Eigenvalues of spin arrays

Alessandro Vindigni

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Array of spins 1/2 coupled via Heisenberg exchange interaction

We consider the Hamiltonian

$$\mathcal{H}_{\text{exch}} = -J \sum_{i=1}^{N} \hat{\mathbf{s}}_i \cdot \hat{\mathbf{s}}_{i+1} \qquad (1)$$

for $s_i = 1/2$, with both **open** and **periodic** boundary conditions. We will express eigenvalues in units of the exchange coupling J (assumed to be positive). In the next tables you will find some sets of **irreducible representations** (IRs) of the SO(3) rotation group, associated with the possible values of total spin and built coupling progressively *intermediate* angular momenta, namely pairing angular momenta as $\hat{\mathbf{S}}_{12} = \hat{\mathbf{s}}_1 + \hat{\mathbf{s}}_2$, $\hat{\mathbf{S}}_{34} = \hat{\mathbf{s}}_3 + \hat{\mathbf{s}}_4$ and so on. Different tables correspond to increasing number of spins in the array (N). The dimensionality of each IR is given in the column **dim**.

Assign the eigenvalues shown below each table to the corresponding IRs and copy them in the proper cell of each table. There are cases in which you can derive an analytic expression for the eigenvalues and thus establish a one-to-one correspondence between the IRs and the eigenstates of the Hamiltonian computed numerically. In other cases this will not be easily feasible. Follow the suggestions case by case in order that you do not engage in lengthy calculations (but alternative approaches are welcome and encouraged).

After having completed the assignment (**even partially!**), try to express with your own words the relationship between IRs of the total spin of the system and the degeneracy of eigenvalues of the spin Hamiltonian (1). If needed, we encourage you to look for external sources to reflect on this relationship (e.g., see the book chapter "CourseLibrary/BookChapters/White_Ch2.pdf" at p. 46 and following).

N = 3 spins 1/2

Open boundary conditions

The spin Hamiltonian is in this case

$$\mathcal{H}_{\text{exch}} = -J\left(\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 + \hat{\mathbf{s}}_2 \cdot \hat{\mathbf{s}}_3\right) = -J\left(\hat{\mathbf{s}}_1 + \hat{\mathbf{s}}_3\right) \cdot \hat{\mathbf{s}}_2 = -J\hat{\mathbf{S}}_{13} \cdot \hat{\mathbf{s}}_2$$

Hint: To determine the eigenvalues analytically, rewrite the scalar product above using the well-known relation

$$\hat{\mathbf{s}}_{13} \cdot \hat{\mathbf{s}}_2 = \frac{1}{2}\left(\hat{\mathbf{S}}^2_{123} - \hat{\mathbf{s}}^2_{13} - \hat{\mathbf{s}}^2_2\right)$$

and express it in terms of the square of the total spin $\hat{\mathbf{S}}^2_{123}$ and the square of the *intermediate* spin $\hat{\mathbf{S}}^2_{13}$.

Answer

$$\mathcal{H}_{\text{exch}}|S_2, S_{13}M_{123}\rangle = -J\hat{\mathbf{S}}_{13}\cdot\hat{\mathbf{S}}_2|S_2, S_{13}M_{123}\rangle = \\ -\frac{J}{2}[S_{123}(S_{123}+1) - S_{13}(S_{13}+1) - s_2(s_2+1)]\,|S_2, S_{13}M_{123}\rangle$$

S_{13}	S_{123}	**dim**	**eigenvalue [J]**
0	1/2	2	0
1	1/2	2	1
1	3/2	4	-1/2

```
number_spins=3
python3 ../05-week/array_spin_eigenvalues.py $number_spins True
```

```
## eigenvalue   degeneracy
## -0.50000     4
## 0.00000      2
## 1.00000      2
##
## Hilbert space dim =      8
```

Periodic boundary conditions

The spin Hamiltonian is in this case

$$\mathcal{H}_{\text{exch}} = -J\left(\hat{\mathbf{s}}_1\cdot\hat{\mathbf{s}}_2 + \hat{\mathbf{s}}_2\cdot\hat{\mathbf{s}}_3 + \hat{\mathbf{s}}_3\cdot\hat{\mathbf{s}}_1\right)$$

Hint: With respect to the previous case, just the coupling between the first and the third spin has been added; this operator can be expressed on the same basis $|S_{13}, s_2, S_{123}\rangle$ by means of the relation

$$\hat{\mathbf{s}}_1\cdot\hat{\mathbf{s}}_3 = \frac{1}{2}\left(\hat{\mathbf{S}}_{13}^2 - \hat{\mathbf{s}}_1^2 - \hat{\mathbf{s}}_3^2\right)\ ,$$

which brings an additional term to the eigenvalues computed before.

