Chapter 2

Dzyaloshinskii-Moriya Interaction

2.1 Introduction

The Heisenberg Hamiltonian in one dimension has been widely studied over the years. For spins $S = 1/2$, the ground state energy and the low-lying excitation spectrum are known exactly for both the ferromagnetic and the antiferromagnetic Hamiltonians. The exact results are obtained using the well-known Bethe Ansatz [1, 2]. The anisotropic Heisenberg Hamiltonian, in which only two of the exchange integrals J_x, J_y and J_z are equal, is also Bethe Ansatz solvable. Other types of anisotropy, besides anisotorpic exchage interaction, may also be present in real systems. Systems like α–Fe_2O_3, NiF_2, $MnCO_3$, $CoCO_3$ etc., which are predominantly antiferromagnetic in nature, exhibit weak ferromagnetism. The sign of the exchange interaction in these substances is negative as seen from the paramagnetic susceptibilities which obey the Curie-Weiss law with negative θ. Neutron diffraction measurements confirm that the spin arrangements in these crystals below the transition points are mainly antiferromagnetic. These phenomena could not be explained in terms of an imbalance between the sublattice magnetizations owing to defects in stoichiometry or in terms of AFM domains with magnetized walls which can be stabilized only by some imperfections of strutural or chemical nature. The problem, whether the weak ferromagnetism can be an intrinsic property of certain crystals, was first studied by Dzyaloshinskii[3]. He proposed a phenomenological theory which suggests that the spin-spin interaction responsible for the weak ferromagnetism of α-Fe_2O_3 is antisymmetrical in nature and is of the type

$$\mathbf{D} \cdot [\mathbf{S_1} \times \mathbf{S_2}]$$

Moriya[4] later provided the microscopic basis of the interaction by extending Anderson's superexchange theory to include the spin-orbit interaction. The bilinear spin-spin coupling between two spins $\mathbf{S_1}$ and $\mathbf{S_2}$ can be written in the most general form as

$$V_{12} = \mathbf{S_1} \cdot \mathbf{K_S} \cdot \mathbf{S_2} + \mathbf{S_1} \cdot \mathbf{K_A} \cdot \mathbf{S_2} \qquad (2.1)$$

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where $\mathbf{K_S}$ and $\mathbf{K_A}$ represent symmetrical and antisymmetrical tensors, respectively. The symmetrical part of the spin coupling can always be expressed in the form

$$K_x\, S_{1x}\, S_{2x} + K_y\, S_{1y}\, S_{2y} + K_z\, S_{1z}\, S_{2z} \tag{2.2}$$

with a suitable choice of the coordinate axes x, y and z. Without loss of generality one can assume that K_z has the largest value among the three coefficients. Then, the most favourable orientation is an antiferromagnetically ordered arrangement of spins pointing in the z-direcrion. Thus the symmetrical part of the spin coupling cannot give rise to the canting of the spins in two-sublattice AFMs. The antisymmetrical part of the spin coupling is generally expressed by the form

$$\mathbf{D} \cdot [\mathbf{S_1} \times \mathbf{S_2}] \tag{2.3}$$

where $\mathbf{D}$ is a constant vector. It is clear that this coupling acts to cant the spins because the coupling energy is minimised when the two spins are perpendicular to each other. The above interaction term is the Dzyaloshinskii-Moriya interaction.

2.2 Origin of the Dzyaloshinskii-Moriya Interaction Term

We treat the localised electron orbital states as unperturbed states and consider the spin-orbit coupling as a perturbation. The second-order energy which is bilinear in the spin-orbit coupling and the exchange interaction is

$$
\begin{aligned}
&\sum_m [\frac{< n|\lambda \mathbf{L_1} \cdot \mathbf{S_1}|m > 2J(mn'nn')\mathbf{S_1} \cdot \mathbf{S_2}}{E_n - E_m} \\
&+ \frac{2J(nn'mn')\mathbf{S_1} \cdot \mathbf{S_2} < m|\lambda \mathbf{L_1} \cdot \mathbf{S_1}|n >}{E_n - E_m}] \\
&+ \sum_{m'} [\frac{< n'|\lambda \mathbf{L_2} \cdot \mathbf{S_2}|m' > 2J(m'nn'n)\mathbf{S_1} \cdot \mathbf{S_2}}{E_{n'} - E_{m'}} \\
&+ \frac{2J(n'nm'n)\mathbf{S_1} \cdot \mathbf{S_2} < m'|\lambda \mathbf{L_2} \cdot \mathbf{S_2}|n' >}{E_{n'} - E_{m'}}]
\end{aligned}
\tag{2.4}
$$

where n, n' represent the ground orbital states and m, m' are the excited orbital states of the two ions 1 and 2 at the positions $\mathbf{R}$ and $\mathbf{R'}$, respectively. $J(nn'mm')$ is the exchange integral

$$J\ (nn'mm') =$$

$$\int\int \phi_n^*(\mathbf{r_1} - \mathbf{R})\phi_{n'}^*(\mathbf{r_2} - \mathbf{R'})\frac{e^2}{r_{12}}\phi_m(\mathbf{r_2} - \mathbf{R})\phi_{m'}(\mathbf{r_1} - \mathbf{R'})d\mathbf{r_1}d\mathbf{r_2} \tag{2.5}$$

and $\phi_n(\mathbf{r} - \mathbf{R})$ is the ground orbital wave function of the ion at $\mathbf{R}$, etc. If the ground orbital state is nondegenerate, the matrix elements of the orbital

angular momentum L in Eq.(2.5) are purely imaginary and we can write the above expression as

$$
\begin{aligned}
& 2\lambda \sum_m \frac{J(nn'mn')}{E_n - E_m} < n|L_1|m > \cdot [S_1, (S_1 \cdot S_2)] \\
& + \ 2\lambda \sum_{m'} \frac{J(nn'nm')}{E_{n'} - E_{m'}} < n'|L_2|m' > \cdot [S_2, (S_1 \cdot S_2)] \\
& = \ 2i\lambda [\sum_m \frac{J(nn'mn')}{E_n - E_m} < n|L_1|m > \\
& - \ \sum_{m'} \frac{J(nn'nm')}{E_{n'} - E_{m'}} < n'|L_2|m' >] \cdot [S_1 \times S_2]
\end{aligned}
\tag{2.6}
$$

From a consideration of superexchange mechanisms, one can replace the exchange integrals in Eq.(2.6) by the respective effective superexchange coupling constants. The expression (2.6) gives the energy associated with the antisymmetric spin-spin interaction. The corresponding Hamiltonian is of the form $D \cdot [S_1 \times S_2]$. Such an interaction exists only when the crystal symmetry is sufficiently low. The following rules determining the direction of D, are obtained from symmetry arguments. Let the spins 1 and 2 be located at the points i and j of the crystal.

(i) If a centre of inversion is located at the midpoint of the line joining i and j, $D = 0$.

(ii) When a mirror plane perpendicular to the line $i j$ bisects it, D is parallel to the mirror plane.

(iii) When there is a mirror plane including i and j, D is perpendicular to the mirror plane.

(iv) When a 2-fold rotation axis is perpendicular to $i j$ and bisects it, D is perpendicular to the two-fold axis.

(v) When there is an n-fold axis $(n \geq 2)$ along $i j$, D is parallel to $i j$.

2.3   Some Recent Examples of Materials with Dzyaloshinskii-Moriya Interaction

The CuO_2 planes of undoped La_2CuO_4 have a small ferromagnetic moment even though the dominant in-plane exchange interaction is antiferromagnetic [5]. The compound undergoes a structural phase transition from the tetragonal to the orthorhombic phase, at $T \approx 500 \, K$. In the orthorhombic phase, the CuO_6 octahedra forming the CuO_2 plane, tilt in a staggered fashion by a small angle of $4°$ around the $\langle 110 \rangle$ axis. This distortion combined with the DM interaction is responsible for a weak ferromagnetic moment in each layer. Thio et.al.,[6] have observed a jump in the magnetization as a function of an external field applied perpendicular to the planes. The canted spins in the planes align in the direction of the magnetic field when it is sufficiently strong, giving rise to a change in the magnetization.

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The spin-Peierls compound $CuGeO_3$ has been extensively studied in recent times. This compound is a linear chain Heisenberg antiferromagnet (AFM) and is the first inorganic compound to undergo spin-Peierls transition at T_{sp} =14 K. Many studies on this compound have been undertaken so far. Among them, the results of electron paramagnetic resonance (EPR) investigations are summarised as follows.

