

Structure and relevant dimension of the Heisenberg model and applications to spin rings

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Abstract

For the diagonalization of the Hamilton matrix in the Heisenberg model relevant dimensions are determined depending on the applicable symmetries. Results are presented, both, by general formulae in closed form and by the respective numbers for a variety of special systems. In the case of cyclic symmetry, diagonalizations for Heisenberg spin rings are performed with the use of so-called magnon states. Analytically solvable cases of small spin rings are singled out and evaluated.

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1 Introduction and summary

As far as their magnetic behaviour is concerned, some recently synthesized molecules like “ferric wheels” of six, eight or ten iron ions of spin $\frac{5}{2}$ [1–4] appear as a limited array of localized single-particle spins which are adequately described by the Heisenberg model [5–8]. The calculation of key quantities like for example the spin-spin correlation function becomes easy once the Heisenberg Hamiltonian has been diagonalized. For a straight forward diagonalization the dimension d of the Hilbert space \mathcal{H} , which for instance is $d = (2s+1)^N$ for N spins with spin quantum number s , may, however, appear prohibitively large even for rather small systems. But the obvious symmetries allow to reduce the problem to a set of less ample problems according to a decomposition of \mathcal{H} into a set of mutually orthogonal subspaces.

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In the case of spin arrays the following symmetry operators may be employed, depending on the degree of symmetry exhibited by the system, i.e. the Hamilton operator under consideration:

- the 3-component of the total spin in the case of axial symmetry,
- the total spin in the case of full rotational symmetry,
- the cyclic shift operator for rings of identical single spins with translationally invariant coupling,
- further discrete symmetries like reflection of the spin ring, reflection of the spin orientation and reflection of time order.

Group theoretical arguments are already used to calculate the spectra of some molecules by means of an irreducible tensor operator approach [6,9]. In the present article an alternative technique is devised. Also, general expressions for the relevant dimension are derived without taking recourse to any specific procedure of diagonalization.

We will generalize considerations by D. Kouzoudis [10,11] who found analytical solutions for special cases of small Heisenberg rings. To this end we are concentrating on the first three symmetries and denote the corresponding simultaneous eigenspaces by $\mathcal{H}(S, M, p)$. After introducing our notation in Sec. 2, we will investigate the various symmetries and their corresponding subspaces in Sec. 3. The dimension of the $\mathcal{H}(S, M, p)$ can be calculated exactly and we derive an explicit formula for the dimension of the subspaces $\mathcal{H}(S, M)$ and $\mathcal{H}(S, M, p)$, which enables the evaluation of the relevant dimension d_r . In Sec. 4 we provide recursion formulae to calculate the Hamilton matrix restricted to the subspaces $\mathcal{H}(S, M, p)$. To this end tools from solid state physics, namely l -magnon states, are utilized [12–14]. Section 5 is devoted to examples and applications. For rings of $N = 5, s = 1$ and $N = 8, s = \frac{1}{2}$ an exact diagonalization of the Heisenberg Hamiltonian with nearest neighbour interaction has been performed using Mathematica[®] [15]. Further we compare the analytical anti-ferromagnetic ground state energies for $N = 2 \dots 8$ with the asymptotic Bethe-Hulthén formula for $N \rightarrow \infty$ [16,17].

2 Heisenberg model

The most general Hamilton operator considered in these investigations consists of a spin-spin interaction term \tilde{H}_0 and a term \tilde{H}_F describing the interaction with an external field which is assumed to point in the 3-direction

$$\tilde{H} = \tilde{H}_0 + \tilde{H}_F = - \sum_{x,y}^N J(x, y) \vec{\xi}(x) \cdot \vec{\xi}(y) - \sum_x^N \mu B \xi^3(x). \quad (1)$$

$x, y \in G = \{1, \dots, N\}$ label the spin sites modulo N and the upper right index denotes the spin component. All spins are defined to be dimensionless vector observables with the commutation relations

$$[\tilde{s}^a(x), \tilde{s}^b(y)] = i \epsilon_{abc} \tilde{s}^c(x) \delta_{xy} . \quad (2)$$

The eigenvalue of $(\tilde{s}^3(x))^2$ is $s(x)(s(x)+1)$, $s(x)$ being the individually fixed quantum number at site x . The possible eigenvalues of any $\tilde{s}^3(x)$ are the magnetic quantum numbers m_x . One may introduce the ladder operators

$$\tilde{s}^\pm(x) = \tilde{s}^1(x) \pm i \tilde{s}^2(x) \quad (3)$$

to reformulate \tilde{H}_0 as

$$\tilde{H}_0 = - \sum_{x,y \in G} J(x,y) \left\{ \tilde{s}^3(x) \tilde{s}^3(y) + \frac{1}{2} [\tilde{s}^+(x) \tilde{s}^-(y) + \tilde{s}^-(x) \tilde{s}^+(y)] \right\} . \quad (4)$$

The total Hilbert space is spanned by the product basis of the single-particle eigenstates of all $\tilde{s}^3(x)$

$$\tilde{s}^3(x) |m_1, \dots, m_x, \dots, m_N\rangle = m_x |m_1, \dots, m_x, \dots, m_N\rangle , \quad (5)$$

which will be a reference basis in our investigations.

