Spintronics and Nanomagnetics

ECS 521/641

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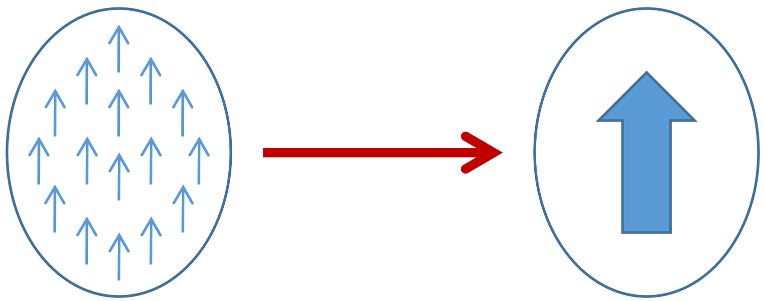
Exchange Interaction

Single-domain nanomagnets

- Exchange interaction
  - ✓ Pauli's exclusion principle
  - ✓ Coulomb repulsion
- Each electron → small magnet
  - ✓ Ferromagnet
  - ✓ Ferrimagnet
  - ✓ Antiferromagnet

W. F. Brown Jr.,
The fundamental theorem of the ferromagnetic particle theory

Magnetic domain formation should be limited to **very small dimensions (100 nm)** because of the competition between the magnetostatic energy and the quantum-mechanical exchange energy, causing nanomagnets to behave like **single giant spins**



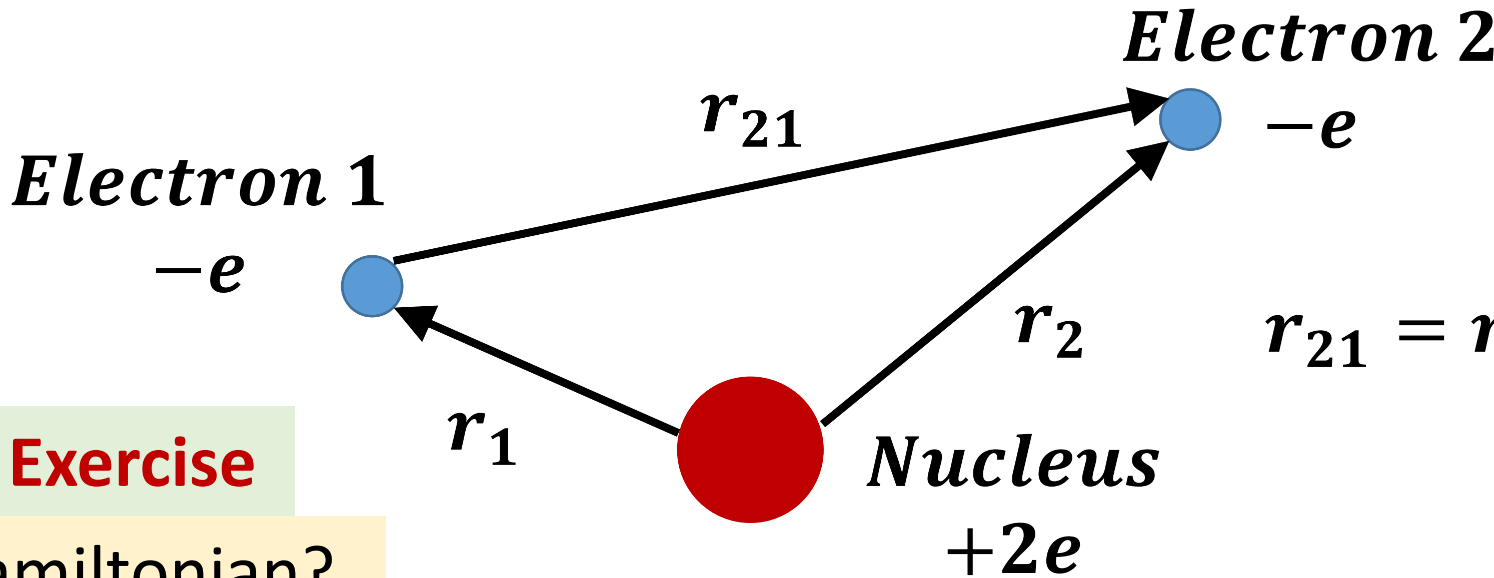
Electron beam lithography (EBL)

Exchange interaction

- Plays the key role in the operation of spin-devices
- **Neglecting spin-orbit interaction**, the state of one single-electron system in an Hydrogen atom is precisely specified
- The multi-electron system cannot be solved exactly
  - Interaction between electrons is unknown
  - Density Functional Theory (Nobel Prize Chemistry, 1998)
- **Pauli's exclusion principle (1924)**
  - No two Fermions, whose wavefunctions have non-zero overlap can have exactly the same set of quantum numbers
  - Explanation of the periodic table
- **Coulomb repulsion** between charged particles
- Symmetry principle says that overall wavefunction must be **antisymmteric** while swapping the indices of any two electrons

Helium atom

- Pauli's exclusion principle was first applied to the simplest many-electron system
  - Two electrons orbiting a nucleus



$$\boldsymbol{r}_{21} = \boldsymbol{r}_2 - \boldsymbol{r}_1$$

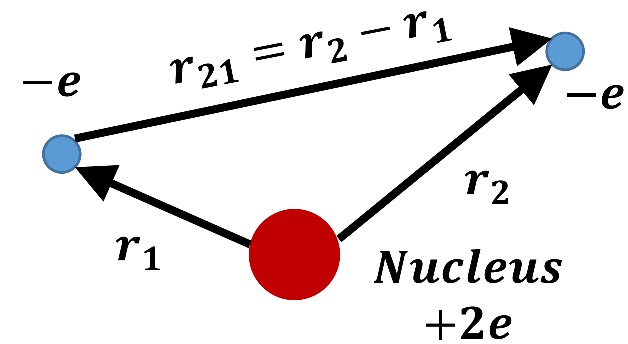
Exercise

Hamiltonian?