The linewidth ΔH which is approximately 1-2 KOe at room temperature decreases very rapidly with decreasing temperature, but it does not increase over the short-range ordering region. In contrast to ΔH versus temperature T, the resonance field H_{res} does not change with T above T_{sp}. To explain this, Yamada et.al.,[8] have suggested that the DM interaction term is present as an antisymmetric perturbation term along with the Heisenberg Hamiltonian. In conventional one dimensional Heisenberg AFMs with spin symmetric perturbations, $\Delta H(T)$ increases with decreasing T over the short range ordering region. Yamada et.al., have shown that, with the DM interaction providing the main perturbation, the results for $\Delta H(T)$ and $H_{res}(T)$, as well as the value of ΔH and the lineshape at high T, are in good agreement with the experimental values. A recent neutron scattering experiment on the quasi-one-dimensional $S = \frac{1}{2}$ AFM Cu-benzoate has shown the existence of a gap in the excitation spectrum induced by an applied magnetic field. Oshikawa and Affleck [11], have attributed the formation of the gap to an effective staggered field. Cu-benzoate has alternating crystal axes, giving rise to an alternating g-tensor. Due to this, a uniform magnetic field produces an effective staggered field on the spin chain. The DM interaction gives an additional contribution to the effective staggered field. The theory provides a successful explanation of the experimental data, including the angle dependence of the gap.

2.4 Ferromagnetic Heisenberg Hamiltonian with DM Interaction

Evidence of the DM interaction has been obtained in real materials in combination with antiferromagnatic spin-spin exchange interaction. There are, however, some theoretical studies [9] on the effect of the DM interaction on the ferromagnetic Heisenberg Hamiltonian. Gwa and Spohn have approximated the noisy Burgers equation by a model involving the asymmetric simple exclusion process. The generator of the relevant master equation is given by the Hamiltonian

$$H = -\frac{1}{4}\sum_{j=1}^{n}[\sigma_j \cdot \sigma_{j+1} - 1 + i\epsilon(\sigma_j^x\sigma_{j+1}^y - \sigma_j^y\sigma_{j+1}^x)], \qquad (2.7)$$

where σ_j is the Pauli spin operator. We recognize the Hamiltonian to be that corresponding to the ferromagnetic Heisenberg spin chain along with a purely DM-type of coupling

$$i[\mathbf{D} \cdot (\sigma_j \times \sigma_{j+1})] \qquad (2.8)$$

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with the vector **D** oriented along the z diection ($D_z = \epsilon$). Alcaraz and Wreszinski [10] have shown that the quantum Heisenberg chain (both FM and AFM) with DM interaction is equivalent to the XXZ Hamiltonian ($J_x = J_y \neq J_z$) with specific boundary conditions

Integrable, nonlinear dynamical models of Heisenberg ferromagnets are known to exhibit an interesting class of localized nonlinear elementary spin excitations such as solitons, domain walls, etc. [12, 13, 14, 15]. Soliton spin excitations have also been identified very recently in one dimensional weak Heisenberg ferromagnetic chains with DM interaction.

In the presence of even a weak DM interaction, the ground state of a classical FM Heisenberg chain changes from the original FM ground state in which the spins have parallel orientations. In this thesis, we include a magnetic field h in the Hamiltonian and assume that the DM interaction strength is less than the FM exchange interaction strength. We find that for a sufficiently strong magnetic field, one can have a fully aligned FM ground state. We study the effect of the DM interaction on the FM spin-wave spectra and show using the Bethe Ansatz that two magnon bound states exist in suitable parameter regimes.

2.5 Ground State for h = 0 and h ≠ 0

The nearest neighbour Heisenberg Hamiltonian with DM interaction is

$$H = -J_1 \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \sum_{i=1}^{N} (\mathbf{S}_i \times \mathbf{S}_{i+1}) \cdot \hat{z}. \tag{2.9}$$

Let the spins be classical vectors in the plane $\mathbf{S}_i = (S_i^x, S_i^y)$, where $S_i^x = \cos \alpha_i$, $S_i^y = \sin \alpha_i$. The first term in the Eq.(2.9) favours parallel neighbouring spin pairs whereas the second has the effect of turning the spins perpendicular to one another. The above Hamiltonian can be written as

$$H = -\sum_{i=1}^{N} [J_1 \cos(\alpha_i - \alpha_{i+1}) + J_2 \sin(\alpha_i - \alpha_{i+1})]. \tag{2.10}$$

Let $\phi = \tan^{-1} \frac{J_2}{J_1}$, $\phi \in [0, \frac{\pi}{2}]$. The Hamiltonian H becomes

$$H = -\frac{J_1}{\cos \phi} \sum_{i=1}^{N} \cos(\alpha_i - \alpha_{i+1} + \phi) \tag{2.11}$$

Since $\frac{J_1}{\cos \phi} \geq 0$ for $\phi \in [0, \frac{\pi}{2}]$, the ground state is given by

$$\alpha_{i+1} - \alpha_i = \phi \tag{2.12}$$

with

$$\alpha_{N+1} = p(\alpha_1 + \phi),$$
$$p = 0, 1 \tag{2.13}$$

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where p=0(1) corresponds to free (angle-dependent) boundary condition. We note that the classical ground state has a canted spin structure, however small be the value of J_2. We now discuss the nature of the quantum mechanical ground state in the presence of a magnetic field.

Ground state for h $\neq$ 0:

The $S = \frac{1}{2}$ Hamiltonian is

$$H = -J_1 \sum_{i=1}^{N} \mathbf{S_i} \cdot \mathbf{S_{i+1}} + J_2 \sum_{i=1}^{N} (\mathbf{S_i} \times \mathbf{S_{i+1}}) \cdot \hat{z} - h \sum_{i=1}^{N} S_i^z. \qquad (2.14)$$

In terms of the spin raising and lowering operators, the Hamiltonian can be written as

$$
\begin{aligned}
H = {} & -J_1 \sum_{i=1}^{N} [S_i^z S_{i+1}^z + \frac{1}{2}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)] \\
& - \frac{iJ_2}{2} \sum_{i=1}^{N} (S_i^- S_{i+1}^+ - S_i^+ S_{i+1}^-) - h \sum_{i=1}^{N} S_i^z.
\end{aligned} \qquad (2.15)
$$

We also assume periodic boundary conditions (PBC). Let us consider a four-spin system. There are three subspaces with $S_{tot}^z = \sum_{i=1}^{4} S_i^z = 0, 1, 2$. In the $S_{tot}^z = 0$ subspace, the basis functions are:

$$
\begin{aligned}
\psi_1 &= \uparrow\uparrow\downarrow\downarrow \\
\psi_2 &= \downarrow\downarrow\uparrow\uparrow \\
\psi_3 &= \uparrow\downarrow\downarrow\uparrow \\
\psi_4 &= \downarrow\uparrow\uparrow\downarrow \\
\psi_5 &= \uparrow\downarrow\uparrow\downarrow \\
\psi_6 &= \downarrow\uparrow\downarrow\uparrow
\end{aligned} \qquad (2.16)
$$

On diagonalization, the eigenvalues are

$$0, 0, -J_1, 2J_1, \frac{J_1 + \sqrt{J_1^2 + 8J_2^2}}{2}, \frac{J_1 - \sqrt{J_1^2 + 8J_2^2}}{2}. \qquad (2.17)$$

If $J_1 > J_2$, the lowest energy is $-J_1$. In the $S_z^{tot} = 1$ subspace the basis functions are:

$$
\begin{aligned}
\psi_1 &= \uparrow\uparrow\uparrow\downarrow \\
\psi_2 &= \uparrow\uparrow\downarrow\uparrow \\
\psi_3 &= \uparrow\downarrow\uparrow\uparrow \\
\psi_4 &= \downarrow\uparrow\uparrow\uparrow
\end{aligned} \qquad (2.18)
$$

The energy eigenvalues are

$$-(J_1 + h), (J_1 - h), -(J_2 + h), (J_2 - h). \qquad (2.19)$$

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The lowest energy is $-(J_1 + h)$. In the $S_z^{tot} = 2$ subspace, there is one basis function

$$\psi_1 = \uparrow\uparrow\uparrow\uparrow \qquad (2.20)$$

The eigenvalue is $-(J_1 + 2h)$.

