Eigenvalues of spin arrays: solution

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Rings of spins 1/2 coupled via Heisenberg exchange interaction

We consider the Hamiltonian

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

for $s_i = 1/2$, with **periodic** boundary conditions. We will express eigenvalues in units of the exchange coupling J (assumed to be positive). In a previous assignment we computed the eigenvalues expressing the Hamiltonian on a suitable basis of **irreducible representations** (IRs) of the SO(3) rotation group, that we built coupling progressively *intermediate* angular momenta (for instance 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). The dimensionality of each IR was given in the column **dim**.

In the present assignment we want to give close look at the symmetry properties of the Hamiltonian $\mathcal{H}$ and the possible basis sets on which it is simultaneously diagonal with the z component of the total spin operator and the translation operator.

N = 3 spins 1/2 with periodic boundary conditions

The spin Hamiltonian is in this case

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

and we have seen in a previous assignment that $\mathcal{H}$ is diagonal on the basis $|S_{13}, s_2, S_{123}\rangle$ with eigenvalues:

$$\mathcal{H}|S_2, S_{13}M_{123}\rangle = -\frac{J}{2}\left[S_{123}\left(S_{123}+1\right) - \frac{9}{4}\right]|S_2, S_{13}M_{123}\rangle$$

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

single-particle basis

We consider the tree operators: $\mathcal{H}$, $\hat{S}^z_{123}$, and the translation operator $\mathcal{T}$ on the *single-particle* basis:

$$\begin{array}{lll} 0 & (000) & |---\rangle \\ 1 & (001) & |--+\rangle \\ 2 & (010) & |-+-\rangle \\ 3 & (011) & |-++\rangle \\ 4 & (100) & |+--\rangle \\ 5 & (101) & |+-+\rangle \\ 6 & (110) & |++-\rangle \\ 7 & (111) & |+++\rangle \end{array}$$

The matrix elements of those 3 operators evaluated on this basis have been computed numerically and (the non-vanishing ones) have been stored in the files in the folder *matrix_el_spin_rings*. With the help of the file *helper.R* we have produced the following matrix representations:

Hamiltonian operator:

$$\mathcal{H} = \begin{bmatrix} -0.75 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.25 & -0.5 & 0 & -0.5 & 0 & 0 & 0 \\ 0 & -0.5 & 0.25 & 0 & -0.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.25 & 0 & -0.5 & -0.5 & 0 \\ 0 & -0.5 & -0.5 & 0 & 0.25 & 0 & 0 & 0 \\ 0 & 0 & 0 & -0.5 & 0 & 0.25 & -0.5 & 0 \\ 0 & 0 & 0 & -0.5 & 0 & -0.5 & 0.25 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.75 \end{bmatrix}$$

z **component of the total spin operator**:

$$\hat{S}^z_{123} = \begin{bmatrix} -1.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -0.5 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -0.5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.5 \end{bmatrix}$$

Translation operator:

$$\mathcal{T} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Question: For which states of this single-particle basis the thee operators $\mathcal{H}$, $\hat{S}^z_{123}$, and $\mathcal{T}$ are simultaneously diagonal?

Answer

The 3 operators are simultaneously diagonal on the states with maximal spin projection along z, namely $|---\rangle$ and $|+++\rangle$.

$\mathcal{H}$-eigenstates

Now we evaluate the matrix elements of the same operators but on the eigenstates of $\mathcal{H}$, say $\mathcal{H}|E,\alpha\rangle = E_\alpha|E,\alpha\rangle$

Hamiltonian operator:

$$\mathcal{H} = \begin{bmatrix} -0.75 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -0.75 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -0.75 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -0.75 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.75 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.75 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.75 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.75 \end{bmatrix}$$

z **component of the total spin operator**:

$$\hat{S}^z_{123} = \begin{bmatrix} -0.44076 & 0 & 0 & -0.23608 & 0 & 0 & 0 & 0 \\ 0 & -1.5 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.5 & 0 & 0 & 0 & 0 & 0 \\ -0.23608 & 0 & 0 & 0.44076 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.44076 & 0.00116 & -0.23607 & 0 \\ 0 & 0 & 0 & 0 & 0.00116 & 0.46124 & 1e-04 & -0.19302 \\ 0 & 0 & 0 & 0 & -0.23607 & 1e-04 & 0.44076 & -0.00095 \\ 0 & 0 & 0 & 0 & 0 & -0.19302 & -0.00095 & -0.46124 \end{bmatrix}$$

Translation operator:

$$\mathcal{T} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.5 & 0.37203 & 0.00183 & 0.78204 \\ 0 & 0 & 0 & 0 & -0.37203 & -0.5 & 0.78204 & -0.00183 \\ 0 & 0 & 0 & 0 & -0.00183 & -0.78204 & -0.5 & 0.37203 \\ 0 & 0 & 0 & 0 & -0.78204 & 0.00183 & -0.37203 & -0.5 \end{bmatrix}$$

Question: Why is $\hat{S}^z_{123}$ not diagonal on this basis?

Answer

Because the numerical routine does not diagonalize subblocks of degenerate M values but rather converges to one of the many possible representations on which $\mathcal{H}$ is diagonal.

Question: What can you say about the $\mathcal{T}$ operator expressed on this basis?

Answer

$\mathcal{T}$ is already diagonal on the subspace associated with the eigenvalue $E = -3/4$. In particular, those 4 states are invariant under translation (i.e., $\kappa = 0$, see later). In fact this is in line with the Weyl theorem: $S = 3/2$ is the multiplet with largest spin and therefore all the states belonging to it are symmetric w.r.t. the excahnge of any pair of particle. A translation is just a special sequence of exchanges between particles, $1^{st} \leftrightarrow 2^{nd}$, $1^{st} \leftrightarrow 3^{rd}$ (if you perform them in sequence).
Simultaneous eigenstates of $\mathcal{H}$ and $\hat{S}^z_{123}$ {-}

Now we evaluate the same matrix elements on simultaneous eigenstates of $\mathcal{H}$ and $\hat{S}^z_{123}$, say $\mathcal{H}|E,\alpha;M,\mu\rangle = E_\alpha|E,\alpha;M,\mu\rangle$ and $\hat{S}^z_{123}|E,\alpha;M,\mu\rangle = M_\mu|E,\alpha;M,\mu\rangle$ and

Hamiltonian operator:

$$\mathcal{H} = \begin{bmatrix} -0.75 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -0.75 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -0.75 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -0.75 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.75 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.75 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.75 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.75 \end{bmatrix}$$

z **component of the total spin operator**:

$$\hat{S}^z_{123} = \begin{bmatrix} -1.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -0.5 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -0.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.5 \end{bmatrix}$$

Translation operator:

$$\mathcal{T} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.5 & -0.86603 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.86603 & -0.5 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -0.5 & -0.86603 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.86603 & -0.5 \end{bmatrix}$$

Question: Finalize the diagonalization of the operator $\mathcal{T}$ and comment the result based on the symmetry properties of the spin Hamiltonian.

Answer

To finalize the diagonalization one needs to consider the last 2 pairs of states associated with $M = 1/2$ and $M = -1/2$. The matrix to be diagonalized is the same in both cases

$$\begin{bmatrix} -0.5 & -0.86603 \\ 0.86603 & -0.5 \end{bmatrix}$$

whose eigenvalues are

$$\lambda_\pm = -0.5 \pm i\,0.86603 = e^{\pm i 2\pi/3}$$

Question: According to the Bloch theorem one expects the eigenvalues of $\mathcal{T}$ to take the form $e^{i\kappa}$. Define in the following table the possible simultaneous eigenstates of the three operators $\mathcal{H}$, $\hat{S}^z_{123}$, and $\mathcal{T}$ labeling them by the relative eigenvalues E, M, and the wave number κ. Once you have assigned those labels, from the knowledge of the analytic result, try to assign also the value of the total spin S_{123} in the first column.

Answer

S_{123}	E [J]	M	κ
$\frac{3}{2}$	$-\frac{3}{4}$	$-\frac{3}{2}$	0
$\frac{3}{2}$	$-\frac{3}{4}$	$-\frac{1}{2}$	0
$\frac{3}{2}$	$-\frac{3}{4}$	$+\frac{1}{2}$	0

S_{123}	E [J]	M	κ
$\frac{3}{2}$	$-\frac{3}{4}$	$+\frac{3}{2}$	0
$\frac{1}{2}^{2\pi/3}$	$\frac{3}{4}$	$-\frac{1}{2}$	$2\pi/3$
$\frac{1}{2}^{-2\pi/3}$	$\frac{3}{4}$	$-\frac{1}{2}$	$-2\pi/3$
$\frac{1}{2}^{2\pi/3}$	$\frac{3}{4}$	$+\frac{1}{2}$	$2\pi/3$
$\frac{1}{2}^{-2\pi/3}$	$\frac{3}{4}$	$+\frac{1}{2}$	$-2\pi/3$

N = 4 spins 1/2 with periodic boundary conditions

The spin Hamiltonian is in this case

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

$\mathcal{H}$-eigenstates

Hamiltonian operator:

$$\mathcal{H} = \begin{bmatrix}
-1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2
\end{bmatrix}$$

z **component of the total spin operator**:

$$\hat{S}^z_{1234} = \begin{bmatrix}
-0.00995 & 0 & 0 & 0.02186 & 0.10154 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.02186 & 0 & 0 & 0.99953 & -0.0022 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0.10154 & 0 & 0 & -0.0022 & -0.98958 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -0.98022 & 0 & -0.0024 & 0.1979 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -0.0024 & 0 & -0.98495 & -0.02382 & 0.00815 & -0.17054 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0.1979 & 0 & -0.02382 & 0.97993 & 1e-04 & -0.00207 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.00815 & 1e-04 & 0.00047 & 0.02472 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.17054 & -0.00207 & 0.02472 & 0.98477 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.98744 & 0.15797 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.15797 & 0.98744 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}$$