$$H_{He} = \frac{|\boldsymbol{p}_1|^2}{2m} + \frac{|\boldsymbol{p}_2|^2}{2m} + \frac{(2e)(-e)}{4\pi\epsilon_0|\boldsymbol{r}_1|} + \frac{(2e)(-e)}{4\pi\epsilon_0|\boldsymbol{r}_2|} + \frac{(-e)(-e)}{4\pi\epsilon_0|\boldsymbol{r}_{21}|}$$

Application of symmetry principle

P operator permutes two identical electrons



$$H_{He}\phi(e_1, e_2) = E\phi(e_1, e_2)$$

$$H_{He} = \frac{|\boldsymbol{p_1}|^2}{2m} + \frac{|\boldsymbol{p_2}|^2}{2m} + \frac{(2e)(-e)}{4\pi\epsilon_0|\boldsymbol{r_1}|} + \frac{(2e)(-e)}{4\pi\epsilon_0|\boldsymbol{r_2}|} + \frac{(-e)(-e)}{4\pi\epsilon_0|\boldsymbol{r_{21}}|}$$

H_{He} is invariant upon permutation $\Rightarrow$ $[H_{He}, P] = 0$

$$e_{1,2} = \boldsymbol{r_{1,2}}, s_{1,2}$$

$$P\phi(e_1, e_2) = E\phi(e_2, e_1) = \lambda\phi(e_1, e_2)$$

$$P^2\phi(e_1, e_2) = \lambda P\phi(e_1, e_2) = \lambda^2\phi(e_1, e_2) = \phi(e_1, e_2)$$

$\lambda^2 = 1$ $\qquad$ $\lambda = \pm 1$

Since electrons are Fermions

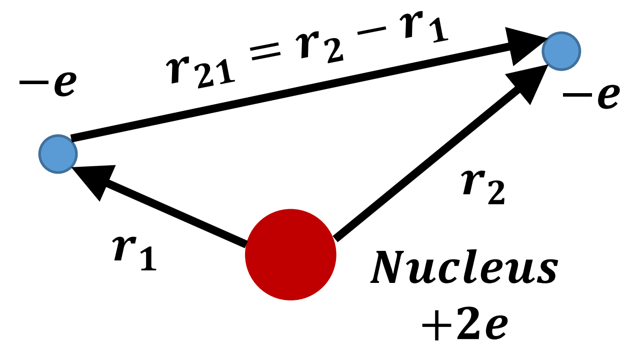
$$\lambda = -1$$

Antisymmetric wavefunction

$$\phi_A(\boldsymbol{r_1}, s_1; \boldsymbol{r_2}, s_2) = \Psi_S\,(\boldsymbol{r_1}, \boldsymbol{r_2})\Xi_A\,(s_1, s_2)$$

or

$$\phi_A(\boldsymbol{r_1}, s_1; \boldsymbol{r_2}, s_2) = \Psi_A\,(\boldsymbol{r_1}, \boldsymbol{r_2})\Xi_S\,(s_1, s_2)$$



$$H_{He} = \frac{|\boldsymbol{p_1}|^2}{2m} + \frac{|\boldsymbol{p_2}|^2}{2m} + \frac{(2e)(-e)}{4\pi\epsilon_0|\boldsymbol{r_1}|} + \frac{(2e)(-e)}{4\pi\epsilon_0|\boldsymbol{r_2}|} + \frac{(-e)(-e)}{4\pi\epsilon_0|\boldsymbol{r_{21}}|}$$

Neglecting spin-orbit interaction

$$\boldsymbol{S} = \boldsymbol{S_1} + \boldsymbol{S_2} \qquad S^2 = \boldsymbol{S}\cdot\boldsymbol{S}$$

Individual $S_i s$ do not commute

$$[S^2, S_z] = 0$$

S^2 is conserved quantity, thus the spinorial part must be eigenstates of these operators

Spinorial part of the wavefunction

$$\phi_A(\boldsymbol{r_1}, s_1; \boldsymbol{r_2}, s_2) = \Psi_S\,(\boldsymbol{r_1}, \boldsymbol{r_2})\Xi_A\,(s_1, s_2)$$

or

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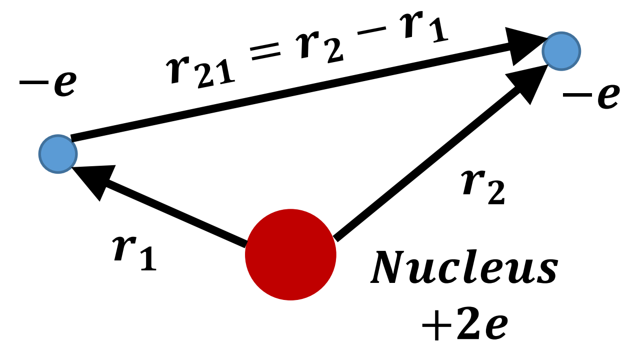

$$\Xi_S\,(s_1, s_2) = |0\rangle_1 |0\rangle_2$$

$$\Xi_S\,(s_1, s_2) = |1\rangle_1 |1\rangle_2$$

$$\Xi_S\,(s_1, s_2) = \frac{1}{\sqrt{2}}(|0\rangle_1 |1\rangle_2 + |1\rangle_1 |0\rangle_2)$$

Triplet states

$$\Xi_A\,(s_1, s_2) = \frac{1}{\sqrt{2}}(|0\rangle_1 |1\rangle_2 - |1\rangle_1 |0\rangle_2)$$