Comparing the lowest energies in the three subspaces, one finds that the ground state is the fully aligned state with $S_z^{tot} = 2$ and energy $-(J_1 + 2h)$ provided $J_1 > J_2$. The ferromagnetic state is the ground state for all values of the magnetic field h. From a numerical diagonalization of six spins and for $J_1 > J_2$, one finds that a ferromagnetic ground state is obtained only for a sufficiently strong magnetic field h. Thus, for $h \neq 0$, there is a region in the $J_1 - J_2 - h$ parameter space in which the ferromagnetic state is the ground state.

2.6 Excitation Spectrum

The ferromagnetic Heisenberg Hamiltonian in the presence of the DM interaction and an external magnetic field is given by

$$H = -J_1 \sum_{i=1}^{N} \mathbf{S_i} \cdot \mathbf{S_{i+1}} + J_2 \sum_{i=1}^{N} (\mathbf{S_i} \times \mathbf{S_{i+1}}) \cdot \hat{z} - h \sum_{i=1}^{N} S_i^z. \qquad (2.21)$$

with $J_1 > 0$ and $J_2 > 0$. In terms of the spin raising and lowering operators, the above Hamiltonian can be written as

$$
\begin{aligned}
H &= -J_1 \sum_{i=1}^{N} [S_i^z S_{i+1}^z + \frac{1}{2}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)] \\
&\quad - \frac{iJ_2}{2} \sum_{i=1}^{N} (S_i^- S_{i+1}^+ - S_i^+ S_{i+1}^-) - h \sum_{i=1}^{N} S_i^z.
\end{aligned} \qquad (2.22)
$$

The ground state ϕ_0 has all spins pointing upwards, i.e.,

$$\phi_0 = \alpha(1)\alpha(2).....\alpha(N),$$

where α denotes an up spin. The ground-state energy $E_g = -J_1 N/4 - hN/2$. One can easily verify that S^z, the z component of the total spin, is a constant of motion, i.e., $[H, S^z] = 0$. We now consider the case in which the r spins deviate from the ground-state spin arrangement, i.e., there are r down spins at the sites $m_1, m_2, ..., m_r$. These spin functions are written as $\Psi(m_1, m_2, ..., m_r)$. The eigenfunction Ψ of H is a linear combination of the $^N C_r$ functions $\Psi(m_1, m_2, ..., m_r)$:

$$\Psi = \sum_{\{m\}} a(m_1, m_2, ..., m_r)\Psi(m_1, m_2, ..., m_r). \qquad (2.23)$$

Each of the numbers $m_1, m_2, ..., m_r$ runs over the possible values 1 to N subject to the condition

$$m_1 < m_2 < ... < m_r \qquad (2.24)$$

to avoid double counting. We write the eigenvalue equation as

$$H\Psi = E\Psi = E \sum_{\{m\}} a\{m\}\Psi(m_1, m_2, ..., m_r).$$ (2.25)

Multiplying (2.25) by a particular $\Psi^*(m_1, m_2, ..., m_r)$ and using orthogonality properties, one obtains

$$
\begin{aligned}
\epsilon a(m_1, m_2, ..., m_r) = & - \frac{J_1 + iJ_2}{2} \sum_{\{m'\}} a(m_1', m_2', ..., m_r') \\
& - \frac{J_1 - iJ_2}{2} \sum_{\{m''\}} a(m_1'', m_2'', ..., m_r'') \\
& + \frac{1}{2}J_1 N' a(m_1, m_2, ..., m_r) + hr a(m_1, m_2, ..., m_r),
\end{aligned}
$$ (2.26)

where $\epsilon = E + J_1 N/4 + hN/2$ is the excitation energy with respect to the ground-state energy E_g and N' is the number of antiparallel spin pairs. The first sum on the right-hand side is over the distributions $m_1', m_2', ..., m_r'$ which arise from a NN exchange of antiparallel spins of the type ↑↓ in $(m_1, m_2, ..., m_r)$ and the second sum is over the distributions $m_1'', m_2'', ..., m_r''$ which arise from an interchange of spins in antiparallel pairs of the type ↓↑ in $(m_1, m_2, ..., m_r)$.

Consider the case of one spin deviation, i.e., $r = 1$. In this case, $N' = 2$ and Eq. (2.26) becomes

$$\epsilon a(m) = -\frac{J_1 + iJ_2}{2}a(m+1) - \frac{J_1 - iJ_2}{2}a(m-1) + J_1 a(m) + ha(m).$$ (2.27)

The solution for $a(m)$ is given by

$$a(m) = e^{ikm}$$

so that

$$\epsilon = J_1(1 - \cos k) + J_2 \sin k + h$$ (2.28)

From the PBC, $k = (2\pi/N)\lambda$, $\lambda = 0, 1, 2, ..., N-1$

Now consider the case $r = 2$, i.e., there are two spin deviations. We distinguish between two cases.
(i) The two down spins are not neighbours, i.e., $m_2 \neq m_1 + 1$. Then from (2.26),

$$
\begin{aligned}
\epsilon a(m_1, m_2) = & - \left[\frac{J_1 + iJ_2}{2}\right][a(m_1 + 1, m_2) + a(m_1, m_2 + 1)] \\
& - \left[\frac{J_1 - iJ_2}{2}\right][a(m_1 - 1, m_2) + a(m_1, m_2 - 1)] \\
& + 2J_1 a(m_1, m_2) + 2ha(m_1, m_2).
\end{aligned}
$$ (2.29)

(ii) The two down spins are neighbours, i.e., $m_2 = m_1 + 1$. Now

$$\epsilon a(m_1, m_1 + 1) = -\left[\frac{J_1 + iJ_2}{2}\right] a(m_1, m_1 + 2)$$
$$- \left[\frac{J_1 - iJ_2}{2}\right] a(m_1 - 1, m_1 + 1)$$
$$+ J_1 a(m_1, m_1 + 1) + 2h a(m_1, m_1 + 1) \qquad (2.30)$$

Eq.(2.29) is satisfied by the Bethe Ansatz [1] (BA)

$$a(m_1, m_2) = C_1 e^{i(k_1 m_1 + k_2 m_2)} + C_2 e^{i(k_2 m_1 + k_1 m_2)} \qquad (2.31)$$

with the eigenvalue

$$\epsilon = J_1[(1 - \cos k_1) + (1 - \cos k_2)] + J_2(\sin k_1 + \sin k_2) + 2h \qquad (2.32)$$

where C_1, C_2, k_1 and k_2 are to be determined. Eq. (2.30) can also be satisfied if C_1 and C_2 are chosen in such a manner that

$$\frac{J_1}{2}[a(m_1, m_1) + a(m_1 + 1, m_1 + 1) - 2a(m_1, m_1 + 1)]$$
$$- \frac{iJ_2}{2}[a(m_1, m_1) - a(m_1 + 1, m_1 + 1)] = 0. \qquad (2.33)$$

The amplitude $a(m, m)$ has no physical meaning, since we are dealing with spin-$\frac{1}{2}$ particles, and are actually defined by Eq.(2.33). Putting Eq.(2.31) into Eq.(2.33), we get

$$\frac{C_2}{C_1} = -\frac{J_1(1 + e^{i(k_1 + k_2)}) - 2J_1 e^{ik_2} - iJ_2(1 - e^{i(k_1 + k_2)})}{J_1(1 + e^{i(k_1 + k_2)}) - 2J_1 e^{ik_1} - iJ_2(1 - e^{i(k_1 + k_2)})}. \qquad (2.34)$$

Choosing $C_1 = e^{(i\phi/2)}$ and $C_2 = e^{(-i\phi/2)}$, one derives the condition

$$\cot\left(\frac{\phi}{2}\right) = \frac{-J_1 \sin \frac{k_1 - k_2}{2}}{J_1 \cos \frac{k_1 - k_2}{2} - J_1 \cos \frac{k_1 + k_2}{2} + J_2 \sin \frac{k_1 + k_2}{2}} \qquad (2.35)$$
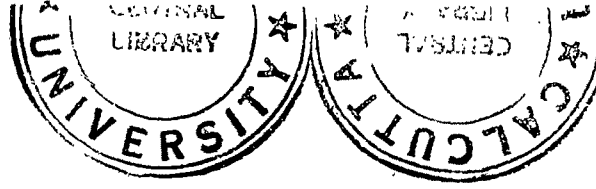
From the PBC, one obtains $a(m_1, m_2) = a(m_2, m_1 + N)$, leading to the relations

$$Nk_1 - \phi = 2\pi \lambda_1$$
$$Nk_2 + \phi = 2\pi \lambda_2$$
$$\lambda_1, \lambda_2 = 0, 1, 2, \ldots \ldots, N - 1 \qquad (2.36)$$

The sum of k_1 and k_2 is a constant of motion by translational symmetry:

$$k = k_1 + k_2 = (2\pi/N)(\lambda_1 + \lambda_2) \qquad (2.37)$$

For real k_1, k_2 and $\phi(-\pi \le \phi \le \pi)$, the eigenvalue spectrum is given by Eq. (2.32) and corresponds to a continuum of scattering states.

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To obtain bound states of two spin deviations, consider k_1, k_2 to be complex, i.e.

$$k_1 = u + iv \qquad (2.38)$$
$$k_2 = u - iv$$

From Eq.(2.36)

$$N(k_1 - k_2) = 2Niv = 2\pi(\lambda_1 - \lambda_2) + 2\phi \qquad (2.39)$$

Put $\phi = \psi + i\chi$ so that

$$\psi = \pi(\lambda_2 - \lambda_1) \quad \chi = Nv \qquad (2.40)$$

For non-zero v, χ is large. So

$$\cot \frac{\phi}{2} = \frac{\sin\psi - i\sinh\chi}{\cosh\chi - \cos\psi} \approx -i \qquad (2.41)$$

From Eq.(2.35), (2.39) and (2.41), one obtains the condition

$$J_1 e^{-v} = J_1 \cos u - J_2 \sin u \qquad (2.42)$$

Thus, from Eq.(2.32), the excitation energy for two spin deviations with complex k_1, k_2 is given by

$$\epsilon_b = J_1 - J_1 \left(\frac{J_1 \cos u - J_2 \sin u}{J_1} \right)^2 + 2h. \qquad (2.43)$$

The possible values of u are given by Eq.(2.42) ($1 \geq e^{-v} \geq 0$). The centre-of-mass momentum wavevector k (defined modulo 2π) $= 2u + 2n\pi$ where n is an integer and is limited to the range $0 \leq k \leq 4\tan^{-1}(J_1/J_2)$. From Eq.(2.32), the continuum of scattering states have bounds ϵ_1 and ϵ_2 given by

$$\epsilon_1 = J_1[2 - 2\cos(k/2)] + 2J_2 \sin(k/2) + 2h$$
$$\epsilon_2 = J_1[2 + 2\cos(k/2)] - 2J_2 \sin(k/2) + 2h \qquad (2.44)$$

Fig.2.1 shows the plots of ϵ_b (the two-magnon bound state energy given by Eq.(2.43)), ϵ_1 and ϵ_2 (Eq.(2.44)) versus $k(0 \leq k \leq 4\tan^{-1}(J_1/J_2))$, for $J_1 = 1.0, J_2 = 0.5$ and $h = 1.0$ and $J_1 = 1.0, J_2 = 0.8$ and $h = 1.0$. One finds that a two-magnon bound state exists in the full range of allowed k-values. There are two points of degeneracy at which $\epsilon_b = \epsilon_1$ or ϵ_2. From Eq.(2.43) and (2.44), the condition for the energies to be the same is

$$J_1 \cos u - J_2 \sin u = J_1 \qquad (2.45)$$

which leads to the relation

$$\sin(u/2)[J_1 \sin(u/2) + J_2 \cos(u/2)] = 0 \qquad (2.46)$$

Thus the two points of degeneracy are

$$u = 2n\pi$$
$$n = 0$$

or integer and

$$\tan u/2 = -J_2/J_1. \qquad (2.47)$$

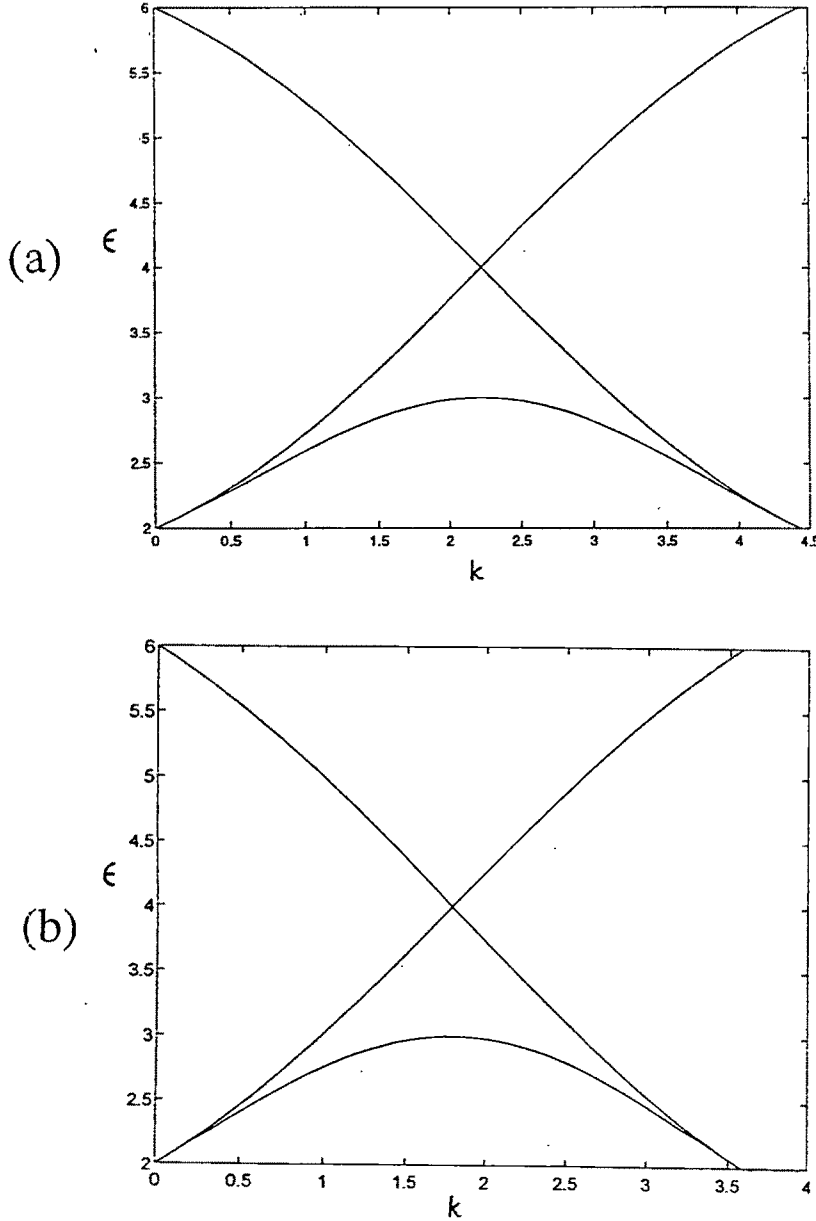Fig.2.1. Two magnon bound state energy ϵ_b and energies of two free magnons, with bounds given by ϵ_1 and ϵ_2, versus k the centre-of-mass momentum wave vector, for (a) $J_1 = 1.0$, $J_2 = 0.5$ and $h = 1.0$ (b) $J_1 = 1.0, J_2 = 0.8$ and $h = 1.0$. The values of k are in the range $0 \leq k \leq 4\tan^{-1}(J_1/J_2)$.

In Fig.2.1, the points correspond to $k = 0$ and $4\tan^{-1}(J_1/J_2)$, respectively, which are the end points of the range of k-values.

For $J_2 = 0$ and $h = 0$, Eqs. (2.42)-(2.44) reduce to those for the isotropic FM Hamiltonian and the values of k are in the range $0 \le k \le 2\pi$. As J_2 increases from zero, the range of k-values decreases. The magnetic field enters only into the energy expressions and has no effect on the k-values. The same linear term $2h$ is contributed by the magnetic field to the energies of the continuum and the bound states. In the FM state, the magnetic field has the largest contribution to the energy equal to $-hN/2$. Since S^z, the z component of the total spin, is a conserved quantity, the other states are obtained by deviating spins from the parallel spin arrangement of the FM state. The FM state has the highest possible value of $S^z = N/2$. The other states have lower values of S^z. For states with low values of S^z, the contribution of the magnetic field to the energy term is much smaller than in the FM state. For one and two spin deviations ($S^z = N/2 - 1$ and $N/2 - 2$, respectively), we have calculated the excitation energies measured with respect to that of the FM state. If these excitation energies are greater than zero for a certain choice of the parameters J_1, J_2 and h, the assumption that the FM state is the ground state is correct.

