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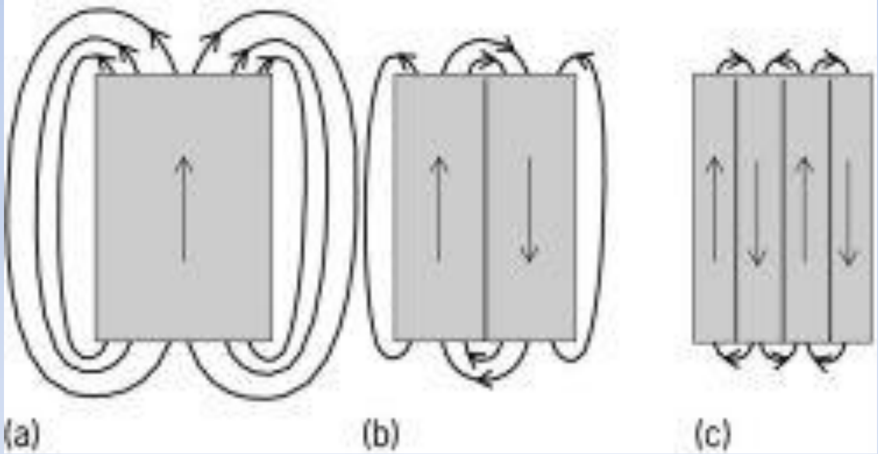
Физика магнетизма и рассеяние поляризованных и неполяризованных нейтронов

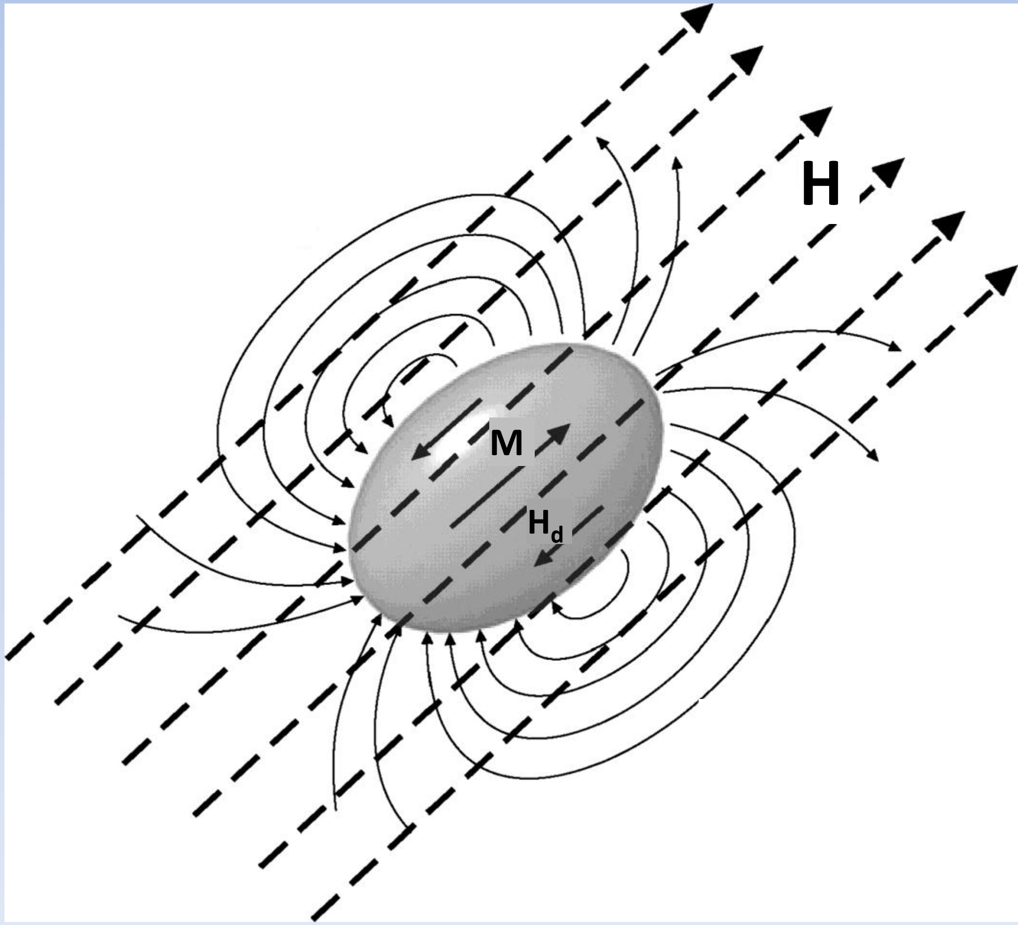
Лекция 5. Взаимодействие магнитных атомов в твердом теле.

Магнитное дипольное взаимодействие

$$\mathcal{H}_{d-d} = \frac{(\boldsymbol{\mu}_1 \cdot \boldsymbol{\mu}_2)\, r^2 - 3(\mathbf{r} \cdot \boldsymbol{\mu}_1)(\mathbf{r} \cdot \boldsymbol{\mu}_2)}{r^5}$$

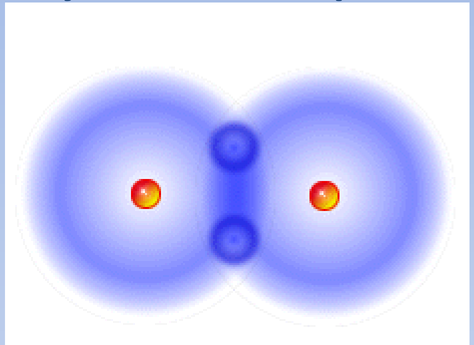
$$\omega_0 = 4\pi \frac{(g\mu_B)^2}{\mathrm{v}_0} \sim 1\,\mathrm{K}$$