Singlet state

Eigenstates of the spinorial part

$$\Xi_S\,(s_1, s_2) = |0\rangle_1|0\rangle_2$$

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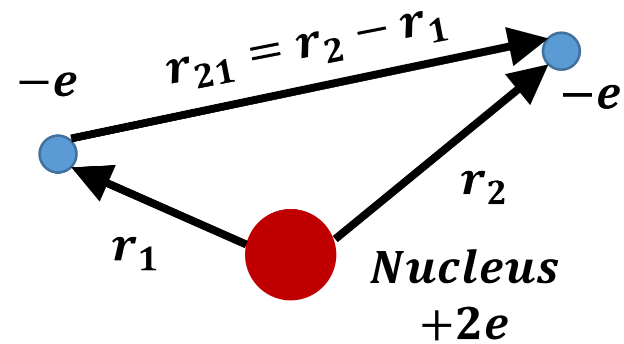

$$\Xi_A\,(s_1, s_2) = \frac{1}{\sqrt{2}}(|0\rangle_1|1\rangle_2 - |1\rangle_1|0\rangle_2)$$

Singlet state

Exercise Determine $S^2|0\rangle_1|0\rangle_2$ and $S_z|0\rangle_1|0\rangle_2$

$$S^2 = \boldsymbol{S}\cdot\boldsymbol{S} = \frac{\hbar^2}{4}(\sigma_1^2 + \sigma_2^2 + 2\boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2}) = \frac{\hbar^2}{2}(3I + \boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2})$$

$$\boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2} = \sigma_{1x}\sigma_{2x} + \sigma_{1y}\sigma_{2y} + \sigma_{1z}\sigma_{2z}$$

$$\boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2}\,\{|0\rangle_1|0\rangle_2\} = |0\rangle_1|0\rangle_2$$

$$\sigma_x|0\rangle = |1\rangle \quad \sigma_y|0\rangle = i|1\rangle \quad \sigma_z|0\rangle = |0\rangle$$

$$\sigma_x|1\rangle = |0\rangle \quad \sigma_y|1\rangle = -i|0\rangle \quad \sigma_z|1\rangle = -|1\rangle$$

Eigenstates of the spinorial part

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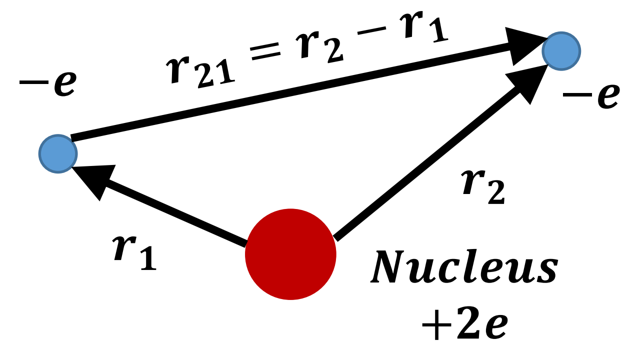
Triplet states



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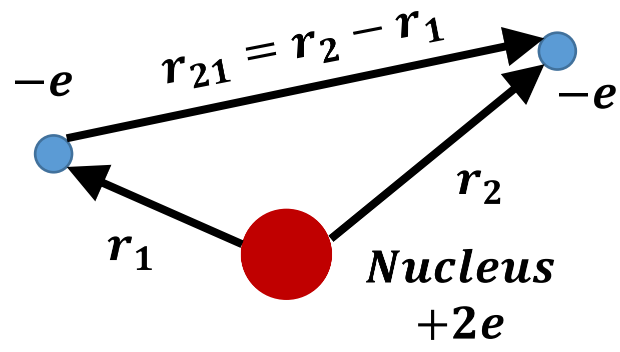
$$S^2\{|0\rangle_1 |0\rangle_2\} = 2\hbar^2 |0\rangle_1 |0\rangle_2 \qquad \boldsymbol{\sigma_1}\cdot\boldsymbol{\sigma_2}\,\{|0\rangle_1 |0\rangle_2\} = |0\rangle_1 |0\rangle_2$$

$$S_z\{|0\rangle_1 |0\rangle_2\} = \frac{\hbar}{2}(\sigma_{1z}|0\rangle_1 |0\rangle_2 + \sigma_{2z}|0\rangle_1 |0\rangle_2) = \hbar\, |0\rangle_1 |0\rangle_2$$

Eigenstates of the spinorial part

$$\Xi_S\,(s_1, s_2) = |0\rangle_1 |0\rangle_2$$
$$\Xi_S\,(s_1, s_2) = |1\rangle_1 |1\rangle_2$$
$$\Xi_S\,(s_1, s_2) = \frac{1}{\sqrt{2}}(|0\rangle_1 |1\rangle_2 + |1\rangle_1 |0\rangle_2)$$

Triplet states



$$\Xi_A\,(s_1, s_2) = \frac{1}{\sqrt{2}}(|0\rangle_1 |1\rangle_2 - |1\rangle_1 |0\rangle_2)$$

Singlet state

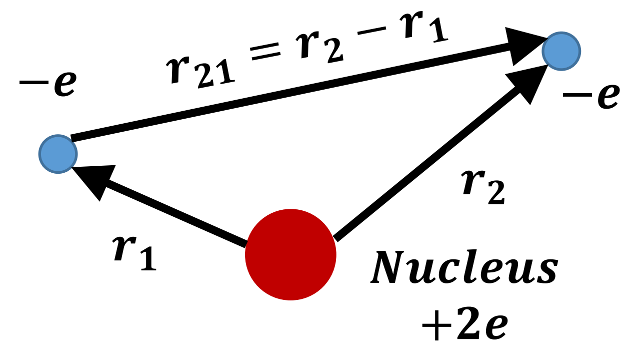
Spinorial part	S_z	S^2
$\|0\rangle_1 \|0\rangle_2$	$\hbar$	$2\hbar^2$
$\|1\rangle_1 \|1\rangle_2$	$-\hbar$	$2\hbar^2$
$(1/\sqrt{2})(\|0\rangle_1 \|1\rangle_2 + \|1\rangle_1 \|0\rangle_2)$	0	$2\hbar^2$
$(1/\sqrt{2})(\|0\rangle_1 \|1\rangle_2 - \|1\rangle_1 \|0\rangle_2)$	0	0

