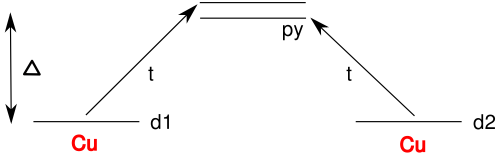
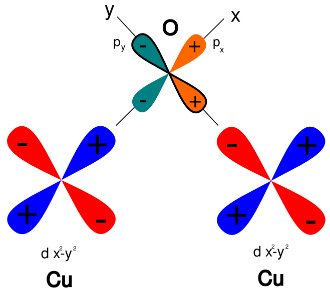
Solid state physics III

Exercise session 3

October 2nd 2025

(A.) In this exercise, we propose to describe an exchange mechanism which, unlike the simple two-site computation, leads to a ferromagnetic coupling. We consider a system composed of two atoms of copper and one atom of oxygen.





Each copper brings an electron to the system (total of two electrons in the system). For reasons of symmetry, one of the electrons can hop only between the orbital d_1 and the orbital p_x while the other can hop only between the orbital d_2 and the orbital p_y. The Hamiltonian that describes such a system is given by

$$\mathcal{H} = \mathcal{H}_\Delta + \mathcal{H}_H + \mathcal{H}_t \tag{1}$$

The term $\mathcal{H}_\Delta$ takes into account that the d levels of copper have a lower energy than the p orbitals of oxygen. H_Δ is written as:

$$\mathcal{H}_\Delta = \Delta\left[n_{p_x,\uparrow} + n_{p_x,\downarrow} + n_{p_y,\uparrow} + n_{p_y,\downarrow}\right] \qquad \Delta > 0 \tag{2}$$

The term $\mathcal{H}_H$ is the Hund coupling between two electrons on the orbitals of oxygen. This is a ferromagnetic Heisenberg coupling. In terms of the of creation and annihilation operators, it takes the form (see previous series):

$$\mathcal{H}_H = -J_H\left[\frac{1}{4}(n_{p_x,\uparrow} - n_{p_x,\downarrow})(n_{p_y,\uparrow} - n_{p_y,\downarrow}) + \frac{1}{2}(p^\dagger_{x,\uparrow}p_{x,\downarrow}p^\dagger_{y,\downarrow}p_{y,\uparrow} + p^\dagger_{x,\downarrow}p_{x,\uparrow}p^\dagger_{y,\uparrow}p_{y,\downarrow})\right] \qquad J_H > 0 \tag{3}$$

The kinetic term $\mathcal{H}_t$ is given by:

$$\mathcal{H}_t = -t\sum_\sigma p^\dagger_{x,\sigma}d_{1,\sigma} + d^\dagger_{1,\sigma}p_{x,\sigma} + p^\dagger_{y,\sigma}d_{2,\sigma} + d^\dagger_{2,\sigma}p_{y,\sigma} \tag{4}$$

In this problem Δ sets the energy scale and we consider the case $t \ll J_H \ll \Delta$. $\mathcal{H}_t$ will thus be treated as a perturbation of $\mathcal{H}_0 = \mathcal{H}_\Delta + \mathcal{H}_H$. In degenerate perturbation theory, the effective Hamiltonian up to 4th order reads:

$$\begin{aligned}\mathcal{H}^{(4)}_{\text{eff}} \quad = \quad & E_0P_0 + P_0VP_0 + P_0VSVP_0 + P_0VSVSVP_0 - \tfrac{1}{2}P_0VP_0VS^2VP_0 - \tfrac{1}{2}P_0VS^2VP_0VP_0 \\ & + P_0VSVSVSVP_0 - \tfrac{1}{2}P_0VS^2VP_0VSVP_0 - \tfrac{1}{2}P_0VSVP_0VS^2VP_0 + \tfrac{1}{2}P_0VP_0VP_0VS^3VP_0 \\ & + \tfrac{1}{2}P_0VS^3VP_0VP_0VP_0 - \tfrac{1}{2}P_0VP_0VS^2VSVP_0 - \tfrac{1}{2}P_0VSVS^2VP_0VP_0 - \tfrac{1}{2}P_0VP_0VSVS^2VP_0 \\ & - \tfrac{1}{2}P_0VS^2VSVP_0VP_0\end{aligned} \tag{5}$$

