loschmidt Echo problem

The Loschmidt echo is a concept that arises in the study of quantum dynamics and quantum information theory, including the dynamics of spin chain models. It provides a measure of the sensitivity of a quantum system's time evolution to perturbations or changes in its initial state. In the context of spin chain models, the Loschmidt echo quantifies how a small perturbation affects the time evolution of the system.

In a spin chain model, the Loschmidt echo is defined as the overlap between the time-evolved state of the system under a perturbed Hamiltonian and the initial state of the system. Mathematically, it can be expressed as:

Certainly! Here is the equation for the Loschmidt echo in LaTeX code:

$$L(t) = \left|\langle\psi(0)|e^{-iH_p t}e^{iH_0 t}|\psi(0)\rangle\right|^2 \tag{5.2.12}$$

where $|\psi(0)\rangle$ is the initial state of the system, H_0 is the unperturbed Hamiltonian governing the system's time evolution, H_p is the perturbed Hamiltonian, and t is the evolution time.

The Loschmidt echo provides information about the stability and robustness of the quantum system. If the initial state is perturbed slightly, a large Loschmidt echo implies that the system's time evolution is highly sensitive to the perturbation. On the other hand, a small Loschmidt echo indicates that the system's evolution remains relatively stable under the perturbation.

The Loschmidt echo has been widely studied in the context of spin chain models, particularly in the investigation of quantum phase transitions, quantum chaos, and many-body localization. It has been used to probe the effects of disorder, interactions, and other perturbations on the dynamics of spin chains, shedding light on the emergence of

long-range correlations, thermalization, and the transition from localized to delocalized behavior.

Furthermore, the Loschmidt echo has connections to other concepts in quantum information theory, such as quantum fidelity and quantum entanglement. It is related to the decay of quantum correlations and the spreading of information in the system. As such, the Loschmidt echo provides insights into the behavior of quantum systems and their response to perturbations, contributing to our understanding of quantum dynamics and information processing.

Given a spin chain with length L and N finite magnons and n magnons at infinity, one can build such transfer matrix as

$$termAGdes(L,N,n,k) = \frac{conjFacdes(N,n)overlapDWdes(N,n)^2 eigenUdes(N,n)^k}{normGdes(L,N,n)} \tag{5.2.13}$$

in which k as the time evolution parameter.

Here

$$conjFacdes(N,n) = \prod_{i=1}^{N}[(\frac{u(k)-\theta}{u(k)-\theta+i})^{\frac{N+n}{2}}(\frac{u(k)+\theta}{u(k)+\theta+i})^{\frac{N+n}{2}}] \tag{5.2.14}$$

calculates the conjugation factor between $\langle u_N|DW_N\rangle$ and $\langle DW_N|u_N\rangle$;

$overlapDWdes(N,n)$ gives the the overlap of the domain wall boundary state and the descendant state with N finite magnons and n magnons at infinity.

$normGdes(L,N,n)$ computes the Gaudin norm of the descendant states of length L and N finite Bethe roots and n roots at infinity.

$eigenUdes(N,n)$ computes the eigenvalue of U with N magnons. The eigenvalue of the descendant state is the same as the primary state.

And after the calculation of the transfer matrix, to convert the Bethe roots to the symmetric sums used in $QQ-relations$, one need to symmetrize all the expressions.

After that, one need to calculate the trace of the companion matrix of the symmetrized transfer matrix, which will be a univariate function to θ.

However it will be extremely hard if one directly computes the trace of the companion matrix with the parameter θ. Since the result will be a rational function of θ, one can

do seeding to the parameter and gain a lot of results in integer form, during which time the finite field technique can be applied. After this, one can perform Thiele's method to lift the result from the numerical results to get the rational function of θ.

One may want to see the time evolution via k. It suffices to calculate the results w.r.t different integer value of k to see it.

Using the method mentioned in 3.2.3[26], one can compute the companion matrix via computing Gröbner basis. Then the following process will be similar to what has been done in the previous section.

Chapter 6 Massively Parallel Computation and Computational Algebraic Geometry

6.1 Introduction to parallelization

6.1.1 Some facts about parallelization

Parallel computation in computational algebraic geometry refers to the use of multiple computing resources, such as processors or machines, to perform computations simultaneously and expedite the solution of problems in algebraic geometry. It aims to leverage the inherent parallelism in algorithms and computations to accelerate the execution time and handle larger and more complex problems.

Parallel computation techniques have been employed in various aspects of computational algebraic geometry, including solving polynomial systems, computing Gröbner bases, analyzing algebraic varieties, and performing numerical algebraic geometry computations. Here are some key aspects and benefits of parallel computation in this field:

1. Speedup and Scalability: Algebraic geometry problems often involve large-scale computations that can be time-consuming and memory-intensive. By utilizing parallel computation, the workload can be distributed across multiple processors or machines, enabling significant speedup and enhanced scalability. This allows researchers to tackle more challenging problems or analyze larger data sets within a reasonable timeframe.
2. Algorithmic Parallelism: Many algorithms in computational algebraic geometry exhibit inherent parallelism. For example, in polynomial system solving or Gröbner basis computations, independent operations can be executed in parallel, such as polynomial multiplication, polynomial division, or elimination steps. Parallelizing these computations reduces the overall execution time by dividing the workload among multiple processors.
3. Divide and Conquer Strategies: Parallel computation techniques often employ divide and conquer strategies to break down a problem into smaller subproblems

that can be solved independently. For instance, in solving large polynomial systems, the problem can be divided into subsets of equations that can be solved in parallel by different processors. The solutions from these subsets can then be combined to obtain the complete solution.

4. Task Parallelism and Task Scheduling: In computational algebraic geometry, parallel computation can also be achieved through task parallelism, where different tasks or operations are executed concurrently. Task scheduling techniques, such as workload balancing and load distribution, play a crucial role in efficiently allocating tasks to available processors and optimizing the overall performance.
5. Parallel Libraries and Frameworks: Various parallel computing libraries and frameworks, such as OpenMP, MPI, or distributed computing platforms, provide tools and programming models to facilitate parallel computations in computational algebraic geometry. These libraries offer functionalities for parallel task execution, data parallelism, communication among processors, and load balancing, simplifying the development and deployment of parallel algorithms.
6. Hybrid Approaches: In some cases, a combination of parallel computation with other techniques, such as symbolic-numeric algorithms or approximation methods, can further enhance the efficiency and accuracy of computational algebraic geometry computations. Parallelization can be combined with adaptive refinement, iterative refinement, or probabilistic sampling techniques to obtain faster and more accurate solutions.

Parallel computation in computational algebraic geometry has become increasingly important as the size and complexity of problems continue to grow. By harnessing the power of parallelism, researchers can tackle challenging computations more effectively, accelerate the solution of problems, and explore new frontiers in algebraic geometry and related areas of mathematics and science.

6.1.2 Mathematical language of parallelization: Petri net

In parallel computation, Petri nets provide a mathematical framework for modeling and analyzing concurrent and distributed systems. They offer a formalism that captures the interactions and dependencies among different computational entities, enabling the study of system behavior, synchronization, and performance.

Mathematically, a Petri net can be defined as a tuple (P, T, F, W, M_0), where:

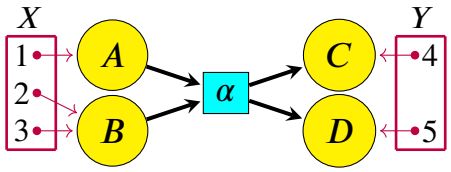
- P is a finite set of places representing the state or condition of the system.
- T is a finite set of transitions representing events or actions that can occur in the system.
- $F \subseteq (P \times T) \cup (T times P)$ is a set of directed arcs connecting places and transitions.
- $W : F \to \mathbb{N}$ is a weight function that assigns a non-negative integer weight to each arc, representing the number of tokens or resources required or produced by the arc.
- $M_0 : P \to \mathbb{N}$ is the initial marking, which specifies the initial distribution of tokens in the places.

The state of the Petri net at any given moment is represented by a marking $M_0 : P \to \mathbb{N}$, which indicates the number of tokens in each place. A marking M is a valid state if it satisfies the following conditions:

1. For each place $p \in P$, $M(p) \geq 0$. 2. For each transition $t \in T$, the number of tokens in its input places is greater than or equal to the number of tokens required by the transition.

The behavior of the Petri net is governed by the firing rule. A transition t can fire and change the state of the system if the marking satisfies the firing condition: for each input place p, the number of tokens in p is greater than or equal to the weight $W(p, t)$. When t fires, it consumes tokens from its input places and produces tokens in its output places, according to the weights specified by the function W.

Here is an example of an open Petri net P from a set X to a set Y



The yellow circles are places and the blue rectangle is a transition. The bold arrows from places to transitions and from transitions to places complete the structure of a Petri net. There are also arbitrary functions from X and Y into the set of places. These indicate points at which tokens could flow in or out, making our Petri net 'open'. We write this open Petri net as $P : X \nrightarrow Y$ for short.

The firing of transitions can occur in parallel, reflecting the concurrent nature of the system. Multiple transitions that satisfy the firing condition can fire simultaneously, leading to different possible next states of the system. The choice of which transitions to fire depends on the specific scheduling policy or strategy employed in the parallel computation.

Through the analysis of Petri nets, various properties of parallel systems can be studied, such as reachability, liveness, deadlock detection, and performance analysis. Reachability analysis examines whether a particular marking can be reached from the initial marking, while liveness analysis investigates the existence of possible firing sequences that can lead to certain states. Deadlock detection focuses on identifying states where no transitions can fire, resulting in a system that cannot progress further. Performance analysis deals with evaluating system throughput, response time, or resource utilization based on the dynamics of the Petri net.

By providing a mathematical framework for modeling and analyzing parallel computation, Petri nets facilitate the understanding, design, and optimization of concurrent and distributed systems. They allow for formal reasoning about system behavior and properties, aiding in the development of efficient and reliable parallel algorithms and architectures.

In this project, the high efficiency Gröbner basis computation is realized by constructing a parallel framework via SINGULAR/GPI-SPACE with self-implemented Buch-

berger algorithm.

6.1.3 SINGULAR/GPI-SPACE framework

GPI-SPACE, which stands for Global-View Parallel Interface Space, is a workflow management system designed for high-performance numerical parallel computing by the Competence Center High Performance Computing of Fraunhofer ITWM. It provides a programming model and a set of tools that simplify the development of parallel applications.

The basic concept behind GPI-SPACE is to provide a global view of the parallel system's data space. This means that instead of explicitly managing the distribution of data across different processes or nodes, users can work with a unified view of the entire data space, regardless of where the data is physically located. This abstraction hides the complexities of parallelism and enables programmers to focus on their algorithms and computations.

Here are the key components and concepts of the GPI-SPACE:

- Data Spaces: In GPI-SPACE, data is organized into data spaces. A data space represents a collection of data elements that are distributed across the parallel system. Each data element is associated with a unique global address, allowing processes to access and manipulate the data seamlessly.
- Data Access: GPI-SPACE provides functions and operations to access and manipulate data in the data spaces. Users can read and modify data elements using their global addresses, without needing to be aware of the underlying distribution or communication details. This allows for transparent access to distributed data, making it easier to develop parallel algorithms.
- Communication: GPI-SPACE abstracts away the communication between processes. It automatically manages the movement of data between processes when necessary, based on the access patterns and dependencies of the application. This communication is performed efficiently using low-level communication libraries or protocols, such as MPI (Message Passing Interface).

- Synchronization: GPI-Space provides synchronization mechanisms to coordinate the execution of parallel processes. Users can specify synchronization points in their code to ensure that processes wait for specific conditions or data dependencies before proceeding. This helps to maintain the correctness and consistency of the parallel execution.
- Load Balancing: GPI-Space incorporates load balancing techniques to distribute the computational workload evenly across the available processes. It dynamically monitors the workload and adjusts the distribution of tasks to optimize performance and resource utilization. Load balancing inGPI-Space helps to minimize idle time and maximize the efficiency of the parallel application.

Here is the basic workflow of GPI-Space

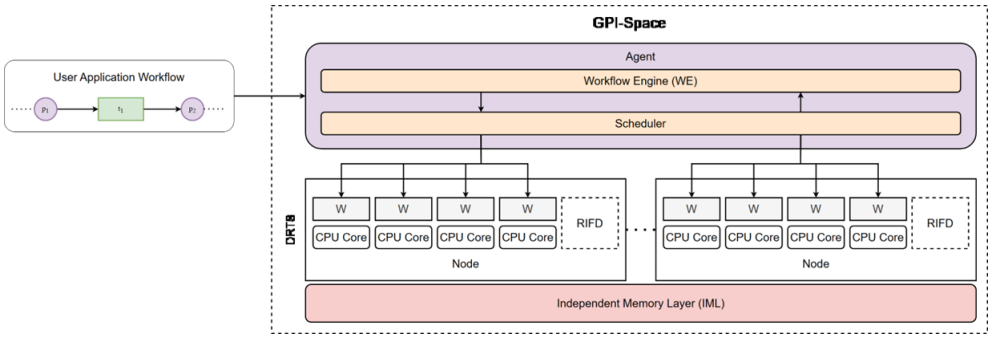


Figure 6.1.1 principle of GPI-Space

GPI-Space supports a wide range of parallel architectures, including shared-memory systems, distributed-memory systems, and hybrid systems. It offers a uniform programming interface that hides the low-level details of the underlying hardware and communication protocols, making it easier to write portable parallel code.

Overall, GPI-Space simplifies the development of parallel applications by providing a global view of the data space, abstracting communication and synchronization, and incorporating load balancing capabilities. It allows users to focus on their algorithms and computations while the framework handles the complexities of parallelism, making it an effective tool for high-performance scientific computing and parallel applications.

And the basic idea of Singular/GPI-Space framework is to combine Singular with GPI-Space to create a way of performing massively parallel computations in computer algebra. Our approach is based on the idea of separating computation and coordina-

tion. While SINGULAR is used as the computational backend, the coordination is done by GPI-SPACE. GPI-Space uses the language of Petri nets to model algorithms in the coordination layer. The SINGULAR/GPI-SPACE framework can be used on anything ranging from a personal computer and compute servers to ultrascale machines. In applications, it scales efficiently up to thousands of cores on HPC clusters. Applications arise, so far, from algebraic geometry (certifying smoothness, resolution of singularities), tropical geometry (computing of tropicalizations with finite symmetries), geometric invariant theory (computing GIT-fans with finite symmetries), high energy physics (computing integration-by-parts identities for Feynman integrals), and condensed matter physics. While relying on GPI-SPACE allows us to apply state-of-the-art parallelization infrastructure when using Singular, our close collaboration has, in turn, also lead to introducing new programming constructs in GPI-SPACE, and to developing an open source version of GPI-SPACE. An Open Source Version of GPI-SPACE has been released by ITWM in Sept. 2020 (this software is actively being tested on CentOS Linux (Versions 6, 7, 8) and Ubuntu (Versions 18.04 LTS, 20.04 LTS), but various other distributions will work as well). A first end user version of the SINGULAR/GPI-SPACE Framework has been released in Dec. 2020, one can find it on the GITHUB.

6.2 Massively parallelization computation of Gröbner basis

6.2.1 Algorithm in Petri nets

The parts that need to be parallelized during the calculation is that:

- calculate the s-polynomials of the s-pairs;
- calculate the normal forms of the s-polynomials.
- judge whether the normal forms is 0 or not.

The input will be a set of polynomials $\{f_1, \ldots, f_n\}$, after change the index set into ordered pairs, one may run the Buchberger computation. The parallelization process will be finished with GPI-SPACE.

Every time for the iteration, there will be 2 transitions to decide whether to add the

corresponding normal forms into the input basis, with adding to m. If it's nonzero, one extends m.

After the iteration, the system outputs the set m, which is the reduced Gröbner basis

.

The Petri net of the algorithm is as follows:

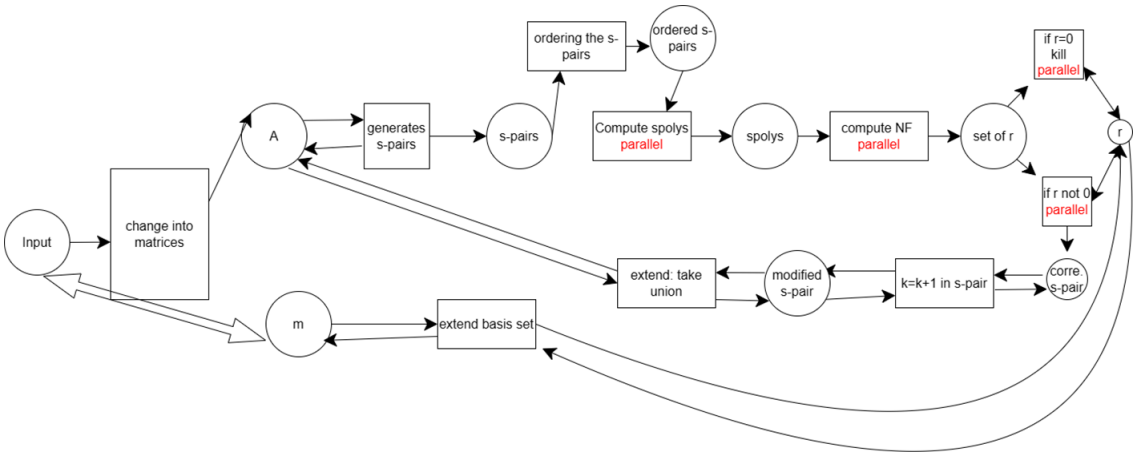


Figure 6.2.2 Petri net of parallel Buchberger algorithm

6.2.2 The structure of the program

The program consists of 3 major parts.

- Framework for Parallelization. See the Petri net above. Each transition is written in XPNET language to define the input and output ports of the workflow. Using Eureka method, it also defines when the computation terminates.
- Functions for calling. To realize the file flow in the framework part, one will need to use the .ssi file format in SINGULAR to improve the efficiency of writing and reading from hard drive. Such control structure can be realized by calling SINGULAR's C++ package *libSingular*. Also, one don't use the real file in the I/O port of the framework, but the file names between the tokens. So there will be a random file name generator. And the most important part, the self-implemented Buchberger algorithm via C++ and SINGULAR, which is a bit faster than the implementation in SINGULAR as "std".
- The interface file. It is written in Python, which is used to call the function in the second part. Change this file, and the parallelization will be changed.

This program has already been published on the GitHub repo, one can download it and give a try.

https://github.com/singular-gpispace/buchberger

6.2.3 Tests for Application I

In the previous chapter, the application of Gröbner basis computation to the completeness of BAEs is mentioned. There are some results cannot be calculated directly with Singular Buchberger computation. Here it is tried with the parallel Buchberger algorithm implemented with Singular/GPI-Space framework.

The test is taken over the same machine as above. The CPU being used is Intel(R) Core(TM) i7-10750H CPU @ 2.60GHz 2.59 GHz with 32GB RAM. The computation is running on 4 cores parallelization.

Here are the time results of computing the Gröbner basis for ideals generated by variables $\{s_1, \ldots, s_n\}$ with respect to the XXX spin chain of length $18 \leq L \leq 20$ and magnons $7 \leq M \leq 10$

Length or magnons	7	8	9	10
18	617.1	1399.3	2001.1	3917.6
19	1427.1	1797.2	3102.9	5221.4
20	3215.4	5121.7	6698.3	8189.4

Table 6.1 Result of parallel Buchberger calculation: Gröbner basis (s)

One can see that, for comparison, the time results of length $18 \leq L \leq 20$ and magnons $7 \leq M \leq 9$ has been shortened by $7 - 8$ times. And the example of length $L = 20$, $M = 10$ can be computed within a reasonable time.

6.2.4 Tests for Application II

Similarly, one can run the second application of this program. The test runs over calculated intermediate results by using Mathematica. The symmetrization process is also performed with Mathematica.

Using 41 CPUs and 144GB RAM on the cluster, the calculation of trace of companion matrices is performed as below. Here the time parameter k is taken to 10, with

the length $6 \leq L \leq 12$ and magnons $0 \leq M \leq 4$. The whole computation process including rational function simplification, trace companion matrix computation over finite fields and lift back to $\mathbb{Q}$ and parallel fitting of the parameter θ. The seeding process takes 20000 seeds in integer values for θ.

Here are the time results for the whole process. The pair (M, m) is the pair of finite magnons and infinite magnons.