Translation operator:

$$\mathcal{T} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.99975 & 0.01212 & -0.01256 & -0.01375 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.00866 & -1e-04 & -0.70687 & 0.01624 & -0.70711 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -0.99975 & 0.00866 & -7e-05 & 0.01403 & -0.00584 & 0.01225 & 0.00612 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -0.01212 & 1e-04 & -0.01403 & 0 & -0.02287 & -0.99957 & 7e-05 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.01256 & 0.70687 & -0.00639 & 0.02272 & -0.49966 & 0.01148 & 0.49983 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.01375 & -0.01624 & -0.01197 & 0.99957 & 0.01148 & -0.00026 & -0.01149 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0.70711 & 0.00612 & 7e-05 & 0.49983 & -0.01149 & -0.5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Question We have seen in a previous assignment that $\mathcal{H}$ is in this case diagonal on the basis $|S_{24}, S_{13}, S_{1234}, M_{1234}\rangle$ with eigenvalues:

$$\mathcal{H}|S_{24}, S_{13}, S_{1234}, M_{1234}\rangle = -\frac{J}{2}[S_{1234}(S_{1234}+1) - S_{24}(S_{24}+1) - S_{13}(S_{13}+1)]\,|S_{24}, S_{13}, S_{1234}, M_{1234}\rangle$$

which allows building the underlying table of eigenvalues. For the $\mathcal{H}$ eigenstates generated by intermediate spin values $S_{24} = S_{13} = 1$, assign the wave number κ associated with the eigenvalue of $\mathcal{T}$ (i.e. the eigenvalue of $\mathcal{T}$ being $e^{i\kappa}$).

Answer

S_{13}	S_{24}	S_{1234}	**dim**	E **[**J**]**	κ
0	0	0	1	0	x
1	0	1	3	0	x
0	1	1	3	0	x
1	1	0	1	2	0
1	1	1	3	1	π
1	1	2	5	-1	0

(we don't expect you to fill cells containing a x).

Simultaneous eigenstates of $\mathcal{H}$ and $\hat{S}^z_{1234}$

Hamiltonian operator:

$$\mathcal{H} = \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix}$$

z **component of the total spin operator**:

$$\hat{S}^z_{1234} = \begin{bmatrix}
-2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}$$

Translation operator:

$$\mathcal{T} = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.3004 & 0.95177 & -0.06237 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.45946 & -0.2017 & -0.86499 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.83585 & 0.23119 & -0.4979 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{bmatrix}$$

Question: Define in the following table the possible simultaneous eigenstates of the three operators $\mathcal{H}$, $\hat{S}^z_{123}$, and $\mathcal{T}$ labeling them by the relative eigenvalues E, M, and the wave number κ (fill only the cells with the question mark "?"). Once you have assigned those labels, from the knowledge of the analytic result, try to assign also the value of the total spin S_{1234} in the first column.

Answer

S_{1234}	E **[**J**]**	M	κ
2	- 1	-2	0
2	- 1	-1	0
2	- 1	0	0
2	-1	+ 1	0
2	-1	+ 2	0
$1^{\pi/2}$	0	-1	$\pi/2$
$1^{-\pi/2}$	0	-1	$-\pi/2$
$1^{\pi/2}$	0	0	$\kappa = \pi/2$ plausible by symmetry with other states with $M = \pm 1$
0	0	0	spin singlet only occurs for N even and necess. gives $\kappa = 0$ (Bethe Ansatz)
$1^{-\pi/2}$	0	0	$\kappa = -\pi/2$ plausible by symmetry with other states with $M = \pm 1$
$1^{\pi/2}$	0	+1	$\pi/2$
$1^{-\pi/2}$	0	+1	$-\pi/2$

S_{1234}	E [J]	M	κ
1^{π}	1	-1	π
1^{π}	1	0	π
1^{π}	1	+1	π
0	2	0	0

N.B.

Given the fact that $\mathcal{H}$ is symmetric under SO(3) rotations in the spin space, we expect that the total spin be also good quantum number.

Question To reduce the computational complexity one could diagonalize $\mathcal{H}$ in the subspaces of the single-particle basis corresponding to the same eigenvalue of M. What would be the dimensionality of the largest subspace (i.e., the maximal degeneracy of M)?

Answer

On the single-particle basis the number of ways to obtain a given value of M can be determined by the number of ways of placing k spins up out of 4. This is just the definition of the binomial

$$\frac{4!}{k!(4-k)!}$$

which takes the maximum value for $k = 2$, yielding 6 possible states associated with $M = 0$. Therefore, the largest subset of M eigenvalues would be this one with 6 degenerate eigenstates.

Take-home message

We have been able to build a basis of common eigenstates of the $\mathcal{H}$, $\hat{S}_T^z$, and $\mathcal{T}$ operators because they commute. Actually, any component of the total spin operator $\hat{\mathbf{S}}_T$ commutes with the other operators. Since the components $\hat{S}_T^\alpha$ ($\alpha = x, y, z$) are the *generators* of rotations in the spin space (of dimension 2^N) these commutation rules reflect the physical fact that the Hamiltonian is invariant under translations of the lattice sites (shifting) and rotations in the spin space.