FIP10604 – Text 06 SPIN HAMILTONIANS

In Text 05, we have seen that virtual processes involving back and forth hopping of one electron between two atoms at well defined positions in a crystal structure gives rise to an effective interaction between the spins of these atoms. The exchange mechanism, discussed in detail in that text, yields an effective Hamiltonian involving only spin operators and an exchange constant that gives the order of magnitude of the interaction energies.

Heisenberg Model

It is reasonable to suppose that what as found for a single pair of atoms should be equally applicable to **all pairs** of "magnetic" atoms or ions (i.e., those with a nonzero spin) in the solid. Then a possible Hamiltonian to describe localized (atomic) magnetic moments on a lattice has the form

$$\mathcal{H} = -\sum_{ij} J_{ij}\, \mathbf{S}_i \cdot \mathbf{S}_j \ , \tag{1}$$

where the sum extends over all lattice sites, and the conditions $J_{ii} = 0$ and $J_{ij} = J_{ji}$ are implied. This is known as the **Heisenberg model**. It belongs to a generic class of models described by ***spin Hamiltonians***, whose sole degrees of freedom are associated to spin.

In lattices with cubic symmetry (or its equivalent in other space dimensions), it is common to use the **nearest-neighbor approximation**,

$$J_{ij} = \begin{cases} J \ , & i,j \text{ neighbors} \\ 0 \ , & \text{other cases} \ . \end{cases} \tag{2}$$

The Hamiltonian then reads

$$\mathcal{H} = -2J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \ , \tag{3}$$

where the sum is now over all **pairs** of nearest-neighbor sites. We can also write

$$\mathcal{H} = -J \sum_{i\delta} \mathbf{S}_i \cdot \mathbf{S}_{i+\delta} \ . \tag{4}$$

In this last sum, i runs over all lattice sites, and δ over the z nearest neighbors of a site i, at positions given by lattice vectors $\mathbf{R}_i + \boldsymbol{\delta}$, for z different vectors $\boldsymbol{\delta}$ that connect a given site to its neighbors (z is known as *coordination number*).

Other models

The Heisenberg Hamiltonian has rotational symmetry in spin space. As seen in Text 04, a crystal field of axial symmetry, together with spin-orbit interaction, introduces a local anisotropy term of the form $D(S_i^z)^2$.

We can then define an anisotropic Heisenberg model,

$$\mathcal{H} = -\sum_{ij} J_{ij}\, \mathbf{S}_i \cdot \mathbf{S}_j - D \sum_i (S_i^z)^2 \,. \tag{5}$$

Remember that the z axis is an *easy axis* for $D > 0$, while the xy plane is an *easy plane* for $D < 0$. Other anisotropic forms are possible and may involve the exchange interactions themselves, which leads to a matrix $\mathbf{J}_{ij}$ in the most general case.

In the limit of very strong anisotropy, we can define two simplified models,

$$\mathcal{H} = -\sum_{ij} J_{ij}\, S_i^z\, S_j^z \qquad \textbf{(Ising Model)} \,; \tag{6}$$

$$\mathcal{H} = -\sum_{ij} J_{ij}\, (S_i^x\, S_j^x + S_i^y\, S_j^y) \qquad \textbf{(}\boldsymbol{XY}\textbf{ Model)} \,. \tag{7}$$

The Ising model is naturally *classical*, since all operators commute, and can be replaced by classical variables that assume two discrete values ($\pm S$, usually rescaled to ± 1). This model can recover a quantum character through the application of a magnetic field along an axis perpendicular to z, yielding the *transverse-field Ising model*.

The XY model is often transformed into a classical model with two-component magnetic moments, which are in-plane vectors of fixed module, so that the Hamiltonian can be rewritten in terms of the orientation angles of these vectors.