3 Symmetry operations and relevant dimensions

Our most general Hamiltonian (1) allows only for invariance with respect to rotations about the 3-axis. Obviously, \tilde{H}_0 as well as \tilde{H}_F commute with the 3-component \tilde{S}^3 of the total spin

$$[\tilde{H}, \tilde{S}^3] = 0 , \quad \tilde{S}^3 = \sum_{x \in G} \tilde{s}^3(x) , \quad (6)$$

the possible eigenvalues of which are the total magnetic quantum numbers

$$M = -S_{\max}, -S_{\max} + 1, \dots, S_{\max} \quad \text{with} \quad S_{\max} = \sum_{x=1}^N s(x) \quad (7)$$

being the maximum total spin quantum number. The total Hilbert space \mathcal{H} for the Heisenberg model is the direct sum of all eigenspaces $\mathcal{H}(M)$ of \tilde{S}^3

$$\mathcal{H} = \bigoplus_{M=-S_{\max}}^{+S_{\max}} \mathcal{H}(M). \quad (8)$$

The problem of diagonalizing \tilde{H} in \mathcal{H} is thus broken up into the corresponding problems in each of the $\mathcal{H}(M)$. This reduces the dimension one has to cope with from

$$d = \dim(\mathcal{H}) = \prod_{x=1}^N (2s(x) + 1) \quad (9)$$

to the respective $\dim(\mathcal{H}(M))$. The relevant dimension d_r then is the maximum of those dimensions, if no other symmetries can be exploited. For given values of M , N and of all $s(x)$ the dimension $\dim(\mathcal{H}(M))$ can be determined as the number of product states (5), which constitute a basis in $\mathcal{H}(M)$, with $\sum_{x \in G} m_x = M$. The solution of this combinatorial problem can be given in closed form.

Theorem:

$$\dim(\mathcal{H}(M)) = \frac{1}{(S_{\max} - M)!} \left[\left(\frac{d}{dz} \right)^{S_{\max} - M} \prod_{x=1}^N \frac{1 - z^{2s(x)+1}}{1 - z} \right]_{z=0}. \quad (10)$$

For equal single-spin quantum numbers $s(1) = \dots = s(N) = s$, and thus a maximum total spin quantum number of $S_{\max} = Ns$, Eq. (10) simplifies to

$$\dim(\mathcal{H}(M)) = f(N, 2s + 1, S_{\max} - M) \quad \text{with} \quad (11)$$

$$f(N, \mu, \nu) = \sum_{n=0}^{[\nu/\mu]} (-1)^n \binom{N}{n} \binom{N - 1 + \nu - n\mu}{N - 1}. \quad (12)$$

In both formulae (10) and (11), M may be replaced by $|M|$ since the dimension of $\mathcal{H}(M)$ equals those of $\mathcal{H}(-M)$. $[\nu/\mu]$ in the sum symbolizes the greatest integer less or equal to ν/μ . Eq. (11) is known as a result of de Moivre [18].

Proof: The proof of (10) and (11) may be accomplished by comparing any product state (5) with the completely aligned state

$$|\Omega\rangle = |m_1 = s(1), m_2 = s(2), \dots, m_N = s(N)\rangle, \quad (13)$$

which is also called magnon vacuum state, see next section. Evidently it is also an eigenstate of \tilde{H} and in the ferromagnetic case a ground state of \tilde{H}_0 . Using the possible decrements $a(x) = s(x) - m_x$ of the magnetic quantum number at each spin site we want to construct a generating function $F(z)$ of the numbers $\dim(\mathcal{H}(M))$ as a polynomial in z

$$F(z) = \sum_{n=0}^{2S_{\max}} \dim(\mathcal{H}(S_{\max} - n)) z^n. \quad (14)$$

The consideration, that the number of product states with fixed magnetic quantum number M corresponds to the related number of sequences of decrements, leads to the following definition

$$F(z) = \prod_{x=1}^N \left(\sum_{a(x)=0}^{2s(x)} z^{a(x)} \right) = \prod_{x=1}^N \frac{1 - z^{2s(x)+1}}{1 - z}. \quad (15)$$

Eq. (10) is then obvious and (11) is easily inferred from (10) by using Leibniz's theorem [19] to calculate multiple derivatives of the product $(1 - z^{2s+1})^N \cdot (1 - z)^{-N}$.

■

In the special case of identical single-particle spins, \tilde{H}_F is proportional to \tilde{S}^3 and therefore commutes with \tilde{H}_0 . The simultaneous eigenstates of \tilde{H}_0 and \tilde{S}^3 are then also eigenstates of \tilde{H}_F . \tilde{H}_F causes a splitting proportional to M of the eigenvalues of \tilde{H}_0 , which otherwise would not depend on M .

In what follows, consideration is alternatively restricted to one of two special cases. In the first case (I) the Hamilton operator is field free, $\tilde{H} = \tilde{H}_0$, and thus invariant under any rotation. In the second case (II) all individual spins are identical.

The total spin quantum number will be denoted by S . It has values in the set $\{0 \leq S_{\min}, S_{\min} + 1, \dots, S_{\max}\}$ and \tilde{S}^2 has eigenvalues $S(S + 1)$. The simultaneous eigenspaces $\mathcal{H}(S, M)$ of \tilde{S}^2 and \tilde{S}^3 are spanned by eigenvectors of \tilde{H} . The one-dimensional subspace $\mathcal{H}(M = S_{\max}) = \mathcal{H}(S_{\max}, S_{\max})$, especially, is spanned by $|\Omega\rangle$. The total ladder operators are

$$\tilde{S}^{\pm} = \tilde{S}^1 \pm i \tilde{S}^2. \quad (16)$$

For $S > M$, \tilde{S}^- maps any normalized \tilde{H} -eigenstate $\in \mathcal{H}(S, M + 1)$ onto an \tilde{H} -eigenstate $\in \mathcal{H}(S, M)$ with norm $\sqrt{S(S + 1) - M(M + 1)}$.