After the $r = 2$ calculation was completed , we noted the similarity of Eq. (2.34) with the corresponding equation in the case of the anisotropic XXZ chain. For the latter, the Hamiltonian is

$$H_{XXZ} = -\sum_{i=1}^{N}(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z) - h\sum_{i=1}^{N} S_i^z. \qquad (2.48)$$

The BA applied to this Hamiltonian leads to the following equation for $\frac{C_2}{C_1}$ (the ratio is the S-matrix of the scattering problem),

$$\frac{C_2}{C_1} = -\frac{1 - 2\Delta e^{ik_2} + e^{i(k_1+k_2)}}{1 - 2\Delta e^{ik_1} + e^{i(k_1+k_2)}} \qquad (2.49)$$

We now show that Eqs.(2.34) and (2.49) are identical in form if the momentum variables are redefined. Let

$$J_2 = J_1 \tan\theta. \qquad (2.50)$$

Then from of Eq.(2.34), we get

$$\frac{C_2}{C_1} = -\frac{1 - 2\cos\theta e^{i(k_2+\theta)} + e^{i(k_1+k_2+2\theta)}}{1 - 2\cos\theta e^{i(k_1+\theta)} + e^{i(k_1+k_2+2\theta)}}. \qquad (2.51)$$

We define the momentum variables as

$$k_1' = k_1 + \theta$$

and

$$k_2' = k_2 + \theta. \qquad (2.52)$$

Also, we put

$$\Delta = \cos\theta \qquad (2.53)$$

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Then Eq.(2.51) reduces to

$$\frac{C_2}{C_1} = -\frac{1 - 2\Delta e^{ik_2'} + e^{i(k_1' + k_2')}}{1 - 2\Delta e^{ik_1'} + e^{i(k_1' + k_2')}} \tag{2.54}$$

The S-matrix in Eq.(2.55) is of the same form as that for the anisotropic XXZ chain (Eq.(2.49)). The excitation spectrum in the two cases should also be similar. The excitation spectrum for one spin deviation is given by Eq.(2.43) as

$$\epsilon = J_1(1 - \cos k_1) + J_2 \sin k_1 + h \tag{2.55}$$

Putting $\frac{J_2}{J_1} = \tan\theta$, we get

$$
\begin{aligned}
\epsilon &= J_1[1 - \cos k_1 + \tan\theta \sin k_1] + h \\
&= \frac{J_1}{\cos\theta}[\Delta - \cos(k_1 + \theta)] + h \\
&= \frac{J_1}{\cos\theta}[\Delta - \cos k_1'] + h
\end{aligned} \tag{2.56}
$$

where $\Delta = \cos\theta$ and $k_1' = k_1 + \theta$ from Eq.(2.53) and Eq.(??). Eq. (2.57) in terms of the new momentum variables k_1' and the anisotropy constant Δ, has the same form,

$$\epsilon = [\Delta - \cos k_1] + h, \tag{2.57}$$

as the excitation spectrum of the XXZ Hamiltonian (Eq.(2.48)), apart from a pre-factor which can be put equal to one by choosing J_1 to be $\cos\theta$.

We next consider the general case of r spin deviations. Again, two cases are to be considered:
(i) No two spin deviations are neighbours.
(ii) Two spin deviations are neighbours.

In case (i), the general eigenvalue (Eq.(2.26)) is satisfied by the full BA

$$a(m_1, \ldots, m_r) = \sum_{P=1}^{r!} e^{[i(\sum_{j=1}^{r} k_{Pj} m_j + \frac{1}{2} \sum_{j<l} \phi_{Pj,Pl})]} \tag{2.58}$$

P is any permutation of r numbers $1, 2, \ldots\ldots r$. Pj is the number obtained by operating P on j. The ϕ-values are the phase shifts in analogy with scattering theory. Eq.(2.31) with $C_1 = e^{i\phi/2}$ $C_2 = e^{-i\phi/2}$ is a special case of Eq.(2.59) for $r = 2$. The eigenvalue equation is given by

$$\epsilon = J_1 \sum_{l=1}^{r}(1 - \cos k_l) + J_2 \sum_{l=1}^{r} \sin k_l + rh \tag{2.59}$$

Eq.(2.28) and (2.32) are special cases of Eq.(2.60) for $r = 1$ and 2, respectively. The wavevectors k_i are determined as before by applying the PBC which leads to the r equations:

$$Nk_i = 2\pi\lambda_i + \sum_j \phi_{ij}, \tag{2.60}$$

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$i = 1, \ldots .r$. The phase shifts ϕ_{ij}'s are determined, as in the case of $r = 2$, by demanding that the BA (Eq.(2.59)) is also a solution for case (ii) (two spin deviations are neighbous). This leads to $\frac{r(r-1)}{2}$ equations similar to Eq.(2.35) since there are as many distinct ϕ's ($\phi_{ij} = -\phi_{ji}$). These equations, together with the r equations, Eq.(2.61), constitute a total number of $\frac{r(r+2)}{2}$ equations in as many unknowns and so are expected to have solutions. The excitation spectrum is governed by Eq. (2.60). The BA can be written in an alternative form as

$$a(m_1, \ldots, m_r) = \sum_P A_P e^{i[\sum_{j=1}^r k_{P_j} m_j]} \qquad (2.61)$$

Associate with each permutation P another permutation P' which differs from P only by the exchange of two adjacent elements:
$P'k = Pk + 1$, $P'k + 1 = Pk$. From the BA equations, one gets

$$\frac{A_P}{A_{P'}} = -\frac{1 + e^{i(k_{Pk}+k_{P'k}+2\theta)} - 2\cos\theta e^{(ik_{Pk}+\theta)}}{1 + e^{i(k_{Pk}+k_{P'k}+2\theta)} - 2\cos\theta e^{(ik_{P'k}+\theta)}} \qquad (2.62)$$

which is a generalization of the expression in Eq.(2.55). Again, the corresponding equations in the case of the XXZ chain have identical forms. Thus the Heisenberg Hamiltonian alongwith the DM interaction has an energy spectrum identical to that of the XXZ chain with appropriate redefinitions of the momentum variables.

After the completion of our work, we came to know of an earlier result obtained by Alcaraz and Wreszinski [10] who mapped the quantum Heisenberg chain with DM interaction onto the XXZ Hamiltonian with a certain type of boundary conditions. For the sake of completeness, we describe the major steps of the mapping. The quantum anisotropic Heisenberg chain with DM interactions is described by the Hamiltonian

$$H_N^{DM}(\Delta, \delta) = H_N^{XXZ}(\delta) + V_N^{DM}(\Delta) \qquad (2.63)$$

where

$$H_N^{XXZ}(\delta) = -\frac{1}{2} \sum_{i=1}^N (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \delta \sigma_i^z \sigma_{i+1}^z) \qquad (2.64)$$

is the XXZ quantum Hamiltonian, with anisotropy δ, and

$$V_N^{DM}(\Delta) = -\frac{\Delta}{2} \sum_{i=1}^N (\sigma_i^x \sigma_{i+1}^y - \sigma_i^y \sigma_{i+1}^x) \qquad (2.65)$$

is the DM interaction. The σ^α's ($\alpha = x, y, z$) are the Pauli matrices. The Hamiltonian (2.64) is rewritten in terms of the following matrices

$$\sigma_i^{\pm 1} = \frac{1}{2}(\sigma_i^x \pm i\sigma_i^y)$$
$$\sigma_i^0 = \sigma_i^z; \quad i = 1, 2, \ldots, N \qquad (2.66)$$