Application of perturbation theory

$$\phi_A(\boldsymbol{r_1}, s_1; \boldsymbol{r_2}, s_2) = \Psi_S\,(\boldsymbol{r_1}, \boldsymbol{r_2})\Xi_A\,(s_1, s_2)$$

or

$$\phi_A(\boldsymbol{r_1}, s_1; \boldsymbol{r_2}, s_2) = \Psi_A\,(\boldsymbol{r_1}, \boldsymbol{r_2})\Xi_S\,(s_1, s_2)$$



$$H_{He} = \frac{|\boldsymbol{p_1}|^2}{2m} + \frac{|\boldsymbol{p_2}|^2}{2m} + \frac{(2e)(-e)}{4\pi\epsilon_0|\boldsymbol{r_1}|} + \frac{(2e)(-e)}{4\pi\epsilon_0|\boldsymbol{r_2}|} + \frac{(-e)(-e)}{4\pi\epsilon_0|\boldsymbol{r_{21}}|}$$

$$H_{He}(\boldsymbol{r_1}, \boldsymbol{r_2})\Psi_{S,A}\,(\boldsymbol{r_1}, \boldsymbol{r_2}) = E\Psi_{S,A}\,(\boldsymbol{r_1}, \boldsymbol{r_2})$$

Perturbation

$$H_0 = H_1 + H_2$$

$$H_1 = \frac{|\boldsymbol{p_1}|^2}{2m} + \frac{(2e)(-e)}{4\pi\epsilon_0|\boldsymbol{r_1}|} \qquad H_2 = \frac{|\boldsymbol{p_2}|^2}{2m} + \frac{(2e)(-e)}{4\pi\epsilon_0|\boldsymbol{r_2}|}$$

Hydrogen atom with $Z = 2e$

Application of perturbation theory

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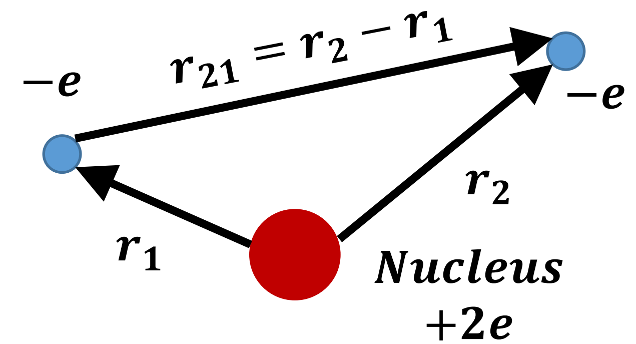

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$$\phi_i(\boldsymbol{r_1})\,\phi_j(\boldsymbol{r_2}) \to \epsilon_i + \epsilon_j$$

$i = j$ $\quad \Psi_S\,(\boldsymbol{r_1}, \boldsymbol{r_2}) = \phi_i(\boldsymbol{r_1})\,\phi_i(\boldsymbol{r_2})$

i, j are orbital states

$i \neq j$

$$\Psi_S\,(\boldsymbol{r_1}, \boldsymbol{r_2}) = \frac{1}{\sqrt{2}}\left[\phi_i(\boldsymbol{r_1})\,\phi_j(\boldsymbol{r_2}) + \phi_i(\boldsymbol{r_2})\,\phi_j(\boldsymbol{r_1})\right]$$

$$\Psi_A\,(\boldsymbol{r_1}, \boldsymbol{r_2}) = \frac{1}{\sqrt{2}}\left[\phi_i(\boldsymbol{r_1})\,\phi_j(\boldsymbol{r_2}) - \phi_i(\boldsymbol{r_2})\,\phi_j(\boldsymbol{r_1})\right]$$

Application of perturbation theory

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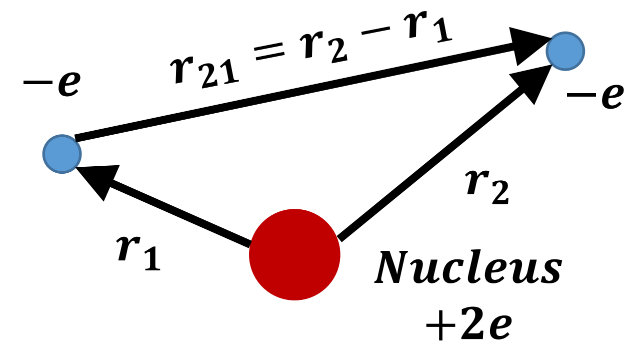

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$$\phi_i(\boldsymbol{r_1})\,\phi_j(\boldsymbol{r_2}) \rightarrow \epsilon_i + \epsilon_j$$

$$i = j \quad \Psi_S\,(\boldsymbol{r_1}, \boldsymbol{r_2}) = \phi_i(\boldsymbol{r_1})\,\phi_i(\boldsymbol{r_2})$$

$$\phi_A(\boldsymbol{r_1}, s_1; \boldsymbol{r_2}, s_2) = \frac{1}{\sqrt{2}}\phi_i(\boldsymbol{r_1})\,\phi_i(\boldsymbol{r_2})(|0\rangle_1|1\rangle_2 - |1\rangle_1|0\rangle_2)$$

$$E_i = 2\epsilon_i + E_C \qquad E_C = \left\langle \phi_A \middle| \frac{(-e)(-e)}{4\pi\epsilon_0|\boldsymbol{r_{21}}|} \middle| \phi_A \right\rangle$$

Application of perturbation theory

$$\phi_A(\boldsymbol{r_1}, s_1; \boldsymbol{r_2}, s_2) = \Psi_S\,(\boldsymbol{r_1}, \boldsymbol{r_2})\Xi_A\,(s_1, s_2)$$

