Session 9 - This session is intended as a quick survey to cover the basics of the origin of magnetic interaction in magnetic systems.

1. **Direct magnetic interaction** The direct magnetic interaction energy between two magnetic dipole moments separated by a distance R is given by (in the SI unit system)

$$\Delta E = \frac{\mu_0}{4\pi} \frac{\mu_1 \cdot \mu_2 - 3(\hat{R} \cdot \mu_1)(\hat{R} \cdot \mu_2)}{R^3}$$

where $\mu_0 = 4\pi \times 10^{-7} N/A^2$ is the vacuum magnetic permittivity, and $\hat{R}$ is the versor of the vector R connecting the two dipoles.

Atoms with net orbital and spin angular momenta L and S have an average magnetic moment $\mu = \mu_L + \mu_S$ where $\mu_L = -\frac{e\hbar}{2m_e}\langle L \rangle = -\mu_B \langle L \rangle$ and $\mu_S = -g_e \mu_B \langle S \rangle$ where the Bohr magneton $\mu_B = 9.274.. \times 10^{-24} \ m^2 A$ and the gyromagnetic factor g_e is ≈ 2.0023.

Estimate the direct magnetic interaction energy between two dipoles of ≈ 1 Bohr magneton separated by a distance of $\approx 1\text{Å}$ and verify that it is way too small to account for the magnetic interaction responsible for the magnetic properties of many materials whose magnetic ordering temperature can reach several hundred K (eg. 860 K in magnetite Fe_2O_3).

2. **Coulomb and kinetic exchange interaction** The direct magnetic interaction being too small magnetism in materials has its origin in electrostatics coupled with Pauli principle.

Electrons are fermions, i.e. their wavefunction is antisymmetric upon exchange. This implies that the probability of finding two electrons with the same spin at the same position must be zero. Hence, electrons with like spins tend to avoid each other more than electrons with opposite spin. Thus the Coulomb energy between electrons depends on their spin, i.e. electrons in orthogonal orbitals that are spin aligned are more energetically favorable. This is known as Coulomb exchange and it is the basis of the first Hund's rule. Kinetic energy gain due to wavefunction delocalization may favor spin pairing; this effect goes under the name of kinetic exchange.

Below we will work with a toy model to understand Coulomb and kinetic exchange.

a) Write the non-relativistic, spinless, Coulomb hamiltonian for two static hydrogen atoms that are far apart such that the overlap of atomic orbitals can be considered small but non-negligible.
b) Assuming the interatomic interaction is perturbatively small, build a basis of symmetric and antisymmetric two-body wavefunctions in order to use in the approximate solution of the above Hamiltonian.
c) Write the Hamiltonian in the basis you have proposed. The matrix representation of this Hamiltonian will have terms that are often called "Coulomb integral" and "Exchange integral". Make an educated guess about which integrals match with these given names.
d) Find the eigenvalues and eigenfunctions of the Hamiltonian. What is the difference between the two eigenvalues?
So far so good but we have not yet done anything with spin!
e) Based on the discussion about fermions above, assign the appropriate spin functions to each eigenvector and rewrite the Hamiltonian operator using the S^2 operator, such that it identifies the energies of respective eigenvectors correctly.
f) Rewrite the above Hamiltonian operator using the rules of angular momentum addition $S^2 = (S_1 + S_2) \cdot (S_1 + S_2)$ so that the final form resembles a Heisenberg spin hamiltonian $H = -JS_1 \cdot S_2$. Give the expression of J in terms of overlap, exchange and coulomb integrals. Do you expect J to be

positive or negative in the case of the hydrogen molecule? Does the expression you have found agree with your expectation? How about two electrons occupying two different 2p levels in an Oxygen atom?

h) Rewrite the same energy operator using this time the Pauli spin-exchange operator whose eigenvalue is 1 for symmetric spin states, -1 for antisymmetric spin states.

Ref.: ch.2 of D.D. Stancil, A. Probhakar, "Spin Waves: Theory and Application", Springer 2009

3. **Superexchange interaction** Magnetic interaction depends on overlap between neighboring atoms.

How is it that magnetism is present in many transition metal oxides where magnetic atoms are far apart, separated by non magnetic oxygen atoms?

How is it that magnetic interaction is sometimes ferromagnetic and sometimes antiferromagnetic ?

Ref.: ch. 7 of E. Pavarini, E. Koch, F. Anders and M. Jarrell, "Correlated Electrons: From Models to Materials Mdelling and Simulation", Vol. 2, ForshungZentrum Juelich 2012, http://www.cond-mat.de/events/correl12

4. **Ferromagnetic spin-$1/2$ chain**

Let us consider a 1D chain of N spin-1/2 particles interacting ferromagnetically as described by the Hamiltonian

$$\mathcal{H} = -2\frac{J}{\hbar^2}\sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}$$

with $J > 0$.

   a) What is the ground state and the associated eigenvalue?

   b) Rewrite the Hamiltonian in terms of the Pauli spin-exchange operator $P_{i,i+1}$.

   c) Consider the basis of states $|m\rangle$ obtained by flipping the mth spin from the ground state. Write the action of the Pauli spin-exchange operator on the basis elements.

   d) Such basis can be argued to be suitable to expand the low lying eigenstates of this Hamiltonian. Using $|\psi\rangle = \sum C_n |n\rangle$ expansion, and the Pauli operator form of the Hamiltonian, obtain an equation for the expansion coefficients C_n. Show that it accepts solutions in the form of waves in periodic media, similar to the ones obtained for lattice vibrations.

   e) Derive the dispersion relation for the eigenvalues. What do the eigenstates look like? (Using the lattice vibration analogy, you can guess that these quasiparticles are called "magnons")

The End.