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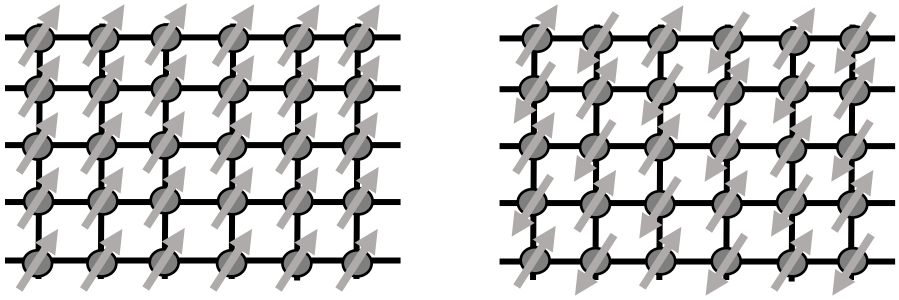
Understanding Ferromagnetism and Antiferromagnetism

Magnets or magnetic material can be found everywhere from your fridge magnets to complex scientific equipment. Despite the ubiquitous nature of magnetic materials, it is likely that very few people know the origins of magnetism and how it comes about. The mathematics behind the theoretical formulation of systems that can be considered magnetic can be quite complex, but from a conceptual standpoint, it is not hard to convince yourself that many types of magnetism are the result of simple Coulombic and magnetic interactions between electrons within a lattice of atoms.

Beginning the discussion on magnetism, it makes sense to view the physical origins of ferromagnetism and antiferromagnetism conceptually through a quantum mechanical lens. The phenomena of ferromagnetism and antiferromagnetism are manifestations of ordered spins of electrons in a lattice of atoms. For simplicity, it may be easiest to read this paper in the context of a 2D square lattice of atoms. This is a very simple, yet surprisingly helpful, configuration one can imagine for a lattice of atoms. In ferromagnetic materials, the spins of the electrons of the atoms align such that they all point in the same direction. In other words, they are parallel. This alignment of magnetic moments usually occurs within specific magnetic domains of the atom. Within these domains, the spins of the constituent atoms align in ferromagnetic materials. At sufficiently low temperatures, or in the presence of an external magnetic field, the moments of these domains will align as well ("Ferromagnetism", 2018). These distance scales of these domains are large enough such that the boundaries of domains can sometimes be determined by observing the material through a microscope. Antiferromagnetism is basically what the name implies. The spins of the constituent atoms in the material become anti-aligned or antiparallel, meaning the spins of nearest neighbor atoms will be opposite. For a 2D square lattice, this means that if the lattice point of interest has spin $m_s = +1/2$, the four nearest neighbors of that lattice site will all have spins $m_s = -1/2$. Again, this antialignment throughout the bulk of the material is only possible at sufficiently low temperatures. Above a certain temperature, antiferromagnetic materials are usually paramagnetic which means the spins of the lattice sites will align themselves antiparallel to an applied magnetic field ("Antiferromagnetism", 2018). Below are representations of ferromagnetic (a) and antiferromagnetic (b) cases:



(a) (b)

Conceptually, these types of magnetism are interesting but don't quite have meaning in physics without some mathematical basis. One very famous quantum mechanical theory of spin interactions in a lattice of atoms is the Heisenberg model. Without delving into the complete derivation of this model, it will suffice to briefly explain the Hamiltonian of this model:

$$H = \frac{1}{2}\sum_{i,j} J_{ij}\left(\boldsymbol{S}_i \cdot \boldsymbol{S}_j\right) \quad (1)$$

Surprisingly, this Hamiltonian is quite simple. The Hamiltonian is the sum of the nearest neighbor spin interactions which is represented by the dot product of the spin operators of nearest neighbor atoms: ($S_i * S_j$). The coefficients that multiply this spin interaction are coefficients that determine the nature of the interaction. For non-nearest neighbors, $J_{ij} = 0$. For nearest neighbors, we can have: $J_{ij} > 0$ or $J_{ij} < 0$, which represent antiferromagnetism and ferromagnetism respectively ("The Heisenberg model", 2018). Trying to understand this Hamiltonian and use it as is would not allow us to derive the specific situations of magnetism. This Hamiltonian must be given some context, or some assumptions must be made that would allow one to determine the coefficients. This can be done by using similar models in conjunction with the Heisenberg model to derive specific magnetic situations. It is not so difficult to do this for the case of antiferromagnetism.