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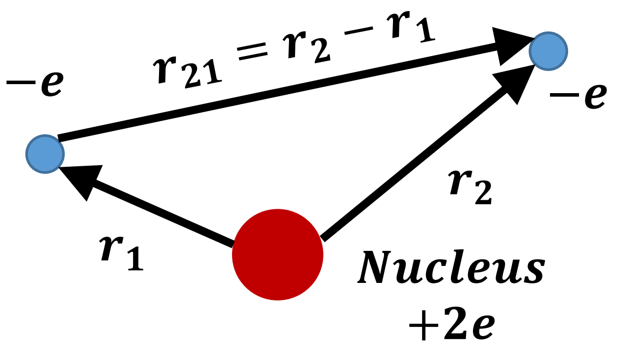

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$$E_C = \left\langle \phi_A \middle| \frac{(-e)(-e)}{4\pi\epsilon_0|\boldsymbol{r_{21}}|} \middle| \phi_A \right\rangle$$

$$E_C = \frac{e^2}{2}\int d\boldsymbol{r_1}\int d\boldsymbol{r_2}({}_1\langle 0|_2\langle 1| - {}_1\langle 1|_2\langle 0|)\left[\frac{|\phi_i(\boldsymbol{r_1})|^2|\phi_i(\boldsymbol{r_2})|^2}{4\pi\epsilon_0|\boldsymbol{r_{21}}|}\right](|0\rangle_1|1\rangle_2 - |1\rangle_1|0\rangle_2)$$

$$({}_1\langle 0|_2\langle 1| - {}_1\langle 1|_2\langle 0|)\,(|0\rangle_1|1\rangle_2 - |1\rangle_1|0\rangle_2) = 2$$

Application of perturbation theory

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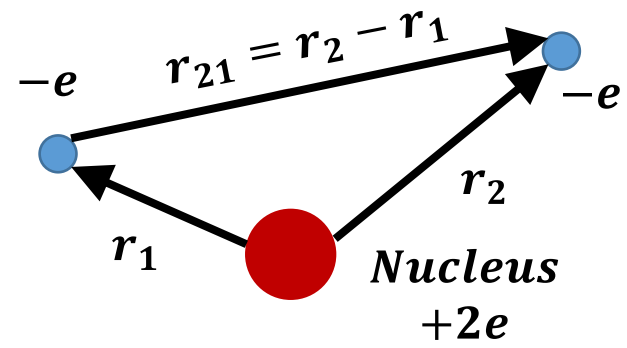

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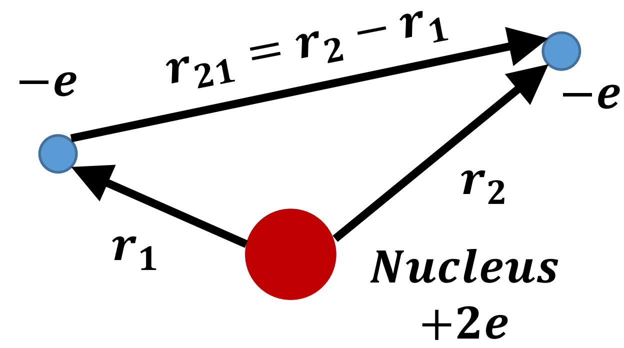
Coulomb repulsion

Coulomb repulsion term ($E_c = K_{1s1s}$)

$$K_{1s1s} = \int d\boldsymbol{r_1} \int d\boldsymbol{r_2} \left[\frac{e|\phi_{1s}(\boldsymbol{r_1})|^2 \, e|\phi_{1s}(\boldsymbol{r_2})|^2}{4\pi\epsilon_0 |\boldsymbol{r_{21}}|} \right]$$



$$\phi_{1s}(r) = \frac{1}{\sqrt{\pi a_{He}^3}} e^{-r/a_{He}}$$

$$a_{He} = a_0/2$$

$$K_{1s1s} = \frac{5e^2}{32\pi\epsilon_0 a_{He}}$$

$$E_{1s}(H\ atom) = -\frac{e^2}{4\pi\epsilon_0 2a_0}$$

Ground state for He

$$\frac{K_{1s1s}}{8E_{1s}} = -\frac{5}{16} = -0.3125$$

Application of perturbation theory

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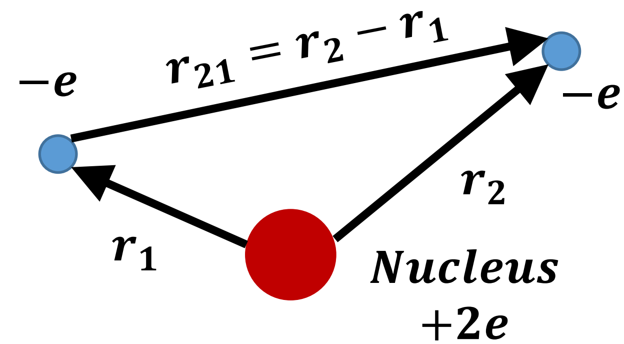

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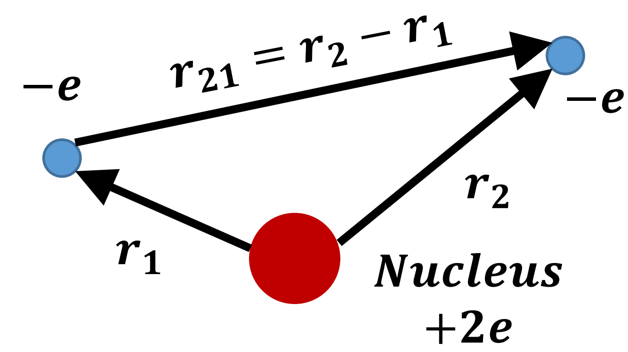
$$\phi_A(\boldsymbol{r_1}, s_1; \boldsymbol{r_2}, s_2) = \Psi_A\,(\boldsymbol{r_1}, \boldsymbol{r_2})\Xi_S\,(s_1, s_2)$$



$$H_{He} = \frac{|\boldsymbol{p_1}|^2}{2m} + \frac{|\boldsymbol{p_2}|^2}{2m} + \frac{(2e)(-e)}{4\pi\epsilon_0|\boldsymbol{r_1}|} + \frac{(2e)(-e)}{4\pi\epsilon_0|\boldsymbol{r_2}|} + \frac{(-e)(-e)}{4\pi\epsilon_0|\boldsymbol{r_{21}}|}$$