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$$H_N^{DM}(\Delta, \delta) =$$

$$-\frac{1}{\cos\phi}\left[\sum_{i=1}^{N-1}(e^{i\phi}\sigma_i^{+1}\sigma_{i+1}^{-1} + e^{-i\phi}\sigma_i^{-1}\sigma_{+1}^{i+1} + \delta\cos\phi\sigma_i^0\sigma_{i+1}^0)\right] + H_S^{p,\Omega}$$

$$(2.67)$$

where

$$-\frac{\pi}{2} < \phi \equiv \tan^{-1}\Delta < \frac{\pi}{2} \qquad (2.68)$$

$H_s^{p,\Omega}$ specifies the boundary condition. The Hamiltonian, minus the surface term $H_s^{p,\Omega}$, commutes with the z-component of the total spin operator $S^z = \sum_{i=1}^N \sigma_i^z$. The most general boundary conditions are

$$\sigma_{N+1}^{\pm 1} = pe^{\pm i\Omega}\sigma_1^{\pm 1}$$
$$\sigma_{N+1}^0 = p\sigma_1^0 \qquad (2.69)$$

where $0 \leq \Omega < 2\pi$ and $p = 0, 1$. The angle Ω denotes a rotation of the spin operator σ_{N+1} with respect to σ_1 around the z-axis. Using these boundary conditions, the surface term $H_s^{p,\Omega}$ in (2.68) becomes

$$H_N^{p,\Omega} =$$

$$-\frac{p}{\cos\phi}(e^{i(\phi-\Omega)}\sigma_N^{+1}\sigma_1^{-1} + e^{-i(\phi-\Omega)}\sigma_N^{-1}\sigma_{+1}^1 + \delta\cos\phi\sigma_N^0\sigma_1^0)$$

$$(2.70)$$

One now makes the canonical transformations

$$\sigma_j^{\pm 1} \to \sigma_j^{\pm 1}e^{\pm i(2j-3)\phi/2}$$
$$\sigma_j^0 \to \sigma_j^0 \qquad (2.71)$$

The Hamiltonian (2.68) becomes

$$H_N^{DM}(\Delta, \delta) = \frac{1}{\cos\phi}H_N^{XXZ}(\delta\cos\phi) \qquad (2.72)$$

where

$$H_N^{XXZ}(\delta\cos\phi) = -\sum_{i=1}^N(\sigma_i^{+1}\sigma_{i+1}^{-1} + \sigma_i^{-1}\sigma_{i+1}^1 + \delta\cos\phi\sigma_i^0\sigma_{i+1}^0)$$

$$-p(e^{i(N\phi-\Omega)}\sigma_N^{+1}\sigma_1^{-1} + e^{-i(N\phi-\Omega)}\sigma_N^{-1}\sigma_{+1}^1 + \delta\cos\phi\sigma_N^0\sigma_1^0)$$

$$(2.73)$$

The Hamiltonian in (2.74) is the quantum XXZ Hamiltonian with anisotropy $\delta\cos\phi$ and boundary condition(see (2.70))

$$\sigma_{N+1}^{\pm 1} = pe^{\pm i(N\phi-\Omega)}\sigma_1^{\pm 1}$$
$$\sigma_{N+1}^0 = p\sigma_1^0 \qquad (2.74)$$

The effect of the DM interaction is to change the anisotrpy constant δ, of the XXZ Hamiltonian, to $\delta\cos\phi = \frac{\delta}{\sqrt{1+\Delta^2}}$ and the boundary conditions $\Omega \to \Omega - N\phi$. With changed boundary conditions, the model is still BA solvable. Also, the new boundary conditions imply modified momentum variables which is seen in our calculations.

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2.7 Dzyaloshinskii-Moriya Interaction in the S=1 Chain

In general, the Bethe Ansatz method has been applied to obtain exact solutions for the ground state energy and the low lying excitation spectrum of one dimensional quantum spin systems. In the Bethe Ansatz method, the S-matrix is the most important quantity which is related to the phase shift in the scattering process between two particles. A model is exactly solvable or integrable, when the many body S-matrix is factorizable as a product of two-body S-matrices and the latter satisfy the Yang-Baxter [17, 18] equation. The ground state properties of the quantum spin chains are of much current interest. However, most of the models are non-integrable and information about the ground state properties is obtained through numerical and approximate analytical techniques. Sato [16] has applied the Bethe Ansatz method to non-integrable systems like spin-S quantum spin chains and has shown that in some cases a model may be partially integrable. This implies that the model contains integrable subspaces. For certain parameter regions, the ground state belongs to an integrable subspace and so the ground state properties can be calculated exactly using the Bethe Ansatz. The exact low-lying states are also obtained in this way. In short, Sato has shown that exact calculation using the Bethe Ansatz is possible even for non-integrable systems. We first outline Sato's method and then apply it to calculate the ground and excited state energies of a non-integrable $S = 1$ chain with DM interaction.

We consider a spin-1 quantum spin chain which can be interpreted as a special case of a n-component quantum lattice gas ($n = S + 1$). At each site of the chain an object with $S^z = m(m = 1, 0, -1)$ is placed. Each object can be considered to have a 'color', specified by the value of S^z. Let N_m be the number of objects with $S^z = m$. We assume that the number N_m is conserved. The bilinear-biquadratic Hamiltonian with DM interaction term, which is studied in the thesis, is

$$
\begin{aligned}
H &= \sum_{i=1}^{L} [\mathbf{S_i} \cdot \mathbf{S_{i+1}} + J_1(\mathbf{S_i} \cdot \mathbf{S_{i+1}})^2 + J_2(\mathbf{S_i} \times \mathbf{S_{i+1}}) \cdot \hat{z} \\
&\quad + J_3[(\mathbf{S_i} \times \mathbf{S_{i+1}}) \cdot \hat{z}]^2 + J_4(s_i^z)^2 + C]
\end{aligned}
\tag{2.75}
$$

In terms of the spin- raising and lowering operators, the above Hamiltonian can be written as

$$
\begin{aligned}
H &= [\sum_{i=1}^{L} s_i^z s_{i+1}^z + J_1(s_i^z)^2(s_{i+1}^z)^2 + J_4(s_i^z)^2 + C \\
&\quad + \frac{1}{2}(s_i^+ s_{i+1}^- + s_i^- s_{i+1}^+) + \frac{iJ_2}{2}(s_i^+ s_{i+1}^- - s_i^- s_{i+1}^+) \\
&\quad + \frac{J_1}{2}(s_i^z s_{i+1}^z(s_i^+ s_{i+1}^- + s_i^- s_{i+1}^+)) \\
&\quad + \frac{J_1}{2}((s_i^+ s_{i+1}^- + s_i^- s_{i+1}^+)s_i^z s_{i+1}^z)
\end{aligned}
$$

$$+ \frac{J_1 + J_3}{2}(s_i^+ s_{i+1}^- s_i^- s_{i+1}^+ + s_i^- s_{i+1}^+ s_i^+ s_{i+1}^-)$$

$$+ \frac{J_1 - J_3}{2}[(s_i^+)^2(s_{i+1}^-)^2 + (s_i^-)^2(s_{i+1}^+)^2] \qquad (2.76)$$

Sato has considered a spin-S quantum spin chain, the Hamiltonian of which can be written as

$$H = \sum_{i=1}^{L} h_{i,i+1} \qquad (2.77)$$

where

$$h_{i,i+1} = const. + \sum_{a \neq b = -s}^{s} f(b,a)e_{ab}^i e_{ba}^{i+1} + \sum_{r=-s}^{s} C(r)e_{rr}^i e_{rr}^{i+1}$$

$$+ \sum_{a,b=-s}^{s} g(a,b)e_{aa}^i e_{bb}^{i+1} \qquad (2.78)$$

In Eq.(2.79), L is the length of a chain and the parameter $f(a,b)$, $c(r)$ and $g(a,b)$ denote the matrix elements of the Hamiltonian. The constant term can be adjusted so that the ground state energy of the system is zero. The operator e_{ab}^i acting on site i corresponds to the $(2s + 1) \times (2s + 1)$ matrix whose (c,d) element is $\delta_{ac}\delta_{bd}$.