Lemma: For $0 \leq M < S_{\max}$, $\mathcal{H}(M)$ can be decomposed into orthogonal subspaces

$$\mathcal{H}(M) = \mathcal{H}(M, M) \oplus \tilde{S}^- \mathcal{H}(M + 1) \quad (17)$$

with

$$\tilde{S}^- \mathcal{H}(M + 1) = \bigoplus_{S \geq M+1} \mathcal{H}(S, M). \quad (18)$$

Proof: The $\mathcal{H}(S, M)$ represent an orthogonal decomposition of $\mathcal{H}(M)$. It is therefore sufficient to identify the orthogonal complement of $\tilde{\mathcal{S}}^- \mathcal{H}(M+1)$ within $\mathcal{H}(M)$ as $\mathcal{H}(M, M)$. This, in turn, is clear if any $|\psi\rangle \neq 0 \in \mathcal{H}(M)$ with $|\psi\rangle \perp \tilde{\mathcal{S}}^- \mathcal{H}(M+1)$ vanishes on application of $\tilde{\mathcal{S}}^+$. The defining property of all such $|\psi\rangle$ is

$$\langle \psi | \tilde{\mathcal{S}}^- | \phi \rangle = 0 \quad \forall |\phi\rangle \in \mathcal{H}(M+1). \quad (19)$$

But then $\tilde{\mathcal{S}}^+ |\psi\rangle \in \mathcal{H}(M+1)$ and $\langle \tilde{\mathcal{S}}^+ \psi | \phi \rangle = 0$ which proves $\tilde{\mathcal{S}}^+ |\psi\rangle = 0$. ■

In consequence, the diagonalization of \tilde{H} in \mathcal{H} has now been traced back to diagonalization in the subspaces $\mathcal{H}(S, S)$, the dimension of which are for $S < S_{\max}$

$$\dim(\mathcal{H}(S, S)) = \dim(\mathcal{H}(M=S)) - \dim(\mathcal{H}(M=S+1)) \quad (20)$$

and can be calculated according to Eq. (10) in case (I) or Eq. (11) in case (II). The relevant dimension d_r is the maximum of the numbers given by Eq. (20).

For many of the systems of interest here, the individual spin quantum numbers are equal, the coupling coefficients J have the special property $J(x, y) = J(|x-y|)$ and the applied magnetic field is homogeneous. This renders the Hamiltonian invariant with respect to translations on the group $G = \{1, \dots, N\}$ of spin sites. Any such translation is represented by the cyclic shift operator \tilde{T} or a multiple repetition. \tilde{T} is defined by its action on the product basis (5)

$$\tilde{T} |m_1, \dots, m_{N-1}, m_N\rangle = |m_N, m_1, \dots, m_{N-1}\rangle. \quad (21)$$

The eigenvalues of \tilde{T} are the N -th roots of unity, $z = \exp\{-ip\}$, where p will be called magnon momentum and can take the following N values modulo 2π from

$$\hat{G} = \left\{ p \mid p = \frac{2\pi k}{N}, k = 0, \dots, N-1 \right\}, \quad (22)$$

where k will be called translational quantum number. Clearly, \tilde{T} commutes now with both Hamiltonian and total spin. Any $\mathcal{H}(S, M)$ is decomposed into simultaneous eigenspaces $\mathcal{H}(S, M, p)$ of $\tilde{\mathcal{S}}^2$, $\tilde{\mathcal{S}}^3$ and \tilde{T} , and diagonalization can be reduced to a diagonalization in the subspaces $\mathcal{H}(S, S, p)$. The according reduction of the relevant dimension can be quantified if the values of p and their degeneracy within $\mathcal{H}(S, S)$ are known. As a rule of thumb one finds a tendency for equal degeneracy and thus

$$d_r \approx \frac{1}{N} \max_S \dim(\mathcal{H}(S, S)). \quad (23)$$

It is, however, possible to determine d_r exactly for any N and s . To this end we introduce the notations of cycles, proper cycles and epicycles. A special decomposition of \mathcal{H} into orthogonal subspaces can be achieved by starting with the product basis (5) and considering the equivalence relation

$$|\psi\rangle \cong |\phi\rangle \Leftrightarrow |\psi\rangle = \tilde{T}^n |\phi\rangle, \quad n \in \{1, 2, \dots, N\} \quad (24)$$

for any pair of states belonging to the product basis. The equivalence relation then induces a complete decomposition of the basis into disjoint subsets, i.e. the equivalence classes. A “cycle” is defined as the linear span of such an equivalence class of basis vectors. The obviously orthogonal decomposition of \mathcal{H} into cycles is compatible with the decomposition of \mathcal{H} into the various $\mathcal{H}(M)$ but not, generally, with the decomposition of $\mathcal{H}(M)$ into its subspaces $\mathcal{H}(S, M)$. Evidently, the dimension of a cycle can never exceed N . Cycles are called “proper cycles” if their dimension equals N , they are termed “epicycles” else. One of the N primary basis states of a proper cycle may arbitrarily be denoted as

$$|\psi_1\rangle = |m_1, \dots, m_x, \dots, m_N\rangle \quad (25)$$

and the remaining ones may be enumerated as

$$|\psi_{n+1}\rangle = \tilde{T}^n |\psi_1\rangle, \quad n = 1, 2, \dots, N - 1. \quad (26)$$

The cycle under consideration is likewise spanned by the states

$$|\chi_k\rangle = \frac{1}{\sqrt{N}} \sum_{\nu=0}^{N-1} \left(e^{i\frac{2\pi k}{N}} \tilde{T} \right)^\nu |\psi_1\rangle \quad (27)$$

which are eigenstates of \tilde{T} with the respective magnon momentum $p(k) = 2\pi k/N$. Consequently, every k (every $p(k)$) occurs once in a proper cycle.

