Mathematics 12: Quantum Spins

Quantum mechanics for a particle in space is controlled by the commutation relations:

$$\left[\hat{x}_i, \hat{p}_j\right] \equiv \hat{x}_i \hat{p}_j - \hat{p}_j \hat{x}_i = i\hbar\delta_{ij}$$

for the different spatial directions labelled by i. If we consider *orbital* motion using the orbital angular momentum:

$$\hat{\mathbf{L}} = \hat{\mathbf{x}} \times \hat{\mathbf{p}}$$

$$\hat{L}_i = \epsilon_{ijk}\hat{x}_j\hat{p}_k$$

then the consequential commutation relations are:

$$\left[\hat{L}_i, \hat{L}_j\right] \equiv \hat{L}_i\hat{L}_j - \hat{L}_j\hat{L}_i = i\hbar\epsilon_{ijk}\hat{L}_k$$

Although orbital motion involves integer values for angular momentum, the electronic *spin* involves half-integral values. We will deal with spin-half here, the smallest permissible value.

The natural representation is 2×2, with:

$$\hat{S}^x = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \hat{S}^y = \frac{\hbar}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \hat{S}^z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

acting on a basis, $\{|\uparrow>, |\downarrow>\}$. You can easily verify the previous commutation relations, and further:

$$\hat{S}^i\hat{S}^j = \frac{\hbar^2}{4}\delta_{ij}\mathbf{1} + \frac{i\hbar}{2}\epsilon_{ijk}\hat{S}_k$$

The 'best' representation is in terms of:

$$\hat{S}^z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \qquad \hat{S}^+ = \hat{S}^x + i\hat{S}^y = \hbar\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \qquad \hat{S}^- = \hat{S}^x - i\hat{S}^y = \hbar\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

the so-called *raising* and *lowering* operators. In terms of our basis, $\hat{S}^+$ 'raises' the spin (ie turns a down into an up) and $\hat{S}^-$ 'lowers' the spin (ie turns an up into a down).

We are interested in interactions between spins:

$$\hat{H}_1 = \sum_{ij} J_{ij}\hat{S}^z_j\hat{S}^z_i = \sum_{ij} J_{ij}\hat{\mathbf{S}}^{\parallel}_i.\hat{\mathbf{S}}^{\parallel}_j$$

the **Ising model**,

$$\hat{H}_2 = \sum_{ij} J_{ij}\{\hat{S}^x_i\hat{S}^x_j + \hat{S}^y_i\hat{S}^y_j\} = \frac{1}{2}\sum_{ij} J_{ij}\{\hat{S}^+_i\hat{S}^-_j + \hat{S}^-_i\hat{S}^+_j\} = \sum_{ij} J_{ij}\hat{\mathbf{S}}^{\perp}_i.\hat{\mathbf{S}}^{\perp}_j$$

the **x-y model**, and

$$\hat{H}_3 = \sum_{ij} J_{ij}\{\hat{S}^x_i\hat{S}^x_j + \hat{S}^y_i\hat{S}^y_j + \hat{S}^z_i\hat{S}^z_j\} = \frac{1}{2}\sum_{ij} J_{ij}\{\hat{S}^+_i\hat{S}^-_j + \hat{S}^-_i\hat{S}^+_j\} + \sum_{ij} J_{ij}\hat{S}^z_i\hat{S}^z_j = \sum_{ij} J_{ij}\hat{\mathbf{S}}_i.\hat{\mathbf{S}}_j$$

the **Heisenberg model**, where J_{ij} are the bond strengths between the i'th and j'th spin. If $J_{ij} < 0$ the spins want to be parallel at low temperature, and if $J_{ij} > 0$ the spins want to be anti-parallel at low temperature.

To understand the action of these interactions we need to consider the basis for a pair of spins:

$$\{|\uparrow\uparrow>, |\uparrow\downarrow>, |\downarrow\uparrow>, |\downarrow\downarrow>\}$$

in terms of which:

$$\hat{S}^z \hat{S}'^z \ |\uparrow\uparrow>= \frac{1}{4} \ |\uparrow\uparrow> \qquad \hat{S}^z \hat{S}'^z \ |\uparrow\downarrow>= -\frac{1}{4} \ |\uparrow\downarrow>$$

$$\hat{S}^z \hat{S}'^z \ |\downarrow\uparrow>= -\frac{1}{4} \ |\downarrow\uparrow> \qquad \hat{S}^z \hat{S}'^z \ |\downarrow\downarrow>= \frac{1}{4} \ |\downarrow\downarrow>$$

for the z-components and we have chosen to scale $\hbar \mapsto 1$. Hence $\hat{H}_1$ is *diagonal* in our chosen basis, for which all spins are either up or down. Also:

$$\hat{\mathbf{S}}^\perp \hat{\mathbf{S}}'^\perp \ |\uparrow\uparrow>= 0 \qquad \hat{\mathbf{S}}^\perp \hat{\mathbf{S}}'^\perp \ |\uparrow\downarrow>= \frac{1}{2} \ |\downarrow\uparrow>$$

$$\hat{\mathbf{S}}^\perp \hat{\mathbf{S}}'^\perp \ |\downarrow\uparrow>= \frac{1}{2} \ |\uparrow\downarrow> \qquad \hat{\mathbf{S}}^\perp \hat{\mathbf{S}}'^\perp \ |\downarrow\downarrow>= 0$$

and so $\hat{H}_2$ and $\hat{H}_3$ makes the spins 'fluctuate'.

In project 2 you can analyse the role of *thermal* fluctuations on the Ising model, $\hat{H}_1$. In project 3 you can analyse the role of *quantum* fluctuations at zero temperature in the x-y model, $\hat{H}_2$, or the Heisenberg model, $\hat{H}_3$.