2.8 Some General Results

The exact two-body matrix is obtained by solving the eigenvalue problem

$$E|\psi> = H|\psi> \qquad (2.79)$$

We consider the fully polarised ferromagnetic state $| + s, +s, +s, \ldots\ldots + s, +s >$ as the vacuum $|0>$ and characterize an object with $s^z = a(a \neq s)$ as a particle 'a'. First, we solve the one-body problem. From Eq. (2.80) with

$$|\psi> = \sum_{m=1}^{L} \psi^a(m)| + s, +s, +s, \ldots\underset{m}{a}\ldots + s, +s >, a = -s, -s+1\ldots..s - 1, \qquad (2.80)$$

we obtain

$$E^a \psi^a(m) = [g(s,a) + g(a,s)]\psi^a(m) + f(a,s)\psi^a(m - 1) + f(s,a)\psi^a(m + 1) \qquad (2.81)$$

Eq.(2.82) has the solution

$$\psi^a(m) = const. \, e^{ikm} \qquad (2.82)$$

and

$$E^a = g(s,a) + g(a,s) + f(s,a)e^{ik} + f(a,s)e^{-ik} \qquad (2.83)$$

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Next we solve the two-body problem. The eigenfunction has the form

$$|\psi> = \sum_{m_1 < m_2}^{L} \Psi(m_1, m_2) | + s, +s, +s, ..., \underset{m_1}{a} + s..., \underset{m_2}{a} ..., +s, +s > \qquad (2.84)$$

where $a, b = -s, -s + 1, ..., s - 1$. This denotes a superposition of states in which particles 'a' and 'b' are located at the sites m_1 and m_2 respectively $(m_1 < m_2)$. The rest of the sites are occupied by the '+s' objects. We now consider two possibilities:

(i) m_1 and m_2 are not NN sites i.e., $(m_2 \neq m_1 + 1)$

(ii) $m_2 = m_1 + 1$, i.e., m_1 and m_2 are nearest neighbour sites

For case(i), we have,

$$
\begin{aligned}
E^{ab}\psi^{ab}(m_1, m_2) &= [g(s, a) + g(a, s) + g(s, b) + g(b, s)]\psi^{ab}(m_1, m_2) \\
&+ f(a, s)\psi^{ab}(m_1 - 1, m_2) + f(s, a)\psi^{ab}(m_1 + 1, m_2) \\
&+ f(b, s)\psi^{ab}(m_1, m_2 - 1) \\
&+ f(s, b)\psi^{ab}(m_1, m_2 + 1).
\end{aligned} \qquad (2.85)
$$

For case(ii), we get for $a \neq b$,

$$
\begin{aligned}
E^{ab}\psi^{ab}(m_1, m_1 + 1) &= [g(s, a) + g(a, b) + g(b, s)]\psi^{ab}(m_1, m_1 + 1) \\
&+ f(a, s)\psi^{ab}(m_1 - 1, m_1 + 1) + f(b, a)\psi^{ab}(m_1 + 1, m_1) \\
&+ f(s, b)\psi^{ab}(m_1, m_1 + 2),
\end{aligned} \qquad (2.86)
$$

and for $a = b$

$$
\begin{aligned}
E^{aa}\psi^{aa}(m_1, m_1 + 1) &= [g(s, a) + g(a, s)]\psi^{aa}(m_1, m_1 + 1) \\
&+ f(s, a)\psi^{aa}(m_1, m_1 + 2) + f(a, s)\psi^{aa}(m_1 - 1, m_1 + 1) \\
&+ c(a)\psi^{aa}(m_1, m_1 + 1).
\end{aligned} \qquad (2.87)
$$

The general solution of the Eq. (2.86) is

$$
\begin{aligned}
\psi^{ab}(m_1, m_2) &= \alpha e^{i(pm_1 + qm_2)} + \beta e^{i(qm_1 + pm_2)} \\
E^{ab} &= E^a + E^b
\end{aligned} \qquad (2.88)
$$

The solution can also be written in a general form as

$$\psi^{a_1 a_2}(m_1, m_2) = \sum_P A^{a_{Q1}, a_{Q2}}(PQ)e^{i(P_{P1} + P_{P2})} \qquad (2.89)$$

where $p = \{P1, P2\}$, $q = \{Q1, Q2\}$ are the permutations of the indices 1 and 2, denoting the momenta and coordinates of the particles. The summation is over all permutations. We now demand that Eq. (2.90) is also a solution of the eigenvalue equation for the case $m_2 = m_1 + 1$. This is true if the amplitudes $A^{ab}(pq)$'s satisfy the following equations

$$A^{ab}(q, p) = \sum_{a', b' = -s}^{s-1} S_{ab}^{a'b'} A^{a'b'}(p, q) \qquad (2.90)$$

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where the nonvanishing matrix elements of the S-matrix are

$$S^{aa}_{aa}(q,p) =$$

$$-\frac{f(a,s) + [g(s,a) + g(a,s) - c(a)]e^{iq} + f(s,a)e^{i(p+q)}}{f(a,s) + [g(s,a) + g(a,s) - c(a)]e^{ip} + f(s,a)e^{i(p+q)}}$$

$$(2.91)$$

$$S^{ab}_{ab}(q,p) =$$

$$-\frac{f(a,s) + [g(a,s) + g(s,b) - g(a,b)]e^{iq} - f(a,b)e^{ip} + f(s,a)e^{i(p+q)}}{f(a,s) + [g(a,s) + g(s,b) - g(a,b)]e^{ip} - f(b,a)e^{ip} + f(s,a)e^{i(p+q)}}$$

$$(2.92)$$

$$S^{ab}_{ba}(q,p) =$$

$$-\frac{f(b,a)(e^{ip} - e^{iq})}{f(a,s) + [g(a,s) + g(s,b) - g(a,b)]e^{ip} - f(a,b)e^{ip} + f(s,a)e^{i(p+q)}}$$

$$(2.93)$$

The S-matrix of the integrable spin-$\frac{1}{2}$ anisotropic Heisenberg model

$$H = -\sum_{i=1}^{L}(S^x_i S^x_{i+1} + S^y_i S^y_{i+1} + \Delta S^z_i S^z_{i+1}) \qquad (2.94)$$

is written as

$$S(q,p) = -\frac{1 - 2\Delta e^{iq} + e^{i(p+q)}}{1 - 2\Delta e^{ip} + e^{i(p+q)}} \qquad (2.95)$$

We note that the S-matrix element $S^{aa}_{aa}(q,p)$ in Eq. (2.92) is of the same form as in Eq. (2.96). This fact is crucial and allows for exact calculations in the case of non-integrable systems.

In general, we cannot exactly solve the l-body problem if $l > 2$. However, the above comparison shows that in the subspace, where $N_m = 0$, except for $m = s$ and a, the eigenvalue problem is just that of the exactly solvable spin-$\frac{1}{2}$ anisotropic Heisenberg chain. Hence, in this subspace, exact calculations are possible and the total energy of the l-body system is equal to the sum of one-particle energies.

In this integrable subspace, each object has one of two colors ($S^z = s$ or a). We shall refer to the subspace as a two-colour sector. In the case of the spin-S system, regarding the state '+s' as the background, there are 2s two-colour sectors ('s − 1' sector, 's − 2' sector,........,'−s' sector). In each of these sectors, we identify an 'a' particle with $S^z = a$ ($a \neq s$) as a 'down spin' in the spin-$\frac{1}{2}$ anisotropic Heisenberg chain. We now apply Sato's method to the Hamiltonian (2.76). The Hamiltonian describes a spin-1 system with bilinear and biquadratic interactions between nearest neighbour spins. The Hamiltonian also includes DM interaction terms of similar nature. The vacuum of the above Hamiltonian is given by

$$|\phi> = |1\,1\,1\,1,........,1\rangle,$$

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with a $S^z = +1$ spin at each site. The energy of the vacuum state is

$$E_0 = N(1 + J_1 + J_4 + C) \tag{2.96}$$

If we demand that $E_0 = 0$, then

$$C = -(1 + J_1 + J_4) \tag{2.97}$$

We now consider two cases in which the excitations are in the '0-sector' or in the '1-sector'.

