

Exploring Quantum Physics

Coursera, Spring 2013 Instructors: Charles W. Clark and Victor Galitski





Guest Lecture: Electron Spin Part IV: Spin Exchange and Magnetism



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Permutation symmetry

• Pauli exclusion principle is the result of Fermion wavefunction antisymmetry upon particle exchange

$$r_{1} \qquad \qquad \text{Indistinguishability:} \qquad \qquad \text{Electrons} \\ \|\Psi(1,2)\|^{2} = \|\Psi(2,1)\|^{2} \\ \Psi(1,2) = \pm \Psi(2,1) \qquad \qquad \qquad \text{Electrons} \\ (\text{fermions}): \qquad \Psi(r_{1},r_{2}) = -\Psi(r_{2},r_{1}) \\ \Psi_{A}(r_{1},r_{2}) = \frac{1}{\sqrt{2}} [\Phi_{a}(r_{1})\Phi_{b}(r_{2}) - \Phi_{b}(r_{1})\Phi_{a}(r_{2})] \\ \Psi_{A}(r_{2},r_{2}) = \frac{1}{\sqrt{2}} [\Phi_{a}(r_{1})\Phi_{b}(r_{2}) - \Phi_{b}(r_{1})\Phi_{a}(r_{2})] \\ \Psi_{A}(r_{2},r_{2}) = \frac{1}{\sqrt{2}} [\Phi_{a}(r_{1})\Phi_{b}(r_{2}) - \Phi_{b}(r_{1})\Phi_{a}(r_{2})] \\ \Psi_{A}(r_{2},r_{2}) = \frac{1}{\sqrt{2}} [\Phi_{a}(r_{2})\Phi_{b}(r_{2}) - \Phi_{b}(r_{2})\Phi_{a}(r_{2})] \\ \Psi_{A}(r_{2},r_{2}) = \frac{1}{\sqrt{2}} [\Phi_{a}(r_{2})\Phi_{a}(r_{2}) - \Phi_{b}(r_{2})\Phi_{a}(r_{2})] \\ \Psi_{A}(r_{2},r_{2}) = \frac{1}{\sqrt{2}} [\Phi_{a}(r_{2})\Phi_{a}(r_{2}) - \Phi_{b}(r_{2})\Phi_{a}(r_{2})] \\ \Psi_{A}(r_{2},r_{2}) = \frac{1}{\sqrt{2}} [\Phi_{a}(r_{2})\Phi_{a}(r_{2}) - \Phi_{b}(r_{2})\Phi_{a}(r_{2})\Phi_{a}(r_{2})] \\ \Psi_{A}(r_{2},r_{2}) = \frac{1}{\sqrt{2}} [\Phi_{A}(r_{2})\Phi_{a}(r_{2})\Phi_{a}(r_{2})\Phi_{a}(r_{2})\Phi_{a}(r_{2})\Phi_{a}(r_{2})\Phi_{a}(r_{2})\Phi_{a}(r_{2})\Phi_{a}(r_{2})\Phi_{a}(r_{2})\Phi_{a}(r_{2})\Phi_{a}(r_{2})\Phi_{a}(r_{2})\Phi_{a}(r_{2})\Phi_{a}(r_{2})\Phi_{a}(r_{2})\Phi_{a}(r_{2})\Phi_{a}(r_{2})\Phi_{a}(r_{2})\Phi_{a}(r_{2})$$

- But the wavefunction includes spatial coordinates *and* spin!
- So we can include a *spatially symmetric* wavefunction if the **spin** components are antisymmetric

$$\Psi_{A}(r_{1},r_{2}) = \frac{1}{\sqrt{2}} [\Phi_{a}(r_{1})\Phi_{b}(r_{2}) - \Phi_{b}(r_{1})\Phi_{a}(r_{2})] \qquad \Psi_{S}(r_{1},r_{2}) = \frac{1}{\sqrt{2}} [\Phi_{a}(r_{1})\Phi_{b}(r_{2}) + \Phi_{b}(r_{1})\Phi_{a}(r_{2})]$$

$$\chi_{S} = \begin{cases} |\uparrow\uparrow\rangle & (1) \\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) & (0) \quad \text{"triplet"} \quad \chi_{A} = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \quad (0) \\ |\downarrow\downarrow\rangle & (-1) \quad \text{"singlet"} \end{cases}$$

Exchange energy

$$\begin{split} \Psi_A(r_1, r_2) &= \frac{1}{\sqrt{2}} [\Phi_a(r_1) \Phi_b(r_2) - \Phi_b(r_1) \Phi_a(r_2)] \\ &\quad \times \chi_S \end{split} \\ \begin{split} \Psi_S(r_1, r_2) &= \frac{1}{\sqrt{2}} [\Phi_a(r_1) \Phi_b(r_2) + \Phi_b(r_1) \Phi_a(r_2)] \\ &\quad \times \chi_A \\ \end{split}$$

A generic example: $H = H_1 + H_2 + H_{12}$ (like in neutral He, where H₁₂ is Coulomb repulsion)

$$\int \Psi^* H \Psi dr_1 dr_2 = E \int \Psi^* \Psi dr_1 dr_2 = E$$

$$\frac{1}{2} \int [\phi_1(r_1)\phi_2(r_2) \pm \phi_1(r_2)\phi_2(r_1)]^* H_1(r_1) [\phi_1(r_1)\phi_2(r_2) \pm \phi_1(r_2)\phi_2(r_1)] dr_1 dr_2 = \frac{1}{2} \int \phi_1(r_1)^* \phi_2(r_2)^* H_1(r_1)\phi_1(r_1)\phi_2(r_2) dr_1 dr_2$$

$$+ \frac{1}{2} \int \phi_1(r_2)^* \phi_2(r_1)^* H_1(r_1)\phi_1(r_2)\phi_2(r_1) dr_1 dr_2$$

$$\pm \frac{1}{2} \int \phi_1(r_2)^* \phi_2(r_2)^* H_1(r_1)\phi_1(r_1)\phi_2(r_1) dr_1 \pm \frac{1}{2} \int \phi_1(r_2)^* \phi_2(r_1)^* H_1(r_1)\phi_1(r_1)\phi_2(r_2) dr_1 dr_2$$

 $E = E_1 + E_2 + E_{12} \pm J$ "Exchange integral"

Magnitude of exchange energy

Because it is coupled to electrostatic configuration, the exchange energy can be very large.... Much larger than direct magnetostatic energy:



This is the same as the interaction between spin and the orbital moments: spin-orbit splitting!

Exchange Hamiltonian

$$H = J \vec{S}_1 \cdot \vec{S}_2$$

$$\vec{S}_1 = \sigma_{x1} \hat{x} + \sigma_{y1} \hat{y} + \sigma_{z1} \hat{z}$$

$$\vec{S}_2 = \sigma_{x2} \hat{x} + \sigma_{y2} \hat{y} + \sigma_{z2} \hat{z}$$
 (os are 2x2 matrices)

Kronecker product:

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B \\ a_{21}B & a_{22}B \end{bmatrix} \qquad H = JS_1 \cdot S_2 = J \left[\sigma_{x1} \otimes \sigma_{x2} + \sigma_{y1} \otimes \sigma_{y2} + \sigma_{z1} \otimes \sigma_{z2} \right]$$

$$H = J\left(\left[\begin{array}{cc} 0 & 1\\ 1 & 0\end{array}\right] \otimes \left[\begin{array}{cc} 0 & 1\\ 1 & 0\end{array}\right] + \left[\begin{array}{cc} 0 & -i\\ i & 0\end{array}\right] \otimes \left[\begin{array}{cc} 0 & -i\\ i & 0\end{array}\right] + \left[\begin{array}{cc} 1 & 0\\ 0 & -1\end{array}\right] \otimes \left[\begin{array}{cc} 1 & 0\\ 0 & -1\end{array}\right]\right)$$

$$H = J\left(\begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \right) = J\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Eigenfunctions of Exchange





- The mean field caused by spin exchange causes a preferred spin orientation a magnetically ordered state – at low temperatures! (J<0: Ferromagnet, J>0: Anti-Ferromagnet)
- This was for localized moments in a lattice: an insulator. What about a metal?





• (Ferro)magnetic metal:



Questions:

- 1. How to transfer this spin asymmetry to nonmagnetic systems?
- 2. What are the processes that govern relaxation back to equilibrium?
- 3. How to manipulate spin asymmetry before equilibrium is obtained?
- 4. How can we engineer devices with unique applications, e.g. logic, interconnects etc.?

Spin Electronics



Figure 2. MR and GMR head structures.



Albert Fert Peter Gruenberg Nobel Prize 2007