The Hubbard model will be used to derive a form of the Heisenberg Hamiltonian that is specific to the antiferromagnetic case. The Hubbard model makes an assumption about the lattice: each lattice site can only support one state (which means each lattice site can only contain a maximum of two electrons) and the Pauli principle asserts that if two electrons occupy the same lattice point, their spin orientations must be opposite (Cleveland, Medina, 1976). The Hamiltonian of the Hubbard model consists of two terms: $H = H_0 + H_1$. The first term, H_0, is a term that represents the Coulomb repulsion of electrons that occupy the same lattice point. The second term, H_1, is a term that represents the kinetic energy of electrons that "hop" from site to site (Cleveland, Medina, 1976). Next, assume that the lattice is in its ground state configuration. In this ground state, the "hopping" term allows for a superposition of electrons on any given lattice point. Think of this electron "hopping" as a sea of electrons that have some probability distribution of their location. Because of this superposition, the Coulomb term of the Hubbard Hamiltonian is large (Cleveland, Medina, 1976). Conversely, we can consider the Coulomb term which prefers one or fewer electrons per site as to reduce the Coulomb repulsion between electrons. We see now that each term in the ground state is in competition to lower the overall energy of the system. Therefore, an approach will be taken that will treat the Hamiltonian as just the H_0 (Coulomb) term and the "hopping" term will be treated as a perturbation (Cleveland, Medina, 1976). This H_0 term looks like:

$$H_0 = \frac{1}{2} I \sum_{i,\sigma} \boldsymbol{n}_{i\sigma}\boldsymbol{n}_{i-\sigma} \quad (2)$$

This term is proportional to the electrostatic energy, *I*. The *n*'s count the number of sites that have two electrons with opposite spin (the *1/2* accounts for double counting). The H_0 term has eigenvalues of *nI* which is the number of sites with two electrons times the electrostatic energy (Cleveland, Medina, 1976). The perturbative Hamiltonian of the "hopping" term looks like:

$$H_{hop} = \sum'_{ij} \sum_{\sigma} T_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} \quad (3)$$

In this Hamiltonian, the double sum is over lattice sites *i* and *j*, and the other sum sums over the allowed values for the spin, σ. The T_{ij} is a coefficient and the *c*'s are operators that create or destroy electrons at lattice sites *i* or *j* with spin σ (Cleveland, Medina, 1976). In the ground state, when a first order perturbation is applied, one sees that the first order perturbation term is zero unless the quantum number *n* (different from the *n* representing number of sites with two electrons) is equal to 1 (which is not the ground state). Then one can attempt to solve the second order perturbation in the ground state. If this second order perturbation calculation is done, the end result will look like (Cleveland, Medina, 1976):

$$H_{eff} = \frac{1}{I} P_0 \left(\sum_{kl} |T_{kl}|^2 \left(2\boldsymbol{S}_k \cdot \boldsymbol{S}_l - \frac{1}{2} \right) \right) P_0 \quad (4)$$

The P_0's are operators that put the constraint on the system such that it is restricted to the subspace of states with quantum number $n = 0$. It is apparent that this Hamiltonian looks just like the Heisenberg Hamiltonian where $J_{ij} = |T_{kl}|^2$. And since $J_{ij} > 0$, the antiferromagnetic case has been derived using the Hubbard model to produce a form of the Heisenberg Hamiltonian in which the values of J_{ij} are known (Cleveland, Medina, 1976).