The reader will easily verify the validity of the following related statements:

- An epicycle of dimension D is spanned by D eigenstates of \tilde{T} with each of the translational quantum numbers $k = 0, N/D, \dots, (D-1)N/D$ occurring exactly once.
- For a primary product state in an epicycle of dimension D , the spin sites are grouped into D “subrings”, each subring having a constant magnetic decrement $s - m_x =: a$ on all of its places. The subring forms a pattern which repeats itself on a cyclic shift of D steps. The total number of spin sites in a subring is N/D .
- Therefore, for $M < S_{\max}$, $\mathcal{H}(M)$ contains a cycle (epi or proper) of dimension D if and only if D is a divisor of N , including $D = 1$ and $D = N$, and $D(S_{\max} - M)/N$ is an integer. The set of such allowed D will be denoted as $C(N, s, M)$.

Let $\mathcal{K}_M(D)$ be the linear span of all cycles of dimension D occurring within $\mathcal{H}(M)$ and let $k_s(N, M, D)$ denote its dimension. According to the above remarks we have

$$\begin{aligned} \dim(\mathcal{H}(M)) &= \sum_{D \in C(N, s, M)} k_s(N, M, D) \\ &= k_s(N, M, N) + \sum_{D \in C(N, s, M); D \neq N} k_s(N, M, D). \end{aligned} \quad (28)$$

Because to each epicycle of dimension D there corresponds exactly one proper cycle with D spin sites and total magnetic quantum number MD/N , and vice versa, (28) may be rewritten as

$$\dim(\mathcal{H}(M)) = k_s(N, M, N) + \sum_{D \in C(N, s, M)} k_s\left(D, \frac{MD}{N}, D\right), \quad (29)$$

which, together with (11), may be used as a recursion relation for the function $k_s(N, M, N)$ and hence also for $k_s(N, M, D)$. This recursion relation can be transformed into an explicit formula which reads

$$k_s(N, M, N) = \sum_{D \in C(N, s, M)} q\left(\frac{N}{D}\right) f\left(D, 2s + 1, \frac{D(S_{\max} - M)}{N}\right) \quad (30)$$

where f is taken over from Eq. (12) and

$$q(\nu) = \begin{cases} (-1)^m & \text{if } \nu \text{ is a product of } m \text{ different primes,} \\ 0 & \text{else.} \end{cases} \quad (31)$$

The proof rests on some elementary combinatorics and will be omitted here. Further we have for the simultaneous eigenspaces $\mathcal{H}(\cdot, M, p(k))$ of \mathcal{S}^3 and \mathcal{T}

$$\dim(\mathcal{H}(\cdot, M, p(k))) = \sum_{\substack{u=1 \\ u|N; u|k}}^N k_s\left(N, M, \frac{N}{u}\right) \frac{u}{N} \quad (32)$$

and

$$\dim(\mathcal{H}(S, M, p)) = \dim(\mathcal{H}(\cdot, S, p)) - \dim(\mathcal{H}(\cdot, S + 1, p)) \quad (33)$$

for $0 \leq S < S_{\max}$ and $|M| \leq S$. This allows the explicit calculation of the relevant dimensions for any given N and s , for examples see table 2.

4 Diagonalization of the Hamiltonian in the magnon basis representation

In this section we consider the Hamiltonian (1) with $J(x, y) = J(|x - y|)$, $B = 0$ and equal single spin quantum numbers

$$\underline{H} = - \sum_{x, y \in G} J(|x - y|) \underline{\vec{s}}(x) \cdot \underline{\vec{s}}(y), \quad \forall x \in G : s(x) = s. \quad (34)$$

In order to calculate the matrix elements of this Hamiltonian restricted to subspaces $\mathcal{H}(S, M, p)$ it is recommendable to use a basis of vectors which are already adapted to the problem. We found it most convenient to work with a basis constructed from so-called magnon states, used for example in [14]. These magnon states should not be confused with those defined by Holstein and Primakoff [13]. The pertinent definitions are the following.

For any function f of spin sites $x \in G$ the discrete Fourier transform is as usual defined by

$$f_p := \frac{1}{\sqrt{N}} \sum_{x \in G} e^{ipx} f(x), \quad p \in \hat{G}. \quad (35)$$

The analogous transformation may be applied to linear operators $\underline{A}(x)$, where $\underline{A}(x)$ for instance may be a single-particle spin component at site x

$$\underline{S}_p^j := \frac{1}{\sqrt{N}} \sum_{x \in G} e^{ipx} \underline{s}^j(x) \quad (36)$$

or a ladder operator (3), which yields

$$\underline{S}_p^\pm = \underline{S}_p^1 \pm i \underline{S}_p^2. \quad (37)$$

Then the Hamiltonian (34) can be written in terms of the \underline{S}_p^\pm and \underline{S}_p^3 as (see [14])

$$\begin{aligned} \underline{H} &= -\sqrt{N} \sum_{p \in \hat{G}} J_p \underline{\vec{S}}_p^* \cdot \underline{\vec{S}}_p \\ &= - \sum_{p \in \hat{G}} \tilde{J}_p \left(\underline{S}_{-p}^+ \underline{S}_p^- + \underline{S}_{-p}^3 \underline{S}_p^3 \right), \quad \tilde{J}_p := \sqrt{N} J_p = \sum_{x \in G} e^{ipx} J(x). \end{aligned} \quad (38)$$

It is straight forward to obtain the following commutation relations

$$[\mathcal{S}_p^+, \mathcal{S}_q^+] = [\mathcal{S}_p^-, \mathcal{S}_q^-] = 0, \quad (39)$$

$$[\mathcal{S}_p^+, \mathcal{S}_q^-] = \frac{2}{\sqrt{N}} \mathcal{S}_{p+q}^3, \quad [\mathcal{S}_p^3, \mathcal{S}_q^\pm] = \pm \frac{1}{\sqrt{N}} \mathcal{S}_{p+q}^\pm \quad (40)$$

from the corresponding commutation relations of the spin operators at site x .