Природа обменного взаимодействия

Молекула водорода



$$\mathcal{H} = \left(\frac{p_1^2}{2m} - \frac{e^2}{\left|\mathbf{R}_a - \mathbf{r}_1\right|} \right) + \left(\frac{p_2^2}{2m} - \frac{e^2}{\left|\mathbf{R}_b - \mathbf{r}_2\right|} \right) + U$$

$$U = e^2 \left(\frac{1}{\left|\mathbf{R}_a - \mathbf{R}_b\right|} + \frac{1}{\left|\mathbf{r}_1 - \mathbf{r}_2\right|} - \frac{1}{\left|\mathbf{R}_b - \mathbf{r}_1\right|} - \frac{1}{\left|\mathbf{R}_a - \mathbf{r}_2\right|} \right)$$

$$\Psi_S(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2(1+\gamma^2)}} \left(\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) + \psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1) \right) \chi_S$$

$$\boxed{\gamma = \int \psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_1)\, d\mathbf{r}_1}$$

$$\Psi_A(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2(1-\gamma^2)}} \left(\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) - \psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1) \right) \chi_A$$

$$\boxed{\begin{aligned} \psi_a(\mathbf{r}) &= \psi(\mathbf{r} - \mathbf{R}_a) \\ \psi_b(\mathbf{r}) &= \psi(\mathbf{r} - \mathbf{R}_b) \end{aligned}}$$

$$\chi_S = \frac{1}{\sqrt{2}} \left(\left|\uparrow\right\rangle_1 \left|\downarrow\right\rangle_2 - \left|\downarrow\right\rangle_1 \left|\uparrow\right\rangle_2 \right)$$

$$\chi_A = \frac{1}{\sqrt{2}} \left(\left|\uparrow\right\rangle_1 \left|\downarrow\right\rangle_2 + \left|\downarrow\right\rangle_1 \left|\uparrow\right\rangle_2 \right); \quad \left|\uparrow\right\rangle_1 \left|\uparrow\right\rangle_2; \quad \left|\downarrow\right\rangle_1 \left|\downarrow\right\rangle_2$$

$$U_S(r) = \int d\mathbf{r}_1 d\mathbf{r}_2 \Psi_S(\mathbf{r}_1,\mathbf{r}_2)\mathcal{H}\Psi_S(\mathbf{r}_1,\mathbf{r}_2) = 2E_0 + \frac{A(r)+B(r)}{1+\gamma^2}$$

$$U_A(r) = \int d\mathbf{r}_1 d\mathbf{r}_2 \Psi_A(\mathbf{r}_1,\mathbf{r}_2)\mathcal{H}\Psi_A(\mathbf{r}_1,\mathbf{r}_2) = 2E_0 + \frac{A(r)-B(r)}{1-\gamma^2}$$

$$A(r) = \int d\mathbf{r}_1 d\mathbf{r}_2 U \psi_a^2(\mathbf{r}_1)\psi_b^2(\mathbf{r}_2)$$ электростатическая энергия

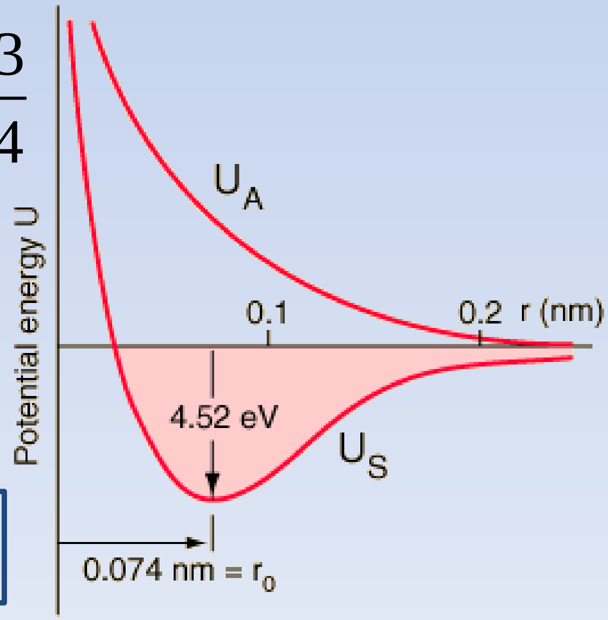
$$B(r) = \int d\mathbf{r}_1 d\mathbf{r}_2 U \psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_1)\psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_2)$$ обменная энергия

$$\boxed{B(r)<0}$$

$$\mathcal{H}_{eff} = J(r)(\mathbf{S}_1\cdot\mathbf{S}_2) + E(r)$$

$$(\mathbf{S}_1\cdot\mathbf{S}_2) = \frac{1}{2}(\mathbf{S}_1+\mathbf{S}_2)^2 - \frac{1}{2}(\mathbf{S}_1^2+\mathbf{S}_2^2) = \frac{1}{2}S(S+1) - \frac{3}{4}$$

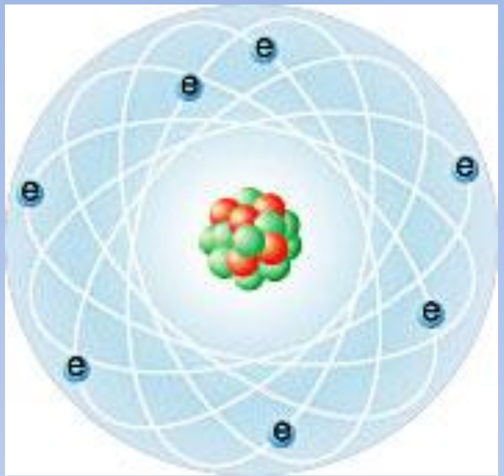
$$\begin{cases} J(r)\frac{1}{4} + E(r) = U_A(r) \\ J(r)\left(-\frac{3}{4}\right) + E(r) = U_S(r) \end{cases}$$



антиферромагнитный обмен

$$\boxed{J(r) = U_A(r) - U_S(r) > 0}$$

Первое правило Хунда. Ферромагнитный обмен.