Answer

$$\mathcal{H}_{\text{exch}}|S_2, S_{13}M_{123}\rangle = -J\hat{\mathbf{S}}_{13}\cdot\hat{\mathbf{S}}_2|S_2, S_{13}M_{123}\rangle - J\hat{\mathbf{s}}_1\cdot\hat{\mathbf{s}}_3|S_2, S_{13}M_{123}\rangle = \\ -\frac{J}{2}[S_{123}(S_{123}+1) - s_1(s_1+1) - s_2(s_2+1) - s_3(s_3+1)]\,|S_2, S_{13}M_{123}\rangle \\ -\frac{J}{2}\left[S_{123}(S_{123}+1) - \frac{9}{4}\right]|S_2, S_{13}M_{123}\rangle$$

S_{13}	S_{123}	**dim**	**eigenvalue [J]**

S_{13}	S_{123}	dim	eigenvalue [J]
0	1/2	2	3/4
1	1/2	2	3/4
1	3/2	4	-3/4

```
number_spins=3
python3 ../05-week/array_spin_eigenvalues.py $number_spins
```

```
##  eigenvalue   degeneracy
##  -0.75000     4
##  0.75000      4
##
##  Hilbert space dim =      8
```

N = 4 spins 1/2

Periodic boundary conditions

The spin Hamiltonian is in this case

$$\mathcal{H}_{\text{exch}} = -J\left(\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 + \hat{\mathbf{s}}_2 \cdot \hat{\mathbf{s}}_3 + \hat{\mathbf{s}}_3 \cdot \hat{\mathbf{s}}_4 + \hat{\mathbf{s}}_4 \cdot \hat{\mathbf{s}}_1\right) \, .$$

Compute its eigenvalues on the basis $|S_{24}, S_{13}, S_{1234}, M_{1234}\rangle$ and copy the values in the table below.

Hint: To determine the eigenvalues analytically, consider the operator

$$\hat{\mathbf{S}}_{13} \cdot \hat{\mathbf{S}}_{24}$$

Answer

$$\mathcal{H}_{\text{exch}}|S_{24}, S_{13}, S_{1234}, M_{1234}\rangle = -J\hat{\mathbf{S}}_{13} \cdot \hat{\mathbf{S}}_{24}|S_{24}, S_{13}, S_{1234}, M_{1234}\rangle =$$
$$-\frac{J}{2}\left[S_{1234}\left(S_{1234}+1\right) - S_{24}\left(S_{24}+1\right) - S_{13}\left(S_{13}+1\right)\right]|S_{24}, S_{13}, S_{1234}, M_{1234}\rangle$$

S_{13}	S_{24}	S_{1234}	dim	eigenvalue [J]
0	0	0	1	0
1	0	1	3	0
0	1	1	3	0
1	1	0	1	2
1	1	1	3	1
1	1	2	5	-1

```
number_spins=4
python3 ../05-week/array_spin_eigenvalues.py $number_spins
```

```
##  eigenvalue   degeneracy
##  -1.00000     5
##  -0.00000     7
##  1.00000      3
##  2.00000      1
##
##  Hilbert space dim =      16
```

Question What would be the ground state for $J < 0$? Which physical state does that IR represents?

Answer

It represents the Néel state in which the spins of sublattices at even sites take their maximal value; the intermediate spins $\hat{\mathbf{S}}_{13}$ *and* $\cdot\hat{\mathbf{S}}_{24}$ *obtained coupling spins with sitting at odd and even sites are paired antiferromagnetically.*

Open boundary conditions

With respect to the previous case, the interaction between the first and the last spin is removed and the Hamiltonian reads

$$\mathcal{H}_{\text{exch}} = -J\left(\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2 + \hat{\mathbf{s}}_2 \cdot \hat{\mathbf{s}}_3 + \hat{\mathbf{s}}_3 \cdot \hat{\mathbf{s}}_4\right) \qquad (2)$$

One possibility to determine the eigenvalues analytically is to diagonalize simulataneously $\mathcal{H}_{\text{exch}}$ for periodic boundary condition and the operator

$$\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_4$$

then subtract the contribution of the latter from the eigenvalues obtained for the array with periodic boundary conditions. This is **not an easy task** in general because there are several *intermediate coupling schemes*

$$\begin{gathered} |S_{24}, S_{13}, S_{1234}, M_{1234}\rangle \\ |S_{12}, S_{34}, S_{1234}, M_{1234}\rangle \\ |S_{14}, S_{23}, S_{1234}, M_{1234}\rangle \\ \cdots \end{gathered}$$

that obviously produce the same set of values for the total spin S_{1234}. In particular, the operator $\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_4$ would be diagonal on the basis set $|S_{14}, S_{23}, S_{1234}, M_{1234}\rangle$ but it is **not diagonal** on the basis $|S_{24}, S_{13}, S_{1234}, M_{1234}\rangle$.
However, that operator is diagonal on the multiplet with maximal spin $S_{1234} = 2$. Thanks to the properties of IRs, it suffices to compute the matrix element

$$\langle S_{24}, S_{13}, S_{1234}, M_{1234}|\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_4|S_{24}, S_{13}, S_{1234}, M_{1234}\rangle$$

on **one state** of the multiplet with $S_{1234} = 2$, to deduce the 5-fold degenerate eigenvalue of the Hamiltonian (2). Compute this eigenvalue analytically and write it down in the proper cell of the underlying table.

