Direct Exchange Interaction using Fermi Operators

Derivation of Heisenberg spin-spin interaction model

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Direct Exchange interaction

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r}$$

$$\left(\frac{e^2}{r_{12}} + \frac{e^2}{r_{ab}} - \frac{e^2}{r_{b1}} - \frac{e^2}{r_{a2}}\right)$$

$$\Delta H$$

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r}$$

$$H = H_0 + \Delta H$$

$$-\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{e^2}{r_{a1}} - \frac{e^2}{r_{b2}} + \left(\frac{e^2}{r_{12}} + \frac{e^2}{r_{ab}} + \frac{e^2}{r_{b1}} + \frac{e^2}{r_{a2}}\right)$$

$\langle a|b\rangle = \int \phi_a^*(\vec{r})\phi_b(\vec{r})dr$ ***is negligible***

Direct Exchange interaction

(Heitler-London model)

$$\Psi_{singlet} = \nu_a(s1, s2) \times \psi_s(\vec{r}_1, \vec{r}_2) \; = \; \frac{1}{\sqrt{2(1 + |\langle a|b\rangle|^2)}}(\phi_a(\vec{r}_1)\phi_b(\vec{r}_2) + \phi_a(\vec{r}_2)\phi_b(\vec{r}_1))$$

$$\Psi_{triplet} = \nu_s(s1, s2) \times \psi_a(\vec{r}_1, \vec{r}_2) \; = \; \frac{1}{\sqrt{2(1 - |\langle a|b\rangle|^2)}}(\phi_a(\vec{r}_1)\phi_b(\vec{r}_2) - \phi_a(\vec{r}_2)\phi_b(\vec{r}_1))$$

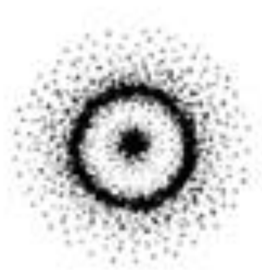
Complete wavefunctions

Spin component

States of coupled atoms as superposition
of states of uncoupled atoms
(zeroth order approximation)

Direct Exchange interaction

(Heitler-London model)



$$\frac{\langle H_s \rangle - \langle H_a \rangle}{2} \quad \text{direct exchange integral}$$

Must always be negative according to the theory of Sturm-Liouville functions (Hamiltonian of this system is of this type)

Heitler-London model breaks down at large distances (> 50a_H)

Direct Exchange interaction

(using Fermi field operators)

Fermi (creation) operator
Creates an electron at $\mathbf{r}_1$

Fermi (annihilation) operator
Destroys an electron at $\mathbf{r}_1$

$$\left\langle \psi(\mathbf{r}) \left| \frac{e^2}{r_{12}} \right| \psi(\mathbf{r}) \right\rangle = \int \psi^*(\mathbf{r}_1)\psi^*(\mathbf{r}_2)\,\frac{e^2}{r_{12}}\,\psi(\mathbf{r}_1)\psi(\mathbf{r}_2)\,d\tau_1 d\tau_2$$

Integral with respect electron's position
and summation over spin state

$\psi^*(\mathbf{r}_1)$ is now replaced with $\psi^\dagger(\mathbf{r}_1)$

Direct Exchange interaction

(using Fermi field operators)

$$\left\langle \psi(\mathbf{r}) \left| \frac{e^2}{r_{12}} \right| \psi(\mathbf{r}) \right\rangle = \int \psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2)\, \frac{e^2}{r_{12}}\, \psi(\mathbf{r}_1)\psi(\mathbf{r}_2)\, d\tau_1 d\tau_2$$

$$\psi(\mathbf{r}) = \sum_{nms} a_{nms}\phi_{nm}(\mathbf{r})\nu(s)$$

Superposition of original atomic wavefunctions

ϕ_{nm} = orbital wavefunction at *nth* lattice site with the component of orbital angular momentum *m*

v(s) = spin wavefunction

Direct Exchange interaction

(using Fermi field operators)

$$H_{coulomb} = \sum_{nms} \left\langle n_1 m_1 s_1, n_2 m_2 s_2 \left| \frac{e^2}{r_{12}} \right| n_3 m_3 s_2, n_4 m_4 s_1 \right\rangle$$

$$= \frac{1}{2} \sum_{nms} \left\langle n_1 m_1, n_2 m_2 \left| \frac{e^2}{r_{12}} \right| n_3 m_3, n_4 m_4 \right\rangle a^\dagger_{n_1 m_1 s_1} a^\dagger_{n_2 m_2 s_2} a_{n_3 m_3 s_2} a_{n_4 m_4 s_1}$$