where P_0 is the projector on the fundamental subspace, $S = \frac{1-P_0}{E_0 - \mathcal{H}_0}$ and $V = \mathcal{H}_t$.
We choose to work in the basis $\mathcal{B} = \left\{ |T^1_{Cu,Cu}\rangle, |T^0_{Cu,Cu}\rangle, |T^{-1}_{Cu,Cu}\rangle, |S_{Cu,Cu}\rangle, |T^1_{Cu,O}\rangle, \dots \right\}$ defined as follows:

$$
\begin{array}{ll}
|T^1_{Cu,Cu}\rangle = d^\dagger_{1,\uparrow} d^\dagger_{2,\uparrow}|0\rangle & |T^1_{Cu,O}\rangle = d^\dagger_{1,\uparrow} p^\dagger_{y,\uparrow}|0\rangle \\
|T^0_{Cu,Cu}\rangle = \frac{1}{\sqrt{2}}(d^\dagger_{1,\uparrow} d^\dagger_{2,\downarrow} + d^\dagger_{1,\downarrow} d^\dagger_{2,\uparrow})|0\rangle & |T^0_{Cu,O}\rangle = \frac{1}{\sqrt{2}}(d^\dagger_{1,\uparrow} p^\dagger_{y,\downarrow} + d^\dagger_{1,\downarrow} p^\dagger_{y,\uparrow})|0\rangle \\
|T^{-1}_{Cu,Cu}\rangle = d^\dagger_{1,\downarrow} d^\dagger_{2,\downarrow}|0\rangle & |T^{-1}_{Cu,O}\rangle = d^\dagger_{1,\downarrow} p^\dagger_{y,\downarrow}|0\rangle \\
|S_{Cu,Cu}\rangle = \frac{1}{\sqrt{2}}(d^\dagger_{1,\uparrow} d^\dagger_{2,\downarrow} - d^\dagger_{1,\downarrow} d^\dagger_{2,\uparrow})|0\rangle & |S_{Cu,O}\rangle = \frac{1}{\sqrt{2}}(d^\dagger_{1,\uparrow} p^\dagger_{y,\downarrow} - d^\dagger_{1,\downarrow} p^\dagger_{y,\uparrow})|0\rangle \\
\\
|T^1_{O,Cu}\rangle = p^\dagger_{x,\uparrow} d^\dagger_{2,\uparrow}|0\rangle & |T^1_{O,O}\rangle = p^\dagger_{x,\uparrow} p^\dagger_{y,\uparrow}|0\rangle \\
|T^0_{O,Cu}\rangle = \frac{1}{\sqrt{2}}(p^\dagger_{x,\uparrow} d^\dagger_{2,\downarrow} + p^\dagger_{x,\downarrow} d^\dagger_{2,\uparrow})|0\rangle & |T^0_{O,O}\rangle = \frac{1}{\sqrt{2}}(p^\dagger_{x,\uparrow} p^\dagger_{y,\downarrow} + p^\dagger_{x,\downarrow} p^\dagger_{y,\uparrow})|0\rangle \\
|T^{-1}_{O,Cu}\rangle = p^\dagger_{x,\downarrow} d^\dagger_{2,\downarrow}|0\rangle & |T^{-1}_{O,O}\rangle = p^\dagger_{x,\downarrow} p^\dagger_{y,\downarrow}|0\rangle \\
|S_{O,Cu}\rangle = \frac{1}{\sqrt{2}}(p^\dagger_{x,\uparrow} d^\dagger_{2,\downarrow} - p^\dagger_{x,\downarrow} d^\dagger_{2,\uparrow})|0\rangle & |S_{O,O}\rangle = \frac{1}{\sqrt{2}}(p^\dagger_{x,\uparrow} p^\dagger_{y,\downarrow} - p^\dagger_{x,\downarrow} p^\dagger_{y,\uparrow})|0\rangle
\end{array}
\tag{6}
$$

1. Show that the states $|S_{\alpha,\beta}\rangle$ $\alpha, \beta \in \{Cu, O\}$ are singlets. This amounts to showing that $(S^-_\alpha + S^-_\beta)|S_{\alpha,\beta}\rangle = 0$ and that $(S^z_\alpha + S^z_\beta)|S_{\alpha,\beta}\rangle = 0$.

