Magnon Excitations and Spin Hamiltonian in Non-collinear Magnetic System

Spin Operators in a Rotating Frame

We already discussed during the lectures how to calculate the magnon dispersion relation of a G-type antiferromagnet using two different basis with the following Heisenberg Hamiltonian:

$$H = -J\sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j \tag{1}$$

Here is another approach, this time using a rotating frame and a **magnetic propagation vector**. The magnetic propagation vector formalism allows a compact description of a periodic magnetic structure [1]. The magnetic moments $\mathbf{m}_j$ on the jth site can be expressed by

$$\mathbf{m}_j = \begin{pmatrix} \cos\mathbf{Q}\cdot\mathbf{r}_j & -\sin\mathbf{Q}\cdot\mathbf{r}_j \\ \sin\mathbf{Q}\cdot\mathbf{r}_j & \cos\mathbf{Q}\cdot\mathbf{r}_j \end{pmatrix}\mathbf{m} = \mathrm{R}\left(\mathbf{Q}\cdot\mathbf{r}_j\right)\mathbf{m}$$

, where $\mathbf{r}_j$ is the position vector and $\mathbf{Q}$ is the magnetic propagation vector. For example, let us consider an antiferromagnetic (AFM) 1D chain with a lattice parameter a. Antiparallel neighboring spins can be described by the magnetic propagation vector of Q=1/2, which corresponds to the rotation angle $(2\pi/a)(1/2)a=\pi$ for a unit lattice.

Similarly, spin operators can also be represented using a rotation matrix:

$$\hat{\mathbf{S}}_j = \begin{pmatrix} \hat{S}_j^x \\ \hat{S}_j^y \\ \hat{S}_j^z \end{pmatrix} = \begin{pmatrix} \cos\mathbf{Q}\cdot\mathbf{r}_j & -\sin\mathbf{Q}\cdot\mathbf{r}_j & 0 \\ \sin\mathbf{Q}\cdot\mathbf{r}_j & \cos\mathbf{Q}\cdot\mathbf{r}_j & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \hat{T}^x \\ \hat{T}^y \\ T^z \end{pmatrix} = \mathrm{R}_z\left(\mathbf{Q}\cdot\mathbf{r}_j\right)\mathbf{T}, \text{ where } \hat{\mathbf{T}} = \begin{pmatrix} \sqrt{S/2}\left(\hat{b}+b^\dagger\right) \\ -i\sqrt{S/2}\left(\hat{b}-b^\dagger\right) \\ S-\hat{b}^\dagger b \end{pmatrix}.$$

(Q1) Consider G-type AFM in a 3D cubic lattice, where spins at all nearest neighbor are antiparallel to each other. Find the propagation vector and derive a dispersion relation of spin waves for the Hamiltonian (1). You will see that the final result is equivalent to one obtained using two basis as discussed in the lecture.

(Q2) Construct a Hamiltonian with two exchange interactions between the nearest and next nearest neighbors, and calculate a dispersion relation. Discuss how the dispersion is affected by whether the exchange interaction is FM or AFM between the next nearest neighbors.

[1] A. Wills, *J. Phys. IV France* **11**, 9-133 (2001)

Antiferromagnet in Triangular Lattice

Let's move to a slightly more complicated system, AFM in the 2D triangular lattice. Consider three spins on the edge of a triangle. If two adjacent spins are placed antiparallel, it is not possible to orient the spin on the third site to satisfy the antiferromagnetic condition with the other two spins. In this case, the system is said to be geometrically frustrated [2]. Fortunately, it is known that spins on a perfect triangular lattice form the 120-degree ordered state: all neighboring spins lie on the same plane with 120 degrees angle between.

Consider the following Hamiltonian in this system:

$$H = -J\sum_{i,j}\mathbf{S}_i \cdot \mathbf{S}_j - K\sum_i \left(\mathbf{S}_i \cdot \hat{\mathbf{z}}\right)^2 \tag{2}$$

, where J is the exchange interaction between the nearest neighbors and K is an easy-plane anisotropy. The anisotropy term forces the spins to lie in the **xy**-plane.

(Q3) Find the propagation vector in this system and derive a dispersion relation using the rotating frame.

(Q4) Derive a dispersion relation using three basis operators. Show that it is equivalent to the result obtained from Q3.

(Q5) Sketch the dispersion relation along the symmetry axes: (1,0,0) and (1,1,0). Find the energy at the zone center and boundary, and describe the effect of the anisotropy term.

[2] Stephen Blundell, *Magnetism in Condensed Matter* (Oxford University Press, Oxford, 2001) pp.166-167

[Advanced topics] Dzyaloshinskii-Moriya interaction

This problem is of more advanced nature and mathematically demanding, but it can be a good exercise for you to learn a physics that is essential to so-called multiferroic materials. The excited state can be produced by the spin-orbit interaction instead of the connected oxygen atoms for a superexchange interaction. Here, we take into account an exchange interaction between the excited state of one ion and the ground state of the other ion. This is known as the **Dzyaloshinskii-Moriya interaction**. It leads to the following term in the Hamiltonian:

$$H_{DM} = \sum_{i,j}\mathbf{D}\cdot\left(\mathbf{S}_i \times \mathbf{S}_j\right).$$

In general, the vector **D** lies parallel or perpendicular to the line connecting the two spins, depending on the symmetry [3].

(Q6) Consider a ferromagnetic 1D chain with the DM vector along the chain. Obtain the ground state of this system and sketch it. Explain the effect of DM interaction.

(Q7) Calculate dispersion relation and sketch it. Find the energy at the zone center and boundary, and describe the effect of the DM term.

[3] Stephen Blundell, *Magnetism in Condensed Matter* (Oxford University Press, Oxford, 2001) p.81