Magnetism in materials

Exercises - Week 02

1. Spin-orbit coupling originates from the interaction between the inherent magnetic moment (spin) of an electron and the magnetic field created by its motion. For a single electron, this interaction is effectively expressed as $A\mathbf{L}\cdot\mathbf{S}$. Show that $[\mathbf{L}\cdot\mathbf{S}, L_x] = i\hbar(\mathbf{L}\times\mathbf{S})_x$. Does $\mathbf{L}\cdot\mathbf{S}$ commute with $\mathbf{L}$ and $\mathbf{S}$? What about $\mathbf{L}^2$ and $\mathbf{S}^2$? Is the total angular momentum operator $\mathbf{J} = \mathbf{L} + \mathbf{S}$ a conserved quantity? Based on the above perspective about conserved quantities, show that the eigenvalues of the spin-orbit Hamiltonian are $\propto j(j+1) - l(l+1) - s(s+1)$.

2. The Brillouin function depends on the angular momentum J and on the variable x which is proportional to B/T.

$$B_J(x) = \frac{2J+1}{2J}\coth\left(\frac{2J+1}{2J}x\right) - \frac{1}{2J}\coth\left(\frac{x}{2J}\right) \tag{1}$$

   Use the Jupiter notebook Ex1.ipynb to plot the function and observe how it changes when you vary J. What is the limit of the function for $J \to \infty$?
   For small x the function is well approximated by a linear trend, find the expression for this line.

3. In the regime in which the Brillouin function can be approximated with linear function the magnetic susceptibility χ follows the Curie law

$$\frac{1}{\chi} = \frac{T}{C} \tag{2}$$

   Use the Jupiter notebook Ex2.ipynb to plot $1/\chi$ vs T and determine when the Curie law is a good approximation. Use the slider to see the effect of the application of a magnetic field B, what deviations from the Curie law can you observe when the field is applied? Explain why when a finite field B is applied and $T \to 0$ the susceptibility does not diverge as predicted by the Curie law.

4. For this exercise, we simulate a measurement of χ at different T and fit the data with the formula

$$\chi(T) = \frac{C}{T} + \chi_0 \tag{3}$$

   where χ_0 accounts for Van-Vleck paramagnetism. Use the Jupiter notebook Ex3.ipynb to generate the data and fit them. Based on what you observed in the previous exercises choose for the fit temperatures range $[T_{start}, T_{stop}]$ in which this expression gives a good approximation. Compare the results you get from the fit with the values of C and χ_0 that you can set through the parameters at the beginning of the script for generating the data. With the last part of the script, you can see how the results of the fit vary when the lower limit of the fitting range is changed keeping constant the upper limit at the highest measured Temperature.

5. Many Uranium compounds are of great current interest as heavy fermion or mixed valent systems. The first thing you want to know is the valence state of uranium and, surprisingly, it is quite difficult to decide whether it is U^{3+} or U^{4+}. You might think that measuring the high-temperature susceptibility which shows a Curie-type behavior, should clinch the point. Let us assume that measurement tells us that the effective moment is $\mu_{\text{eff}} = 3.6\mu_B$, with 1% accuracy. Can you decide whether the valence state is U^{3+} or U^{4+} ?

   Hint The orbital configuration for U^{3+} and U^{4+} are respectively $5f^3$ and $5f^2$. The effective moment μ_{eff} is such that we can rewrite the Curie law :

$$\chi = \frac{n\mu_0\mu_{\text{eff}}^2}{3k_BT}$$

6. SmB_6 is a mixed valent material, containing about 60% trivalent and 40% divalent samarium. Let us assume that only the Sm 4f-electrons contribute to the magnetic susceptibility, ,and that the Sm-ions can be treated as independent (it is a good approximation from $T \approx 100K$ upwards). The Van-Vleck susceptibility is given in this case by :

$$\chi_{VV} = \frac{n\mu_0 2(L+1)S\mu_B^2}{3(J+1)\Delta}$$

   With $\Delta = E_{J+1}^0 - E_J^0$ equal to $\Delta/k_B \approx 410K$ for Sm^{2+} ion and $\Delta/k_B \approx 1450K$ for Sm^{3+} ion. $\mathbf{Sm}^{3+}$ and $\mathbf{Sm}^{2+}$ have electronic configuration $[\text{Xe}]4f^5$ and $[\text{Xe}]4f^6$ respectively. What is the relative importance of the Curie and Van-Vleck terms at room temperature?

7. Oxygen molecules present molecular orbitals as shown in figure 1. Indicates how these orbitals are filled in the ground state. What consequences does this have on the magnetic behaviour of O_2 ?

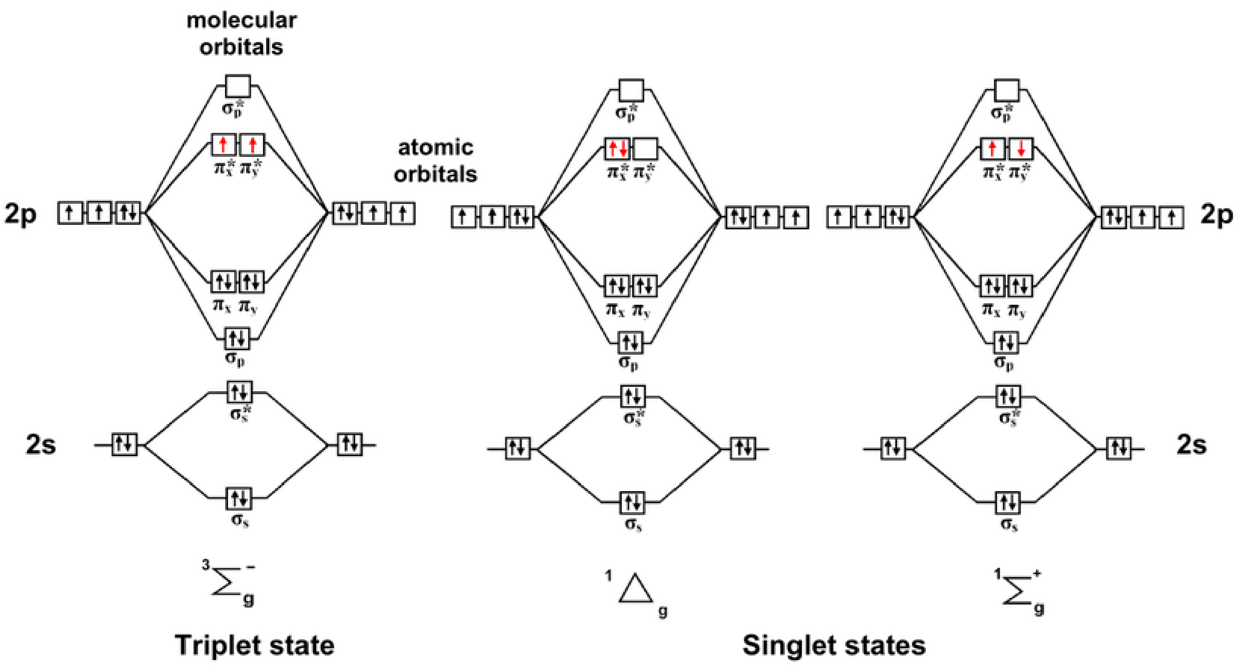
molecular
orbitals
atomic
orbitals
2p
2s
Triplet state
Singlet states

Figure 1: