Solid State Physics IV: Magnetism

Problem set: Lectures 1-7

November 5th, 2022, Version 1.0

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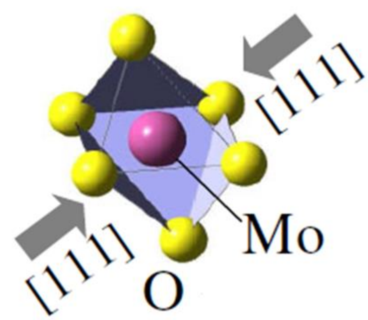
Instructions: Please solve the problem and return it to me (hirschberger@ap.t.u-tokyo.ac.jp) by **November 28th, 2022 at 17:30 Japanese Standard Time** at the latest. Please include your U. Tokyo student ID number. Written comments should be in English, but you can type the solution or hand-write it as you choose.

Problem 1:

Consider the oxide $Y_2Mo_2O_7$, where nonmagnetic Y^{3+} and O^{2-} ions determine the charge of the Molybdenum ion, by charge neutrality. What is the charge and valence electron configuration of the Molybdenum ion? Please write the shell configuration in the form (example: hydrogen atom) $1s^1$.

Further, if the crystal field environment on the Mo-site is octahedral, please sketch the 4d energy levels, and "place" electrons in the electronic orbitals as we did in the lecture. What is the total expected spin angular momentum of the Molybdenum ion?



Bonus: in real-world $Y_2Mo_2O_7$, a trigonal distortion lifts the degeneracy of the ground state 4d manifold (cartoon). This corresponds to a squeezing of the octahedral environment, as in the picture. How do you expect t_{2g} states to split in presence of this distortion? Do you expect the ground state, with trigonal distortion, to be singly or doubly degenerate?

Problem 2:

Conventionally, the Dzyaloshinskii-Moiya interaction is written as $\mathcal{H}_{DMI} = \frac{1}{2}\sum_{ij} \boldsymbol{D}_{ij}(\boldsymbol{S}_i \times \boldsymbol{S}_j)$, where the sum is over all pairs of atoms at sites *i*, *j* on the lattice and the factor of (1/2) corrects for double-counting of pairs; $\boldsymbol{D}_{ij}$ is the Dzyaloshinskii-Moriya "vector", which is specific to each bond $\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$. Rewrite the Hamiltonian in the form

$$\mathcal{H}_{DMI} = \sum_{ij} \boldsymbol{S}_i \begin{pmatrix} J_{ij}^{11} & J_{ij}^{12} & J_{ij}^{13} \\ J_{ij}^{21} & J_{ij}^{22} & J_{ij}^{23} \\ J_{ij}^{31} & J_{ij}^{32} & J_{ij}^{33} \end{pmatrix} \boldsymbol{S}_j$$

with an exchange matrix $\bar{J}_{ij}$ that you have to express in terms of elements of $\boldsymbol{D}_{ij}$. Comment on the name "antisymmetric exchange" for this spin-spin interaction. Why is it OK commute (interchange) the operators S_i^α and S_j^β, if $i \neq j$?

Problem 3:

Recall the expression from Lecture 2 for the magnetic moment in terms of a loop current $\boldsymbol{j}_{mag} = -\boldsymbol{m} \times \nabla f(|\boldsymbol{r} - \boldsymbol{R}|)$, with a normalized and spatially localized function *f*. Confirm the relations $\nabla \cdot \boldsymbol{j}_{mag} = 0$ and $\boldsymbol{m} = \frac{1}{2}\int d^3r\,(\boldsymbol{r} - \boldsymbol{R}) \times \boldsymbol{j}_{mag}$. Here, $\boldsymbol{m}$ is a constant that does not depend on position $\boldsymbol{r}$.