Exchange interaction [tln94]

A brief history:

- The formulation of classical electrodynamics culminated in the achievements of Faraday and Maxwell in the 19$^{\text{th}}$ century.

- The origin of microscopic magnetic moments and the cooperative phenomena of magnetism in condensed matter (diamagnetism, paramagnetism, ferromagnetism, ...) remained a mystery until much later.

- The theorem of Bohr and (independently) van Leeuven made the failure of classical physics in this effort quite clear:

  > *At any finite temperature and in all finite applied electric or magnetic fields, the net magnetization of a collection of charged particles in thermal equilibrium vanishes identically.*

- Classical theories of paramagnetism by Langevin (1905) and of ferromagnetism by Curie and Weiss (1907) assumed (with no basis for justification) the existence of elementary magnetic moments.

- The discovery of spin quantization by Stern and Gerlach (1922) and the postulation of the electron spin by Uhlenbeck and Goudsmit (1925) lead the way toward understanding atomic magnetism.

- The strongest known force between magnetic moments – the magnetic dipole interaction – was too weak by orders of magnitude to explain ferromagnetism as observed in matter.

- The formulation of quantum mechanics by Heisenberg, Born, Schrödinger, Dirac, and others (beginning in 1925) provided the basis for cooperative magnetism.

- Heisenberg and Dirac (1926) identified a strong indirect interaction between the spins of electrons with overlapping wave functions.

- This *exchange* interaction is caused by the combined effects of electrostatic repulsion and the symmetry requirement for the wave function.

- The exchange coupling is captured by the Heisenberg model,

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j,$$

  for unpaired electron spins of nearest-neighbor ions on a lattice.

- The Ising model, proposed earlier (1920) by Lenz on phenomenological grounds, gained justification as a simplified version.

Exchange coupling of electron spins in molecular hydrogen:

  – The two-electron-wave function of H_2 must be antisymmetric on account of the fact that electrons are fermions.

  – Writing it as a product of two factors,

$$\Psi_S = \psi_s(\mathbf{r}_1, \mathbf{r}_2)\chi_S, \quad \Psi_T = \psi_a(\mathbf{r}_1, \mathbf{r}_2)\chi_T,$$

  where $\psi_s(\mathbf{r}_1, \mathbf{r}_2)$ and $\psi_a(\mathbf{r}_1, \mathbf{r}_2)$ are symmetric and antisymmetric spatial parts, respectively, and χ_S and χ_T describe an (antisymmetric) spin singlet and a (symmetric) spin triplet, respectively.

  – The splitting of the lowest two energy levels is due to the different charge distribution in ψ_s and ψ_a, not due to different interactions between parallel or antiparallel electronic magnetic moments.

  – In the case of H_2, ψ_a produces a higher electrostatic potential energy than ψ_s does, due to a combination of stronger repulsion between the two electrons and weaker attraction between electrons and protons.

  – In consequence, Ψ_S has a lower energy than Ψ_T. For modeling purposes, this energy difference can be attributed to the electron spins as an effective exchange interaction.

  – A spin flip from singlet to triplet necessitates as witch from ψ_s to ψ_a. It costs energy as encoded in an effective spin Hamiltonian of the form,

$$\mathcal{H} = -J\mathbf{S}_1 \cdot \mathbf{S}_2.$$

  – In the case of H_2, the exchange energy J is negative, which favors the singlet energetically as is experimentally established.

A more quantitative analysis of the exchange interaction is provided in a course on *Electricity and Magnetism*.