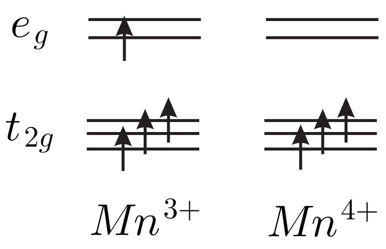

Figure 6.12:

solid, each having the same "core" spin S, and sharing a single itinerant e_g electron, that has a tight-binding matrix element

$$t = < \phi_{e_g}(\mathbf{r}-\mathbf{R}_i)|H|\phi_{e_g}(\mathbf{r}-\mathbf{R}_j) > \tag{6.35}$$

for hopping from site to site.

Explain the origin of the terms

$$H_{int} = -J\sum_i \hat{\mathbf{s}}_i \cdot \mathbf{S}_i + J_x \sum_{ij} \mathbf{S}_i \cdot \mathbf{S_j} \quad , \tag{6.36}$$

in the total Hamiltonian ($\hat{\mathbf{s}}_i$) is the spin of the e_g electron) and suggest relative magnitudes of U, $J$and J_x.[9]

(d) Consider two neighbouring core spins $\mathbf{S}_i$ $\mathbf{S}_j$ that are at a relative angle θ_{ij}. By considering that the spin wavefunction of the itinerant electron must, for $J \gg t$, be always aligned with the local core spin $\mathbf{S}$, explain why the Schrödinger equation for the itinerant electron can be simplified to one in which the tight-binding hopping matrix element from site i to site j is replaced by

$$t_{eff} = t\cos(\frac{\theta_{ij}}{2}) \quad . \tag{6.37}$$

To do this, you may wish to note that under a rotation by an angle θ, the spin wavefunction transforms as

$$\begin{pmatrix} |\uparrow'> \\ |\downarrow'> \end{pmatrix} = \begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \\ -\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \begin{pmatrix} |\uparrow> \\ |\downarrow> \end{pmatrix} \tag{6.38}$$

(e) Sketch the density of states of the itinerant electrons for different alignments of the core spins $\mathbf{S}$:
ferromagnetic (all core spins aligned),
antiferromagnetic (all neighbouring core spins anti-aligned),

[9] In second-quantised notation, the full Hamiltonian can be written as

$$H = t\sum_{ij=n.n.,\sigma} \hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + U\sum_i \hat{n}_{i\sigma}\hat{n}_{i-\sigma} - J\sum_i \hat{\mathbf{s}}_i\cdot\mathbf{S}_i + J_x\sum_{ij}\mathbf{S}_i\cdot\mathbf{S_j} \quad .$$