$i \neq j$

$$\Psi_S\,(\boldsymbol{r_1}, \boldsymbol{r_2}) = \frac{1}{\sqrt{2}}\left[\phi_i(\boldsymbol{r_1})\,\phi_j(\boldsymbol{r_2}) + \phi_i(\boldsymbol{r_2})\,\phi_j(\boldsymbol{r_1})\right]$$

$$E_i = \epsilon_i + \epsilon_j + E_S$$

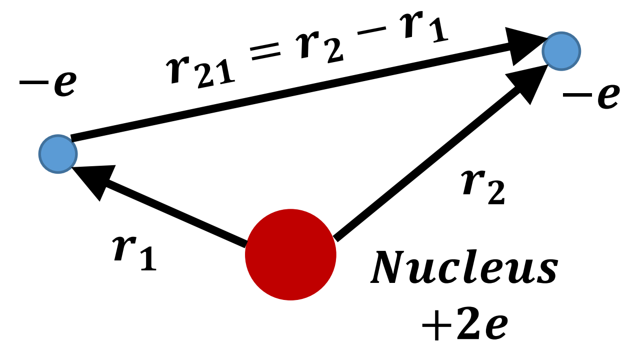
$$E_S = \frac{e^2}{2}\int d\boldsymbol{r_1}\int d\boldsymbol{r_2}\left[\frac{\left(\phi_i^*(\boldsymbol{r_1})\,\phi_j^*(\boldsymbol{r_2}) + \phi_i^*(\boldsymbol{r_2})\,\phi_j^*(\boldsymbol{r_1})\right)\left(\phi_i(\boldsymbol{r_1})\,\phi_j(\boldsymbol{r_2}) + \phi_i(\boldsymbol{r_2})\,\phi_j(\boldsymbol{r_1})\right)}{4\pi\epsilon_0|\boldsymbol{r_{12}}|}\right]$$

$$\langle \Xi_A\,(s_1, s_2)|\Xi_A\,(s_1, s_2)\rangle$$

$$E_S = K_{ij} + J_{ij}$$

Application of perturbation theory

$$\phi_A(\boldsymbol{r_1}, s_1; \boldsymbol{r_2}, s_2) = \Psi_S\,(\boldsymbol{r_1}, \boldsymbol{r_2})\Xi_A\,(s_1, s_2)$$



or

$$\phi_A(\boldsymbol{r_1}, s_1; \boldsymbol{r_2}, s_2) = \Psi_A\,(\boldsymbol{r_1}, \boldsymbol{r_2})\Xi_S\,(s_1, s_2)$$

$i \neq j$

$$\Psi_S\,(\boldsymbol{r_1}, \boldsymbol{r_2}) = \frac{1}{\sqrt{2}}\left[\phi_i(\boldsymbol{r_1})\,\phi_j(\boldsymbol{r_2}) + \phi_i(\boldsymbol{r_2})\,\phi_j(\boldsymbol{r_1})\right]$$

$$E_S = \frac{e^2}{2}\int d\boldsymbol{r_1}\int d\boldsymbol{r_2}\left[\frac{\left(\phi_i^*(\boldsymbol{r_1})\,\phi_j^*(\boldsymbol{r_2}) + \phi_i^*(\boldsymbol{r_2})\,\phi_j^*(\boldsymbol{r_1})\right)\left(\phi_i(\boldsymbol{r_1})\,\phi_j(\boldsymbol{r_2}) + \phi_i(\boldsymbol{r_2})\,\phi_j(\boldsymbol{r_1})\right)}{4\pi\epsilon_0|\boldsymbol{r_{21}}|}\right]$$

$$\langle\Xi_A\,(s_1, s_2)|\Xi_A\,(s_1, s_2)\rangle$$

$$E_S = K_{ij} + J_{ij}$$

$$K_{ij} = \int d\boldsymbol{r_1}\int d\boldsymbol{r_2}\left[\frac{e|\phi_i(\boldsymbol{r_1})|^2\,e\left|\phi_j(\boldsymbol{r_2})\right|^2}{4\pi\epsilon_0|\boldsymbol{r_{21}}|}\right]$$

Coulomb repulsion

Exchange interaction

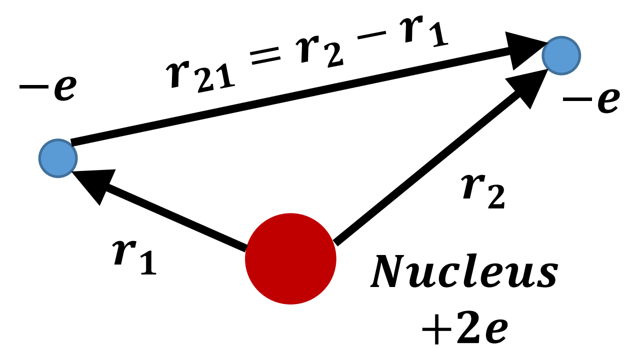
$$J_{ij} = e^2\int d\boldsymbol{r_1}\int d\boldsymbol{r_2}\left[\frac{\phi_i^*(\boldsymbol{r_1})\phi_j^*(\boldsymbol{r_2})\phi_i(\boldsymbol{r_2})\,\phi_j(\boldsymbol{r_1})}{4\pi\epsilon_0|\boldsymbol{r_{21}}|}\right]$$

