Consider a system of three spin-1/2 moments, $\vec{S}_1, \vec{S}_2, \vec{S}_3$. The permutation operator $P_{12}$ exchanges spin 1 and 2:

$$P_{12}\,|\sigma_1, \sigma_2, \sigma_3\rangle = |\sigma_2, \sigma_1, \sigma_3\rangle$$

where $\sigma_{1,2,3} = \pm 1/2$ are the eigenvalues of $S_1^z, S_2^z, S_3^z$. The permutation operator $P_{123}$ performs a cyclic permutation on spins 1, 2, and 3 so that $2 \to 1$, $1 \to 3$, $3 \to 2$

$$P_{123}\,|\sigma_1, \sigma_2, \sigma_3\rangle = |\sigma_2, \sigma_3, \sigma_1\rangle$$

(a) Express $P_{12}$ in terms of the spin operators $\vec{S}_1, \vec{S}_2$.

(b) Express $P_{123}$ in terms of the spin operators $\vec{S}_1, \vec{S}_2, \vec{S}_3$.

See Prof. Chakravarty's lecture notes p. 38–41:

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

so $\vec{\sigma}_1 \cdot \vec{\sigma}_2 = (\sigma_x^1 \sigma_x^2 + \sigma_y^1 \sigma_y^2 + \sigma_z^1 \sigma_z^2)$

and $\vec{\sigma}_1 \cdot \vec{\sigma}_2 \uparrow\uparrow = (\cancel{\downarrow\downarrow} + \underbrace{(i\downarrow)(i\downarrow)}_{-\cancel{\downarrow\downarrow}} + \uparrow\uparrow) = \uparrow\uparrow$

$$\vec{\sigma}_1 \cdot \vec{\sigma}_2 \uparrow\downarrow = (\downarrow\uparrow + \underbrace{(i\downarrow)(-i\uparrow)}_{\downarrow\uparrow} + \uparrow(-\downarrow)) = 2\downarrow\uparrow - \uparrow\downarrow$$

$$\vec{\sigma}_1 \cdot \vec{\sigma}_2 \downarrow\uparrow = (\uparrow\downarrow + \underbrace{(-i\uparrow)(i\downarrow)}_{\uparrow\downarrow} - \downarrow\uparrow) = 2\uparrow\downarrow - \downarrow\uparrow$$

$$\vec{\sigma}_1 \cdot \vec{\sigma}_2 \downarrow\downarrow = (\cancel{\uparrow\uparrow} + \underbrace{(-i\uparrow)(-i\uparrow)}_{-\cancel{\uparrow\uparrow}} + (-\downarrow)(-\downarrow)) = \downarrow\downarrow$$

In summary:

$$\vec{\sigma}_1 \cdot \vec{\sigma}_2 \begin{Bmatrix} \uparrow\uparrow \\ \uparrow\downarrow \\ \downarrow\uparrow \\ \downarrow\downarrow \end{Bmatrix} = \begin{Bmatrix} \uparrow\uparrow \\ 2\downarrow\uparrow - \uparrow\downarrow \\ 2\uparrow\downarrow - \downarrow\uparrow \\ \downarrow\downarrow \end{Bmatrix}$$

Try $P_{12} = \frac{1}{2}(\mathbb{1} + \vec{\sigma}_1 \cdot \vec{\sigma}_2) = \frac{1}{2}(\mathbb{1} + \frac{4}{\hbar^2}\vec{S}_1 \cdot \vec{S}_2)$ or $2(\frac{\mathbb{1}}{4} + \vec{S}_1 \cdot \vec{S}_2)$

$$P_{12}\ \uparrow\uparrow = \frac{1}{2}(\uparrow\uparrow + \uparrow\uparrow) = \uparrow\uparrow$$

$$P_{12}\ \uparrow\downarrow = \frac{1}{2}(\uparrow\downarrow + 2\downarrow\uparrow - \uparrow\downarrow) = \downarrow\uparrow$$

$$P_{12}\ \downarrow\uparrow = \frac{1}{2}(\downarrow\uparrow + 2\uparrow\downarrow - \downarrow\uparrow) = \uparrow\downarrow$$

$$P_{12}\ \downarrow\downarrow = \frac{1}{2}(\downarrow\downarrow + \downarrow\downarrow) = \downarrow\downarrow$$