Hint: Use the fact that

$$\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_4 | ++++\rangle = \hat{s}_1^z \hat{s}_4^z | ++++\rangle \tag{3}$$

Answer

The contribution to add to the energy obtained for periodic boundary conditions is

$$J\hat{s}_1^z \hat{s}_4^z | ++++\rangle = \frac{J}{4}$$

which yields

$$\mathcal{H}_{\text{exch}} | ++++\rangle = -\frac{3}{4}J$$

S_{13}	S_{24}	S_{1234}	**dim**	**eigenvalue [J]**
0	0	0	1	?
1	0	1	3	?
0	1	1	3	?
1	1	0	1	?
1	1	1	3	?
1	1	2	5	-3/4

```
number_spins=4
python3 ../05-week/array_spin_eigenvalues.py $number_spins True
```

```
##  eigenvalue   degeneracy
##  -0.75000     5
##  -0.45711     3
##  -0.11603     1
##  0.25000      3
##  0.95711      3
##  1.61603      1
##
##  Hilbert space dim =      16
```

N = 5 spins 1/2

Open boundary conditions

The spin Hamiltonian is in this case

$$\mathcal{H}_{\text{exch}} = -J\left(\hat{\mathbf{s}}_1\cdot\hat{\mathbf{s}}_2 + \hat{\mathbf{s}}_2\cdot\hat{\mathbf{s}}_3 + \hat{\mathbf{s}}_3\cdot\hat{\mathbf{s}}_4 + \hat{\mathbf{s}}_4\cdot\hat{\mathbf{s}}_5\right) \,.$$

Using the same trick as in Eq. (3), determine the eigenvalues associated with the multiplet $S_{12345} = 5/2$ and transfer the computed value in the relative cell of the table below.

Answer

One can proceed as in the last part of the previous exercise

$$\begin{aligned}\mathcal{H}_{\text{exch}}|++++\rangle &= -J\left(\hat{\mathbf{s}}_1\cdot\hat{\mathbf{s}}_2 + \hat{\mathbf{s}}_2\cdot\hat{\mathbf{s}}_3 + \hat{\mathbf{s}}_3\cdot\hat{\mathbf{s}}_4 + \hat{\mathbf{s}}_4\cdot\hat{\mathbf{s}}_5\right)|++++\rangle \\ &= -J\left(\hat{s}_1^z\hat{s}_2^z + \hat{s}_2^z\hat{s}_3^z + \hat{s}_3^z\hat{s}_4^z + \hat{s}_4^z\hat{s}_5^z\right)|++++\rangle = -J\end{aligned}$$

S_{12}	S_{34}	S_{1234}	S_{12345}	**dim**	**eigenvalue [J]**
0	0	0	1/2	2	?
1	0	1	1/2	2	?
1	0	1	3/2	4	?
0	1	1	1/2	2	?
0	1	1	3/2	4	?
1	1	0	1/2	2	?
1	1	1	1/2	2	?
1	1	1	3/2	4	?
1	1	2	3/2	4	?
1	1	2	5/2	6	-1

```
number_spins=5
python3 ../05-week/array_spin_eigenvalues.py $number_spins True
```

```
##  eigenvalue   degeneracy
##  -1.00000     6
##  -0.80902     4
##  -0.58870     2
##  -0.30902     4
##  -0.20711     2
##  0.30902      4
##  0.66082      2
##  0.80902      4
##  1.20711      2
##  1.92789      2
##
##  Hilbert space dim =      32
```

Symmetry and eigenvalue degeneracy

How does the degeneracy of the eigenvalues computed numerically in the previous sections relates to the dimensionality of the IRs reported in all the tables?

Answer

The degeneracy of computed eigenvalues is at least equal to the dimensionality of the IRs of SO(3).

Provide an argument to justify why eigenvalues computed assuming periodic boundary conditions show generally a higher degree of **degeneracy.**

Answer

The system is more symmetric when periodic boundary conditions are assumed. In fact, also translational symmetry of lattice indeces holds in this case, besides the rotational symmetry in the spin space. Generally, a more symmetric system has a more degenerate eigenvalues spectrum. A clear example is the case of d levels (5-fold degenerate) for the free ion that split into the t_{2g} *(3-fold degenerate) and* eg *(2-fold degenerate) multiplet when the symmetry of the environment is lowered from SO(3) to* O_h.

Hint It is instructive to read the paragraph *Symmetry Representations* of the book chapter White_Ch2 (/rstudio/files/magnetismcourse/HS2021/CourseLibrary/BookChapters/White_Ch2.pdf) at p. 46 and following.