Asymmetric interactions

The models analyzed so far contain exchange interactions which are symmetric with respect to the order of spins for a given interacting pair. However, if we consider a *superexchange* mechanism (described in Text 05), taking into account the possibility of *hopping* between different orbitals and including the spin-orbit interaction, we can obtain an asymmetric exchange interaction known as *Dzyaloshinsky-Moryia interaction*,[1] which is described by a Hamiltonian term of the form

$$\mathcal{H}_{DM} = \sum_{ij} \mathbf{d}_{ij} \cdot \mathbf{S}_i \times \mathbf{S}_j \,. \tag{8}$$

In general, the vector $\mathbf{d}_{ij}$, which has the property $\mathbf{d}_{ji} = -\mathbf{d}_{ij}$, has significantly lower magnitude than the exchange constants J_{ij}. This interaction is not very common because there is a number of symmetry restrictions that it must satisfy to be nonzero. Nevertheless, it may have an important role in particular situations, giving rise to *non-colinear* magnetic orderings (e.g., a helical pattern of spins, magnetic skyrmions,etc.).

[1] Original Article: T. Moryia, Physical Review **120**, 91 (1960)

Effect of interactions

Having built models in which the localized magnetic moments interact with each other, we will study the effects of interactions, especially in connection to (i) existence and nature of magnetic order at low temperatures, and (ii) general behavior of the magnetic susceptibility as a function of temperature.

This study will be done in several steps. The problem is complex because it involves a many-body interacting system. Therefore, there is no exact solution, except in very special cases (as we will see later).

We will focus on the Heisenberg model with nearest-neighbor interactions, initially seeking to determine the nature of the ground state, in order to verify whether the presence of interactions gives rise to spontaneous magnetic order or not.

Ground state of the Heisenberg model

The Heisenberg Hamiltonian with nearest-neighbor interactions, Eq. (3), may be written as

$$\mathcal{H} = -2J \sum_{\langle ij \rangle} \left[S_i^z \, S_j^z + \tfrac{1}{2} \left(S_i^+ \, S_j^- + S_i^- \, S_j^+ \right) \right] \ . \tag{9}$$

– Ferromagnetic (FM) case

For $J > 0$, by analogy with an equivalent classical model [viewing the spins as classical magnetic moments in Eq. (3)], we would expect a ground state with all the spins aligned in parallel. Associating to this state a *ket* $|F\rangle$, we have

$$S_i^z |F\rangle = S|F\rangle \ . \tag{10}$$

Notice that the choice of z axis is arbitrary.

Applying each of the three terms inside the summation in Eq. (9) on the state $|F\rangle$ gives $S_i^z \, S_j^z |F\rangle = S^2 |F\rangle$, $S_i^+ \, S_j^- |F\rangle = 0$, $S_i^- \, S_j^+ |F\rangle = 0$. Thus,

$$\mathcal{H}|F\rangle = -NzJS^2|F\rangle \ , \tag{11}$$

where N is the total number of lattice sites.

We have found that $|F\rangle$ is an eigenvector of $\mathcal{H}$ and corresponds to the lowest energy. Therefore, the ground state of the Heisenberg model for $J > 0$ presents long-range FM order.

– Antiferromagnetic (AF) case

For $J < 0$, a classical analogy yields the so-called *Néel state*, in which neighboring spins have opposite orientations. This would imply a quantum-mechanical state represented by a *ket* $|N\rangle$ defined by

$$S_i^z|N\rangle = \begin{cases} +S|N\rangle\ , & i \text{ belonging to sublattice } A \\ -S|N\rangle\ , & i \text{ belonging to sublattice } B\ . \end{cases} \tag{12}$$

Here we suppose the lattice can be divided into two interpenetrating sublattices, such that all the neighbors of a site on sublattice A belong to sublattice B and *vice versa* (lattices with this property are called *bipartite*).

This hypothesis, based on a classical analogy, works with the Ising model: $|N\rangle$ is an eigenvector of the Ising Hamiltonian, and corresponds to the lowest energy for $J < 0$. However, $|N\rangle$ **is not an eigenvector of the Heisenberg Hamiltonian** (and therefore is not the ground state), since the transverse terms (with S^+ and S^-) change the orientations of pairs of neighboring spins (although conserving the total spin).

The problem of determining the ground state of the AF Heisenberg model is complex. We will come back to it later.