(b) The effect of $P_{123}$ can be gotten by applying $P_{12}$ and then $P_{23}$ on $|\sigma_1, \sigma_2, \sigma_3\rangle$

$$P_{12}\,|\overset{1}{\sigma_1}, \overset{2}{\sigma_2}, \overset{3}{\sigma_3}\rangle = |\overset{1}{\sigma_2}, \overset{2}{\sigma_1}, \overset{3}{\sigma_3}\rangle \Rightarrow P_{23}\,|\overset{1}{\sigma_2}, \overset{2}{\sigma_1}, \overset{3}{\sigma_3}\rangle = |\overset{1}{\sigma_2}, \overset{2}{\sigma_3}, \overset{3}{\sigma_1}\rangle$$

which is what $P_{123}|\sigma_1, \sigma_2, \sigma_3\rangle = |\sigma_2, \sigma_3, \sigma_1\rangle$

so $P_{123} = P_{23}P_{12} = \frac{1}{4}(\mathbb{1} + \frac{4}{\hbar^2}\vec{S}_2 \cdot \vec{S}_3)(\mathbb{1} + \frac{4}{\hbar^2}\vec{S}_1 \cdot \vec{S}_2)$

or $4(\frac{\mathbb{1}}{4} + \vec{S}_2 \cdot \vec{S}_3)(\frac{\mathbb{1}}{4} + \vec{S}_1 \cdot \vec{S}_2)$

$p_z$ dispersions are degenerate, and they disperse the same way as the $s$ state (Why?). Of course, atoms could contain both $s$- and $p$-orbitals, in which case we have to include them both in our model. These states can also mix to form a more complex dispersion.

The generalization to three dimensions is simple. The equation for the amplitudes are

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}C(x, y.z, t) = E_0C(x, y.z, t) &- A_xC(x+b, y.z, t) - A_xC(x-b, y.z, t) \\ &- A_yC(x, y+b, z, t) - A_yC(x, y-b, z, t) \\ &- A_zC(x, y, z+b, t) - A_yC(x, y, z-b, t), \end{aligned} \tag{1.172}$$

where we have assumed a cubic lattice with a lattice spacing of $b$, but have assumed for generality that the matrix elements are different for the electron hopping in different directions. The energy spectrum is given by

$$E_k = E_0 - 2A_x \cos k_x b - 2A_y \cos k_y b - 2A_z \cos k_z b, \tag{1.173}$$

while the amplitudes are given by

$$C(x, y, z, t) = e^{-E_k t/\hbar} e^{-i\mathbf{k}\cdot\mathbf{r}}. \tag{1.174}$$

### 1.5.2 Spin Waves

A magnetic Hamiltonian that can describe ferromagnetism is the ferromagnetic spin-1/2 Heisenberg model, where the nearest spins interact via a spin-spin interaction

$$H = -J\sum_n \boldsymbol{\sigma}_n \cdot \boldsymbol{\sigma}_{n+1}. \tag{1.175}$$

For simplicity, I have absorbed the factor $(\hbar/2)^2$ in the coupling $J$, and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector made of the Pauli matrices. The Hamiltonian is for a one-dimensional chain of spins, but you can easily generalize it to higher dimensions. First, define the raising and the lowering operators

$$\sigma_n^+ = \frac{\sigma_n^x + i\sigma_n^y}{2} \tag{1.176}$$

$$\sigma_n^- = (\sigma_n^+)^\dagger = \frac{\sigma_n^x - i\sigma_n^y}{2}. \tag{1.177}$$

Remember that the Pauli matrices are Hermitian and that $\sigma^+|+\rangle = 0$, $\sigma^+|-\rangle = |+\rangle$, $\sigma^-|-\rangle = 0$, and $\sigma^-|+\rangle = |-\rangle$. Now, the interaction for a pair of spins can be written as

$$\boldsymbol{\sigma}_n \cdot \boldsymbol{\sigma}_{n+1} = 2[\sigma_n^+ \sigma_{n+1}^- + \sigma_n^- \sigma_{n+1}^+] + \sigma_n^z \sigma_{n+1}^z, \tag{1.178}$$

where we have used the fact that the Pauli matrices belonging to distinct sites commute. The interaction can also be written in terms of a permutation operator $P_{n,n+1}$ that permutes the spins on the sites $n$ and $n+1$. To check this, define the kets for two spins as $|\pm,\pm\rangle$, where the first entry is for the first spin and the second entry is for the second spin. Then,

$$\left(2[\sigma_n^+ \sigma_{n+1}^- + \sigma_n^- \sigma_{n+1}^+] + \sigma_n^z \sigma_{n+1}^z\right) |{+}{+}\rangle = |{+}{+}\rangle \tag{1.179}$$

$$\left(2[\sigma_n^+ \sigma_{n+1}^- + \sigma_n^- \sigma_{n+1}^+] + \sigma_n^z \sigma_{n+1}^z\right) |{-}{-}\rangle = |{-}{-}\rangle \tag{1.180}$$

$$\left(2[\sigma_n^+ \sigma_{n+1}^- + \sigma_n^- \sigma_{n+1}^+] + \sigma_n^z \sigma_{n+1}^z\right) |{+}{-}\rangle = 2\,|{-}{+}\rangle - |{+}{-}\rangle\,, \tag{1.181}$$

$$\left(2[\sigma_n^+ \sigma_{n+1}^- + \sigma_n^- \sigma_{n+1}^+] + \sigma_n^z \sigma_{n+1}^z\right) |{-}{+}\rangle = 2\,|{+}{-}\rangle - |{-}{+}\rangle\,. \tag{1.182}$$

