Spin Orbital Exchange in Mott Insulator [Mostovoy]

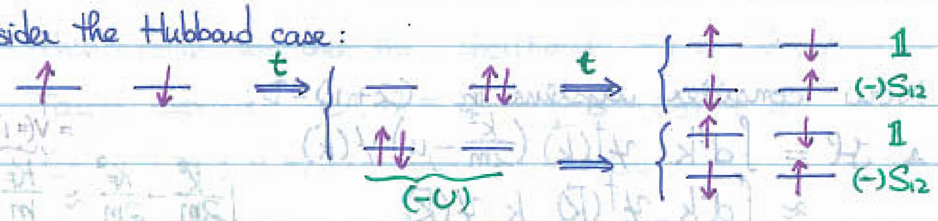
$$\mathcal{H} = -t\sum(c^\dagger_{i\sigma}c_{j\sigma} + h.c.) + U\sum n_{i\uparrow}n_{i\downarrow} \quad ; \langle n_i\rangle = 1,\ U > \underbrace{W}_{\text{band width}}$$

Neglecting t, ground state highly degenerate.

Perturbation theory $\Longrightarrow$ $\mathcal{H}_{eff} = J\sum \vec{S}_i \cdot \vec{S}_j$ $[J \propto t^2]$

But in real problems we have multi-band, hence both orbital and spin degeneracies.

Consider the Hubbard case:



$$\Longrightarrow \mathcal{H}_{12} = -\frac{2t^2}{U}(\mathbb{1} - S_{12})$$

In spin space, $S_{12} = P_{S=1} - P_{S=0} = 2(\vec{S}_1 \cdot \vec{S}_2) + \frac{1}{2}$

Combining, $\mathcal{H}_{eff} = \frac{4t^2}{U}(\vec{S}_1 \cdot \vec{S}_2 - \frac{1}{4})$

Next consider 3d transition metals.

Spherical harmonics broken down by lattice structure:

$\{Y^3_m\} \longrightarrow \{e_g\} + \{t_{2g}\}$

e_g : $3z^2 - r^2$; $x^2 - y^2$

t_{2g} : xy ; yz ; xz

$\{e_g\}$ and $\{t_{2g}\}$ are irreps under cubic symmetry group.

e.g. $4_z : (x,y,z) \mapsto (y,-x,z)$; $3_{[111]} : (x,y,z) \mapsto (z,x,y)$

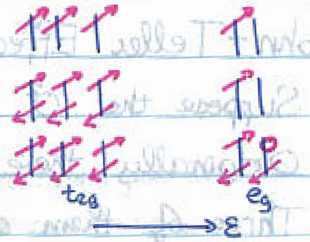
For octahedral anion coordination $\mathcal{E}_{e_g} > \mathcal{E}_{t_{2g}}$.

For tetrahedral anion coordination $\mathcal{E}_{t_{2g}} > \mathcal{E}_{e_g}$

Examples: Mn^{3+} (d^4) in $LaMnO_3$

Ni^{3+} (d^7) in $NaNiO_2$

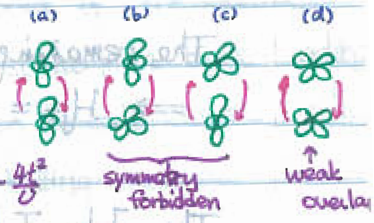
Cu^{2+} (d^9) in $KCuF_3$



[Hund's fa...

These are e_g materials with orbital degeneracy.

Now consider $e_g - e_g$ magnetic exchanges:



$$\mathcal{H}_a = -\frac{4t^2}{U}\left(\frac{1}{2}+T_1^z\right)\left(\frac{1}{2}+T_2^z\right)\left(\frac{1}{4}-\vec{S}_1\cdot\vec{S}_2\right)$$

where $T^z|3z^2-r^2\rangle = \frac{1}{2}|3z^2-r^2\rangle$; $T^z|x^2-y^2\rangle = -\frac{1}{2}|x^2-y^2\rangle$

For (b) and (c) there is virtual level interaction:

$$\mathcal{H}_{b+c} = -\frac{t^2}{U'-J_H\left(\frac{3}{4}+\vec{S}_1\cdot\vec{S}_2\right)}\left[\left(\frac{1}{2}-T_1^z\right)\left(\frac{1}{2}+T_2^z\right)+(1\leftrightarrow 2)\right]$$

$$\approx \left[-\frac{t^2}{U'}-\frac{t^2J_H}{U'^2}\left(\frac{3}{4}+\vec{S}_1\cdot\vec{S}_2\right)\right]\left[\left(\frac{1}{2}-T_1^z\right)\left(\frac{1}{2}+T_2^z\right)+(1\leftrightarrow 2)\right]$$

Note $\mathcal{H}_a$ is antiferro while $\mathcal{H}_{b+c}$ is ferro.

Using x-basis and y-basis for pseudo-spin, we can analyze the x-axis and y-axis exchange.

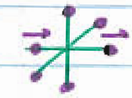
Turns out: $\begin{cases} I^x = -\frac{1}{2}T^z - \frac{\sqrt{3}}{2}T^x \\ I^y = -\frac{1}{2}T^z + \frac{\sqrt{3}}{2}T^x \\ I^z = T^z \end{cases}$ with $\begin{cases} T^z = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \\ T^x = \frac{1}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\end{cases}$

$$\Rightarrow \mathcal{H} = \frac{4t^2}{U}\sum_n\sum_{\alpha=x,y,z}\left(\frac{1}{2}+I_n^\alpha\right)\left(\frac{1}{2}+I_{n+\alpha}^\alpha\right)\left(\vec{S}_n\cdot\vec{S}_{n+\alpha}-\frac{1}{4}\right)$$
$$+\sum_{n,\alpha}\left(-\frac{2t^2}{U}\right)\left(1+\frac{J_H}{U}\vec{S}_n\cdot\vec{S}_{n+\alpha}\right)\left(\frac{1}{4}-I_n^\alpha I_{n+\alpha}^\alpha\right)$$

NOTE: We don't have  since the virtual hop is always between two 's.

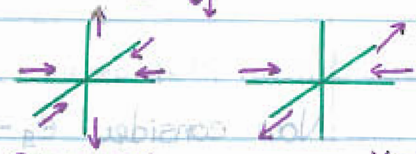
John-Teller Effect.

Suppose the O^{2-} atom moves only along radial axis.
Originally there will be 6 degree of freedom.
Three of them are ferroelectric: $w_\alpha = \frac{1}{\sqrt{2}}(u_x - u_{-\alpha})$



For the remaining, one is a breathing mode

The remaining are compatible with E_g:



$Q_z = \frac{2v_z - v_x - v_y}{\sqrt{6}}$ $\quad$ $Q_x = \frac{v_y - v_x}{\sqrt{2}}$

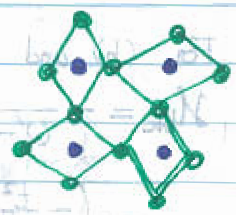
$$\Longrightarrow \mathcal{H}_{JT} = -g(T^z Q_z + T^x Q_x)$$

The John-Teller effect is then captured by:

$$E = g(T^z Q_z + T^x Q_x) + \frac{K}{2}(Q_z^2 + Q_x^2)$$

There can be cooperative John-Teller effect:

$$H_{eff} = \frac{2g^2}{3K} T_1^z T_2^z$$



- Unlike the e_g orbital, in t_{2g} orbital, orbital exchange can occur.