$$\mathcal{H}=\left(\frac{p_1^2}{2m}+\frac{p_2^2}{2m}+\hat{U}(\mathbf{r}_1,\mathbf{r}_2)\right)+\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}$$

$$\Psi_S(\mathbf{r}_1,\mathbf{r}_2)=\left(\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2)+\psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1)\right)\chi_S/\sqrt{2}$$

$$\Psi_A(\mathbf{r}_1,\mathbf{r}_2)=\left(\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2)-\psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1)\right)\chi_A/\sqrt{2}$$

$$U_S=\int d\mathbf{r}_1 d\mathbf{r}_2 \Psi_S(\mathbf{r}_1,\mathbf{r}_2)\mathcal{H}\Psi_S(\mathbf{r}_1,\mathbf{r}_2)=\varepsilon_a+\varepsilon_b+A+B$$

$$U_A=\int d\mathbf{r}_1 d\mathbf{r}_2 \Psi_A(\mathbf{r}_1,\mathbf{r}_2)\mathcal{H}\Psi_A(\mathbf{r}_1,\mathbf{r}_2)=\varepsilon_a+\varepsilon_b+A-B$$

$$\boxed{J=U_A-U_S=-2B<0}$$

$$A=\int d\mathbf{r}_1 d\mathbf{r}_2\left|\psi_a(\mathbf{r}_1)\right|^2\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}\left|\psi_b(\mathbf{r}_1)\right|^2$$

$$B=\int d\mathbf{r}_1 d\mathbf{r}_2 \psi_a(\mathbf{r}_1)\psi_b^*(\mathbf{r}_1)\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}\psi_a^*(\mathbf{r}_2)\psi_b(\mathbf{r}_2)$$

$$=\frac{4\pi e^2}{V}\sum_{\mathbf{k}}\frac{1}{k^2}\left|\int d\mathbf{r}\,\psi_a(\mathbf{r})\psi_b^*(\mathbf{r})e^{i\mathbf{k}\mathbf{r}}\right|^2>0$$

$$\boxed{\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}=\frac{1}{V}\sum_{\mathbf{k}}\frac{4\pi e^2}{k^2}e^{i\mathbf{k}(\mathbf{r}_1-\mathbf{r}_2)}}$$

Обменное взаимодействие в кристалле

$$\mathcal{H}=\sum_{\alpha=1}^{N}\frac{p_\alpha^2}{2m}-\sum_{i,\alpha}\frac{e^2}{\left|\mathbf{R}_i-\mathbf{r}_\alpha\right|}+\frac{1}{2}\sum_{\alpha,\beta}\frac{e^2}{\left|\mathbf{r}_\alpha-\mathbf{r}_\beta\right|}$$

$$\left[\frac{p_\alpha^2}{2m}-\frac{e^2}{\left|\mathbf{R}_i-\mathbf{r}_\alpha\right|}\right]\psi_i\left(\mathbf{r}_\alpha\right)=E_0\psi_i\left(\mathbf{r}_\alpha\right)$$

$$-\frac{1}{2}J_{ij}=\int d\mathbf{r}_\alpha d\mathbf{r}_\beta \psi_i^*\left(\mathbf{r}_\alpha\right)\psi_j^*\left(\mathbf{r}_\alpha\right)\left(\frac{e^2}{\left|\mathbf{r}_\alpha-\mathbf{r}_\beta\right|}-\frac{e^2}{\left|\mathbf{R}_j-\mathbf{r}_\alpha\right|}-\frac{e^2}{\left|\mathbf{R}_i-\mathbf{r}_\beta\right|}\right)\psi_i\left(\mathbf{r}_\beta\right)\psi_j\left(\mathbf{r}_\beta\right)$$

$$\boxed{\mathcal{H}=\frac{1}{2}\sum_{i\neq j}J_{ij}\left(\mathbf{S}_i\cdot\mathbf{S}_j\right)}$$

$$\mathbf{S}=\sum_i\mathbf{S}_i \qquad \mathcal{H}\mathbf{S}=\mathbf{S}\mathcal{H}$$

Критерий ферромагнетизма

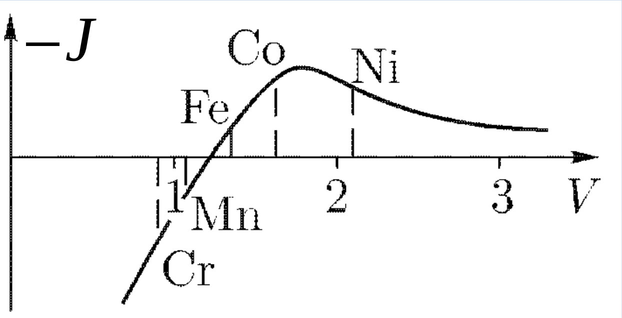
$$-\frac{1}{2}J_{i,j}=\int d\mathbf{r}_\alpha d\mathbf{r}_\beta \psi_i^*(\mathbf{r}_\alpha)\psi_j^*(\mathbf{r}_\alpha)\left(\frac{e^2}{|\mathbf{r}_\alpha-\mathbf{r}_\beta|}-\frac{e^2}{|\mathbf{R}_j-\mathbf{r}_\alpha|}-\frac{e^2}{|\mathbf{R}_i-\mathbf{r}_\beta|}\right)\psi_i(\mathbf{r}_\beta)\psi_j(\mathbf{r}_\beta)$$

$$J_{i,j}<0$$

$$\int d\mathbf{r}_\alpha d\mathbf{r}_\beta \psi_i^*(\mathbf{r}_\alpha)\psi_j^*(\mathbf{r}_\alpha)\frac{e^2}{|\mathbf{r}_\alpha-\mathbf{r}_\beta|}\psi_i(\mathbf{r}_\beta)\psi_j(\mathbf{r}_\beta)>$$

$$>\int d\mathbf{r}_\alpha d\mathbf{r}_\beta \psi_i^*(\mathbf{r}_\alpha)\psi_j^*(\mathbf{r}_\alpha)\left(\frac{e^2}{|\mathbf{R}_j-\mathbf{r}_\alpha|}+\frac{e^2}{|\mathbf{R}_i-\mathbf{r}_\beta|}\right)\psi_i(\mathbf{r}_\beta)\psi_j(\mathbf{r}_\beta)$$