Exchange interaction: Overlap charge density

$$\phi_A(\boldsymbol{r_1}, s_1; \boldsymbol{r_2}, s_2) = \Psi_S\,(\boldsymbol{r_1}, \boldsymbol{r_2})\Xi_A\,(s_1, s_2)$$

or

$$\phi_A(\boldsymbol{r_1}, s_1; \boldsymbol{r_2}, s_2) = \Psi_A\,(\boldsymbol{r_1}, \boldsymbol{r_2})\Xi_S\,(s_1, s_2)$$



$i \neq j$

$$\Psi_S\,(\boldsymbol{r_1}, \boldsymbol{r_2}) = \frac{1}{\sqrt{2}}\left[\phi_i(\boldsymbol{r_1})\,\phi_j(\boldsymbol{r_2}) + \phi_i(\boldsymbol{r_2})\,\phi_j(\boldsymbol{r_1})\right]$$

$$E_S = \frac{e^2}{2}\int d\boldsymbol{r_1}\int d\boldsymbol{r_2}\left[\frac{\left(\phi_i^*(\boldsymbol{r_1})\,\phi_j^*(\boldsymbol{r_2}) + \phi_i^*(\boldsymbol{r_2})\,\phi_j^*(\boldsymbol{r_1})\right)\left(\phi_i(\boldsymbol{r_1})\,\phi_j(\boldsymbol{r_2}) + \phi_i(\boldsymbol{r_2})\,\phi_j(\boldsymbol{r_1})\right)}{4\pi\epsilon_0|\boldsymbol{r_{21}}|}\right]$$

$$\langle \Xi_A\,(s_1, s_2) | \Xi_A\,(s_1, s_2)\rangle$$

$$E_S = K_{ij} + J_{ij}$$

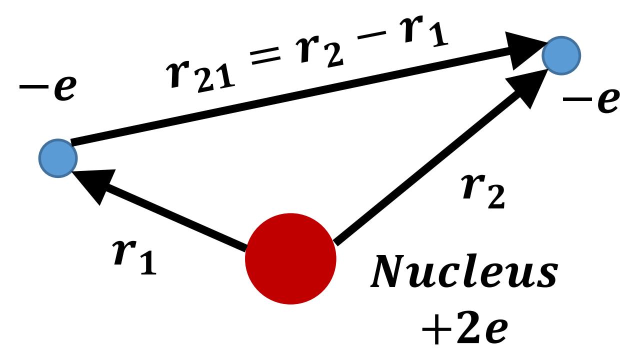
$$\rho_{ij}(\boldsymbol{r_1}) = \phi_i^*(\boldsymbol{r_1})\,\phi_j(\boldsymbol{r_1})$$

$$\rho_{ij}(\boldsymbol{r_2}) = \phi_j^*(\boldsymbol{r_2})\,\phi_i(\boldsymbol{r_2})$$

$$J_{ij} = e^2\int d\boldsymbol{r_1}\int d\boldsymbol{r_2}\left[\frac{\rho_{ij}(\boldsymbol{r_1})\rho_{ij}(\boldsymbol{r_2})}{4\pi\epsilon_0|\boldsymbol{r_{21}}|}\right]$$

$$J_{ij} = e^2\int d\boldsymbol{r_1}\int d\boldsymbol{r_2}\left[\frac{\phi_i^*(\boldsymbol{r_1})\phi_j^*(\boldsymbol{r_2})\phi_i(\boldsymbol{r_2})\,\phi_j(\boldsymbol{r_1})}{4\pi\epsilon_0|\boldsymbol{r_{21}}|}\right]$$

Heisenberg model of ferromagnetism



$$\phi_A(\boldsymbol{r_1}, s_1; \boldsymbol{r_2}, s_2) = \Psi_S\,(\boldsymbol{r_1}, \boldsymbol{r_2})\Xi_A\,(s_1, s_2)$$

or

$$\phi_A(\boldsymbol{r_1}, s_1; \boldsymbol{r_2}, s_2) = \Psi_A\,(\boldsymbol{r_1}, \boldsymbol{r_2})\Xi_S\,(s_1, s_2)$$

$i \neq j$

$$\Psi_A\,(\boldsymbol{r_1}, \boldsymbol{r_2}) = \frac{1}{\sqrt{2}}\left[\phi_i(\boldsymbol{r_1})\,\phi_j(\boldsymbol{r_2}) - \phi_i(\boldsymbol{r_2})\,\phi_j(\boldsymbol{r_1})\right]$$

Singlet state

$$E_S = K_{ij} + J_{ij}$$

Triplet states

$$E_T = K_{ij} - J_{ij}$$

$$\rho_{ij}(\boldsymbol{r_1}) = \phi_i^*(\boldsymbol{r_1})\,\phi_j(\boldsymbol{r_1})$$

$$\rho_{ij}(\boldsymbol{r_2}) = \phi_j^*(\boldsymbol{r_2})\,\phi_i(\boldsymbol{r_2})$$