We define “ l -magnon states” with momenta p_1, \dots, p_l as

$$|\Omega_{\vec{p}}\rangle = |\Omega_{p_1, \dots, p_l}\rangle := \mathcal{S}_{p_1}^- \mathcal{S}_{p_2}^- \cdots \mathcal{S}_{p_l}^- |\Omega\rangle \quad (41)$$

for $p_\nu \in \hat{G}$, $\nu = 1, \dots, l$ and $l = 0, \dots, 2Ns$, $|\Omega\rangle$ being the magnon vacuum state as given in Eq. (13). For $l > 2Ns$ $|\Omega_{\vec{p}}\rangle$ will be the zero vector. Since the $\mathcal{S}_{p_\nu}^-$ commute, a unique representation of (41) may be achieved by postulating $p_1 \leq p_2 \leq \dots \leq p_l$.

One-magnon states $|\Omega_p\rangle$ are orthogonal

$$\langle \Omega_p | \Omega_q \rangle = 2s \delta_{p,q}, \quad (42)$$

which follows from (40) and

$$\mathcal{S}_p^3 |\Omega\rangle = \sqrt{N} s \delta_{p,0} |\Omega\rangle. \quad (43)$$

Moreover, the one-magnon states are already eigenvectors of \tilde{H} and \tilde{T}

$$\tilde{H} |\Omega_p\rangle = E_p |\Omega_p\rangle, \quad E_p = 2s \tilde{J}_p + s(Ns - 2) \tilde{J}_0, \quad (44)$$

$$\tilde{T} |\Omega_p\rangle = e^{-ip} |\Omega_p\rangle. \quad (45)$$

The last relation may be derived from

$$\tilde{T}^x \mathcal{S}_p^\pm = e^{-ipx} \mathcal{S}_p^\pm \tilde{T}^x \quad \forall x \in G, \forall p \in \hat{G}. \quad (46)$$

For $l > 1$ the l -magnon states are in general no longer orthogonal or linearly independent. But they span the total Hilbert space \mathcal{H} and they behave nicely with respect to the ladder operator \mathcal{S}^- , namely

$$\mathcal{S}^- |\Omega_{p_1, \dots, p_l}\rangle = \sqrt{N} |\Omega_{0, p_1, \dots, p_l}\rangle, \quad (47)$$

and they span the subspaces $\mathcal{H}(M, p)$, which follows from

$$\tilde{T} |\Omega_{p_1, \dots, p_l}\rangle = \exp \left\{ -i \sum_{\nu=1}^l p_\nu \right\} |\Omega_{p_1, \dots, p_l}\rangle \quad (48)$$

$$\tilde{\mathcal{L}}_0^3 |\Omega_{p_1, \dots, p_l}\rangle = (Ns - l) |\Omega_{p_1, \dots, p_l}\rangle. \quad (49)$$

Let the magnon states $|\Omega_{\vec{p}}\rangle$ be ordered as follows

$$\begin{aligned} & |\Omega\rangle \\ & |\Omega_0\rangle, |\Omega_1\rangle, \dots, |\Omega_{N-1}\rangle \\ & |\Omega_{00}\rangle, |\Omega_{11}\rangle, \dots, |\Omega_{N-1, N-1}\rangle \\ & \vdots \end{aligned} \quad (50)$$

where each row is ordered lexicographically. We will call the basis of \mathcal{H} generated by applying the well-known Gram-Schmidt orthonormalization procedure to the sequence (50) “magnon basis”. Note that the Gram-Schmidt procedure will sometimes produce zero vectors, because the $|\Omega_{\vec{p}}\rangle$ are linearly dependent. The main result of this section is then the following proposition.

Proposition: The magnon basis contains a subspace for each subspace $\mathcal{H}(S, M, p)$, $S = Ns, Ns - 1, \dots, |M|$; $p \in \hat{G}$.

Proof: Since the $|\Omega_{\vec{p}}\rangle$ span the subspaces $\mathcal{H}(M, p)$ and different $\mathcal{H}(M, p)$ are orthogonal, the magnon basis spans $\mathcal{H}(M, p)$, too. The subspace with maximal $S = Ns$ is spanned by the magnon states

$$|\Omega\rangle, |\Omega_0\rangle, |\Omega_{00}\rangle, \dots, |\Omega_{(2Ns)\text{zeros}}\rangle, \quad (51)$$

which also occur in the magnon basis up to normalization. These vectors also span the one-dimensional spaces $\mathcal{H}(S, M, p)$ with $S = Ns$; $M = -S, \dots, S$; $p = 0$. Hence the proposition holds for $S = Ns$. We then may proceed by induction. Under the assumption that the proposition holds for all $S > S_0$, we have to show that it holds for $S = S_0$. Consider the subspaces $\mathcal{H}(M)$ with $M = S_0$. According to (18) we have

$$\mathcal{H}(S_0) = \tilde{\mathcal{L}}^- \mathcal{H}(S_0 + 1) \oplus \mathcal{H}(S_0, S_0). \quad (52)$$