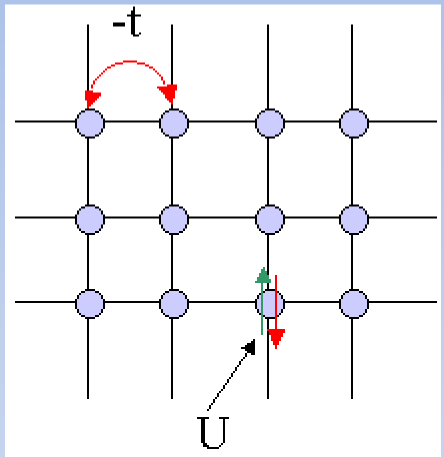
Металл	Незаполненная оболочка	V	Температура Кюри, К
Ti	$3d$	1,12	
Cr	$3d$	1,13	
Mn	$3d$	1,47	
Fe	$3d$	1,63	1040
Co	$3d$	1,82	1400
Ni	$3d$	1,97	630
Mo	$4d$	0,92	
Gd	$4f$	3,1	290
W	$5d$	0,79	
Pt	$5d$	1,23	



Модель Хаббарда

$$\mathcal{H} = -t\sum_{s=\uparrow,\downarrow}\left(c_{1s}^{+}c_{2s} + c_{2s}^{+}c_{1s}\right) + U\sum_{i=1,2} n_{i\uparrow}n_{i\downarrow} \qquad n_{is} = c_{is}^{+}c_{is}$$

основные состояния: $\left|\uparrow,\downarrow\right\rangle \quad \left|\downarrow,\uparrow\right\rangle \quad \left|\uparrow,\uparrow\right\rangle \quad \left|\downarrow,\downarrow\right\rangle$



возбужденные состояния: $\left|\uparrow\downarrow,0\right\rangle \quad \left|0,\uparrow\downarrow\right\rangle$

$$\Delta E_1 = 0$$

$$\Delta E_2 : \qquad \sum_n \left\langle\downarrow,\uparrow\right|\mathcal{H}^t\left|n\right\rangle \frac{1}{-U}\left\langle n\right|\mathcal{H}^t\left|\uparrow,\downarrow\right\rangle$$

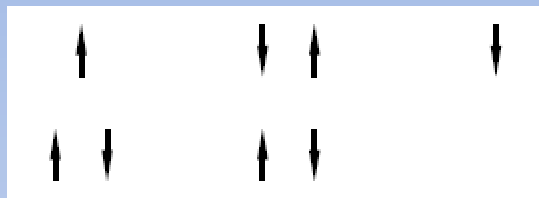
$$-\frac{2t^2}{U}\begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix} = \varepsilon\begin{pmatrix}a\\ b\end{pmatrix} \quad \Rightarrow \quad \varepsilon = 0, \begin{pmatrix}1\\ 1\end{pmatrix} \qquad \varepsilon = -\frac{4t^2}{U}, \begin{pmatrix}1\\ -1\end{pmatrix}$$

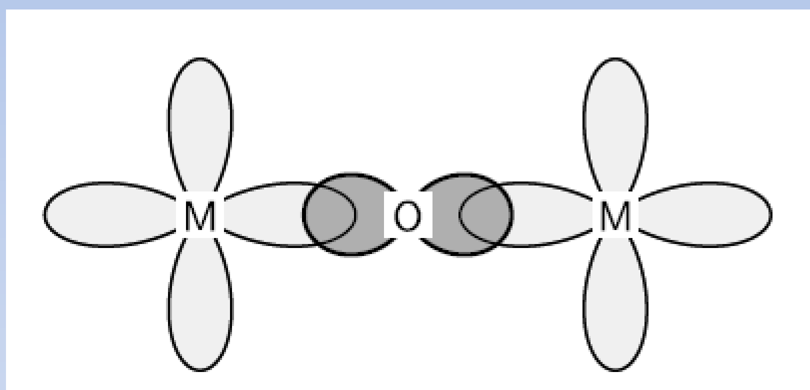
$$\mathcal{H}_{eff} = J\left(\mathbf{S}_1\cdot\mathbf{S}_2\right) \qquad J = \frac{4t^2}{U}$$

$$\frac{t^4}{U^3}\left(\mathbf{S}_1\cdot\mathbf{S}_2\right)^2$$

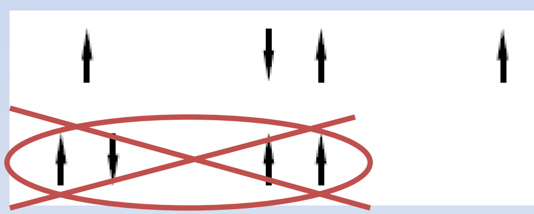
Косвенный обмен (superexchange)