Therefore, as announced earlier,

$$\boldsymbol{\sigma}_n \cdot \boldsymbol{\sigma}_{n+1} = 2P_{n,n+1} - 1. \tag{1.183}$$

What is the ground state of the ferromagnetic Heisenberg model? Since the coupling constant $J$, also called the exchange constant, is positive, a pair of nearest neighbor spins like to be parallel to the each other. So, perhaps, the groundstate is that state in which they are all lined up parallel to each other. This is clearly an infinitely degenerate state because it does not matter which direction in space they point as long as they are parallel to each other. Let us check that the assumed state is the lowest energy state. Note that the Hamiltonian acting on the presumed ground state is

$$-J\sum_n (2P_{n,n+1} - 1)\,|{+}{+}{+}\ldots\rangle = -JN\,|{+}{+}{+}\ldots\rangle\,. \tag{1.184}$$

The state $|{+}{+}{+}\ldots\rangle$ is definitely an eigenstate; physically it is clear that it is also the lowest energy state, but, with a little bit more effort, you can also show that there are no other eigenstates of energy lower than $-JN$, where $N$ is the total number of spins in the lattice. As the temperature is raised, thermal fluctuations will create excited states, which will disorder the spins. There will be a temeperature $T_c$ at which the system will loose its average magnetization and a phase transition will take place. It can be rigorously shown that $T_c = 0$ for dimensions $d \leq 2$, but it is finite at $d = 3$. This proof is slightly off our track, so I won't give it to you here.

What do the excited states look like? Let us redefine the zero of energy by subtracting the ground state energy, so that

$$H - E_0 = -2J \sum_n (P_{n,n+1} - 1). \tag{1.185}$$

It is easy to guess that the first excited state would be one where one of the spins is flipped. We need to invent a nice notation to denote this. For example, if the $4th$ spin is flipped, we will label that state as

$$|x_4\rangle = |+++-+++\ldots\rangle . \tag{1.186}$$

What is the action of the Hamiltonian on this state? If the permutation operator does not involve the $4th$ spin, the state is unchanged. If it involves the $4th$ spin, it will either permute it with the spin on the right, or on the left, so that

$$P_{34}\,|x_4\rangle = |x_3\rangle , \tag{1.187}$$

$$P_{45}\,|x_4\rangle = |x_5\rangle . \tag{1.188}$$

The terms in the Hamiltonian that survive are

$$[-2J(P_{34} - 1) - 2J(P_{45} - 1)]\,|x_4\rangle = 4J\,|x_4\rangle - 2J\,|x_3\rangle - 2J\,|x_5\rangle . \tag{1.189}$$

In general,

$$H\,|x_n\rangle = 4J\,|x_n\rangle - 2J\,|x_{n+1}\rangle - 2J\,|x_{n-1}\rangle . \tag{1.190}$$

This is identical to the problem we solved for an electron in a periodic lattice. The schrödinger equation is given by

$$i\hbar \frac{\partial}{\partial t} C_n(t) = \sum_{n'} \langle n|H|n'\rangle\, C_{n'}(t), \tag{1.191}$$

where the only matrix elements of the Hamiltonian are

$$H_{n,n} = 4J, \tag{1.192}$$

$$H_{n,n+1} = H_{n-1,n} = -2J. \tag{1.193}$$

The set of linear difference equations can once again be solved by the choice

$$C_n(t) = \frac{1}{\sqrt{N}} e^{-ikx_n} e^{-iEt/\hbar}. \tag{1.194}$$

Then, the energy spectrum is given by

$$E_k = 4J(1 - \cos kb). \tag{1.195}$$

The definite energy solutions correspond to waves of a flipped spin whose amplitude at a given site $n$ is determined by the wavevector $k$ lying within the first Brillouin zone between $\frac{-\pi}{b}$ and $\frac{\pi}{b}$. The energy dispersion at long wavelengths is that of a free particle, a magnon, of an effective mass $m_{\text{eff}} = \hbar^2/(4Jb^2)$.

Once we start examining the problem of two flipped spins, we discover that the spin waves interact when they approach each other. The interaction may in fact give rise to bound states. Although the two spin wave problem can still be solved eaxctly with some effort, we may argue that if there is a small density of such excited states, or spin waves, at low temperatures, they can be approximated to be independent. Such an independent particle approximation reproduces many low temperature properties of ferromagnets. In the independent particle approximation, the excited state energy $\varepsilon(k_1, k_2, \ldots)$ is then given by

$$\varepsilon(k_1, k_2, \ldots) \approx E_{k_1} + E_{k_2} + \ldots \tag{1.196}$$