Length or magnons	(0,0)	(1,1)	(2,0)	(0,2)	(2,2)	(3,1)	(1,3)	(0,4)	(4,0)
6	0.0	0.0	3.4	3.7	N/A	N/A	N/A	N/A	N/A
8	0.0	1.3	9.9	10.1	67.4	433.7	417.2	231.8	215.7
10	0.0	10.1	299.1	278.4	1300.2	1973.1	1937.4	719.8	762.4
12	0.0	37.8	771.5	723.6	1701.4	2619.0	2903.1	2003.4	1998.9

Table 6.2 Result of parallel Buchberger calculation: companion matrix (s)

Here "N/A" means the example does not exist.

One can see the complete results of length $6 \leq L \leq 12$ and magnons $0 \leq M \leq 4$ with $k = 10$ can be calculated within reasonable time. Notice that previously the results of $L = 12$, $(M, m) = (3, 1)$ and $(1, 3)$ cannot be calculated directly with SINGULAR within acceptable time limit.

Chapter 7 Summary and Outlook

7.1 Summary

In terms of research direction, this project mainly focuses on topics related to quantum integrable systems. In recent years, quantum integrable system models have played an important role in various areas of mathematics and physics, particularly in revealing the characteristics and critical behavior of highly nonlinear and strongly correlated physical systems far from the perturbative regime. The precise solutions of integrable models are often required for such research, but the process can be challenging. Exploring and developing efficient methods for solving the relevant equations is a key issue in this field.

In terms of research objects, this project focuses on the application of computational algebraic geometry methods in integrable spin chain models. Computational algebraic geometry methods, which have evolved from the study of algebraic equation solutions, have become mature and efficient mathematical tools over the years. In the study of integrable spin chains, the most important problem is the precise solution of the Bethe Ansatz equations (algebraic equations). The compatibility between the two makes the application of computational algebraic geometry methods in solving integrable spin chains a promising research direction, and remarkable achievements have already been made by research groups both domestically and internationally. In this process, solving the corresponding Gröbner basis is the most crucial step. Improving the methods for solving Gröbner basis is a key aspect of this research.

The research process of this project mainly focuses on the selection and improvement of methods for solving Gröbner basis . After extensive testing and comparison, one method, namely the Buchberger algorithm, was chosen from the two main methods. And it had been re-implemented by hand in C++ and SINGULAR language. The SINGULAR/GPI-SPACE framework was introduced to enhance parallel computing, resulting in improved computational efficiency.

The resulting program, namely ”paraBuchberger”, is applied to 2 certain problems:

counting solutions of BAEs in XXX spin chain model and finding the sum of solutions for Loschmidt problem in XXZ spin chain model. And both have been proved to be efficient to some degree. Some results that cannot be computed previously is now solved with the new method.

However, due to time and computational resource limitations, this research project was unable to test integrable system models on a larger scale, and the testing process was also simplified. For example, the testing of algorithm selection used existing algorithm implementations, which may not be as efficient as developing one's own. The final comparative testing was only conducted on a few representative calculations due to time constraints, and there were some limitations in controlling variables. These aspects can be further improved.

In conclusion, the results of this project have achieved the expected outcomes to some extent. The algorithmic roadmap was designed and followed according to the planned timeline. The program itself was developed and subjected to reliability testing. A series of programming errors were identified and fixed through compilation testing. Finally, by computing a few finite-scale instances, the proposed method in this project was compared with traditional methods, demonstrating its superiority.

7.2 Outlook

From the final run test results, it can be seen that the proposed parallel Buchberger method in this research significantly improves the computational efficiency of Gröbner bases. This has implications for several fields:

1. In the context of the studied integrable spin chain computations, this method can be attempted for solving larger-scale integrable spin chain Bethe Ansatz Equation (BAE) problems, providing a clearer understanding of spin chain models.
2. In high-energy physics, it is possible to apply computational algebraic geometry methods, such as computing Gröbner bases, to address reduction problems in Feynman integrals. By identifying the corresponding syzygy equations through the module associated with the reduction, one can use the module intersection

method to search for partial integration relations and thereby reduce integrals. In this process, the computation of Gröbner bases can also benefit from the parallel method mentioned in this study to enhance computational efficiency.

3. Basic mathematical problems also involve the calculation of Gröbner bases on modules, particularly in finite fields, as well as the verification of Gröbner bases' correctness. This is helpful in areas such as combinatorics, quantum groups, algebraic geometry, and complex geometry.

And so on.

Therefore, the proposed approach in this research still holds untapped potential, awaiting further exploration and implementation in physics, mathematics, and other fields.

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