Now that the antiferromagnetic case has been derived, deriving the ferromagnetic case is a natural next step. To describe the ferromagnetic case, the Hubbard model will not be needed, only the Heisenberg model. To begin, there are a couple assumptions that must be made: the spin interactions in the lattice are the dominating interactions, the particles of interest are fermions, and the spin interactions are anisotropic (Muller, Timm, 2015). Now that some of the assumptions have been enumerated, it is possible to re-write the Heisenberg Hamiltonian:

$$H = \frac{1}{2} \sum_{ij} J_{ij} \left(S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \right) \quad (5)$$

In this equation, it can be shown that the *x*, *y*, or *z* components of spin do not commute with each other. Therefore, the total spin, *S*, is defined as:

$$\boldsymbol{S} = \sum_i S_i \quad (6)$$

Defining the total spin this way shows that equations (1) and (5) are equal. Using the fact that a single component of the total spin will commute with at least one component of the Hamiltonian,

it is possible to define a state that is an eigenstate of H, S^2, and S_z (the z component was chosen because it is convention) (Muller, Timm, 2015). Now consider the state in which all the spins are aligned which results in the maximum value for the total spin. The state is just the product of each individual electron state at its maximum spin value:

$$|\psi> = |S_1, m_1> \cdot |S_2, m_2> \cdot |S_3, m_3> \cdots \quad (7)$$

Next, the Hamiltonian (5) above can act on this wavefunction. It is possible to rearrange the x and y spin dot products into raising and lowering operators for the spin quantum number m_s. The z spin dot product is left unaltered. Once this operation is carried out, the result is produced:

$$H|\psi> = -\frac{1}{2}S^2 \sum_{ij} J_{ij}|\psi> \quad (8)$$

Remember, this is true for a state which has maximized spin for each state and each spin is aligned parallel with its nearest neighbor (Muller, Timm 2015). Now considering a state $|\psi>$, not necessarily having maximum total spin, it is necessary take the expectation value of H with this state:

$$<\psi|H|\psi> = -\frac{1}{2}\sum_{ij} J_{ij}\left(\frac{1}{2}<\psi|S_i^+ S_j^-|\psi> + \frac{1}{2}<\psi|S_i^- S_j^+|\psi> + <\psi|S_i^z S_j^z|\psi>\right) = -\frac{1}{2}\sum_{ij} J_{ij} m_i m_j \quad (9)$$

If $J_{ij} \geq 0$ for all i and j then $J_{ij}m_i m_j \leq J_{ij}S^2$. And since the states described are states with eigenvalues that are less than the maximum possible eigenvalues, $-(1/2)S^2\sum_{ij}J_{ij}$, and since we assumed that $J_{ij} \geq 0$ (exchange interactions are positive), we have described the ground state of the Heisenberg model in the ferromagnetic case (Muller, Timm, 2015). (Note: I said earlier that if $J_{ij} > 0$, this means the system is antiferromagnetic, but since there is a (-) sign in this expectation value, then $J_{ij} < 0$ which is the ferromagnetic case).

From a theoretical standpoint, these quantum models of ferromagnetisms and antiferromagnetism are interesting, but what determines if a certain material is ferromagnetic, antiferromagnetic, paramagnetic, diamagnetic, or some other type of magnetism? One way of determining the type of magnetism in a material is to measure the magnetic susceptibility of the material. This magnetic susceptibility, which will now be referred to as χ_m, is a measure of the internal magnetic response of the material to an externally applied magnetic field. In paramagnetic materials, the internal magnetic field aligns itself in the direction of the externally applied magnetic field. In diamagnetic materials, the internal magnetic field aligns itself opposite the direction of the externally applied magnetic field. The case is slightly more complicated for ferromagnetic and antiferromagnetic materials, although the general idea still applies.

In ferromagnetic material, the magnetic susceptibility can be written as:

$$\chi_m = \frac{C}{T - C\lambda/\mu_0} \tag{10}$$

In this equation, T is the temperature of the material, λ is a constant that represents the strength of the exchange interaction between electrons in the lattice, and the C is the Curie constant given by:

$$C = \frac{N\mu_B^2\mu_0}{k_B} \tag{11}$$

where N is the number of magnetic particles per volume, μ_B is the Bohr magneton, μ_0 is the vacuum permeability, and k_B is the Boltzmann constant (Morton, 2012). It is obvious from this equation that as temperature of the material increases, the magentic susceptibility decreases. Classically this makes sense because as the temperature of the material increases, the atoms in the lattice have greater kinetic energy and therefore, are vibrating very rapidly in the solid. This rapid vibration makes it difficult for the spins of the electrons of an atom to align. To make an analogy, it is like having a row of archers that are trying to hit a target. It is easy for them to hit the target if they are not moving around a lot. One can think of the archers' steady aim being disrupted by an earthquake. In this analogy, the archer's ability to hit the target is like the electrons ability to align their spins, and the magnitude of the earthquake is like the magnitude of the thermal energy of the atoms. Speaking in terms of energy, above a certain temperature, commonly referred to as the Curie-Weiss temperature, ferromagnetism will no longer be observed in the material. This temperature can be expressed as:

$$\theta_W = \frac{N\mu_B^2\lambda}{k_B} = \frac{J}{2k_B} \tag{12}$$

In the final form of the expression, the J stands for the exchange interaction energy between electrons in the lattice. This exchange interaction energy is the same energy that governs the magnetic ordering in the material. It is the J_{ij} from earlier. Therefore, the Curie-Weiss temperature is a measure of when the thermal energy becomes comparable to the mean exchange energy of the electrons (Morton, 2012). All this makes sense because if the thermal energy dominates over this exchange energy, the ferromagnetic effects will be greatly reduced by the thermal energy.

Similar arguments can be made about antiferromagnetism. The expression for the magnetic susceptibility of antiferromagnetic material can be written as:

$$\chi_m = \frac{C}{T + \theta_N} \tag{13}$$

Again, in this equation, C is the Curie constant, T is the temperature of the material, and θ_N is the Neel temperature. Below this temperature, the susceptibility will depend on the orientation of the

field to the crystal but will typically fall to a net magnetization of zero as the temperature trends towards zero (Morton, 2012).

Now that the quantum origins of magnetism in ferromagnetic and antiferromagnetic objects have been mathematically described, and the dependence on temperature of the magnetic ordering is understood, one may ask: how are materials probed to find out what kind of magnetic ordering they have? One cannot simply look at a metal and determine whether it is a ferromagnet or an antiferromagnet. One way to probe the magnetic structure of materials is to reflect (specularly) neutrons off the layers of the lattice structure of a material. Since neutrons have intrinsic spin, their spin moments will interact with the spins of the electrons in the lattice. Based upon the intensity of the reflected neutron beam, it is possible to determine the intensity of the magnetic ordering in the metal and what kind of magnetic ordering is present (Berk, Majkrzak, O'Donovan, 2004). This method of probing magnetic materials (specifically magnetic thin films) is called polarized neutron reflectometry (PNR). It is "polarized" because the incident neutrons are either all spin up (+) or spin down (-). Based on the type of material, the reflected neutrons will have either spin up or spin down. We refer to the intensity of the reflected beams as R(++), R(--), R(+-), or R(-+). The first plus or minus stands for the spins of the incident neutrons, and the second symbol is the spins of the reflected neutrons. From the signs in the brackets, one can see that materials can cause the spin of the incident neutron to "flip" (Berk, Majkrzak, O'Donovan, 2004). Not surprisingly, this is referred to as the "spin-flip channel". Whether or not the material allows for a spin-flip channel will also give insight into the magnetic properties of the material. Although there are more ways to probe the magentic structure of materials, this is the way in which my research group probes magnetic thin films.

Even though magnets are common household items and even though people begin to learn about and play with magnets as early as kindergarten, magnetic ordering in materials comes about through complex quantum mechanical interactions within a lattice of atoms. The information presented in this paper gives a theoretical idea of what might be happing at the smallest distance scales in this material. Moreover, the information in this paper only scratches the surface of only two types of magnetism. The term "magnetism" covers a wide range of specific phenomena in crystal lattices. As mentioned earlier, there are more types of magnetism than just ferromagnetism or antiferromagnetism. There is plenty of theory to describe all these types of magnetism and experimental work is always being done in order to find more exotic magnetic materials that will hopefully illuminate some of the hidden mysteries of magnetism in condensed matter.

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