Hence $\mathcal{H}(S_0, S_0)$ is spanned by vectors from the magnon basis and the same holds for every $\mathcal{H}(S_0, S_0, p)$, $p \in \hat{G}$. For the other subspaces $\mathcal{H}(S_0, M, p)$, $M < S_0$, we have

$$\mathcal{H}(S_0, M, p) = \left(\tilde{\mathcal{L}}^- \right)^{S_0 - M} \mathcal{H}(S_0, S_0, p) \quad (53)$$

and we know that the restrictions

$$\mathcal{S}^- : \mathcal{H}(M+1) \longrightarrow \mathcal{H}(M), \quad M \geq 0, \quad (54)$$

are isometries up to a factor $\sqrt{S(S+1) - M(M+1)}$. Hence \mathcal{S}^- maps vectors from the magnon basis onto vectors from the magnon basis (up to a factor), which concludes the proof. \blacksquare

We are left with two tasks. First, in order to calculate the magnon basis, we need a formula for the inner product between magnon states. We have no explicit formula, but using the commutation relations (39) and (40) we derived a recursion relation, which is sufficient for computer algebraic calculations. Similarly, we can express the matrix elements of the Hamiltonian between two magnon states by finite sums containing only inner products of magnon states, which completes the second task. The results are

$$\begin{aligned} \langle \Omega_{p_1, \dots, p_l} | \Omega_{q_1, \dots, q_l} \rangle &= 2s \sum_{\nu=1}^l \delta_{q_\nu, p_1} \langle \Omega_{p_2, \dots, p_l} | \Omega_{q_1, \dots, \check{q}_\nu, \dots, q_l} \rangle \\ &\quad - \frac{2}{N} \sum_{1 \leq \nu < \mu \leq l} \langle \Omega_{p_2, \dots, p_l} | \Omega_{q_1, \dots, \check{q}_\nu, \dots, (q_\mu \mapsto (q_\mu + q_\nu - p_1)), \dots, q_l} \rangle, \end{aligned} \quad (55)$$

where the symbol \check{q}_ν denotes deletion of the index q_ν and $(q_\mu \mapsto (q_\mu + q_\nu - p_1))$ denotes replacement of the index q_μ by the given expression which has to be understood modulo N . Further

$$\begin{aligned} &\langle \Omega_{p_1, \dots, p_l} | \tilde{H} | \Omega_{q_1, \dots, q_l} \rangle \quad (56) \\ &= \sum_{p \in \hat{G}} \tilde{J}_p \langle \Omega_{p, p_1, \dots, p_l} | \Omega_{p, q_1, \dots, q_l} \rangle + \tilde{J}_0 \langle \Omega_{p_1, \dots, p_l} | \Omega_{q_1, \dots, q_l} \rangle \left(s^2 N - 2sl + \frac{l^2}{N} \right) \\ &\quad + \sum_{p \in \hat{G}, p \neq 0} \tilde{J}_p \frac{1}{N} \sum_{\nu, \mu=1}^l \langle \Omega_{p_1, \dots, (q_\nu \mapsto (q_\nu + p)), \dots, p_l} | \Omega_{q_1, \dots, (q_\mu \mapsto (q_\mu + p)), \dots, q_l} \rangle. \end{aligned}$$

Now we have all what is required in order to write a program [15] which reduces the diagonalization of \tilde{H} to the diagonalization of the submatrices of \tilde{H} with respect to the magnon basis of the relevant subspaces $\mathcal{H}(S, M, p)$. The final diagonalization can be done numerically or in the few cases, where the relevant dimension is less or equal 4, analytically. Table 2 shows in bold face for which cases analytical solution will be possible. Two examples for eigenvalues and multiplicities are given in the next section. The complete routine, which also presents the eigenvectors, may be downloaded from the internet [15]. It may be possible to exactly solve other cases if the discrete symmetries mentioned in the introduction are taken into account. The cases $N = 2, 3, 4$ can, in principle, also be solved by Clebsch-Gordan decomposition of the Hilbert space.

| | k | | | | | |
|-------|-------|-------|-----|-------|-----|-------|
| | 0 | 1 | 2 | 3 | 4 | 5 |
| S | 3 1 0 | 2 1 0 | 2 1 | 2 1 0 | 2 1 | 2 1 0 |
| 3 | 1 | | | | | |
| 2 | 1 | 1 | 1 | 1 | 1 | 1 |
| 1 | 1 2 | 1 1 | 1 2 | 1 1 | 1 2 | 1 1 |
| M 0 | 1 2 1 | 1 1 1 | 1 2 | 1 1 2 | 1 2 | 1 1 1 |
| -1 | 1 2 | 1 1 | 1 2 | 1 1 | 1 2 | 1 1 |
| -2 | 1 | 1 | 1 | 1 | 1 | 1 |
| -3 | 1 | | | | | |

Table 1

Dimensions of the subspaces $\mathcal{H}(S, M, p(k))$ for $N = 6$, $s = \frac{1}{2}$. Each column can be created by applying the ladder operator (16) yielding $(2S+1)$ -dimensional subspaces. One realizes a discrete symmetry between columns for k and $6 - k$.