2. Show that the states $|T^\gamma_{\alpha,\beta}\rangle$ $\alpha, \beta \in \{Cu, O\}$, $\gamma \in \{1, 0, -1\}$ are triplets. This amounts to showing that:

$$
\begin{aligned}
&(S^z_\alpha + S^z_\beta)|T^1_{\alpha,\beta}\rangle = |T^1_{\alpha,\beta}\rangle \\
&(S^z_\alpha + S^z_\beta)|T^{-1}_{\alpha,\beta}\rangle = -1|T^{-1}_{\alpha,\beta}\rangle \\
&(S^z_\alpha + S^z_\beta)|T^0_{\alpha,\beta}\rangle = 0 \quad \text{and} \quad \langle S_{\alpha,\beta}|T^0_{\alpha,\beta}\rangle = 0.
\end{aligned}
\tag{7}
$$

3. Show that in the $\mathcal{B}$ basis, the Hamiltonian $\mathcal{H}_0$ is diagonal. What are the eigen energies and eigen vectors.

4. Convince yourself that:

$$
\begin{array}{lcl}
V|T^\alpha_{Cu,Cu}\rangle = -t\left(|T^\alpha_{O,Cu}\rangle + |T^\alpha_{Cu,O}\rangle\right) & \text{and that} & V|S_{Cu,Cu}\rangle = -t\left(|S_{O,Cu}\rangle + |S_{Cu,O}\rangle\right) \\
V|T^\alpha_{Cu,O}\rangle = -t\left(|T^\alpha_{O,O}\rangle + |T^\alpha_{Cu,Cu}\rangle\right) & & V|S_{Cu,O}\rangle = -t\left(|S_{O,O}\rangle + |S_{Cu,Cu}\rangle\right) \\
V|T^\alpha_{O,Cu}\rangle = -t\left(|T^\alpha_{O,O}\rangle + |T^\alpha_{Cu,Cu}\rangle\right) & & V|S_{O,Cu}\rangle = -t\left(|S_{O,O}\rangle + |S_{Cu,Cu}\rangle\right) \\
V|T^\alpha_{O,O}\rangle = -t\left(|T^\alpha_{Cu,O}\rangle + |T^\alpha_{O,Cu}\rangle\right) & & V|S_{O,O}\rangle = -t\left(|S_{Cu,O}\rangle + |S_{O,Cu}\rangle\right)
\end{array}
\tag{8}
$$

5. In the previous question it has been shown that the perturbation does not couple the ground subspace to itself. Show that $P_0 V P_0 = 0$ and that the terms of order 3 in V in (5) vanish. The effective Hamiltonian is reduced to:

$$
\mathcal{H}^{(4)}_{\text{eff}} = E_0 P_0 + P_0 V S V P_0 + P_0 V S V S V S V P_0 - \frac{1}{2}(P_0 V S^2 V P_0 V S V P_0 + P_0 V S V P_0 V S^2 V P_0) \tag{9}
$$

6. Calculate $\mathcal{H}^{(2)}_{\text{eff}} = P_0 V S V P_0$

7. Calculate $P_0 V S^2 V P_0 V S V P_0$ and by symmetry $P_0 V S V P_0 V S^2 V P_0$

8. Calculate $P_0 V S V S V S$

9. Deduce $\mathcal{H}^{(4)}_{\text{eff}}$. What are the spin configurations that are favored?

(B.) Holstein-Primakoff bosons: The Holstein-Primakoff transformation is given by

$$\begin{cases} S_+ = \left(\sqrt{2s - b^\dagger b}\right) b \\ S_- = b^\dagger \left(\sqrt{2s - b^\dagger b}\right) \\ S_z = s - b^\dagger b \end{cases} \tag{10}$$

with $b^\dagger$ (b) bosonic creation (annihilation) operators:

$$[b, b^\dagger] = 1 \ , \ [b, b] = [b^\dagger, b^\dagger] = 0$$

These operators act in the Fock space $\{|n\rangle | n = 0, 1, 2, \cdots\}$ as follows

$$\begin{aligned} b^\dagger |n\rangle &= \sqrt{n+1}|n+1\rangle \\ b|n\rangle &= \sqrt{n}|n-1\rangle \end{aligned}$$

1. Show that the operators obtained by the Holstein-Primakoff transformation satisfy the commutation relations for the spin operators:

$$[S_+, S_-] = 2S_z \tag{11}$$

$$[S_z, S_\pm] = \pm S_\pm \tag{12}$$

2. Show that S_z and $S_\pm$ given by Eq. (10) act on the Fock space as

$$\begin{aligned} S_z|n\rangle &= (s-n)|n\rangle \\ \boldsymbol{S}^2|n\rangle &= s(s+1)|n\rangle \end{aligned}$$

   Deduce that

$$|s, m\rangle = |n = s - m\rangle$$

   and that only the states of the Fock space satisfying

$$n \leq 2s$$

   are physical states.