АФ

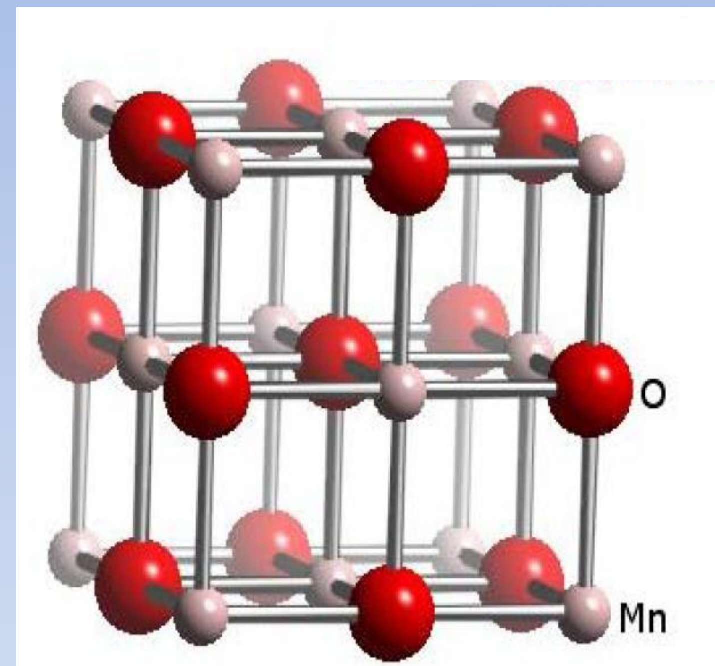




ФМ



MnO

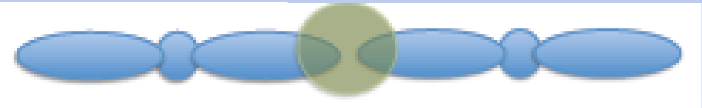


$$J = \frac{2t_{MM}^2}{U}$$

Правила Гуденафа-Канамори (Goodenough-Kanamori rules)

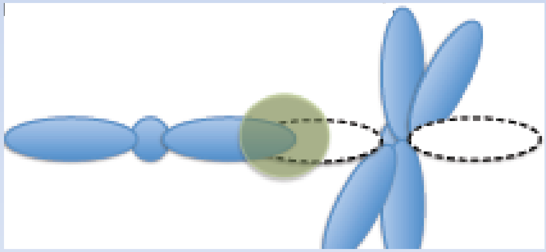
Между двумя магнитными ионами, взаимодействующими друг с другом через немагнитный ион, реализуется

1) **сильный антиферромагнитный обмен**, если орбитали ионов заполнены наполовину,

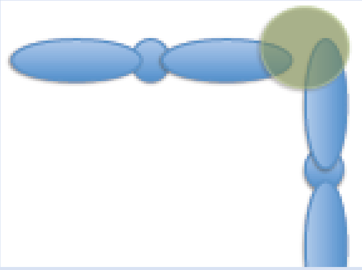


2) **слабый ферромагнитный обмен** в случаях заполнения орбиталей

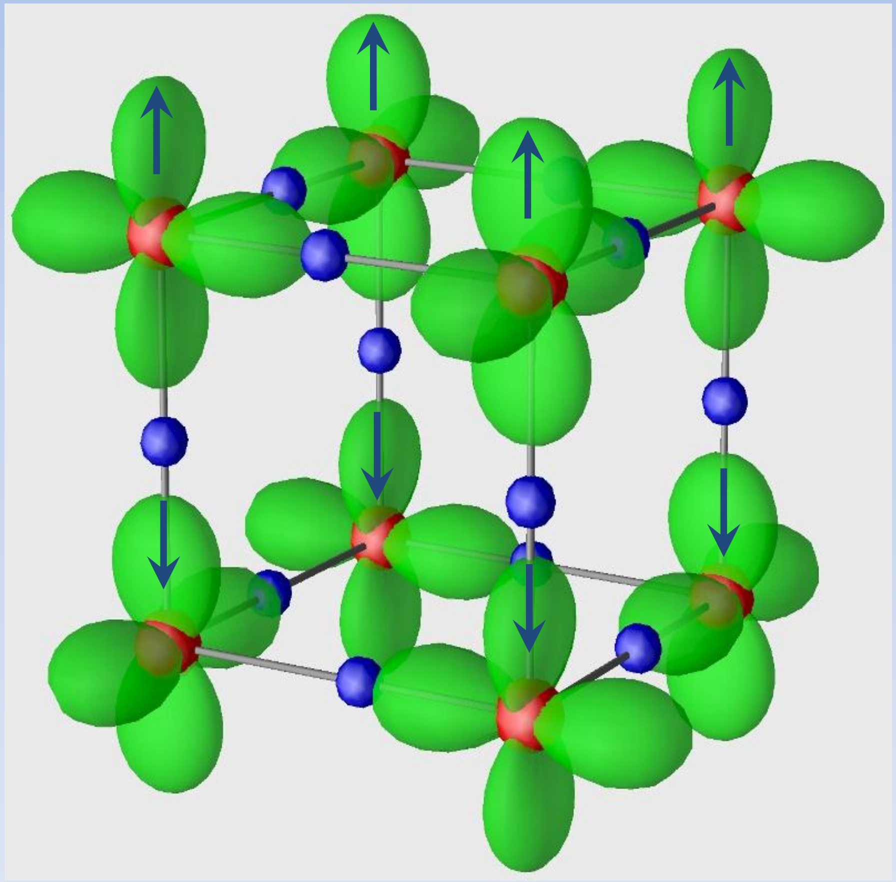
a) полностью ⇔ наполовину ⇔ пустая



b) наполовину, 90°



Квази-1D АФ
$KCuF_3$

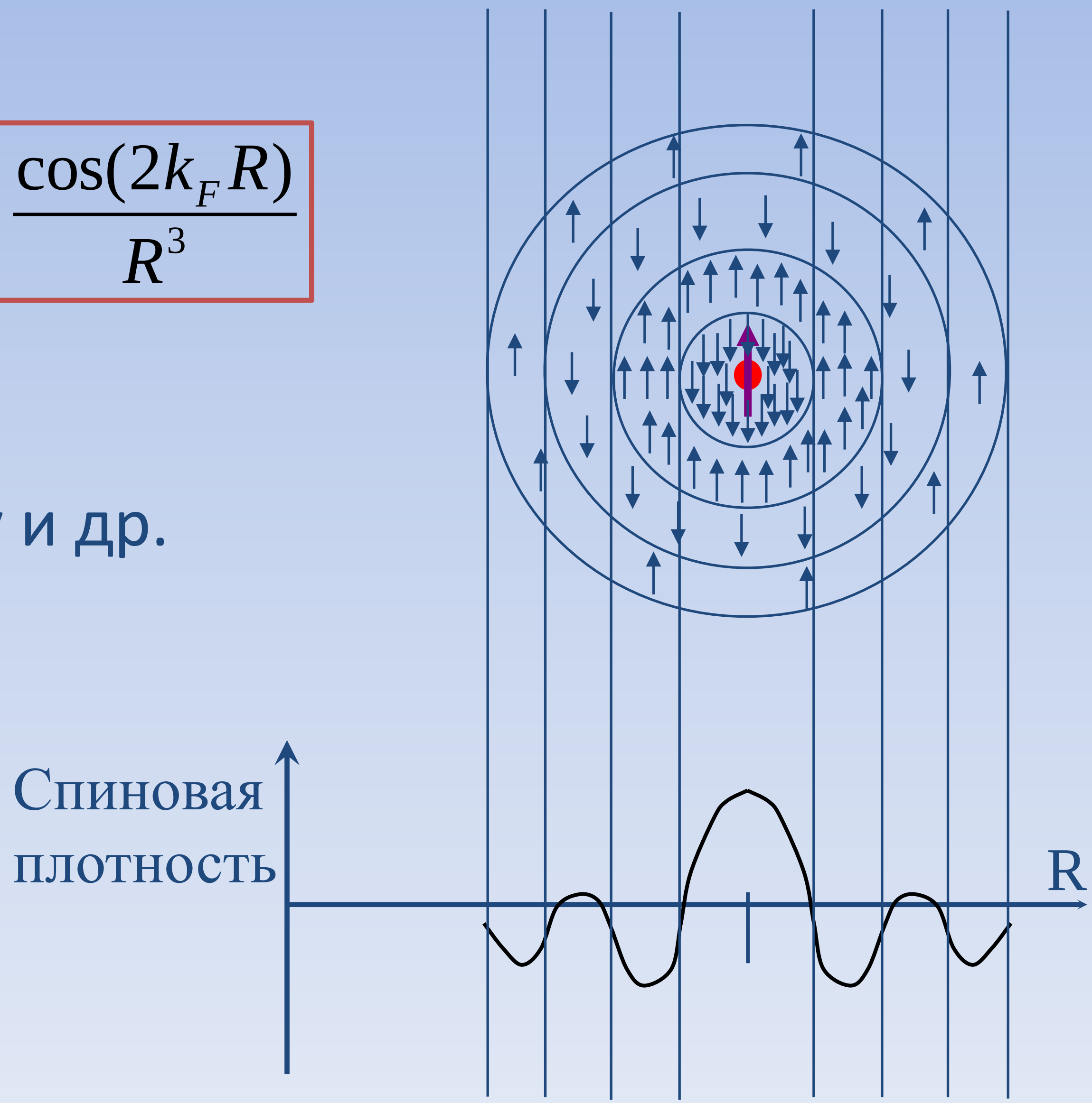


Косвенный обмен в металлах

Взаимодействие RKKY (Ruderman, Kittel, Kasuya, Yosida).

$$J_{RKKY}(R) \sim \frac{\cos(2k_F R)}{R^3}$$

Пример: Ho, Dy и др.