5 Examples

5.1 Relevant dimension of spin rings

In order to illustrate the above considerations let us discuss the example $N = 6$, $s = \frac{1}{2}$, which has been solved by D. Kouzoudis [11]. The decomposition (8) yields the following relation between the dimensions of the involved Hilbert spaces

$$\dim(\mathcal{H}) = 2^6 = 1 + 6 + 15 + 20 + 15 + 6 + 1 = \sum_{M=-S_{\max}}^{S_{\max}} \dim(\mathcal{H}(M)) \quad .(57)$$

Obviously, $|\Omega\rangle = |+++++\rangle$ spans the one-dimensional space $\mathcal{H}(M)$ with $M = S_{\max} = Ns = 3$, which is an epicycle of dimension $D = 1$. $\mathcal{H}(M = 2)$ consists of the proper cycle generated e.g. by $| - + + + + \rangle$ and hence is six-dimensional. It is spanned by the six eigenstates of \tilde{T} and \tilde{H} given in Eq. (27), which are one-magnon states. The next space $\mathcal{H}(M = 1)$ consists of two proper cycles generated e.g. by $| - - + + + \rangle$ and $| - + - + + \rangle$, respectively, and one three-dimensional epicycle generated by $| - + + - + \rangle$. Hence $\dim(\mathcal{H}(M = 1)) = 6 + 6 + 3 = 15$. Note that the last mentioned epicycle corresponds to the proper cycle generated by $| - + + \rangle$ with $N = 3$, $M = \frac{1}{2}$. The largest space $\mathcal{H}(M = 0)$ is spanned by three proper cycles generated by $| - - + - + \rangle$, $| + + - + - \rangle$, $| + + + - - \rangle$ and one two-dimensional epicycle generated by $| + - + - + \rangle$.

| | | N | | | | | | | | |
|---|---------------|----------|----------|----------|----------|----------|----------|----------|-------|--------|
| | | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| s | $\frac{1}{2}$ | 1 | 2 | 3 | 5 | 9 | 14 | 28 | 48 | 90 |
| | $\frac{1}{2}$ | 1 | 1 | 1 | 1 | 2 | 2 | 4 | 6 | 10 |
| | 1 | 1 | 3 | 6 | 15 | 40 | 105 | 280 | 750 | 2025 |
| | 1 | 1 | 1 | 2 | 3 | 8 | 15 | 37 | 84 | 207 |
| | $\frac{3}{2}$ | 1 | 4 | 11 | 36 | 120 | 426 | 1505 | 5300 | 19425 |
| | $\frac{3}{2}$ | 1 | 2 | 4 | 8 | 23 | 61 | 192 | 590 | 1956 |
| | 2 | 1 | 5 | 17 | 70 | 295 | 1260 | 5620 | 25200 | 113706 |
| | 2 | 1 | 2 | 5 | 14 | 53 | 180 | 712 | 2800 | 11403 |
| | $\frac{5}{2}$ | 1 | 6 | 24 | 120 | 609 | 3150 | 16576 | 88900 | 484155 |
| | $\frac{5}{2}$ | 1 | 2 | 7 | 24 | 105 | 450 | 2085 | 9884 | 48483 |

Table 2

Relevant dimension assuming only invariance with respect to rotations (upper rows) and assuming also invariance with respect to cyclic shifts (lower rows).

Consequently, $\dim(\mathcal{H}(M=0)) = 6 + 6 + 6 + 2 = 20$. The remaining spaces $\mathcal{H}(M)$ with $M < 0$ have the same cycle structure as $\mathcal{H}(|M|)$ due to the symmetry $+ \leftrightarrow -$.

The dimensions of the subspaces $\mathcal{H}(S, M, p(k))$ are given in table 1. Note that in accordance with the rule of thumb (23) the numbers $\dim(\mathcal{H}(\cdot, M, p))$ are almost uniformly distributed with respect to p . The deviations from the uniform distribution for $|M| = 0, 1$ can be explained by the extra eigenvalues of \tilde{T} produced by the mentioned epicycles of dimensions three and two.

The next table 2 shows the relevant dimensions for a wide variety of N and s . The ratio of upper-row to lower-row entries is roughly N in accordance with the rule of thumb, Eq. (23). Dimensions less than five are given in bold, these cases can be solved analytically. Two examples are presented in the next subsection.

5.2 Exactly solvable systems

Analytical solutions are for instance possible in the cases $N = 5, s = 1$ and $N = 8, s = \frac{1}{2}$, which to our knowledge have not yet been published. Table 3 contains the exact eigenvalues and multiplicities for the Heisenberg Hamiltonian Eq. (34) with nearest neighbour interaction and $N = 5, s = 1$ and Fig. 1 shows the same

| | | | | | | | | | |
|--------|--|------------------|--------------------------------|--|---|--------------------|--------------------|------------------|-------------------|
| E/J | -10 | -4 | 2 | $2 \pm 2\sqrt{2}$ | 4 | $4 \pm 2\sqrt{11}$ | $5 \pm 2\sqrt{65}$ | $5 \pm \sqrt{5}$ | $-5 \pm \sqrt{5}$ |
| deg(E) | 11 | 7 | 12 | 15 | 3 | 3 | 1 | 2 | 18 |
| E/J | $-3 \pm \sqrt{5}$ | $1 \pm \sqrt{5}$ | $2 \pm \sqrt{5} \pm \sqrt{13}$ | $\frac{2}{3} (6 \pm [\sqrt{5} + 2\sqrt{23} \cos(\alpha)])$ | | | | | |
| deg(E) | 14 | 14 | 10 | 6 | | | | | |
| E/J | $\frac{2}{3} (6 \pm [\sqrt{5} - \sqrt{23} \cos(\alpha)] \pm \sqrt{69} \sin(\alpha))$ | | | | | | | | |
| deg(E) | 6 | | | | | | | | |

Table 3

Eigenvalues and degeneracies for the Heisenberg Hamiltonian Eq. (34) with nearest neighbour interaction and $N = 5, s = 1$. The value of α is $\alpha = \frac{1}{3} \arctan \left[\sqrt[3]{\frac{1338}{5}}/5 \right]$

