

# Integrability in Classical and Quantum Systems

## Part I The Heisenberg Spin Chain

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This document details the Heisenberg XXX Spin Chain and its solution using the Algebraic Bethe Ansatz. It is intended as the first instalment (Part I) of a two-part document, with Part II (published at a later date) to cover the classical, non-linear Korteweg de Vries equation. Whilst the Heisenberg Spin Chain and Korteweg de Vries equation may seem disparate subjects, they are both examples of integrable systems that have, in more modern mathematical times, been solved by broadly similar methods. In addition, and perhaps more importantly, they give rise to similar physical concepts in terms of stable solutions with a particle interpretation and associated scattering properties. It is the commonality of methods and physical phenomenology that concludes the document upon Part II completion.

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## Acronyms and Abbreviations

Only acronyms unique to the subject matter are listed, common Physics terms such as  $SU(2)$  are not.

ABA : Algebraic Bethe Ansatz  
BAE : Bethe Ansatz Equations  
CBA : Coordinate Bethe Ansatz  
FCR : Fundamental Commutation Relation  
HSC : Heisenberg Spin Chain  
KdV : Korteweg de Vries  
QS : Quantum System  
YBE : Yang-Baxter Equation

## 1 Introduction

### 1.1 Preamble

This document is Part I of an intended two-part document on the general subject of *Integrability in Classical and Quantum System via KdV and the Heisenberg Spin Chain*. This first part addresses the quantum integrable model known as the Heisenberg Spin Chain (HSC) [1], with part II dedicated to the KdV equation, and finishing with a comparison of both HSC and KdV models.

This Part I starts with a general introduction to integrable systems. Primarily classical, but ending by extension of the same concepts to integrable quantum systems [2]. The HSC is one such quantum system, but its modern algebraic solution has similarities to both classical models and other quantum integrable models. The HSC is solved using a modern mathematical method known as the *Algebraic Bethe Ansatz* (ABA) due to Faddeev [3]. Beforehand, there are quite a lot of mathematical preliminaries to define matrix operators, that are also common to other integrable systems. Once defined, the physics of the spin chain starts with the simplest, but very illustrative, case of a one-magnon spin chain solved by an earlier, more intuitive method, called the *Coordinate Bethe Ansatz* (CBA) [4],[5] due to Bethe [6] 1931. This then sets the scene for a solution to the multiple magnon spin chain, thereby completing the document. A common feature across all sections is the Hamiltonian and Spin, for which the Appendices also give some simple background on standard  $SU(2)$  spin multiplets.

Key sources of information for the work are Faddeev [3],[7], primarily for the ABA method, whilst Nepomechie [5], was motivation for the initial idea, and covers both the CBA and ABA, albeit in not so much detail for the ABA, which is the only method used herein to solve the HSC. There is also excellent coverage of CBA and ABA due to Beisert [4], especially with regard to a more pictorial understanding of the algebra involved. Two other very useful, and relatively elementary papers on quantum integrability, are Lamers [8] and Doikou et al [2]. All aforementioned references, as would be expected, offer something different - which unfortunately also includes notation (particularly indexing symbols). In this regard, the algebra herein contains a mix of what the author considered the clearest.

### 1.2 Integrability in Dynamical Systems

A loose, intuitive definition of an integrable dynamical system is one in which its equations of motion have been solved. A dynamical system, itself, can be broadly defined as a set of one or more interacting objects, likely subject to internal and external forces, whose behaviour evolves, usually over time, according to a set of differential equations describing the system.

The simplest example of a dynamical system is just a single particle moving in a straight line, possibly subject to a force acting along its line of motion. By Newton II, the acceleration can be determined from the force, integrated once to get the velocity, and integrated a second time to get its position, providing that the force can, in principle, be integrated (a numeric integration is allowed). If so, then given two constants for its initial velocity and position, its motion is completely determined thereafter and it is thus an integrable system, albeit rather simple.

A more complicated, familiar example is the rigid body motion of a gyroscope (or spinning top), spinning around its z-axis, which is pitched over from the vertical and, due to gravity, the spin axis precesses around the z-axis in azimuth, whilst possibly periodically nodding (termed nutation) under a perturbing force on the spin axis. This system can be completely solved for the angular velocities and integrated (albeit using elliptic integrals) to give the attitude angles - it is also an integrable system, see Goldstein [9].

Such an example brings us nicely to a more academic definition of integrability, namely a system that possesses as many *first integrals of motion* as it has degrees of freedom. The gyroscope's position is specified by three 'Euler' angles (roll, pitch, yaw) and has three degrees of freedom. To completely specify its motion, both three positions and three body rates (spin, precession and nutation) are required. However, by specifying the initial positions and angular velocities, only three (not six) first integrals of motion are required. These *first integrals* are obtainable as functions of both the angles and their rates. In fact, the functions are equations of conservation of angular momentum and energy. The point here is that the three first integrals are closely tied to three conserved quantities. In effect, three functions of the body rates and angles can be found such that the time-derivative of these functions is zero, and integrating them with respect to time gives a constant of motion for each.

In general, for a dynamical system with  $n$ -degrees of freedom, if  $n$  first integrals of motion can be found, equivalent to  $n$  conserved quantities, then the system is considered integrable. Invariably one of these first integral functions is the Hamiltonian representing the energy conservation equation; angular momentum (and/or spin) is usually another.

In the field of Hamiltonian dynamics, the independence of first integral functions translates to two of them at a time possessing a zero *Poisson Bracket*. In this case, two such functions are then said to be in *involution*, i.e. their Poisson bracket is zero. Integrability then becomes a matter of finding  $n$  functions in involution. In a sense they commute, which then leads to a similar notion in the quantum world.

Whilst the above is all classical theory, Hamiltonian dynamics beautifully spans both the classical and quantum world. It is no coincidence that a fundamental operator in Quantum Mechanics (QM) is *The Hamiltonian*. The Poisson bracket of two functions translates very simply to the commutator of their QM operator forms. The classical statement of integrability then translates to QM very nicely, i.e. if  $n$  commuting operators can be found (one of which is invariably the Hamiltonian) then the Quantum system (QS) is integrable. Unfortunately, the notion of integrability in QM is not universally defined but, nevertheless, obtaining commuting operators is invariably where a solution to a QS starts, and it thus forms the working definition used herein. Most importantly, it translates to finding  $n$  eigenstates of a QS, such as the Heisenberg Spin Chain, that forms the example of quantum integrability in this document.

### 1.3 The Heisenberg XXX Spin Chain

The quantum-mechanical model of magnetism as a spin chain was proposed by Werner Heisenberg in 1928 [1], and later solved by Hans Bethe 1931 [6] using his method now known as the CBA, albeit, as mentioned, the method used herein is due to Faddeev [3],[7], developed much later in the 1970s.

The HSC model comprises a one dimensional lattice of sites (*the chain*), and each site can have a quantum spin state of up or down, as mathematically represented by a  $\mathbb{C}^2$  spinor. Hence it is a quantum model with just two discrete states specified at each lattice site. For  $N$  sites, the mathematical model operates in a  $\mathbb{C}^{2N}$  Hilbert space, and operators and state vectors are given as tensor products,  $\mathbb{C}^{2N} \times \mathbb{C}^{2N}$  for the matrix operators, and  $\mathbb{C}^{2N}$  for states. The algebraic preliminaries for these operators and states is given in the next section.

The number of sites  $N$  is generally large (e.g. Avogadro's number) but generally treated as infinite as an asymptotic limit, with consequent exact integrability. The work herein treats the chain as open-ended, albeit it could be closed, infinite or not. As such, the asymptotic limits assume site interactions vanish in the limit, i.e. the scattering potential is zero at both spatial and temporal times  $\pm\infty$ . A bit more discussion is given for the one-magnon example, Section (3).

## 2 Matrix Operators and Tensor Products

### 2.1 Two-site 4x4 matrix forms

Before giving the full,  $N$ -site tensor product forms for all matrix operators, it is instructive to give a brief overview of some of the key two-site,  $4 \times 4$  matrix forms ( $\mathbb{C}^4 \otimes \mathbb{C}^4$ ). This is especially so because, whilst the full  $N$ -site, tensor product acts on a much larger  $\mathbb{C}^{2N}$  spinor space, the operators (generally  $\mathbb{C}^{2N} \otimes \mathbb{C}^{2N}$ ) only act non-trivially on two spinor sites at a time, so they can be thought of (in a sense) as  $4 \times 4$  matrices. Equally importantly, the integrability of this HSC and many other non-linear models only needs to consider the action on two sites, because all higher cases can be factored into two-site scattering processes, see Section (2.2.6).

Note that only the permutation ( $\mathcal{P}$ ) and Lax matrices ( $R, L$ ) are given here, but there are other important operators, namely the *monodromy* ( $T$ ) and *transfer* ( $t$ ), that are only detailed later when discussing the full tensor product forms, Section (2.2). Indeed, more information on the matrices  $\mathcal{P}$ ,  $R$  and  $L$  is also given in Section (2.2)

#### 2.1.1 Permutation matrix $\mathcal{P}$

The permutation matrix  $\mathcal{P}$  is given by

$$\mathcal{P} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (1)$$

This matrix acts on the tensor product  $u \otimes d$  of two spinors  $u$  and  $d$ , by swapping (or permuting, transposing) their positions, i.e.

$$\mathcal{P}(u \otimes d) = (d \otimes u)$$

The permutation matrix acts as a single transposition, exactly as per a two-cycle in the permutation group  $S_n$ , i.e. a transposition  $(ab)$  swaps (permutes)  $a$  and  $b$ , and is its own inverse, that is  $(ab)(ab) = I$ , just as  $\mathcal{P}^2 = I$  above. This association between the permutation matrix and transposition comes into its own when moving to  $N$ -site tensor products and multiple, consecutive permutations; more details are given in Section (2.2.3).

Matrix  $\mathcal{P}$  is symmetric, hermitian and unitary, i.e.

$$\begin{aligned} \mathcal{P} &= \mathcal{P}^T = \mathcal{P}^* \\ \mathcal{P}^\dagger &= \mathcal{P}^{-1} \quad \mathcal{P}^2 = I \end{aligned}$$

The eigenvalues and eigenvectors of the permutation matrix  $\mathcal{P}$  are basically those of the  $SU(2)$  spin multiplets (triplet and a singlet for a two-site spin system), which are also those of the other matrix operators. The spin eigenvectors and eigenvalues are provided in the Appendices for background information, but the eigenvectors are not required further.

### 2.1.2 The R Matrix

The ‘R’ matrix (a form of Lax matrix, see next), is defined in terms of the permutation matrix, the  $2 \times 2$  identity matrix  $I$ , and a *spectral parameter*  $\lambda$  (also known as a *deformation parameter*), by

$$R(\lambda) = \lambda I \otimes I + i\mathcal{P} \quad (2)$$

Expanding in full  $4 \times 4$  form, using  $\mathcal{P}$  (above), this is

$$R = \begin{pmatrix} \lambda + i & 0 & 0 & 0 \\ 0 & \lambda & i & 0 \\ 0 & i & \lambda & 0 \\ 0 & 0 & 0 & \lambda + i \end{pmatrix}$$

A useful relation, used much later, is the derivative of  $R$  with respect to  $\lambda$ , which is simply the identity, i.e.

$$\frac{dR}{d\lambda} = I \quad (3)$$

Also useful for later, it is noted that for a zero spectral parameter, i.e.  $\lambda = 0$ , the  $R$  matrix becomes the permutation matrix, multiplied by  $i$  as in

$$R(0) = i\mathcal{P} \quad (4)$$

### 2.1.3 The Lax Matrix $L$

The Lax matrix is defined in terms of  $R$  and the spectral parameter  $\lambda$  by

$$L(\lambda) = R(\lambda - \frac{i}{2}) \quad (5)$$

Substituting for  $R$  then  $L$  becomes

$$L = \begin{pmatrix} \lambda + i/2 & 0 & 0 & 0 \\ 0 & \lambda - i/2 & i & 0 \\ 0 & i & \lambda - i/2 & 0 \\ 0 & 0 & 0 & \lambda + i/2 \end{pmatrix}$$

The  $L$  matrix has a more intuitive form, when given in terms of the spin operators  $S_z$ ,  $S_+$  and  $S_-$ , as the following block matrix, where each element is itself a  $2 \times 2$  matrix (in the  $4 \times 4$  case, but they are tensor product for larger order matrices):

$$L = \begin{pmatrix} \lambda I + iS_z & iS_- \\ iS_+ & \lambda I - iS_z \end{pmatrix} \quad (6)$$

This spin-operator form is very similar to the block matrix form of the monodromy matrix, Section (2.2.7), whose elements are spin operators, and used to construct eigenstates of the spin chain. In particular, the off-diagonal  $S_+$  operator is used to create down spins by flipping up-spins at a lattice site.

Given the definition of  $L$  in terms of  $R$  (5) then, for spectral parameter  $\lambda = i/2$ ,

$$L(i/2) = R(0) = i\mathcal{P} \quad \lambda = i/2 \quad (7)$$

This is also useful for later.

## 2.2 N-site tensor product forms

The aforementioned two-site,  $4 \times 4$  ( $\mathbb{C}^4 \times \mathbb{C}^4$ ) matrix operators, i.e.  $\mathcal{P}$ ,  $R$ ,  $L$  plus  $H$ ,  $S$ , further below, all have equivalent N-site  $\mathbb{C}^{2N} \times \mathbb{C}^{2N}$  forms. Indeed, these N-site forms still act ‘non-trivially’ on only two specific sites, i.e. the sub-space  $\mathbb{C}^4 \times \mathbb{C}^4$ , and, otherwise, act trivially on all other  $N - 2$  sites (the identity operator occupies the other  $N - 2$  locations in the tensor product). The identification of the two-specific sites is given by a 2-letter subscript, e.g.  $H_{ij}$  acts on sites  $i$  and  $j$ , similarly for  $\mathcal{P}_{ij}$  etc.. Note that a one-letter subscript, such as  $\bar{\sigma}_i$  (next section), pertains to an operator acting non-trivially on only a single site  $i$ .

### 2.2.1 Pauli Matrices

For an N-site Hamiltonian chain, the spin operator (barring the  $\hbar/2$  factor) at site  $i$  is given by the tensor product of  $\bar{\sigma}$  (96) with the  $2 \times 2$  identity  $I$  as follows:

$$\bar{\sigma}_i = I_1 \otimes \cdots \bar{\sigma}_i \cdots \otimes I_N, \quad I \in \mathbb{C}^2 \times \mathbb{C}^2$$

Likewise, for the spin at site  $j$ ,  $j \neq i$ :

$$\bar{\sigma}_j = I_1 \otimes \cdots \bar{\sigma}_j \cdots \otimes I_N$$

The multiplicative product of the site  $i$  and  $j$  spins is thus

$$\begin{aligned} \bar{\sigma}_i \bar{\sigma}_j &= I_1 \otimes \cdots \bar{\sigma}_i \cdots \bar{\sigma}_j \cdots \otimes I_N \\ \bar{\sigma}_j \bar{\sigma}_i &= I_1 \otimes \cdots \bar{\sigma}_i \cdots \bar{\sigma}_j \cdots \otimes I_N \end{aligned}$$

From these it is seen that the operators at different sites commute, i.e.

$$\bar{\sigma}_i \bar{\sigma}_j = \bar{\sigma}_j \bar{\sigma}_i \Rightarrow [\bar{\sigma}_i \bar{\sigma}_j] = 0$$

This is not the same as the commutator relations (95) for each matrix, as given by  $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$ . Remember, the algebra here is that of tensor products of spin operators.

Note that, for tensor products, the notation used for the square of a vector (98) extends as follows:

$$\begin{aligned} \bar{\sigma}_i^2 &= \bar{\sigma}_i \bar{\sigma}_i = \bar{\sigma}_i \cdot \bar{\sigma}_i = \bar{\sigma}^i \cdot \bar{\sigma}_i \\ \bar{\sigma}_i \bar{\sigma}_j &= \bar{\sigma}_i \cdot \bar{\sigma}_j = \bar{\sigma}^i \cdot \bar{\sigma}_j = \bar{\sigma}_i \cdot \bar{\sigma}^j \end{aligned} \tag{8}$$

Two-site operators, such as  $\bar{\sigma}_i \bar{\sigma}_j$ , are act non-trivially on sites  $i$  and  $j$ , whilst they act trivially on all other sites, i.e. leaving them as is due to the use of the identity operator at these sites.

If  $i = j$ , and treating the squared product  $\bar{\sigma}_i^2$  as an inner product, see (97), then

$$\bar{\sigma}_i^2 = I_1 \otimes \cdots \cdots 3I_i \cdots \otimes I_N = 3I^{\otimes N}$$

### 2.2.2 The Hamiltonian and Spin Operator

By defining the spin operator  $\bar{S}_i$  for the  $i$ th site as

$$\bar{S}_i = \frac{\hbar}{2} \bar{\sigma}_i \tag{9}$$

and the two-site ( $i$  and  $j$ ) Hamiltonian  $H_{ij}$  as

$$H_{ij} = J \bar{S}_i \cdot \bar{S}_j \tag{10}$$

then the Hamiltonian for the N-site, *completely isotropic* (explanation follows) open spin chain is ordinarily given by the total spin interaction across all sites  $i$  and  $j$  as in the sum

$$H = J \sum_{i=1, i < j}^N H_{ij} = J \sum_{i=1, i < j}^N \bar{S}_i \cdot \bar{S}_j \quad (11)$$

This is a sum over all two-site interactions, where  $J$  is an exchange energy constant, discussed again shortly.

The *completely isotropic* nature of this Hamiltonian alludes to the fact that the interactions of spin in all three  $x, y, z$  axes are assumed to have the same energy scaling factor  $J$ . Mathematically this means that the Hamiltonian commutes with all three component spin operators at all sites, i.e.  $[\bar{S}, H] = 0$ , where  $\bar{S} = (S_x, S_y, S_z)$ , and that the exchange constant  $J$ , which would ordinarily be the vector  $J = (J_x, J_y, J_z)$ , is now the single value  $J$  (strictly speaking, the vector  $J(1, 1, 1)$ ), and can be moved outside of the sum as the single constant factor  $J$ . See Lamers [8] for some more details on  $J$ . Because of this isotropy, the model is referred to as the XXX spin-chain model, as opposed to the next, more-involved, XXZ model, which has X and Y directions isotropic with consequent  $J_y = J_x$ , but  $J_z \neq J_x$ .

Whilst XXX is isotropic, as usual in QM, a choice has to be made as to the spin-alignment axis. Since the choice has been made herein to align along the z-axis, in accord with common convention, it is thus rather unfortunate that the model is referred to as XXX and not ZZZ!

The sign of  $J$  may be positive or negative. The case  $J < 0$  in the XXX model corresponds to ferromagnetism, whereby the spins are parallel. In this case the ground state is very simply constructed and the excitations can be found with the help of Bethe's ansatz. Conversely, when  $J > 0$ , this corresponds to anti-ferromagnetism, where anti-parallel spins are energetically preferred. In the case of an electron, for example, since parallel spins cannot occupy the same position, by the Exclusion Principle, they are actually further apart than anti-parallel spins, which can occupy the same position. As a consequence, due to their distance, parallel spins have a lower Coulomb potential than anti-parallel spins with a smaller separation.

Although  $J$  is referred to as the an energy exchange constant, from the Hamiltonian definition (units of energy, i.e. Joules), and the spin vector squared (units of  $\hbar^2$ , i.e. Joule<sup>2</sup>secs<sup>2</sup> as per the 'action'), then  $J$  is seemingly inversely proportional to the energy. Nevertheless, the quadratic factor sec<sup>2</sup> in the definition of  $\hbar$  actually makes the units of  $J$  equal to  $M^{-1}L^{-2}$  (M=mass, L = length). As such, it can be seen related to an inverse square law ( $1/L^2$  - ignoring the mass term). This gives some hint to its Coulomb interaction background of  $J$ .

For a simple model, it suffices to consider only the nearest neighbour interactions so that the condition  $i < j$  becomes  $j = i + 1$  and  $H$  then becomes

$$H = J \sum_{i=1}^N \bar{S}_i \cdot \bar{S}_{i+1} \quad (12)$$

As an example, the simplest, two-site model ( $N = 2$ ) has only one term for  $i = 1, j = 2$ , in which case this Hamiltonian (now denoted  $H_{12}$ ) becomes a single term with no sum as in

$$H = H_{12} = J \bar{S}_1 \cdot \bar{S}_2, \quad N = 2 \quad (13)$$

and using  $\bar{S}_1 = \bar{S} \otimes I$  and  $\bar{S}_2 = I \otimes \bar{S}$  then

$$H_{12} = J(\bar{S} \otimes \bar{S})$$



However, to keep things general for now, the two sites  $i$  and  $j$  will not be constrained as neighbouring until necessary, and the Hamiltonian will be treated as per its first definition (10).

The combined, total spin operator  $\bar{S}_{ij}$  for spins at the two unique sites  $i$  and  $j$  is

$$\bar{S}_{ij} = \bar{S}_i + \bar{S}_j \quad (14)$$

To obtain the total squared spin (that with the familiar QM eigenvalues  $S(S+1)$ ) then, using (14),

$$\bar{S}_{ij}^2 = \bar{S}_i^2 + \bar{S}_j^2 + 2\bar{S}_i \cdot \bar{S}_j$$

Since  $\bar{S}_i = (\hbar/2)\bar{\sigma}_i$  (9), and using the above results  $\bar{\sigma}_i^2 = \bar{\sigma}_j^2 = 3I^{\otimes N}$  this becomes

$$\bar{S}_{ij}^2 = \frac{3}{2}\hbar^2 I^{\otimes N} + 2\bar{S}_i \cdot \bar{S}_j \quad (15)$$

By rearranging to give the inner product  $\bar{S}_i \cdot \bar{S}_j$  in terms of the squared spin  $\bar{S}_{ij}^2$  i.e.

$$\bar{S}_i \cdot \bar{S}_j = \frac{1}{2}(\bar{S}_{ij}^2 - \frac{3}{2}\hbar^2 I^{\otimes N})$$

and substituting for  $\bar{S}_i \cdot \bar{S}_j$  into the Hamiltonian  $H_{ij}$  (10), then

$$H_{ij} = \frac{J}{2}(\bar{S}_{ij}^2 - \frac{3}{2}\hbar^2 I^{\otimes N}) \quad (16)$$

This is not quite in the desired form and requires some adjustment to achieve a zero energy, spin chain ground state. To determine this, an all-up spins, ground state  $\Omega_u$  is defined as follows:

$$\Omega_u = |\uparrow\uparrow \cdots \uparrow\rangle = |u_1, u_2, \cdots u_N\rangle$$

Keeping in mind that  $\bar{S}_{ij}^2 \sim \bar{S}^2$ , and that in QM  $\bar{S}^2\psi = S(S+1)\psi$  then, for the all up state,  $\Omega_u$ , the eigenvector equation  $H_{ij}\Omega_u = E\Omega_u$  is

$$H_{ij}\Omega_u = \frac{J}{2}(S(S+1) - \frac{3}{2})\hbar^2\Omega_u = -2J\hbar^2\Omega_u, \quad S = 1$$

It is desirable to have the ground state energy zero (convention only) and, given the freedom to arbitrarily raise or lower the eigenvalues (so long as it is by the same amount for all eigenvalues), the Hamiltonian can easily be adjusted to achieve this by altering the identity term, changing it from  $3/2$  to  $2$  to give

$$H_{ij} = \frac{J}{2}(\bar{S}_{ij}^2 - 2\hbar^2 I^{\otimes N}) \quad (17)$$

Since  $S(S+1) = 2$  (for two sites  $i$  and  $j$ ,  $S = 1$ ), this now gives a zero energy ground state for the all up ( $\Omega_u$ ) spin state as in

$$H_{ij}\Omega_u = \frac{J}{2}(S(S+1) - 2)\hbar^2\Omega_u = 0, \quad S = 1$$

It is preferred to work with the Pauli spin matrices  $\bar{\sigma}_i$ , instead of spin operators  $\bar{S}_i$ , because the permutation matrix is also defined in terms of them (further below), and so the Hamiltonian and Permutation matrix can easily be related. To do this, the squared operator  $\bar{S}_{ij}^2$  is replaced by the product  $\bar{\sigma}_i \bar{\sigma}_j$  (which is intentionally not the same as  $\bar{\sigma}_{ij}^2$ )

Reverting back to an earlier relation (15), and using the definitions  $\bar{S}_i = (\hbar/2)\bar{\sigma}_i$  and  $\bar{S}_j = (\hbar/2)\bar{\sigma}_j$  to write  $\bar{S}_i \cdot \bar{S}_j$  in terms of  $\bar{\sigma}_i \cdot \bar{\sigma}_j$ , then

$$\bar{S}_{ij}^2 = \frac{3}{2}\hbar^2 I^{\otimes N} + \frac{1}{2}\hbar^2 \bar{\sigma}_i \cdot \bar{\sigma}_j$$

Substituting for  $\bar{S}_{ij}^2$  into  $H_{ij}$  above gives

$$H_{ij} = \frac{J}{4} \hbar^2 (\bar{\sigma}_i \cdot \bar{\sigma}_j - I^{\otimes N}) \quad (18)$$

**From here onward,  $\hbar$  will be set to unity, and natural units used.**

### 2.2.3 The Permutation Matrix $\mathcal{P}$

The two-site permutation  $\mathcal{P}_{ij}$  matrix acts by swapping the spinors at sites  $i$  and  $j$  ( $i \neq j$ ).

The swapping action is at the heart of the translation operator as exhibited by the matrices  $L$  and  $R$ , given they both contain the permutation matrix - the permute acts as a translation, and consecutive permutations can be used to translate across consecutive sites, as will be seen in the ABA algebra. With this in mind, its action can be thought of as a discrete momentum operator - momentum being the generator of translation in QM - see Section (2.2.8).

The algebra of permutation matrices is identical to that of single transpositions (two-cycles) in the permutation group  $S_N$ , i.e.  $P_{ij} \sim (ij)$ . For example, if  $(ab)$  is the transposition swapping (permuting)  $a$  and  $b$ , and  $(bc)$  swapping  $b$  and  $c$ , then the compound operation  $(bc)(ab)$ , whereby convention dictates  $(ab)$  is performed first followed by  $(bc)$ , is equivalent to  $a \rightarrow c$ ,  $b \rightarrow a$  and  $c \rightarrow b$ , and identical to the permutation matrix multiplication  $\mathcal{P}_{bc}\mathcal{P}_{ab}$ . Indeed, this is equivalent to a three cycle  $(acb)$  albeit, for the algebra herein, only decomposition into two-cycles, i.e. consecutive transpositions, or consecutive multiplications of the two-site permutation matrix, is required and/or useful. To this end, matrices operating on three-sites, such as  $\mathcal{P}_{abc}$ , are not used herein. This last case actually has relevance to three-particle scattering, and such interactions are considered to always be factorizable into consecutive, two-particle scattering events - see Section (2.2.6) for more details.

Some index permutation relations are now given that are very useful for the ABA algebra that follows later in Section (4). Also see Section (2.2.4) for *Auxiliary* site notation and use of  $a$  and  $b$  as subscript indices - briefly,  $1 \leq i, j, n \leq N$  and  $a$  and  $b$  lie outside this  $N$ -site quantum space, i.e.  $a, b \notin \{1 \dots N\}$ .

This first relation simply states that transposition is its own inverse, i.e.  $(ab) = (ba)$  and  $(ab)(ba) = I$

$$\mathcal{P}_{ab} = \mathcal{P}_{ba}, \quad \mathcal{P}_{ab}\mathcal{P}_{ba} = I^{\otimes N} \quad (19)$$

Since distinct transpositions commute, i.e.

$$(ab)(cd) = (cd)(ab), \quad a \neq c, d \quad b \neq c, d$$

then two permutations that act on different sites also commute

$$[\mathcal{P}_{ij}, \mathcal{P}_{kl}] = 0, \quad i \neq k, l \quad j \neq k, l \quad (20)$$

For example

$$[\mathcal{P}_{12}, \mathcal{P}_{34}] = 0$$

Because all other operators are built from the permutation matrix and the identity, this commutation property applies to these operators too, and is usefully applied in further proofs.

Every permutation three-cycle  $(abn)$ , by cyclic rotation, has three equivalent forms

$$(abn) = (nab) = (bna)$$

and given that every three-cycle can be decomposed into two, two-cycles, i.e. two transpositions, then the above three-cycles are equivalent to the following transposition combinations:

$$(abn) = (an)(ab) = (nb)(na) = (ba)(bn)$$

Thus, in terms of the permutation operator, the following products of permutation matrices are all identical

$$\mathcal{P}_{an}\mathcal{P}_{ab} = \mathcal{P}_{nb}\mathcal{P}_{na} = \mathcal{P}_{ba}\mathcal{P}_{an} \quad (21)$$

Using the symmetry of transpositions, i.e.  $(nb) = (bn)$ ,  $(na) = (an)$  and  $(ba) = (ab)$ , these can also be written as

$$\mathcal{P}_{an}\mathcal{P}_{ab} = \mathcal{P}_{bn}\mathcal{P}_{an} = \mathcal{P}_{ab}\mathcal{P}_{bn} \quad (22)$$

This notation also makes clear that it matters not whether the auxiliary sites  $a$  and  $b$  come before the quantum space or after it, e.g.  $(an)$  or  $(na)$ . Equally, it is pseudo convention that  $a$  comes before  $b$ , but algebraically immaterial -  $(ab)$  or  $(ba)$ .

It is of note that decomposition of transportation of spin over lattice sites into transpositions and their equivalent  $\mathcal{P}$  operator products relates to the subject of scattering section, Section (2.2.6), which also decomposes scattering events into successive two-particle interactions (transpositions). With some additional considerations of commutation, as enforced by the Yang-Baxter equation, Section (2.2.6), this then leads to the concept of factorised scattering and, ultimately, integrability of the HSC XXX model.

Moving on, the two-site permutation matrix  $\mathcal{P}_{ij}$  can be written in terms of the Pauli spin matrix<sup>1</sup> as follows:

$$\mathcal{P}_{ij} = \frac{1}{2}(\bar{\sigma}_i\bar{\sigma}_j + I^{\otimes N}) \quad (23)$$

Furthermore, because of the shared term  $\bar{\sigma}_i\bar{\sigma}_j$ , between  $\mathcal{P}_{ij}$  and the Hamiltonian  $H_{ij}$ , above, the Hamiltonian can be written in terms of the permutation matrix as

$$H_{ij} = \frac{J}{2}(\mathcal{P}_{ij} - I^{\otimes N}) \quad (24)$$

Summing over all  $i, j$ ,  $i < j$  gives the full Hamiltonian

$$H = \frac{JN}{2} \sum_{i,j=1,i<j}^N \mathcal{P}_{ij} - \frac{JN}{2} I^{\otimes N} \quad (25)$$

Suffice to say,  $\mathcal{P}$  plays an enormous role in the ABA algebra that follows later.

#### 2.2.4 Auxiliary Space

The two-site auxiliary space is the  $\mathbb{C}^4 \otimes \mathbb{C}^4$  tensor product space bolted on to the front or end of the  $\mathbb{C}^{2N} \otimes \mathbb{C}^{2N}$  quantum space.

The auxiliary space doesn't have a physical existence, i.e. it isn't part of the the spin lattice sites  $1 \dots N$ , that are covered by the  $\mathbb{C}^{2N} \otimes \mathbb{C}^{2N}$  quantum space and have an up/down z-axis spinor on each site

The two auxiliary sites serve as a convenient mathematical intermediary - they are 'traced' over when forming the transfer matrix, Section (2.2.8), which is one of the desired commuting operators for the integrable solution. As such, the auxiliary sites do not appear in the final solution.

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<sup>1</sup>that this is so seems quite remarkable

Only two auxiliary sites are required since the algebra is always reduced to two-particle scattering as in factorized scattering. Indeed, all operators only act non-trivially on two sites such as permuting them via  $\mathcal{P}$ .

The notation for their use is best given by way of some examples, as follows.

**Example 1. Nepomechie [5]  $00'$  notation**

The subscripts 0 and  $0'$  represent two auxiliary sites at the front of the chain, before the first lattice site, index 1, which is the first site in the  $\mathbb{C}^{2N} \otimes \mathbb{C}^{2N}$  quantum space. For example, the tensor product operator  $R$  acting on the auxiliary space, is given by

$$R_{00'} = I_0 \otimes I_{0'} \otimes I_1 \otimes \cdots \otimes I_n \cdots \otimes I_N \quad (26)$$

By its  $00'$  subscripted definition, it is considered to only act non-trivially on the auxiliary space but, otherwise, acts trivially on the quantum space.

Faddeev [3] uses the indices  $a$  and  $b'$  as in, for example  $R_{ab}$  (see below), and they can be at the front or back of the lattice chain, but it seems they are at the back in the reference. Front or back, it matters not so long as they are used consistently.

In addition, the subscript/auxiliary-site ordering of 0 and  $0'$ , i.e.  $00'$  or  $0'0$  (or  $ab$ ,  $ba$ ) is immaterial so long as the ordering is consistently adhered to (of course).

The convention adopted herein is to use subscripts  $a$  and  $b$  (not 0 and  $0'$ ), with the, largely irrelevant assumption that the auxiliary sites are at the beginning of the chain. The only reason for this choice is that it avoids hard-to-see superscript primes as in  $0'$ , and removes use of zero twice in the subscript (even if one is primed) -  $a$  and  $b$  is considered clearer.

**Example 2. (Faddeev [3]  $ab$  notation)**

Two auxiliary sites  $a$  and  $b$  at the front of the chain as in

$$R_{ab} = I_a \otimes I_b \otimes I_1 \otimes \cdots \otimes I_n \cdots \otimes I_N$$

or two auxiliary sites at the rear of the chain, after the last lattice site  $N$

$$R_{ab} = I_1 \otimes \cdots \otimes I_n \cdots \otimes I_N \otimes I_a \otimes I_b, \quad (27)$$

$$a = N + 1, b = N + 2$$

End of examples

In the ABA formulation, Section(4),  $R$  actually acts only on auxiliary lattice sites, the  $L$  operators (which are identical to  $R$  to within the spectral parameter  $\lambda$  anyhow), usually act on one auxiliary site and one quantum site. In both the  $R$  and  $L$  cases, plus operators  $H$  and  $T$ , the important point is that these operators always act on two sites, wherever these sites may be, as indexed by their subscripts. The exception is the transfer matrix  $t(\lambda)$ , which is ‘traced-over’ the auxiliary space, and acts only in the  $\mathbb{C}^{2N} \otimes \mathbb{C}^{2N}$  quantum space, generally indexed by letters  $n, i, j$  where  $i, j, k \in 1 \dots N$ .

Excepting the transfer matrix, operators indexed like  $L_{na}$  operate on the lattice site  $n$  and auxiliary space  $a$ .

Whatever the case, keep in mind that every operator with two subscripts acts on two  $\mathbb{C}^2$  sites, and since all operators contain the permutation matrix, then the operator action invariably permutes spinors between these two sites amongst its other action - see the specific matrix forms for the exact details.

### 2.2.5 The Lax Matrix $L$

Before defining the Lax matrix operator  $L$ , the following pre-requisite definitions are given, where  $\alpha, \beta, \gamma, \delta$  are 2x2, complex matrices, as per the earlier definitions of  $S_z, S_+, S_-$ , and the N-site tensor products  $\alpha_n, \beta_n, \gamma_n, \delta_n$ , defined in terms of them

$$\alpha = \lambda I + iS_z \quad \beta = iS_- \quad \gamma = iS_+ \quad \delta = \lambda I - iS_z \quad (28)$$

$$\begin{aligned} \alpha_n &= I_1 \otimes \cdots \otimes \alpha_n \cdots \otimes I_N \\ \beta_n &= I_1 \otimes \cdots \otimes \beta_n \cdots \otimes I_N \\ \gamma_n &= I_1 \otimes \cdots \otimes \gamma_n \cdots \otimes I_N \\ \delta_n &= I_1 \otimes \cdots \otimes \delta_n \cdots \otimes I_N \end{aligned} \quad (29)$$

The N-site Lax matrix  $L$  is now written in the following block form, whereby each element is actually an N-fold tensor product of dimension  $2^N$  by  $2^N$ . The matrix itself, as shown, is thus  $2^{2N+1} \times 2^{2N+1}$ , albeit, it will be modified when an extra ‘auxiliary’ space is introduced (in fact two, see Section (2.2.4)). For notational clarity,  $L$  is often written in the following 2x2 form:

$$L(\lambda) = \begin{pmatrix} \alpha_n & \beta_n \\ \gamma_n & \delta_n \end{pmatrix} \quad (30)$$

but it is actually used later, Section (4), in the following expanded, pseudo  $4 \times 4$  form, where each element is really a  $2N \times 2N$  matrix (hence *pseudo* acting non-trivially on  $\mathbb{C}$  site  $n$  (subscript  $n$ ) of the N-site quantum space; subscript  $a$  denotes auxiliary space  $a$ , and  $b$  denotes auxiliary space  $b$ ).

$$L_{an}(\lambda) = L(\lambda) \otimes I \quad (31)$$

$$L_{an}(\lambda) = \begin{pmatrix} \alpha_n(\lambda) & 0 & \beta_n(\lambda) & 0 \\ 0 & \alpha_n(\lambda) & 0 & \beta_n(\lambda) \\ \gamma_n(\lambda) & 0 & \delta_n(\lambda) & 0 \\ 0 & \gamma_n(\lambda) & 0 & \delta_n(\lambda) \end{pmatrix} \quad (32)$$

$$L_{bn}(\lambda) = I \otimes L(\lambda) \quad (33)$$

$$L_{bn}(\lambda) = \begin{pmatrix} \alpha_n(\lambda) & \beta_n(\lambda) & 0 & 0 \\ \gamma_n(\lambda) & \delta_n(\lambda) & 0 & 0 \\ 0 & 0 & \alpha_n(\lambda) & \beta_n(\lambda) \\ 0 & 0 & \gamma_n(\lambda) & \delta_n(\lambda) \end{pmatrix} \quad (34)$$

$L$  can also be written terms of spin operators, see (6), and also in terms of  $R$ , i.e.  $L(\lambda) = R(\lambda - i/2)$  (5). Because  $R$  is defined in terms of the permutation matrix and the identity  $R(\lambda) = \lambda I \otimes I + i\mathcal{P}$  (2), and given the commutation rule (20), then  $L$  also satisfies this commutation rule, i.e.

$$[L_{ai}, L_{bj}] = 0, \quad i \neq j, \quad a \neq b \quad (35)$$

### 2.2.6 Yang-Baxter Equation

The matrix operator  $L$  and those that follow next ( $R$  and monodromy  $T$ ) satisfy a key equation (key to the integrability of the HSC and other integrable systems), known as the *Yang-Baxter Equation*<sup>2</sup> [10].

$$S_{12}(p_1, p_2)S_{13}(p_1, p_3)S_{23}(p_2, p_3) = S_{23}(p_2, p_3)S_{13}(p_1, p_3)S_{12}(p_1, p_2) \quad (36)$$

This equation is best described in its physical interpretation as a form of commutation relation amongst three scattering matrices  $S(12)$ ,  $S(23)$  and  $S(13)$ , where each represents a two-particle scattering process, e.g.  $S(12)$  is for particles 1 and 2.

In effect, the YBE expresses the fact that, if the scattering is such that interactions (12) followed by (13) followed by (23), in time-ordered sequence, is the same as the reverse ordered process, i.e. (23) followed by (13) followed by (12), then the underlying system is integrable.

Note that this is a special case of three-particle scattering. In general, the three-particle interaction potential  $U(x, t)$  (a function of position and possibly time), is of a form such that the YBE does not hold true. However, at least for the integrable HSC model, this is (must be) satisfied. In effect it means a three body (or more) scattering process can be factorised into two-body processes, and is thus known as *factorized scattering*.

Alternatively stated, the YBE expresses the equivalence of two different ways to factorise a three-particle scattering matrix into a product of three, two-particle matrices

The YBE, as actually given in terms of the operators used herein, is given shortly (40) but, in brief, if  $R$  and  $T$  satisfy the YBE then the HSC is integrable.

The algebra above is that of permutations, specifically two-cycle transpositions, and one can apply the same rules, see Section (2.1.1) for more details on this aspect. There are also geometric-equivalent, pictorial representations of the YBE given in, for example, [4].

It should be noted that general  $R$  matrices and the YBE pervade many integrable systems in physics, and there is a nice introduction to YBE and general  $R$  matrices in [10], and [11]. There is also, of course, an abundance of freely available, high quality literature on the web, search *Yang-Baxter*.

### 2.2.7 Monodromy Matrix $T$

The Monodromy matrix is defined as the following product of all  $N$  Lax matrices  $L_{ai}, i = 1 \dots N$ :

$$T_a(\lambda) = L_{aN}(\lambda)L_{aN-1}(\lambda) \dots L_{a2}(\lambda)L_{a1}(\lambda) \quad (37)$$

As for the Lax matrix  $L$ , further above, for notational clarity this is often written in the following 2x2 form

$$T_a(\lambda) = \begin{pmatrix} A(\lambda) & C(\lambda) \\ B(\lambda) & D(\lambda) \end{pmatrix} \quad (38)$$

but it is actually used, Section (4) in the following expanded pseudo  $4 \times 4$  form, where each element is really a  $2N \times 2N$  matrix - the term *pseudo* meaning that each element actually acts non-trivially on  $\mathbb{C}$  site  $n$  of an  $N$ -site tensor product (AKA the *quantum space*). Reminder: subscript  $a$  denotes auxiliary space  $a$ , and  $b$  (below) denotes auxiliary space  $b$ .

$$T_a(\lambda) = T(\lambda) \otimes I \quad (39)$$

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<sup>2</sup>This is also known as the Fundamental Commutation Relation (FCR)

$$T_a(\lambda) = \begin{pmatrix} A(\lambda) & 0 & B(\lambda) & 0 \\ 0 & A(\lambda) & 0 & B(\lambda) \\ C(\lambda) & 0 & D(\lambda) & 0 \\ 0 & C(\lambda) & 0 & D(\lambda) \end{pmatrix} \quad (40)$$

$$T_b(\lambda) = I \otimes T(\lambda) \quad (41)$$

$$T_b(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) & 0 & 0 \\ C(\lambda) & D(\lambda) & 0 & 0 \\ 0 & 0 & A(\lambda) & B(\lambda) \\ 0 & 0 & C(\lambda) & D(\lambda) \end{pmatrix} \quad (42)$$

Looking at the original Lax matrix form (6), it can be seen that the diagonal matrix elements  $A$  and  $D$  represent Cartan operators, e.g.  $S_z$ , whilst the two non-diagonal elements  $B$  and  $C$  are akin to creation  $S_-$  and annihilation  $S_+$  operators, respectively.

The monodromy matrix obeys the Yang-Baxter Equation, i.e., for two unique spectral parameters  $\lambda_a$  and  $\lambda_b$ , then

$$R_{ab}(\lambda_a - \lambda_b)T_a(\lambda_a)T_b(\lambda_b) = T_b(\lambda_b)T_a(\lambda_a)R_{ab}(\lambda_a - \lambda_b) \quad (43)$$

A proof of this for three-sites,  $N = 3$  follows, but is illustrative enough for the full  $N$ -site proof to easily be seen by extension.

Using the definition (37) of the monodromy matrix in terms of operator  $L$  then, for three sites,  $N = 3$ ,  $T_a$  and  $T_b$  expand as follows, where the spectral parameters have been omitted for clarity:

$$\begin{aligned} T_a &= L_{a3}L_{a2}L_{a1}, \quad N = 3 \\ T_b &= L_{b3}L_{b2}L_{b1} \end{aligned}$$

Substituting for  $T_a$  and  $T_b$  into the left term of the YBE (43) gives

$$R_{ab}L_{a3}L_{a2}L_{a1}L_{b3}L_{b2}L_{b1}$$

Using the  $L$  operator commutation rule  $[L_{ai}, L_{bj}] = 0, i \neq j$  (35) then the two middle terms can be swapped, i.e.  $L_{a1}L_{b3} = L_{b3}L_{a1}$  to give

$$R_{ab}L_{a3}L_{a2}L_{b3}L_{a1}L_{b2}L_{b1}$$

similarly,  $L_{b3}$  can be swapped with  $L_{a2}$ , and  $L_{b2}$  swapped with  $L_{a1}$  to give

$$R_{ab}L_{a3}L_{b3}L_{a2}L_{b2}L_{a1}L_{b1}$$

The three matrix product  $R_{ab}L_{a3}L_{b3}$  can now easily be replaced using the YBE, i.e.  $R_{ab}L_{a3}L_{b3} = L_{b3}L_{a3}R_{ab}$  to obtain

$$L_{b3}L_{a3}R_{ab}L_{a2}L_{b2}L_{a1}L_{b1}$$

Applying the YBE again, i.e.  $R_{ab}L_{a2}L_{b2} = L_{b2}L_{a2}R_{ab}$ , gives

$$L_{b3}L_{a3}L_{b2}L_{a2}R_{ab}L_{a1}L_{b1}$$

and a final application of YBE for  $R_{ab}L_{a1}L_{b1} = L_{b1}L_{a1}R_{ab}$  gives

$$L_{b3}L_{a3}L_{b2}L_{a2}L_{b1}L_{a1}R_{ab}$$

Lastly, swapping  $L_{b2}$  with  $L_{a3}$ , and rippling  $L_{b1}$  left using the commutation rule, this becomes

$$L_{b3}L_{b2}L_{b1}L_{a3}L_{a2}L_{a1}R_{ab}$$

Comparing with the starting term, it is seen that

$$R_{ab}L_{a3}L_{a2}L_{a1}L_{b3}L_{b2}L_{b1} = L_{b3}L_{b2}L_{a3}L_{a2}R_{ab}L_{a1}L_{b1}$$

which, back in terms of monodromy matrices, is

$$R_{ab}T_aT_b = T_bT_aR_{ab}$$

This is just the YBE for the monodromy matrices (43) and hence, for  $N = 3$ , it is proven that the monodromy matrices satisfy the YBE. By repeated application of the commutation rule and YBE, this proof easily extends to any number of sites  $N$ .

### 2.2.8 Transfer Matrix $t$

The Transfer matrix is defined as the trace of the monodromy matrix over the auxiliary space

$$t(\lambda) = \text{tr}_a T_a(\lambda) \quad (44)$$

It acts on the  $N$ -site quantum space  $2^{2N} \times 2^{2N}$  and taking the trace over the auxiliary space effectively removes it from the final solution, which is purely given in the physical, quantum space.

The trace is effectively a block sum of the two block diagonal elements of  $T_a$  (40), i.e.

$$t(\lambda) = A(\lambda) + D(\lambda)$$

The transfer matrix commutes for two different spectral parameters, here  $\lambda$  and  $\lambda'$ , i.e.

$$[t(\lambda), t(\lambda')] = 0$$

This is easily proven: using the identity  $R_{ab}^{-1}R_{ab} = I$ , then the trace of  $T_aT_b$  can be written as

$$\text{tr}(T_aT_b) = \text{tr}(R_{ab}^{-1}R_{ab}T_aT_b)$$

and by the cyclicity of the trace, this is the same as

$$\text{tr}(T_aT_b) = \text{tr}(R_{ab}T_aT_bR_{ab}^{-1})$$

Using Yang-Baxter (43) then

$$R_{ab}T_aT_b = T_bT_aR_{ab}$$

and so

$$\text{tr}(T_aT_b) = \text{tr}(T_bT_aR_{ab}R_{ab}^{-1})$$

finally, since  $R_{ab}R_{ab}^{-1} = I$  then the result follows:

$$\text{tr}(T_aT_b) = \text{tr}(T_bT_a)$$

Note too that the trace  $\text{tr}(T_aT_b) \equiv \text{tr}(T_a)\text{tr}(T_b)$  since they act on different auxiliary spaces

The transfer matrix, for specific spectral parameter  $\lambda = i/2$  (see further), relates to the Hermitian momentum operator  $P$  via

$$e^{iP} = i^{-N}t(i/2) \quad (45)$$



and can thus be interpreted as a unitary translation (*shift*) operator  $U$ . Before showing this, a quick, pertinent refresher in QM.

**QM Aside.** With the momentum operator  $P$  given in the usual QM form as

$$P = -i\hbar\partial x$$

then the shift operator  $U$ , for a finite translation  $\Delta a$ , is thus

$$U = e^{iPa/\hbar} = e^{\Delta a\partial x} \quad (46)$$

If  $\Delta a$  now represents the small, finite distance between consecutive spin sites, then a spin state  $\psi(x)$  at site  $x$ , is translated to site  $x + \Delta a$  by the action of  $U$  on  $\psi(x)$

$$U\psi(x) = e^{iP\Delta a}\psi(x) \approx (1 + \Delta a\partial_x)\psi(x) = \psi(x) + \Delta a\partial_x\psi = \psi(x + \Delta a) \quad (47)$$

For an operator  $G_n$  acting on site  $n$ , say, the equivalent action of  $U$  to translate  $G$  to the next site  $n + 1$ , denoted by  $G_{n+1}$ , is given in the usual operator transformation form

$$UG_nU^{-1} = G_{n+1} \quad (48)$$

**End of QM aside.**

Relating back to the monodromy matrix  $T$ , as given in (37), a key point regarding the transfer matrix is that, for spectral parameter  $\lambda = i/2$ , the monodromy matrix is the product of  $N$  permutation matrices  $\mathcal{P}$ . This is easily shown as follows, given the definition (5) of the Lax matrix  $L$  in terms of  $R$ , then for  $\lambda = i/2$ ,  $L(i/2)$  is simply  $R(0)$ , which itself is just  $i\mathcal{P}$  by (2), hence

$$L(i/2) = R(0) = i\mathcal{P}$$

Thus, the Lax matrix terms  $L_{aN}$ ,  $L_{aN-1}$  etc.. in the monodromy matrix definition (37) are

$$L_{aN}(i/2) = i\mathcal{P}_{aN}, \quad L_{aN-1}(i/2) = i\mathcal{P}_{aN-1}, \text{ etc.}$$

and the monodromy matrix  $T_a(i/2)$  is therefore

$$T_a(i/2) = i^N \mathcal{P}_{aN} \mathcal{P}_{aN-1} \dots \mathcal{P}_{a2} \mathcal{P}_{a1} \quad (49)$$

The combination of permutations on the right can be manipulated into a more useful form to obtain the trace of  $T_a(i/2)$  (further below), as given by the following identity:

$$\mathcal{P}_{aN} \mathcal{P}_{aN-1} \dots \mathcal{P}_{a2} \mathcal{P}_{a1} = \mathcal{P}_{12} \mathcal{P}_{23} \dots \mathcal{P}_{N,N-1} \mathcal{P}_{Na} \quad (50)$$

and verified as follows:

Evaluating the lhs permutation, working right to left, gives

$$\begin{aligned} a &\rightarrow 1 \\ 1 &\rightarrow a \rightarrow 2 \\ 2 &\rightarrow a \rightarrow 3 \\ &\vdots \\ N-1 &\rightarrow a \rightarrow N \end{aligned}$$

And so, by the theory of permutations, the LHS comprises  $N$  transpositions and can be written as the following single  $N$ -cycle:

$$\mathcal{P}_{aN} \mathcal{P}_{aN-1} \dots \mathcal{P}_{a2} \mathcal{P}_{a1} = (a12 \dots N-1, N)$$

Similarly, evaluating the rhs permutation, working right to left, gives

$$\begin{aligned}
N &\rightarrow a \\
a &\rightarrow N \rightarrow N-1 \dots \rightarrow 1 \\
N-1 &\rightarrow N \\
N-2 &\rightarrow N-1 \\
&\vdots \\
2 &\rightarrow 3 \\
1 &\rightarrow 2
\end{aligned}$$

and this too can be written as the single N-cycle

$$\mathcal{P}_{12}\mathcal{P}_{23}\dots\mathcal{P}_{N,N-1}\mathcal{P}_{Na} = (Na12\dots N-2, N-1)$$

By cyclic permutation, i.e. rotate one to the left,

$$(Na12\dots N-1) \rightarrow (a12\dots N-1, N)$$

this becomes identical to the original permutation, thus verifying that the two forms of permutation are equivalent.

The key point about the second permutation form is that the auxiliary site, index  $a$ , now only appears in a single permutation term, i.e.  $\mathcal{P}_{Na}$  and simplifies the calculation of the trace, as required next in the evaluation of the transfer matrix. Specifically, the trace of  $\mathcal{P}_{Na}$  over the auxiliary space is just the identity, i.e.

$$tr_a(\mathcal{P}_{Na}) = I^{\otimes N}$$

By (50),

$$tr_a(\mathcal{P}_{aN}\mathcal{P}_{a,N-1}\dots\mathcal{P}_{a2}\mathcal{P}_{a1}) = tr_a(\mathcal{P}_{12}\mathcal{P}_{23}\dots\mathcal{P}_{N,N-1}\mathcal{P}_{Na})$$

and since the trace is over the auxiliary space only, all permutations (on the rhs above) not in the auxiliary space, i.e. all but  $\mathcal{P}_{a,N}$ , can be ignored so that

$$tr_a(\mathcal{P}_{12}\mathcal{P}_{23}\dots\mathcal{P}_{N,N-1}\mathcal{P}_{Na}) = \mathcal{P}_{12}\mathcal{P}_{23}\dots\mathcal{P}_{N,N-1}tr_a(\mathcal{P}_{Na})$$

Finally, since  $tr_a(\mathcal{P}_{Na})$  is just the identity, as given above, then

$$\mathcal{P}_{12}\mathcal{P}_{23}\dots\mathcal{P}_{N,N-1}tr_a(\mathcal{P}_{Na}) = \mathcal{P}_{12}\mathcal{P}_{23}\dots\mathcal{P}_{N,N-1} \quad (51)$$

Using the form of the monodromy matrix (49) then, by definition (44), the transfer matrix is given by

$$t(i/2) = tr_a T_a(i/2) = i^N \mathcal{P}_{12}\mathcal{P}_{23}\dots\mathcal{P}_{N,N-1} \quad (52)$$

The sequence of permutations on the rhs above is equivalent to the unitary translation (or *shift*) operator  $U$  given earlier (46), i.e.

$$U = \mathcal{P}_{12}\mathcal{P}_{23}\dots\mathcal{P}_{N,N-1} \quad (53)$$

Using this, the expression for the transfer matrix now simplifies to

$$t(i/2) = i^N U \quad (54)$$

Alternatively,  $U$  is expressed in terms of the transfer matrix, by simple rearrangement as in

$$U = i^{-N} t(i/2) \quad (55)$$

and so  $t(i/2)$  is thus a translation through  $N$  sites resulting in the single permutation effectively swapping site 1 with site  $N$  (multiplied by  $i^N$ )

## 2.3 The Hamiltonian Revisited

Armed with the transfer matrix derived in the previous section, this section now shows that it relates to the Hamiltonian and, most importantly, commutes with it. To get there, the work starts back with the monodromy matrix (37), reproduced below

$$T_a(\lambda) = L_{aN}(\lambda)L_{aN-1}(\lambda) \dots L_{a2}(\lambda)L_{a1}(\lambda)$$

Differentiating  $T_a(\lambda)$  (37), which introduces a summation, and evaluating at  $\lambda = i/2$  so that  $L = i\mathcal{P}$ , gives

$$\left. \frac{dT_a(\lambda)}{d\lambda} \right|_{\lambda=i/2} = i^{N-1} \sum_{n=1}^N \mathcal{P}_{aN}\mathcal{P}_{aN-1} \dots \widehat{\mathcal{P}}_{an} \dots \mathcal{P}_{a2}\mathcal{P}_{a1} \quad (56)$$

where  $\widehat{\mathcal{P}}_{an}$  denotes the term is omitted, hence each term in the sum is a product of  $N - 1$  permutation operators, but there remain  $N$  terms in the total summation.

Using the permutation identity (50) and the trace of the permutation sequence (51), the above expression can be recast as

$$\left. \frac{dt(\lambda)}{d\lambda} \right|_{\lambda=i/2} = i^{N-1} \sum_{n=1}^N \mathcal{P}_{12}\mathcal{P}_{23} \dots \mathcal{P}_{n-1,n+1}\mathcal{P}_{N-1,N} \quad (57)$$

To clear most of the permutations on the rhs, the inverse of the transfer matrix (54) is required, as follows:

$$t(i/2)^{-1} = i^{-N}U^{-1} \quad (58)$$

where the inverse of the unitary shift matrix  $U$  (53) is

$$U^{-1} = \mathcal{P}_{N,N-1} \dots \mathcal{P}_{23} \dots \mathcal{P}_{12} \quad (59)$$

Multiplying the above derivative expression  $dt/d\lambda$  by the inverse, and utilising the inverse shift operator definition  $U^{-1}$  clears nearly all of the permutations in the summation and, after some algebraic manipulation, gives

$$\left. \frac{dt(\lambda)}{d\lambda} t(\lambda)^{-1} \right|_{\lambda=i/2} = -i \sum_{n=1}^N \mathcal{P}_{n,n+1} \quad (60)$$

The derivative term on the left also simplifies to give

$$\left. \frac{d}{d\lambda} \ln t(\lambda) \right|_{\lambda=i/2} = -i \sum_{n=1}^N \mathcal{P}_{n,n+1} \quad (61)$$

In accordance with (25), the full spin-chain Hamiltonian for neighbouring site interactions only  $(n, n + 1)$ , is

$$H = \frac{J}{2} \sum_{n,n+1}^N \mathcal{P}_{n,n+1} - \frac{JN}{2} I^{\otimes N} \quad (62)$$

and equating this with the previous derivative term to clear the summation gives

$$H = \frac{iJ}{2} \left. \frac{d}{d\lambda} \ln t(\lambda) \right|_{\lambda=i/2} - \frac{JN}{2} I^{\otimes N} \quad (63)$$

In this form, it can now be deduced that the Hamiltonian actually commutes with the transfer matrix. Although perhaps not obvious, the commutation hinges on the fact that if two operators

$F$  and  $G$  commute, then any polynomial function (*power series*) of  $G$  will also commute with  $F$ , formally stated as

If  $[F, G] = 0$  then  $[F, f(G)] = 0$  where  $f(G) = \sum_{m=0}^M a_m G^m$  for constant coefficients  $a_m$

This includes the case where the maximum degree  $M$  goes to infinity and so, since the natural logarithm function has such an infinite degree power series expansion, then it can be concluded that if an operator  $F$  commutes with  $G$ , then it commutes with  $\ln(G)$ . In fact here it has to commute with the derivative, i.e.  $d/d\lambda \ln(G)$ , where  $G \sim t(\lambda)$ . However, the derivative of a power series is just another power series, so the derivative is superfluous.

Thus, if the Hamiltonian  $H$  can be written in terms of  $t(\lambda)$ , as demonstrated above, then since  $t(\lambda)$  commutes with itself, and by extension the power series  $d/d\lambda \ln(t(\lambda))$ , then  $H$  must also commute with  $t(\lambda)$ . Note too that this result is independent of the spectral parameter  $\lambda$ .

### 3 A one-magnon spin chain

Consider the  $N$ -site ground state  $\Omega_u$

$$\Omega_u = |\uparrow\uparrow \cdots \uparrow\rangle = |u_1, u_2, \cdots u_n \cdots u_N\rangle$$

To this a single spin site  $n$  is to be flipped from up to down, which will create the following new state,  $\psi_n$

$$\psi_n = |\uparrow \cdots \uparrow \downarrow \uparrow \cdots \uparrow\rangle = |u_1, u_2, \cdots d_n \cdots u_N\rangle$$

and denoted by the  $N$ -site tensor product

$$\psi_n = u_1 \otimes \cdots d_n \cdots \otimes u_N, \quad u, d \in \mathbb{C}^2, \psi_n \in \mathbb{C}^{2N}$$

To find the energy of this state, as in standard QM, it is operated on by the Hamiltonian, e.g.

$$H\psi_n = E\psi_n$$

For the HSC, this is the two-site form  $H_{ij}$  (24), given in terms of the permutation matrix, reproduced below

$$H_{ij} = \frac{J}{2}(\mathcal{P}_{ij} - I), \quad i < j, I \equiv I^{\otimes N} \quad (64)$$

Convention has it that  $i < j$

As written, the Hamiltonian acts on all pairs  $(i, j)$  of sites  $i$  and  $j$ , which would ordinarily give a sum of  ${}^N C_2$  terms. For example, in a three-site case, it would be a sum of  $H$  acting on the three site pairs  $(1, 2)$ ,  $(1, 3)$  and  $(2, 3)$ . However, as noted, only nearest neighbour sites are considered, with the energy exchange between a flipped site being zero for any swap of an up and down spinor separated by one or more sites, i.e.  $j > i + 1$ . In the above example, the three site pairs therefore reduce to just the two  $(1, 2)$  and  $(2, 3)$ , and adjacent sites are thus indexed  $j = i + 1$ , i.e.  $(i, i + 1)$ , so that  $H_{ij}$  now becomes  $H_{i, i+1}$ . Thus, to obtain the total energy of the one-flipped spin state, the two-site Hamiltonian becomes

$$H = \sum_i^N H_{i, i+1} \psi_n \quad (65)$$

Firstly, the action of  $H_{ij}$  on a pair of consecutive up spins, as given by example in the smallest, non trivial, two-site case,  $N = 2$ , is given by

$$H_{12}|u_1, u_2\rangle = (\mathcal{P}_{12} - I)|u_1, u_2\rangle$$

Expanding out each term on the right gives

$$\mathcal{P}_{12}|u_1, u_2\rangle = |u_2, u_1\rangle = |u_1, u_2\rangle, \quad u_1 = u_2 = u$$

$$I|u_1, u_2\rangle = |u_1, u_2\rangle$$

It is seen that, since the two spins are identically up, the permutation and identity operator just return the original input state, with the result that the difference is zero, i.e.

$$H_{12}|u_1, u_2\rangle = 0, \quad E = 0$$

This should be no surprise since  $|u_1, u_2\rangle$  is a ground state, and the Hamiltonian was intentionally constructed (adjusted) to give a ground state energy of zero. Most importantly, this result extends to any pair of consecutive spins with the same alignment (up or down) - exchanging them gives no change in energy. Thus, if only one site  $n$ , as in eigenstate  $\psi_n$ , is a down-spin, with all the rest up, the energy sum reduces to terms with index  $n-1, n$  and  $n+1$ , i.e.

$$H\psi_n = \frac{J}{2}(\mathcal{P}_{n-1,n} - I)\psi_n + \frac{J}{2}(\mathcal{P}_{n,n+1} - I)\psi_n$$

Each term on the right evaluates as

$$\begin{aligned} \mathcal{P}_{n-1,n}\psi_n &= \psi_{n-1}, & I\psi_n &= \psi_n \\ \mathcal{P}_{n,n+1}\psi_n &= \psi_{n+1}, & I\psi_{n+1} &= \psi_{n+1} \end{aligned}$$

and putting them together gives

$$H\psi_n = \frac{J}{2}(\psi_{n-1} - 2\psi_n + \psi_{n+1}) \quad (66)$$

Note, some texts use a negative factor  $-J$  that is compensated by reversing the signs in the right bracket, thus giving the same result, i.e.  $H\psi_n = -(J/2)(-\psi_{n-1} + 2\psi_n - \psi_{n+1})$

As seen,  $H\psi_n$  is not an energy eigenvector equation since the rhs is not a simple eigenvalue multiple of the state  $\psi_n$  on the left. However, this can be made a momentum eigenstate  $\psi(p)$  by transforming to momentum space using a Fourier transform, again, standard QM,

$$H\psi(p) = \frac{J}{2} \sum_{-\infty}^{\infty} (\psi_{n-1} - 2\psi_n + \psi_{n+1}) e^{ipn}$$

where the momentum wave state  $\psi(p)$  is given by

$$\psi(p) = \sum_{-\infty}^{\infty} \psi_n e^{ipn} \quad (67)$$

This is not quite the desired form yet, and more follows. However, a couple of points beforehand:

1. This is actually a discrete Fourier transform for a lattice with an infinite number of sites ( $N \rightarrow \infty$ ), hence the summation limits. This assumption gives both a continuous momentum spectrum and zeros any edge effects as the state is assumed to go to zero at infinity i.e.  $\psi_n \rightarrow 0$   $n \rightarrow \infty$  (an *asymptotic* boundary condition). Because  $N$  is very large in practice, e.g. a 1d crystal lattice has approximate order Avogadro number of sites, it is a very good approximation and safe assumption. For a finite  $N$ , the momentum is quantised (just like the QM case of a particle in a finite size (length  $N$ ) infinite square-well potential), with quantisation  $\Delta p = 2\pi i/N$ .

This quantisation is also the case for a closed chain of  $N$  sites, but now the boundary conditions are periodic and  $p$  restricted to modulo  $2\pi$  as in  $e^{ip} = 1$ .

2. What would normally be the  $x$  position coordinate on the right (i.e.  $e^{ipx}$ ) is simply the lattice site index  $n$ . If the lattice spacing were  $\Delta$ , then  $x = n\Delta$ , so  $\Delta$  has effectively been set to unity and the  $x$ -coordinate position is just the index.

Returning to the Fourier transform, the infinite limits also permit a legitimate relabelling of the position index  $n$  in each of the three bracket terms on the right (this is also acceptable for large  $N$ , as mentioned above)

$$H\psi(p) = \frac{J}{2} \sum_{-\infty}^{\infty} \psi_n e^{ip(n+1)} - 2\psi_n e^{ipn} + \psi_n e^{ip(n-1)}$$

This relabelling is actually the clever part, because now the states on the right are all the same, so what looked like three individual states is now just the one  $\psi_n$ . Factoring  $\psi_n$  and common factor  $e^{ipn}$  gives

$$H\psi(p) = \frac{J}{2} \sum_{-\infty}^{\infty} (e^i - 2 + e^{-i}) e^{ipn} \psi_n$$

The bracketed term simplifies to the following trigonometric form

$$(e^i - 2 + e^{-i}) = 2(\cos p - 1) = -4 \sin^2(p/2)$$

and can be removed from the summation (since it is not over  $p$ ) leaving

$$H\psi(p) = -\frac{J}{2} 4 \sin^2(p/2) \sum_{-\infty}^{\infty} e^{ipn} \psi_n$$

Lastly, the summation term on the right is just  $\psi(p)$  (67) so

$$H\psi(p) = -\frac{J}{2} 4 \sin^2(p/2) \psi(p) \tag{68}$$

which shows that  $\psi(p)$  is an energy eigenstate for eigenvalue  $(-J/2)4 \sin^2(p/2)$ .

**Discussion.** It is hoped the reader can appreciate just how neat this bit of trickery using the Fourier transform is. It has converted an operator equation in position space, that results in a superposition of linear states (but not eigenstates), i.e. (66), into an eigenvector equation in momentum space. In other words, there was an eigenvector equation always present, just in the momentum space, not position space, and not visible at first (or second) glance.

Furthermore, this now just looks like a standard QM particle with momentum  $p$  - positive means it is travelling to the right. What was initially a static lattice problem, with one spin flipped, now has a *quasi*-particle interpretation. In fact, from a mathematical standpoint, the result (68) is unequivocally a particle, because one wouldn't know otherwise if shown this eigenvector equation and asked to deduce the problem from which it arose. This single particle (there is only one momentum  $p$ ) is termed a *magnon*, and when two flipped spins are introduced, two magnons with momentum  $p$  and  $q$  are seen - a bit more on this shortly.

The Fourier transform method, as above, for transforming a position space solution to momentum space, and thereby obtaining an eigenstate (where there was none before), is actually a common trick in physics, equivalent to a change of basis to diagonalise a problem. As an example, see the *Tight Binding Model* in condensed matter physics.

The general  $M$  ( $M < N$ ) magnon eigenvector states were determined by Bethe [6] in 1931 by essentially guessing the general solution (devising by much physical insight is a more accurate description), and the method has become known as the *Coordinate Bethe Ansatz* (CBA).

It is not the intention of this document to pursue the CBA method further because much later mathematical developments (Faddeev 1971 [3], [7]) led to another method, known as the *Algebraic Bethe Ansatz* (ABA). The ABA is common to many non-linear systems, classical and quantum, and is the method used herein to solve the same quantum HSC problem. Part II of this document details the solution to the classical Korteweg de Vries (KdV) non-linear equation (a third order PDE). Solving the KdV and this quantum HSC share similar, modern mathematical developments, and also have some remarkable physical commonality. To which end, this brief section, essentially an *introduction to magnons*, closes with a quick mention of the two-magnon CBA, that introduces two particles and leads to concepts of scattering and dispersion - two very physical areas that are of relevance to both KdV soliton solutions and Magnons. For more details of the CBA solution, see the accounts by Beisert [4] for the one, two and three magnon solutions. Nepomechie [5] also gives a good but less-detailed account. The ABA is the domain of Faddeev [3], [7] and detailed further herein.

### The CBA Two-magnon Solution

The two magnon eigenstate has the following form, where  $p$  and  $q$  denote the magnon's momentum (one  $p$  and one  $q$ )

$$\psi(p, q) = k(p, q) \sum_{n < m, -\infty}^{\infty} e^{ipn} e^{iqm} + S(p, q) e^{ipm} e^{iqn} \quad (69)$$

and corresponding eigenvalue

$$E = E(p) + E(q) \quad (70)$$

There are the usual approximations here, but consider it an infinite, open-ended (not closed) chain - see Beisert [4] for more details.

The sum, as before, runs from  $-\infty$  to  $+\infty$ , and the  $n < m$  condition really means that the particle position  $n$  lies to the left of position  $m$ . However, because both  $n, m$  can be positive or negative, the sign in the exponential can mean that the magnons move to the left and right.

More explicitly, the first term has  $p$  to the left of  $q$ , with  $p$  is moving to the right,  $q$  to the left. In the second term,  $q$  is now to the left of  $p$ , still moving to the left, and  $p$  is thus to the right of  $q$ , also still moving to the right. At some stage, they scatter as they pass, and this is reflected (no pun) in the *scattering factor*  $S(p, q)$ .

The energy eigenvalue is seen to be the sum of the individual, one-magnon solution energies - the scattering has not affected the solution. In fact, the scattering factor  $S(p, q)$  is just a complex phase shift of unit magnitude.

The solution is stable, there is no dispersion - the individual momenta  $p, q$  remain unchanged after scattering - the momentum *wave* (hint KdV) is unaffected by the scattering, bar a QM phase shift, and QM observables are invariant to a phase shift.

This is qualitatively as per a soliton solution to the KdV equation. Colliding solitons can merge, change their form whilst under the influence of their position and time-dependent potential, but travel through each other and emerge the same shape as they entered (the scattering potential region). The potential term decays to zero as times and positions go to  $\pm\infty$  as in the asymptotic solution.

This retention of final form (post scattering) is a feature of linear superposition. For example, electromagnetic waves in free space can be decomposed into the same Fourier components before and after they electromagnetically interfere (scatter). But KdV is distinctly non-linear, so such a stable, integrable solution to a non-linear problem was unexpected, but led to many further developments in solving non-linear problems.

## 4 Algebraic Bethe Ansatz

### 4.1 Eigenstates of the Spin chain

This section derives the eigenstates of the transfer matrix. Since the transfer matrix commutes with the Hamiltonian, these states are basically the solutions to the integrable system known as the Heisenberg XXX spin chain model. The Monodromy matrix in block form (40) is

$$T_a(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}$$

and obeys the Yang-Baxter Equation (43),

$$R_{ab}(\lambda_a - \lambda_b) T_a(\lambda_a) T_b(\lambda_b) = T_b(\lambda_b) T_a(\lambda_a) R_{ab}(\lambda_a - \lambda_b) \quad (71)$$

The  $R$  matrix, defined in 4x4 form (2), is reproduced below with its entries used to define constants  $a, b, c$  as on the right

$$R(\lambda) = \begin{pmatrix} \lambda + i & 0 & 0 & 0 \\ 0 & \lambda & i & 0 \\ 0 & i & \lambda & 0 \\ 0 & 0 & 0 & \lambda + i \end{pmatrix} = \begin{pmatrix} a & 0 & 0 & 0 \\ 0 & b & c & 0 \\ 0 & c & b & 0 \\ 0 & 0 & 0 & a \end{pmatrix}$$

and hence  $a, b, c$  are formally defined as

$$a = \lambda + i, \quad b = \lambda, \quad c = i \quad (72)$$

Note that constant  $c$  is rather trivially defined as just the imaginary unit  $i$ . Also note that the  $a$  and  $b$  constants are not related to the subscripts on the spectral parameters  $\lambda_a$  and  $\lambda_b$  (an unfortunate clash of notation).

Although not shown here, see [3], by applying the block form of the monodromy matrix to the YBE, the following key *exchange relations* (three of a possible sixteen) in  $A, B, C, D$  are obtained

$$[B(\lambda_a)B(\lambda_b)] = 0 \quad (73)$$

$$A(\lambda_a)B(\lambda_b) = \frac{a(\lambda_b - \lambda_a)}{b(\lambda_b - \lambda_a)} B(\lambda_b)A(\lambda_a) - \frac{c}{b(\lambda_b - \lambda_a)} B(\lambda_a)A(\lambda_b) \quad (74)$$

$$D(\lambda_a)B(\lambda_b) = \frac{a(\lambda_a - \lambda_b)}{b(\lambda_a - \lambda_b)} B(\lambda_b)D(\lambda_a) - \frac{c}{b(\lambda_a - \lambda_b)} B(\lambda_a)D(\lambda_b)$$

Denoting the ground state wave-function by  $\Omega_u$  for the all spin-up ground state (hence  $u$  subscript), then  $\Omega_u$  is a simultaneous eigenstate of  $A$  and  $D$  for the  $N$ -site spin chain, i.e.

$$\begin{aligned} A(\lambda)\Omega_u &= \left(\lambda + \frac{i}{2}\right)^N \Omega_u \\ D(\lambda)\Omega_u &= \left(\lambda - \frac{i}{2}\right)^N \Omega_u \end{aligned} \quad (75)$$

The eigenvalues are defined by the constants  $\alpha_N$  and  $\delta_N$ , for an  $N$ -site chain, as per [3] notation

$$\alpha_N(\lambda) = \left(\lambda + \frac{i}{2}\right)^N \quad \delta_N(\lambda) = \left(\lambda - \frac{i}{2}\right)^N \quad (76)$$

and so the  $A$  and  $D$  eigenvector equations are now written more concisely as

$$A(\lambda)\Omega_u = \alpha_N(\lambda)\Omega_u \quad (77)$$

$$D(\lambda)\Omega_u = \delta_N(\lambda)\Omega_u \quad (78)$$



Operator  $C$  is a raising operator and hence annihilates the all-up spin, ground state  $\Omega_u$

$$C(\lambda)\Omega_u = 0 \quad (79)$$

Operator  $B$  is a lowering operator and acts as a creation operator to create down-spin states by flipping up-spin states at individual sites in the spin chain. These states, containing one or more down spins in a spin chain, are called Bethe states.

Note that the association of  $A, B, C, D$  as spin operators,  $S_z, S_-, S_+, S_z$  respectively, is given in accordance with the form of Lax matrix  $L$  (6).

It is seen from the above  $A, D$  eigenvector equations that, since  $\Omega_u$  is a simultaneous eigenstate of  $A$  and  $D$ , it is also an eigenstate of their sum  $A + D$ , and given that the transfer matrix is the trace of the monodromy matrix (40) over the auxiliary space ( $a$  here), i.e.

$$t(\lambda) = \text{tr}(T_a(\lambda)) = A(\lambda) + D(\lambda) \quad (80)$$

then  $\Omega_u$  is also an eigenstate of the transfer matrix ( $t(\lambda)$  (2.2.8) ), i.e.

$$t(\lambda)\Omega_u = (\alpha_N(\lambda) + \delta_N(\lambda))\Omega_u \quad (81)$$

This is important since the transfer matrix commutes with the Hamiltonian, and therefore  $\Omega_u$  is a Bethe state, albeit the ground state. However, as is the case in QM, once a ground state is obtained, successive states can be generated using a creation operator. Since ground and higher states of the transfer matrix are in involution, i.e. they all commute with each other and the Hamiltonian, then obtaining all  $N$  of them for an  $N$ -site spin chain gives the *completely-integrable* solution to the HSC, which is the ultimate goal, i.e. using the ABA to obtain the solution to the HSC.

To create a state of  $M$  flipped spins ( $M$  sites with spin down, all others spin up), the operator  $B$  is applied  $M$  times to the ground state  $\Omega_u$ , with a unique spectral parameter  $\lambda_i, i = 1 \dots M$  assumed for each application of  $B$ .

Each operation of  $B$  adds another flipped spin to a unique site, presumed also to have prior been in the up state, i.e. no flipping of spins already flipped.

For example, the single flipped spin state, denoted by  $|\lambda_1\rangle$  ( $M = 1$ ) is obtained by a single application of  $B$  as in

$$|\lambda_1\rangle = B(\lambda_1)\Omega_u \quad (82)$$

Note that the state vector  $|\lambda_1\rangle$  does not show the state of all the other  $N - 1$  lattice sites since they are all ground state, up spins, and superfluous notation.

Similarly, the two-flipped spin state is given by

$$|\lambda_1, \lambda_2\rangle = B(\lambda_1, \lambda_2)\Omega_u \quad (83)$$

and the general,  $M$ -flipped spin state is given by applying  $B$  to the ground state,  $M$  times, and written as

$$|\lambda_1, \dots, \lambda_M\rangle = B(\lambda_1) \cdots (\lambda_M)\Omega_u \quad (84)$$

The actual algebraic details of using operator  $B$ , in conjunction with the exchange relations (74) to create new states, is given in [3], albeit the level of detail is overview-only for the general case of a state with  $M$  flipped spins. As such, the algebra for the simplest case of one flipped spin,  $M = 1$ , is given in detail next.

Because the algebra is quite involved, and notationally arduous, the process is given in very small steps - patience might be required.

## 4.2 One flipped-spin solution

Before commencing, the spectral parameters  $\lambda_a$  and  $\lambda_b$  are renamed as  $\lambda$  and  $\lambda_1$  respectively - the latter denoting  $M = 1$  for the one-down spin case

$$\lambda_a \rightarrow \lambda$$

$$\lambda_b \rightarrow \lambda_1$$

Using these revised names, the exchange equations (74) become

$$\begin{aligned} A(\lambda)B(\lambda_1) &= \frac{a(\lambda_1 - \lambda)}{b(\lambda_1 - \lambda)}B(\lambda_1)A(\lambda) - \frac{c}{b(\lambda_1 - \lambda)}B(\lambda)A(\lambda_1) \\ D(\lambda)B(\lambda_1) &= \frac{a(\lambda - \lambda_1)}{b(\lambda - \lambda_1)}B(\lambda_1)D(\lambda) - \frac{c}{b(\lambda - \lambda_1)}B(\lambda)D(\lambda_1) \end{aligned} \quad (85)$$

Reminder the  $a, b, c$  constants are

$$a = \lambda + i, \quad b = \lambda, \quad c = i$$

and the following new constants are defined from them

$$\begin{aligned} a_1 &= a(\lambda_1 - \lambda) = \lambda_1 - \lambda + i \\ a_2 &= a(\lambda - \lambda_1) = \lambda - \lambda_1 + i \\ b_1 &= b(\lambda_1 - \lambda) = \lambda_1 - \lambda \end{aligned} \quad (86)$$

Substituting these constants into the  $A$  and  $D$  exchange equations gives

$$\begin{aligned} A(\lambda)B(\lambda_1) &= \frac{a_1}{b_1}B(\lambda_1)A(\lambda) - \frac{c}{b_1}B(\lambda)A(\lambda_1) \\ D(\lambda)B(\lambda_1) &= \frac{a_2}{-b_1}B(\lambda_1)D(\lambda) - \frac{c}{-b_1}B(\lambda)D(\lambda_1) \end{aligned} \quad (87)$$

and resolving the minus signs in  $D$  gives

$$D(\lambda)B(\lambda_1) = -\frac{a_2}{b_1}B(\lambda_1)D(\lambda) + \frac{c}{b_1}B(\lambda)D(\lambda_1)$$

Multiplying throughout by  $b_1$  gives  $A$  and  $D$  in the forms required for the next stage.

$$\begin{aligned} b_1 A(\lambda)B(\lambda_1) &= a_1 B(\lambda_1)A(\lambda) - c B(\lambda)A(\lambda_1) \\ b_1 D(\lambda)B(\lambda_1) &= -a_2 B(\lambda_1)D(\lambda) + c B(\lambda)D(\lambda_1) \end{aligned}$$

Apply the  $A$  equation to the ground state

$$b_1 A(\lambda)B(\lambda_1)\Omega_u = a_1 B(\lambda_1)A(\lambda)\Omega_u - c B(\lambda)A(\lambda_1)\Omega_u$$

and using the eigenvectors equations for  $\Omega_u$  (75), then

$$b_1 A(\lambda)|\lambda_1\rangle = a_1 B(\lambda_1)\alpha_N(\lambda)\Omega_u - c B(\lambda)\alpha_N(\lambda_1)\Omega_u$$

Rearranging constant terms

$$b_1 A(\lambda)|\lambda_1\rangle = a_1 \alpha_N(\lambda)B(\lambda_1)\Omega_u - c \alpha_N(\lambda_1)B(\lambda)\Omega_u$$

and reapplying the eigenvector equation for  $B$  (82) gives

$$b_1 A(\lambda)|\lambda_1\rangle = a_1 \alpha_N(\lambda)|\lambda_1\rangle - c \alpha_N(\lambda_1)B(\lambda)\Omega_u$$

Note that the term on the rhs involving  $B(\lambda)\Omega_u$  is left undefined - it will later be set to zero as a condition.

Now do the same as above for the  $D$  equation

$$b_1 D(\lambda) B(\lambda_1) \Omega_u = -a_2 B(\lambda_1) D(\lambda) \Omega_u + c B(\lambda) D(\lambda_1) \Omega_u$$

$$b_1 D(\lambda) |\lambda_1\rangle = -a_2 B(\lambda_1) \delta_N(\lambda) \Omega_u + c B(\lambda) \delta_N(\lambda_1) \Omega_u$$

$$b_1 D(\lambda) |\lambda_1\rangle = -a_2 \delta_N(\lambda) B(\lambda_1) \Omega_u + c \delta_N(\lambda_1) B(\lambda) \Omega_u$$

$$b_1 D(\lambda) |\lambda_1\rangle = -a_2 \delta_N(\lambda) |\lambda_1\rangle + c \delta_N(\lambda_1) B(\lambda) \Omega_u$$

The final forms of the  $A$  and  $D$  equations are thus

$$b_1 A(\lambda) |\lambda_1\rangle = a_1 \alpha_N(\lambda) |\lambda_1\rangle - c \alpha_N(\lambda_1) B(\lambda) \Omega_u \quad (88)$$

$$b_1 D(\lambda) |\lambda_1\rangle = -a_2 \delta_N(\lambda) |\lambda_1\rangle + c \delta_N(\lambda_1) B(\lambda) \Omega_u \quad (89)$$

Adding the two equations

$$b_1 (A(\lambda) + D(\lambda)) |\lambda_1\rangle = (a_1 \alpha_N(\lambda) - a_2 \delta_N(\lambda)) |\lambda_1\rangle + c (\delta_N(\lambda_1) - \alpha_N(\lambda_1)) B(\lambda) \Omega_u$$

and re-writing the lhs using the fact that  $A + D$  is simply the transfer matrix  $t(\lambda)$  (80), gives

$$b_1 (t(\lambda)) |\lambda_1\rangle = (a_1 \alpha_N(\lambda) - a_2 \delta_N(\lambda)) |\lambda_1\rangle + c (\delta_N(\lambda_1) - \alpha_N(\lambda_1)) B(\lambda) \Omega_u \quad (90)$$

Defining constants  $\lambda_t$  and  $d$  as

$$\lambda_t(\lambda) = \frac{1}{b_1} (a_1 \alpha_N(\lambda) - a_2 \delta_N(\lambda)) \quad (91)$$

$$d = \delta_N(\lambda_1) - \alpha_N(\lambda_1) \quad (92)$$

then this equation in the transfer matrix becomes

$$t(\lambda) |\lambda_1\rangle = \lambda_t |\lambda_1\rangle + c d B(\lambda) \Omega_u \quad (93)$$

The action of  $B$  on the ground state, as given by the term  $B(\lambda)\Omega_u$ , is not defined, but if the entire term was zero then it is easily seen that the state  $|\lambda_1\rangle$  is, indeed, an eigenvector of the transfer matrix, i.e. a Bethe state, and thus the eigenvector solution for a single flipped spin HSC. Of course, this is subject to the  $B$  term disappearing. Given  $B(\lambda)\Omega_u \neq 0$ , i.e.  $B$  does not annihilate the ground state (which it doesn't since it is a creation operator) then, for the term to disappear, the constant  $d$  must be zero ( $c$  is the non-zero imaginary unit  $i$ ). This then puts a constraint on  $\lambda_1$

$$d = 0 \Rightarrow \delta_N(\lambda_1) = \alpha_N(\lambda_1)$$

Expanding out the constants  $\alpha_N$  and  $\delta_N$  for parameter  $\lambda_1$  shows  $\lambda_1$  must be a root of an  $N$ th order polynomial (for an  $N$ -site chain), i.e.

$$(\lambda_1 - \frac{i}{2})^N = (\lambda_1 + \frac{i}{2})^N \quad (94)$$

Comparing with Faddeev [3], there is some reassurance this is the correct answer given the full condition for an M-spin (Faddeev uses  $l$  in place of  $M$  here),  $N$ -site chain is the following rather-involved form

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

The aforementioned reassurance derives from the fact that the lhs of this condition matches (94) if the rhs is unity. The rhs is a continued product, but note it is only strictly valid for two-flipped spins ( $M \geq 2$ ) since the product has the condition  $k \neq j$ , and because  $M = 1$  and  $j = 1$ , there are no terms in the product, in which case it is taken to be unity.

$$\left(\frac{\lambda_j + i/2}{\lambda_j - i/2}\right)^N = 1, \quad M = 1$$

This condition is a polynomial in  $\lambda_1$  of highest degree  $N - 1$ , because the  $\lambda_i^N$  terms cancels. In principle, then, there  $N - 1$  solutions for  $\lambda_1$ . The values for the simplest two-site and three-site cases,  $N = 2$  and  $N = 3$  respectively, are

$$M = 1, N = 2, \lambda_1 = 0 \text{ repeated}$$

$$M = 1, N = 3, \lambda_1 = \pm \frac{1}{2\sqrt{3}}$$

Using the earlier definitions of the constants  $a_1, b_1, c_1$  (86), reproduced below

$$a_1 = \lambda_1 - \lambda + i, \quad a_2 = \lambda - \lambda_1 + i, \quad b_1 = \lambda_1 - \lambda$$

For  $M = 1, N = 2, \lambda_1 = 0$

$$a_1 = -\lambda + i, \quad a_2 = \lambda + i, \quad b_1 = -\lambda$$

then the Bethe state eigenvalue (91) is

$$\lambda_t(\lambda) = \frac{1}{-\lambda}((-\lambda + i)\alpha_N(\lambda) - (\lambda + i)\delta_N(\lambda))$$

Furthermore, using the definitions of  $\alpha_N(\lambda)$  and  $\delta_N(\lambda)$  (76), also reproduced below

$$\alpha_N(\lambda) = \left(\lambda + \frac{i}{2}\right)^N, \quad \delta_N(\lambda) = \left(\lambda - \frac{i}{2}\right)^N$$

then the Bethe state eigenvalue (91) can be simplified to the following quadratic polynomial for  $N = 2$

$$\lambda_t(\lambda) = 2\lambda^2 + \frac{3}{2}, \quad M = 1, N = 2$$

This is reassuringly real-valued, as required for physical observables in QM, and a natural property of Hermitian operators.