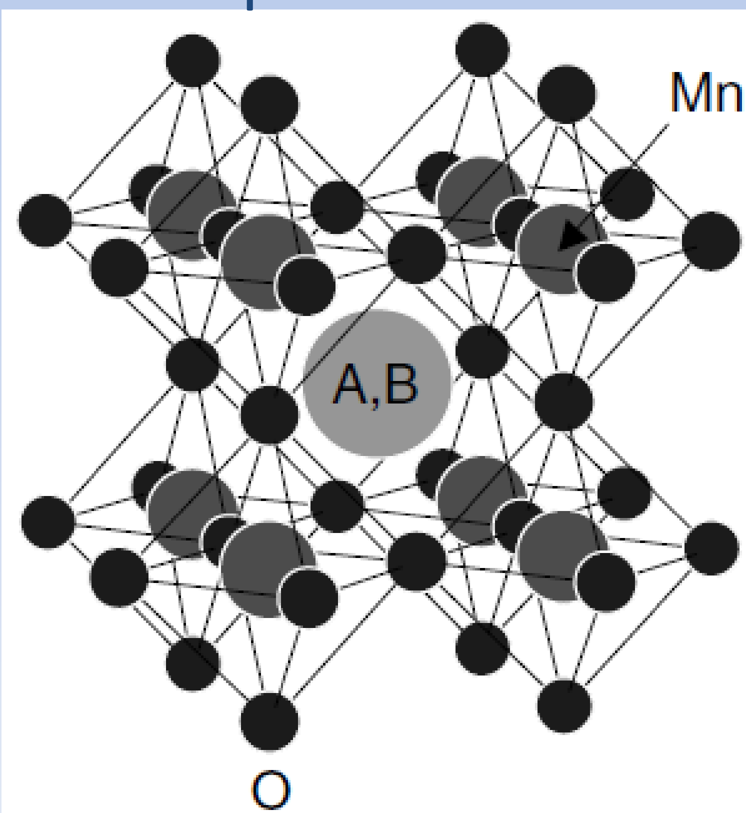


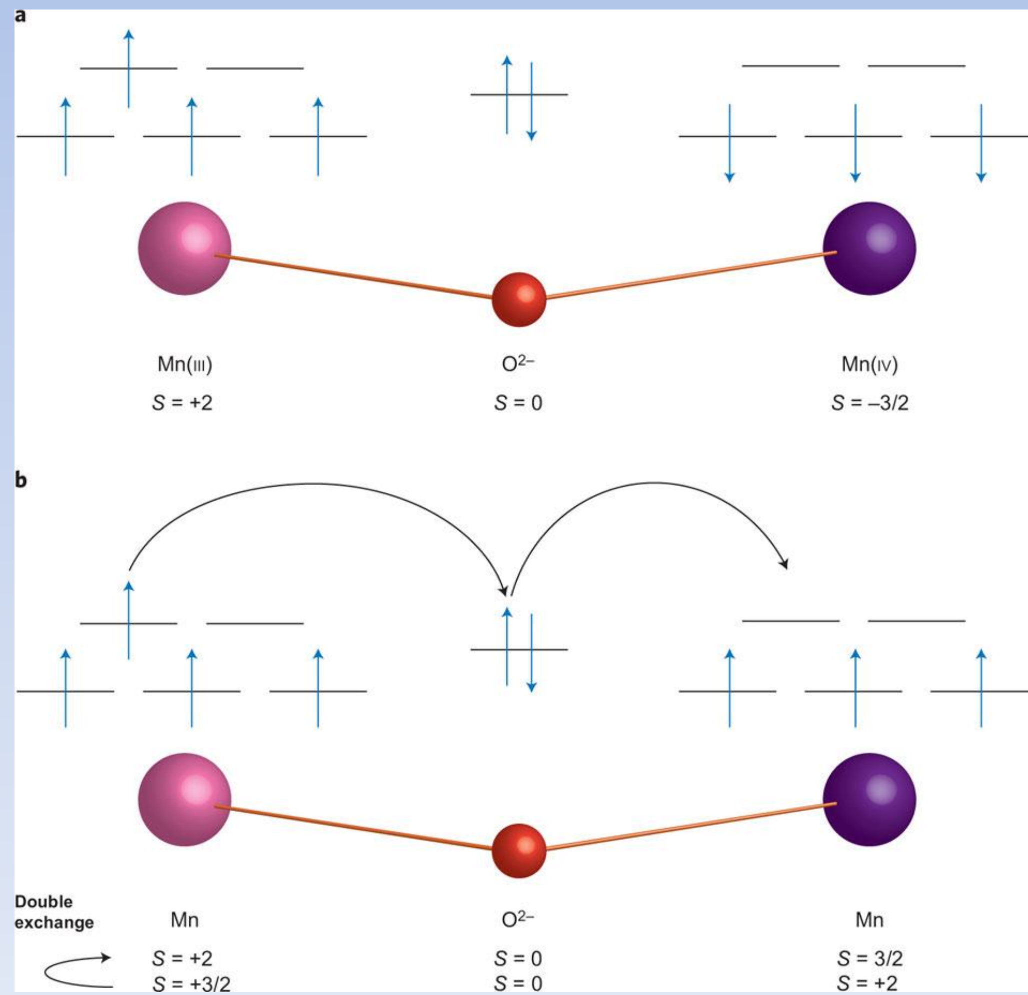
Двойной обмен (double exchange)

Вещества с магнитными ионами **смешанной валентности** (mixed valency) такие, как Mn, Fe и др.

<u>Пример:</u> $La_{1-x}Sr_xMnO_3$ при x>0.175, где Sr^{2+}, La^{3+} и Mn^{3+}, Mn^{4+}

При x=0 и x=1 – АФ изолятор

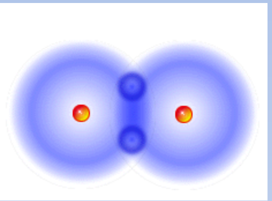




Анизотропный обмен

$$\mathcal{H} = \frac{1}{2}\sum_{i\neq j} J_{ij}\left(\mathbf{s}_i \cdot \mathbf{s}_j\right) \qquad \mathbf{S} = \sum_i \mathbf{s}_i \qquad \mathcal{H}\mathbf{S} = \mathbf{S}\mathcal{H}$$

$$\mathcal{H}_{aniso} = \frac{1}{2}\sum_{i\neq j}\left(J_{ij}^{xx} s_i^x s_j^x + J_{ij}^{yy} s_i^y s_j^y + J_{ij}^{zz} s_i^z s_j^z\right) \qquad \mathcal{H}_{aniso}\mathbf{S} \neq \mathbf{S}\mathcal{H}_{aniso}$$



$$\mathcal{H} = \lambda\left(\mathbf{L}_1 \cdot \mathbf{S}_1\right) + \lambda\left(\mathbf{L}_2 \cdot \mathbf{S}_2\right) + U\left(\mathbf{r}_1, \mathbf{r}_2\right)$$

$$\Delta E_3 = \lambda^2 \sum_{n_1, m_1} \frac{\langle g_1 g_2 | \mathbf{L}_1 \cdot \mathbf{S}_1 | n_1 g_2 \rangle \langle n_1 g_2 | U | m_1 g_2 \rangle \langle m_1 g_2 | \mathbf{L}_1 \cdot \mathbf{S}_1 | g_1 g_2 \rangle}{\left(E_{n_1} - E_{g_1}\right)\left(E_{m_1} - E_{g_1}\right)}$$

$$+\left(1 \leftrightarrow 2\right)$$

$$\Psi_{Snm}\left(\mathbf{r}_1, \mathbf{r}_2\right) = \frac{1}{\sqrt{2\left(1 + \left|\gamma_{nm}\right|^2\right)}}\left(\psi_n\left(\mathbf{r}_1\right)\psi_m\left(\mathbf{r}_2\right) + \psi_n\left(\mathbf{r}_2\right)\psi_m\left(\mathbf{r}_1\right)\right)\chi_S$$

$$\gamma_{nm} = \int \psi_n^*\left(\mathbf{r}_1\right)\psi_m\left(\mathbf{r}_1\right) d\mathbf{r}_1$$