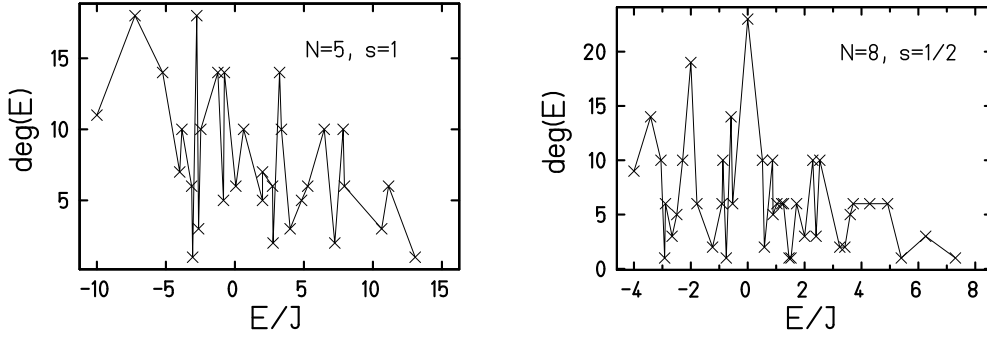


Fig. 1. Eigenvalues and degeneracies for the Heisenberg Hamiltonian Eq. (34) with $N = 5, s = 1$ (l.h.s.) and $N = 8, s = \frac{1}{2}$ (r.h.s.). The lines are drawn as a guide for the eye.

information graphically, but also for $N = 8, s = \frac{1}{2}$. The analytical, but rather lengthy expressions for the latter case may be evaluated using a Mathematica[®] script we provide [15]. Here we would like to present only the eigenvalue which in the antiferromagnetic case corresponds to the ground state energy

$$E_0/J = \frac{4}{3} \left\{ 2 + \sqrt{13} \cos \left[\frac{1}{3} \arctan \left(\frac{3\sqrt{3}}{5} \right) \right] \right\} \text{ for } N = 8, s = \frac{1}{2}. \quad (58)$$

In order to clarify the structure of the energy spectrum we calculate the smoothed density of states. To this end the degeneracy of an energy eigenvalue E_n is first divided by the mean distance to the neighbouring eigenvalues, then the resulting function is linearly interpolated and convoluted with a characteristic function of width 1. This density of states $\rho(E)$, which is displayed for the Heisenberg Hamiltonian Eq. (34) in Fig. 2 for $N = 5, s = 1$ (l.h.s.) and $N = 8, s = \frac{1}{2}$ (r.h.s.), shows an interesting band structure.

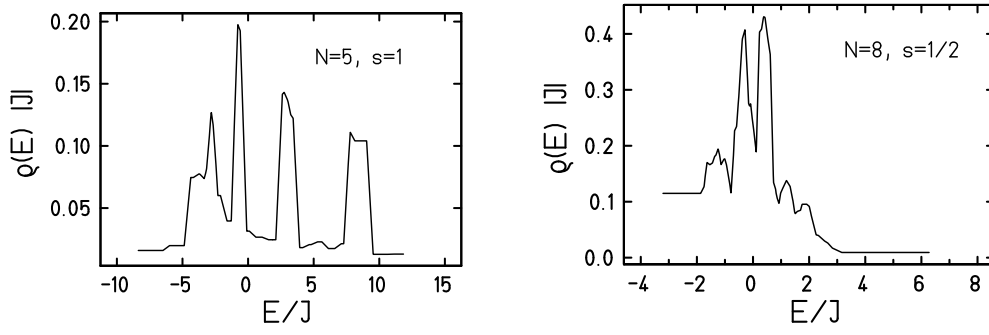


Fig. 2. Smoothed density of states $\rho(E)$ for the Heisenberg hamiltonian Eq. (34) with $N = 5, s = 1$ (l.h.s.) and $N = 8, s = \frac{1}{2}$ (r.h.s.).

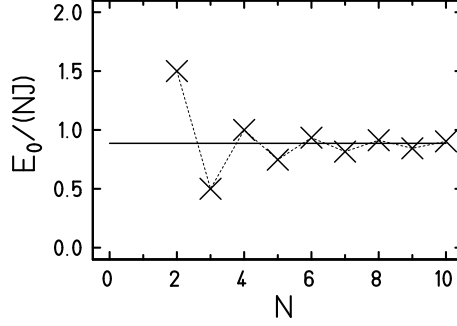


Fig. 3. Comparison of analytical ($N \leq 8$) and numerical ($N > 8$) ground state energies (symbols) for antiferromagnetic coupling with the large N limit (solid line) of Bethe and Hulthén [16,17].

5.3 Bethe-Hulthén

The calculated eigenvalues, Table 3 and Figure 1, correspond to the ferromagnetic case for $J > 0$ and to the antiferromagnetic case for $J < 0$. Thus our data also contain the antiferromagnetic ground state energy $E_0(N)$ and we can compare $E_0(N)/(NJ)$ with the exact limit

$$\lim_{N \rightarrow \infty} \frac{E_0(N)}{NJ} = 2 \ln(2) - \frac{1}{2} \quad (59)$$

known as the Bethe-Hulthén formula [12,16,17]. In Fig. 3 analytical ($N \leq 8$) and numerical ($N > 8$) ground state energies are displayed by symbols and the large N limit by a solid line. It turns out that the limit is approached from above for even N and from below for odd N and that the approach is faster for even values of N . This shows the effect of spin frustration.

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