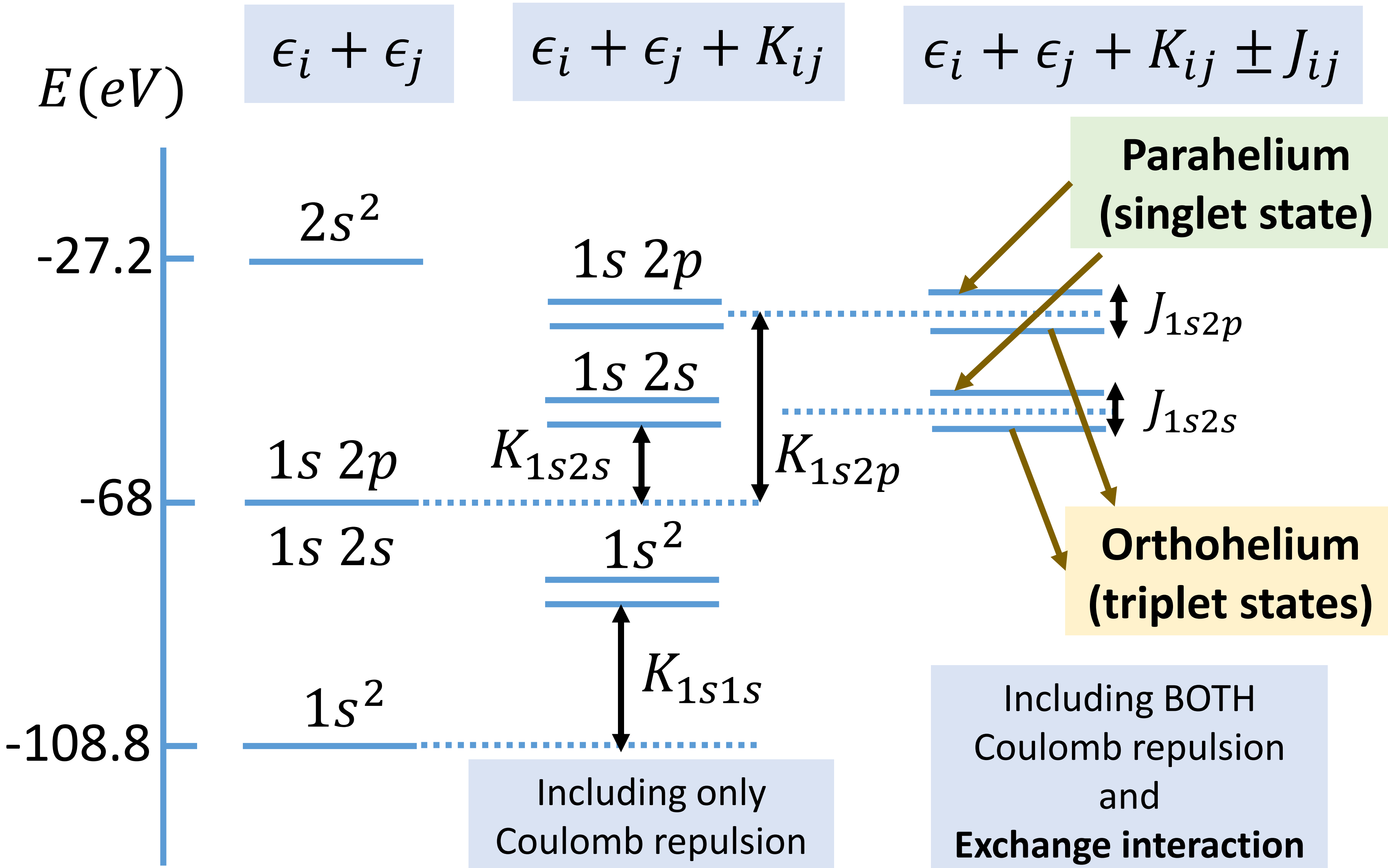
$$J_{ij} = e^2 \int d\boldsymbol{r_1} \int d\boldsymbol{r_2} \left[\frac{\rho_{ij}(\boldsymbol{r_1})\rho_{ij}(\boldsymbol{r_2})}{4\pi\epsilon_0 |\boldsymbol{r_{21}}|}\right]$$

$$E_T - E_S = -2J_{ij}$$

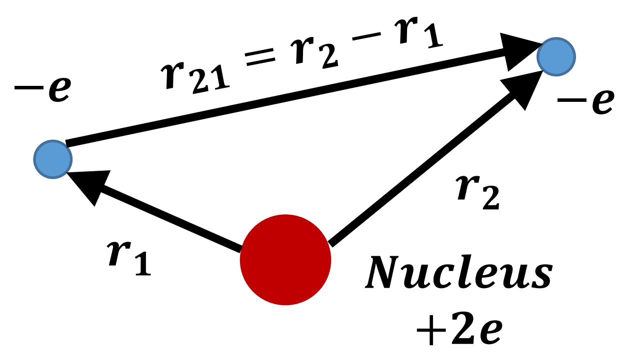
$$H_{ij} = -2J_{ij}\boldsymbol{S_1} \cdot \boldsymbol{S_2}$$

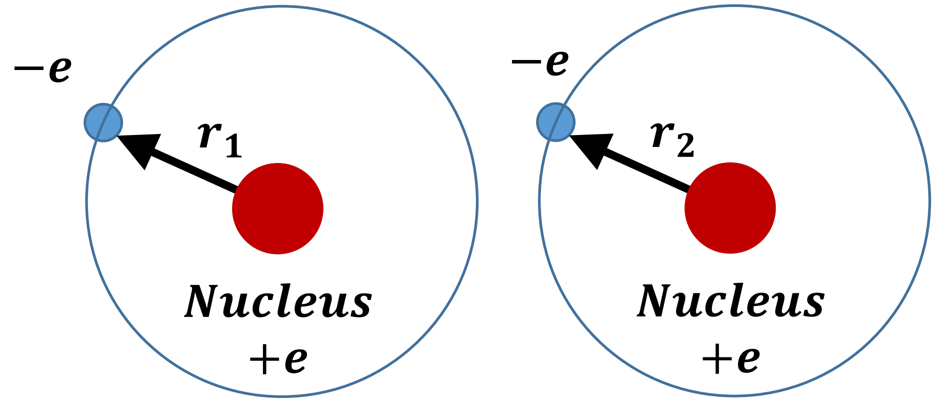
J_{ij} positive → ferromagnetism

Energy levels of Helium atom



Helium atom versus Hydrogen molecule





ONE confining potential

TWO confining potential

Parahelium (singlet state)

Orthohelium (triplet states)

Orthohydrogen (triplet states)

Parahydrogen (singlet state)

Hydrogen molecule: Singlet state is at the lower energy state