Note, as mentioned above, there are  $N - 1$  values of  $\lambda_1$  obtained by solving the polynomial condition (94). This will accordingly give  $N - 1$  eigenvalues (and corresponding eigenvectors) of the transfer matrix for  $\lambda_t(\lambda)$ . An  $N$ 'th eigenstate can be obtained from the Spin [3], [5].

This completes the ABA solution of the Heisenberg Spin Chain and, indeed, Part I of this document.

## 5 Summary and Conclusions

A solution for the one-dimensional Heisenberg Spin Chain (HSC) [1] has been detailed, obtained by the method known as the Algebraic Bethe Ansatz (ABA) due to Faddeev [3]. Whilst this method is physically less intuitive than the *Coordinate Bethe Ansatz* (CBA), devised by Bethe [6] nearly half a century earlier, it is based upon a relatively modern, general method of finding commuting operators that also commute with the Hamiltonian, and thereby generate constants of motion. Specifically, these commuting operators are known as *transfer* matrices, derived from the trace of the *monodromy* matrix, itself derived from the product of *Lax* operators - all these operators having analogues in the solution of other non-linear, classical and quantum systems. For this  $N$ -site HSC, a complete solution has been obtained by showing the ABA gives  $N - 1$  such commuting transfer matrices - the additional spin operator makes up the set of  $N$  commuting operators that all commute with the Hamiltonian. In other words, the quantum equivalent of the classical requirement to obtain  $N$  first integrals of motion of a dynamical system is achieved and the HSC solved, i.e. it is a quantum *integrable system*.

Whilst the HSC model is one of spins at spatially separated lattice sites, when transformed to the Fourier domain the system is seen to be equivalent to particles of a given momentum, known as *magnons*. With this particle interpretation comes a more physical interpretation of the equations in terms of particle scattering. Most importantly, the multiple particle scattering can be factored into two-particle scattering processes, which is actually the key to the HSC integrability given it permits numerous simplifications via operator commutation properties that wouldn't ordinarily arise under a complex multi-particle interaction.

The magnon particle interpretation and associated scattering properties then nicely relate to what is the intended Part II of this document. This second part will detail the solution to the classical, non-linear Korteweg de Vries (KdV) equation, that has algebraic analogues to the ABA. In addition, from a physical perspective, the KdV equation is famed for its soliton solutions, that also have a particle interpretation with related scattering properties as per magnons and numerous other quasi-particles that are appearing in many branches of physics, not least condensed matter physics and field theory.

## 6 References

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## 7 Appendices

### 7.1 Pauli Matrices and Spin Operators

#### 7.1.1 Pauli Matrices

At the heart of the algebra is the standard SU(2) Pauli spin matrix representation (below) for spin aligned ('up') or anti-aligned ('down') along the z-axis, as per common convention - some texts use the x-axis instead.

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

That the z-axis is chosen can be seen by the fact that  $\sigma_z$  is diagonalised with the +1 (up) and -1 down eigenvalues.

Each Pauli matrix squares to the identity

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I$$

The matrices satisfy the SU(2) algebra, as given by the commutation relations

$$[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k \quad (95)$$

A vector of 2x2 Pauli matrices  $\vec{\sigma}$  is defined as

$$\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z) \quad (96)$$

and its square (inner product with itself - see below) is thus, using the above, just a multiple of the identity matrix

$$\vec{\sigma}^2 = \vec{\sigma} \cdot \vec{\sigma} = \sigma_x^2 + \sigma_y^2 + \sigma_z^2 = 3I \quad (97)$$

Note that many texts treat the square of a vector (here a 'vector' of matrices) as the inner product of the vector with itself as in  $\vec{\sigma}_i^2 = \vec{\sigma}_i \cdot \vec{\sigma}_i$ , with an implied summation over  $i$  so that the following four forms all have the same meaning, i.e.

$$\vec{\sigma}^2 = \vec{\sigma} \vec{\sigma} = \vec{\sigma} \cdot \vec{\sigma} \quad (98)$$

#### 7.1.2 Spin Operators

The  $S_x, S_y, S_z$  spin operators are defined as the following  $\hbar/2$  scaled forms of the Pauli matrices, where the re-scaling is to give the spin eigenvalues as  $\pm\hbar/2$ :

$$S_x = \frac{\hbar}{2}\sigma_x \quad S_y = \frac{\hbar}{2}\sigma_y \quad S_z = \frac{\hbar}{2}\sigma_z$$

The matrices satisfy the following, standard SU(2) commutation relations, where  $x = 1, y = 2, z = 3$  for  $i, j, k$  in range 1 to 3:

$$[S_i, S_j] = i\hbar\epsilon_{ijk}S_k \quad (99)$$

The spin raising  $S_+$  and lowering  $S_-$  operators are defined as

$$S_+ = S_x + iS_y \quad S_- = S_x - iS_y \quad S_+ = S_+^*$$

which expand in full as the following 2x2 matrices:

$$S_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad S_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

These matrices also satisfy the standard SU(2) commutation relations

$$[S_z, S_+] = \hbar S_+ \quad [S_z, S_-] = -\hbar S_- \quad [S_+, S_-] = 2\hbar S_z \quad (100)$$

The total spin vector  $\bar{S}$ , just like  $\bar{\sigma}$  further above, is defined as

$$\bar{S} = (S_x, S_y, S_z)$$

and, since the spin matrices are just scaled versions of the Pauli matrices, the squared spin is as per  $\bar{\sigma}^2$  but with scale-factor  $3\hbar/4$  as in

$$\bar{S}^2 = \frac{3}{4}\hbar^2 I$$

A useful relation between  $S_z$  and the raising and lowering operators,  $S_+$  and  $S_-$  respectively, is

$$\bar{S}^2 = S_z^2 + \frac{1}{2}(S_+S_- + S_-S_+)$$

The spinors  $u \in \mathbb{C}^2$  ( up) and  $d \in \mathbb{C}^2$  (down) are defined as

$$u = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad d = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

These are, not surprisingly, the spin-up and spin-down eigenvectors of the spin z-component matrix  $S_z$ , i.e.

$$S_z u = (\hbar/2)u \quad S_z d = (-\hbar/2)d \quad (101)$$

with the standard raising and lowering relations

$$S_+ u = 0 \quad S_+ d = u \quad S_- u = d \quad S_- d = 0$$

These 2x2 matrix forms and two-element spinors are now used as the building block for the simple tensor product forms.

## 7.2 Two-particle SU(2) Multiplets

### 7.2.1 Permutation Matrix

The eigenvectors of the permutation matrix  $\mathcal{P}$  are the same as the two-site  $R$  matrix, Lax matrix  $L$  and Hamiltonian  $H$ , since these latter three are just a linear combination of  $\mathcal{P}$  and the identity matrix. However, given they all comprise different linear multiples of the identity, the eigenvalues are only the same to within an additive constant. Most importantly, as noted in the main text, Section (2.2.3), the two-site permutation matrix  $\mathcal{P}_{ij}$  can be written in terms of the Pauli spin matrices as follows:

$$\mathcal{P}_{ij} = \frac{1}{2}(\bar{\sigma}_i \bar{\sigma}_j + I^{\otimes N})$$

Consequently, the eigenvectors of  $\mathcal{P}_{ij}$  are those of SU(2) spin multiplets (a triplet and a singlet) for a two-site spin system N=2.

Being Hermitian,  $\mathcal{P}$  has real-valued eigenvalues comprising the three-degenerate values +1 (the symmetric SU(2) *triplet* state - next), and a single -1 eigenvalue (the anti-symmetric *singlet* state).

$$\text{eigenvalues of } \mathcal{P} = \{1, 1, 1, -1\}$$



Using the tensor product of spinors  $u$  and  $v$ , the four normalised eigenvectors of  $\mathcal{P}$ , denoted by  $u_1, u_2, u_3$  and  $d_1$ , are

$$\begin{aligned} u_1 &= u \otimes u \quad u, v \in \mathbb{C}^2 \quad \text{eigenvalue } 1 \\ u_2 &= \frac{1}{\sqrt{2}}(u \otimes d + d \otimes u) \quad \text{eigenvalue } 1 \\ u_3 &= d \otimes d \quad \text{eigenvalue } 1 \\ d_1 &= \frac{1}{\sqrt{2}}(u \otimes d - d \otimes u) \quad \text{eigenvalue } -1 \\ u_1, u_2, u_3, d_1 &\in \mathbb{C}^2 \otimes \mathbb{C}^2 \end{aligned} \tag{102}$$

The eigenvectors  $u_1, u_2, u_3$  and  $d_1$  thus satisfy the following eigenvector equations:

$$\begin{aligned} \mathcal{P}u_1 &= u_1 \quad \mathcal{P}u_2 = u_2 \quad \mathcal{P}u_3 = u_3 \\ \mathcal{P}d_1 &= -d_1 \end{aligned}$$

The first three eigenvector equations represent the degenerate *triplet* state for eigenvalue  $+1$ , and the last  $d_1$  is the single, *singlet* state, for eigenvalue  $-1$ . Note that the  $-1$  singlet eigenvalue is obviously not the standard QM value of zero (see next section), but is  $-1$  here due to the addition of the identity matrix term in the permutation matrix definition above.

The eigenvectors are expanded in full component form as

$$u_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad u_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} \quad u_3 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad d_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ -1 \\ 1 \\ 0 \end{pmatrix}$$

These four eigenvectors are both normalised and orthogonal, and therefore form an orthonormal basis for the  $4 \times 4$  representation of  $\text{SU}(2)$ .

### 7.2.2 Spin matrix - z-axis

By defining a two-site (sites 1 and 2), z-axis spin operator  $S_{12}^z$  as the following  $\mathbb{C}^2 \otimes \mathbb{C}^2$  tensor product:

$$S_{12}^z = (S_z \otimes I + I \otimes S_z)$$

and defining the eigenvectors, upper case  $U$  in terms of the above, lower case  $u$  variants as

$$U_+ = u_1 \quad U_0 = u_2 \quad U_- = u_3 \quad D_0 = d_1$$

then the eigenvectors  $U_+, U_0, U_-$  and  $D_0$  satisfy the following eigenvector equations:

$$\begin{aligned} S_{12}^z U_+ &= \hbar U_+ \\ S_{12}^z U_0 &= 0 \\ S_{12}^z U_- &= -\hbar U_- \\ S_{12}^z D_0 &= 0 \end{aligned} \tag{103}$$

As an example of obtaining the above, the eigenvector action of  $S_{12}^z$  on  $U_+$  is detailed following.

Using the above definitions

$$U_+ = u_1 = u \otimes u, \quad S_{12}^z = (S_z \otimes I + I \otimes S_z)$$

then

$$S_{12}^z U_+ = (S_z \otimes I + I \otimes S_z) u \otimes u$$

Multiplying out the bracket gives

$$S_{12}^z U_+ = S_z u \otimes u + u \otimes S_z u$$

and using  $S_z u = (\hbar/2)u$  (101), then the above  $S_{12}^z$  action on  $u_1$  is verified, i.e.

$$S_{12}^z U_+ = \hbar u \otimes u = \hbar U_+$$

From the above four eigenvector relations (103), it is seen that the eigenvectors are now so-named  $U_+$ ,  $U_0$ ,  $U_-$  and  $D_-$  because, the subscript matches their eigenvalue to the tensor product spin matrix  $S_z$ . For reference, the  $4 \times 4$  spin operator  $S_z$  is expanded in full as

$$S_z = \hbar \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

The above eigenvector relations can be confirmed using this matrix and the eigenvectors, as also expanded in full further above.

In quantum mechanics, the triplet spin states represent the two-particle state for total spin eigenvalue  $S = 1$  with ‘magnetic’ spin quantum number  $m_s = 1, 0, -1$ . These have a symmetric spin wave-function, as can be seen by swapping the  $u$  and  $d$  spinors in the above eigenvector definitions for  $u_+$ ,  $u_0$ ,  $u_-$ . The singlet state is the anti-symmetric spin wave-function with spin state  $S = 0$  and consequently  $m_s = 0$  also.