$$\Psi_{Anm}\left(\mathbf{r}_1, \mathbf{r}_2\right) = \frac{1}{\sqrt{2\left(1 - \left|\gamma_{nm}\right|^2\right)}}\left(\psi_n\left(\mathbf{r}_1\right)\psi_m\left(\mathbf{r}_2\right) - \psi_n\left(\mathbf{r}_2\right)\psi_m\left(\mathbf{r}_1\right)\right)\chi_A$$

$$\int d\mathbf{r}_1 d\mathbf{r}_2 \Psi^*_{Sn_1g_2}(\mathbf{r}_1,\mathbf{r}_2) U(\mathbf{r}_1,\mathbf{r}_2) \Psi_{Sm_1g_2}(\mathbf{r}_1,\mathbf{r}_2) = \frac{A(n_1g_2;m_1g_2)+B(n_1g_2;m_1g_2)}{1+|\gamma_{nm}|^2}$$

$$\int d\mathbf{r}_1 d\mathbf{r}_2 \Psi^*_{An_1g_2}(\mathbf{r}_1,\mathbf{r}_2) U(\mathbf{r}_1,\mathbf{r}_2) \Psi_{Am_1g_2}(\mathbf{r}_1,\mathbf{r}_2) = \frac{A(n_1g_2;m_1g_2)-B(n_1g_2;m_1g_2)}{1-|\gamma_{nm}|^2}$$

$$A(n_1g_2;m_1g_2) = \int d\mathbf{r}_1 d\mathbf{r}_2 \psi_{m_1}(\mathbf{r}_1)\psi^*_{n_1}(\mathbf{r}_1) U(\mathbf{r}_1,\mathbf{r}_2) \left|\psi_{g_2}(\mathbf{r}_2)\right|^2$$

$$B(n_1g_2;m_1g_2) = \int d\mathbf{r}_1 d\mathbf{r}_2 \psi_{g_2}(\mathbf{r}_1)\psi^*_{n_1}(\mathbf{r}_1) U(\mathbf{r}_1,\mathbf{r}_2) \psi^*_{g_2}(\mathbf{r}_2)\psi_{m_1}(\mathbf{r}_2)$$

$$\boxed{\Delta E_3 \to \mathcal{H}_{aniso} = \sum_{\mu\nu}\left(S_1^\mu \Gamma^{(1)}_{\mu\nu}(\mathbf{S}_1\cdot\mathbf{S}_2) S_1^\nu + S_2^\mu \Gamma^{(2)}_{\mu\nu}(\mathbf{S}_1\cdot\mathbf{S}_2) S_2^\nu\right)}$$

$$\Gamma^{(1)}_{\mu\nu} \cong \lambda^2 \sum_{n_1,m_1} \frac{\langle g_1g_2|L_1^\mu|n_1g_2\rangle J(n_1g_2;m_1g_2)\langle m_1g_2|L_1^\nu|g_1g_2\rangle}{(E_{n_1}-E_{g_1})(E_{m_1}-E_{g_1})}$$

$$\boxed{S=\frac{1}{2} \qquad \mathcal{H}_{aniso} = \frac{1}{4}\sum_{\mu,\nu}\sum_{i=1,2}\left[\left(\Gamma^{(i)}_{\mu\nu}+\Gamma^{(i)}_{\nu\mu}\right)-\delta_{\mu\nu}\left(\Gamma^{(i)}_{xx}+\Gamma^{(i)}_{yy}+\Gamma^{(i)}_{zz}\right)\right]S_2^\nu S_1^\mu}$$

Взаимодействие Дзялошинского-Мориа

$$\mathcal{H}_{DM} = -\lambda \sum_{n_1} \frac{\langle g_1 | \mathbf{L}_1 \cdot \mathbf{S}_1 | n_1 \rangle \langle n_1 g_2 | U | g_1 g_2 \rangle + \langle g_1 g_2 | U | n_1 g_2 \rangle \langle n_1 | \mathbf{L}_1 \cdot \mathbf{S}_1 | g_1 \rangle}{E_{n_1} - E_{g_1}}$$

$$-\lambda \sum_{n_2} \frac{\langle g_2 | \mathbf{L}_2 \cdot \mathbf{S}_2 | n_2 \rangle \langle g_1 n_2 | U | g_1 g_2 \rangle + \langle g_1 g_2 | U | g_1 n_2 \rangle \langle n_2 | \mathbf{L}_2 \cdot \mathbf{S}_2 | g_2 \rangle}{E_{n_2} - E_{g_2}}$$

$$\cong 2\lambda \sum_{\mu} \sum_{n_1} \frac{J\left(n_1 g_2; g_1 g_2\right) \langle g_1 | L_1^{\mu} | n_1 \rangle \left[S_1^{\mu}, (\mathbf{S}_1 \cdot \mathbf{S}_2) \right]}{E_{n_1} - E_{g_1}}$$

$$+2\lambda \sum_{\mu} \sum_{n_2} \frac{J\left(g_1 n_2; g_1 g_2\right) \langle g_2 | L_2^{\mu} | n_2 \rangle \left[S_2^{\mu}, (\mathbf{S}_1 \cdot \mathbf{S}_2) \right]}{E_{n_2} - E_{g_2}}$$

$$\left[\mathbf{S}_2, (\mathbf{S}_1 \cdot \mathbf{S}_2) \right] = i \left[\mathbf{S}_1 \times \mathbf{S}_2 \right]$$

$$\boxed{\mathcal{H}_{DM} = \mathbf{D} \cdot \left[\mathbf{S}_1 \times \mathbf{S}_2 \right]}$$

$$\mathbf{D} = -2i\lambda \left(\sum_{n_1} \frac{J\left(n_1 g_2; g_1 g_2\right) \langle g_1 | \mathbf{L}_1 | n_1 \rangle}{E_{n_1} - E_{g_1}} - \sum_{n_2} \frac{J\left(g_1 n_2; g_1 g_2\right) \langle g_2 | \mathbf{L}_2 | n_2 \rangle}{E_{n_2} - E_{g_2}} \right)$$