'0'-sector:

The first excited state is given as

$$\psi = \sum_{m=1}^{L} \psi^0(m)|1\,1\,1\,1\ldots,\underset{m}{0}\ldots\ldots,1,> \tag{2.98}$$

The eigenvalue equation is given by

$$
\begin{aligned}
E^0\psi^0(i) \quad &= [N_2 + J_1(N-2) + J_4(N-1) + CN]\psi^0(i) \\
&\quad +2(J_1 + J_3)\psi^0(i) + (1 - iJ_2)\psi^0(i+1) + (1 + iJ_2)\psi^0(i-1) \\
&= [-2 - J_4 + 2J_3]\psi^0(i) + (1 + iJ_2)\psi^0(i+1) + (1 - iJ_2)\psi^0(i-1)
\end{aligned}
\tag{2.99}
$$

Comparing with Eq. (2.81), one gets

$$
\begin{aligned}
[g(1,0) + g(0,1)] &= -2 - J_4 + 2J_3 \\
f(1,0) &= (1 - iJ_2) \\
f(0,1) &= (1 + iJ_2)
\end{aligned}
\tag{2.100}
$$

With the choice

$$\psi^0(m) = const.e^{ikm} \tag{2.101}$$

we have the excited state energy as

$$E^0 = -(2 + J_4 - 2J_3) + 2\cos k + 2J_2 \sin k \tag{2.102}$$

The state with two excitations is described by the wave function

$$|\psi^{00}\rangle = \sum_{m_1 < m_2 = 1}^{L} \psi^{00}(m_1, m_2)|1,1,1,\ldots\ldots,\underset{m_1}{0}\ldots,\underset{m_2}{0}\ldots,11 > \tag{2.103}$$

The general solution for $\psi^{00}(m_1, m_2)$ is

$$\psi^{00}(m_1, m_2) = \alpha e^{i(m_1 p + m_2 q)} + \beta e^{i(m_2 p + m_1 q)} \tag{2.104}$$

For $m_2 \neq m_1 + 1$,

$$
\begin{aligned}
E^{00}\psi^{00}(m_1, m_2) &= -4(1 - J_3 + \frac{J_4}{2})\psi(m_1, m_2) \\
&\quad + (1 - iJ_2)[\psi^{00}(m_1 + 1, m_2) + \psi^{00}(m_1, m_2 + 1)] \\
&\quad + (1 + iJ_2)[\psi^{00}(m_1 - 1, m_2) + \psi^{00}(m_1, m_2 - 1)]
\end{aligned}
\tag{2.105}
$$

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For $m_2 = m_1 + 1$,

$$E^{00}\psi^{00}(m_1, m_1 + 1) =$$
$$[N - 3 + J_1(N - 3) + J_4(N - 2) + cN + 2(J_1 + J_3)]\psi^{00}(m_1, m_1 + 1)$$
$$+ \quad (1 - iJ_2)\psi^{00}(m_1, m_1 + 2) + (1 + iJ_2)\psi^{00}(m_1 - 1, m_1 + 1)$$

$$(2.106)$$

Again comparing with equation (2.87) of Sato's general formalism,

$$g(1, 0) + g(0, 1) + C(0, 0) = -3 - 3J_1 - 2J_4 + 2(J_1 + J_3) \qquad (2.107)$$

or, from (2.100)

$$C(0, 0) = -(1 + J_1 + J_4) \qquad (2.108)$$

Proceeding exactly as in Sato's formalism, the two body scattering matrix is determined as

$$S^{00}_{00} = -\frac{1 - 2\Delta e^{iq'} + e^{i(p'+q')}}{1 - 2\Delta e^{ip'} + e^{i(p'+q')}} \qquad (2.109)$$

where

$$\Delta = -\frac{J_1 + 2J_3 - 1}{2}\cos\theta, \quad \cdots$$
$$p' = p - \theta,$$
$$q' = q - \theta,$$
$$\theta = \tan^{-1}J_2. \qquad (2.110)$$

The excited state energy is

$$E^{00} = 2E^0$$
$$= -2(2 + J_4 - 2J_3) + 2(\cos p + \cos q) + 2J_2(\sin p + \sin q) \qquad (2.111)$$

from Eq.(2.102). With $J_2 = \tan\theta$,

$$E^{00} = -2(2 + J_4 - 2J_3)$$
$$+ \sec\theta(\cos\theta\cos p + \cos\theta\cos q + \sin\theta\sin p + \sin\theta\sin q)$$
$$= -2(2 + J_4 - 2J_3) + 2\sec\theta(\cos p' + \cos q') \qquad (2.112)$$

'−1'-sector

The eigenvalue equation for ψ^{-1} is

$$E^{-1}\psi^{-1}(i) = (-4 + 2(J_1 + J_3))\psi^{-1}(i)$$
$$(J_1 - J_3)\psi^{-1}(i + 1) + (J_1 - J_3)\psi^{-1}(i - 1) \qquad (2.113)$$

Comparing with Eq. (2.81), we get

$$g(1, -1) + g(-1, 1) = -4 + 2(J_1 + J_3) \qquad (2.114)$$

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and

$$f(-1,1) = f(1,-1) = J_1 - J_3 \qquad (2.115)$$

With the choice,

$$v^{-1}(m) = const.\ e^{ikm} \qquad (2.116)$$

the eigenvalue E^{-1} is given by

$$E^{-1} = -4 + 2(J_1 + J_3) + 2(J_1 - J_3)\cos k \qquad (2.117)$$

The eigenfunction for the excited state with two excitations is given by

$$\psi^{-1-1} = \sum_{m_1 < m_2} \psi^{-1-1}(m_1, m_2)|111.., \underset{m_1}{-1} ..., 11.., \underset{m_2}{-1} ..., 1> \qquad (2.118)$$

Proceeding as in the case of the '0'-sector, the two body S-matrix is given by

$$S_{-1-1}^{-1-1}(q,p) = -\frac{1 - 2\Delta e^{iq} + e^{i(p+q)}}{1 - 2\Delta e^{ip} + e^{i(p+q)}} \qquad (2.119)$$

where

$$\Delta = \frac{2 - (J_1 + J_3)}{J_1 - J_3} \qquad (2.120)$$

There is no redefinition of the momentum variables when the S-matrix is compared with that of the XXZ chain. Also,

$$C(-1,-1) = 0 \qquad (2.121)$$

The energy is given by

$$E^{-1,-1} = 2(J_1 - J_3)(-2\Delta + \cos p + \cos q) \qquad (2.122)$$

In both the '0' and '-1' sectors, one makes use of the 'reduced' Bethe Ansatz, to obtain the transcendal equations for $\{p_j\}$;

$$e^{ip_j L} = -\prod_{i}^{M} S_{aa}^{aa}(p_i, p_j), \quad a = 0, 1. \qquad (2.123)$$

This equation is identical in form to that in the case of the $S = 1/2$ anisotropic Heisenberg chain [18]. We take the logarithm of (2.122) to obtain the coupled algebraic equations

$$Lp_j = 2\pi I_j - i\sum_{i=1}^{M} lnS_{aa}^{aa}(p_i, p - j), \qquad 1 \le M \qquad (2.124)$$

The equations determine the momenta p_j. The I_j's are integers or half-odd integers depending on whether M is odd or even respectively and are given by

$$I_1, I_2, ..., I_M = \left(-\frac{M-1}{2}\right), \left(-\frac{M-1}{2}+1\right), ..., \left(\frac{M-1}{2}\right) \qquad (2.125)$$

Using the solutions of (2.125), the total energy of each sector is given by the sum of the one-particle energies. For example, in the ' − 1'-sector, the total energy is

$$E = \sum_{j=1}^{M} E(p_j) = (J_1 - J_3) \sum_{j=1}^{M} 2(-\Delta + \cos p_j). \tag{2.126}$$

(Eq.(2.122) is the expression for the energy E for $M = 2$.)

One can compare the reduced Bethe Ansatz calculations (Eqs.(2.124) and (2.126)) with the results of the exact diagonalization of finite systems. In a certain parameter regime of the Hamiltonian, the ground state energy is given by that in the '−1'-sector. This again is identical to twice the ground state energy of the $S = 1/2$ XXZ chain with the anisotropic parameter Δ (after the factor $(J_1 - J_3)$ in Eq.(2.126) is absorbed in the energy E). For the ground state, $M = L/2$ and from the known Bethe Ansatz result for the ground state energy of the $S = 1/2$ XXZ chain in the thermodynamic limit [18], the ground state energy of the spin-1 model under consideration is

$$E_g = \frac{\Delta}{2} - \sinh \lambda \left(1 + 4 \sum_{n=1}^{\infty} \frac{1}{1 + e^{2n\lambda}} \right), \tag{2.127}$$

where $\Delta = \cosh \lambda$. Table 2.1 compares the exact diagonalization results for $L = 12$ with the ground state energies obtained from Eq.(2.127) for various values of the anisotropy parameter Δ (Eq.(2.121)).

Table 2.1

Δ	$E_g(Eq.(2.127))$	Exact diagonalization(L=12)
4	−2.1230	−2.1239
5	−2.5990	−2.5993
6	−3.0827	−3.0828
7	−3.5711	−3.5711
8	−4.0623	−4.0622

In the parameter regime under consideration, the lowest excited state also belongs to the '−1'-sector. The spectrum can be obtained in the same manner as that for the XXZ chain, with appropriate modification of the I_j's in (2.124). The anisotropy parameter Δ has to be large (>3.5) in order that the equivalence with the XXZ chain holds true.

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