To simplify the expression above, we assume non-degenerate states.
And, n_3 (or n_4) = n_1, n_4 (or n_3) = n_2 :

$$H_{coulomb} = \frac{1}{2} \sum_{ns} \left\langle n_1 n_2 \left| \frac{e^2}{r_{12}} \right| n_2 n_1 \right\rangle a^\dagger_{n_1 s_1} a^\dagger_{n_2 s_2} a_{n_2 s_2} a_{n_1 s_1}$$

$$\Downarrow$$

$$H_{coulomb} = \sum_{s_1 s_2} \left\langle n_1 n_2 \left| \frac{e^2}{r_{12}} \right| n_2 n_1 \right\rangle a^\dagger_{n_1 s_1} a_{n_1 s_1} a^\dagger_{n_2 s_2} a_{n_2 s_2} - \sum_{s_1 s_2} \left\langle n_1 n_2 \left| \frac{e^2}{r_{12}} \right| n_1 n_2 \right\rangle a^\dagger_{n_1 s_1} a_{n_1 s_2} a^\dagger_{n_2 s_2} a_{n_2 s_1}$$

Coulomb interaction between two electrons localized at n_1 and n_2

Quantum effect due to the property of Fermi operators (spin-spin exchange)

Direct Exchange interaction

(using Fermi field operators)

$$H_{coulomb} = \sum_{s_1 s_2} \left\langle n_1 n_2 \left| \frac{e^2}{r_{12}} \right| n_2 n_1 \right\rangle a^\dagger_{n_1 s_1} a_{n_1 s_1} a^\dagger_{n_2 s_2} a_{n_2 s_2} - \sum_{s_1 s_2} \left\langle n_1 n_2 \left| \frac{e^2}{r_{12}} \right| n_1 n_2 \right\rangle a^\dagger_{n_1 s_1} a_{n_1 s_2} a^\dagger_{n_2 s_2} a_{n_2 s_1}$$

$$H_{coulomb} = K_{n_1 n_2} - J_{n_1 n_2} \left(\sum_{s_1 s_2} a^\dagger_{n_1 s_1} a_{n_1 s_2} a^\dagger_{n_2 s_2} a_{n_2 s_1} \right)$$

$$-J_{n_1 n_2} \left(\sum_{s_1 s_2} a^\dagger_{n_1 s_1} a_{n_1 s_2} a^\dagger_{n_2 s_2} a_{n_2 s_1} \right)$$

$$\begin{aligned}
= \quad & J_{n_1 n_2} \Big[\frac{1}{2} (a^\dagger_{n_1 \uparrow} a_{n_1 \uparrow} + a^\dagger_{n_1 \downarrow} a_1 \downarrow)(a^\dagger_{n_2 \uparrow} a_{n_2 \uparrow} + a^\dagger_{n_2 \downarrow} a_{n_2 \downarrow}) \\
+ \quad & \frac{1}{2} (a^\dagger_{n_1 \uparrow} a_{n_1 \uparrow} - a^\dagger_{n_1 \downarrow} a_{n_1 \downarrow})(a^\dagger_{n_2 \uparrow} a_{n_2 \uparrow} - a^\dagger_{n_2 \downarrow} a_{n_2 \downarrow}) \\
+ \quad & a^\dagger_{n_1 \uparrow} a_{n_1 \downarrow} a^\dagger_{n_2 \downarrow} a_{n_2 \uparrow} + a^\dagger_{n_1 \downarrow} a_{n_1 \uparrow} a^\dagger_{n_2 \uparrow} a_{n_2 \downarrow}
\end{aligned}$$

$$\begin{aligned}
s_{nz} &= \frac{1}{2} (a^\dagger_{n_1 \uparrow} a_{n_1 \uparrow} - a^\dagger_{n_1 \downarrow} a_{n_1 \downarrow} \\
s_{n+} &= s_{nx} + i s_{ny} = a^\dagger_{n_1 \uparrow} a_{n_1 \downarrow} \\
s_{n-} &= s_{nx} - i s_{ny} = a^\dagger_{n_1 \downarrow} a_1 \uparrow
\end{aligned}$$

$$- \; J_{n_1 n_2} \left(\frac{1}{2} + 2 s_{n_1} \cdot s_{n_2} \right)$$

$$H_{coulomb} = \frac{1}{2} \sum_{ns} \left\langle n_1 n_2 \left| \frac{e^2}{r_{12}} \right| n_2 n_1 \right\rangle a^{\dagger}_{n_1 s_1} a^{\dagger}_{n_2 s_2} a_{n_2 s_2} a_{n_1 s_1}$$

$$\Downarrow$$

$$K_{n_1 n_2} - J_{n_1 n_2} \left(\frac{1}{2} + 2 s_{n_1} \cdot s_{n_2} \right)$$

Spin-spin direct exchange interaction

Heisenberg supposed this to be the origin of ferromagnetism

Thank you