

Assignment 1: Crystal field interaction, diamagnetism and Pauli paramagnetism

1. Show that in the high temperature approximation, $k_B T \gg E - \mu$, the Pauli paramagnetism of a sea of electrons is equal to the paramagnetic susceptibility of isolated electrons which is given by

$$\chi = \frac{\mu_o \mu_B^2 n}{k_B T}. \quad (1)$$

Hint: Find the total number of electrons in the band filled up to the Fermi level and assume that the statistics approach the Maxwell-Boltzmann distribution in the high temperature limit.

2. An electron with angular momentum \mathbf{L} moves in a classical Bohr-like orbit of radius r in the xy plane. A field \mathbf{B} is imposed in the z direction. Use Faraday's law, the force on the electron, torque and change in angular momentum to predict the induced magnetic moment. Calculate the diamagnetic susceptibility and discuss whether it matches the quantum mechanical calculation done in class.
3. Consider the single electron states $\psi_{n=2,l=1}$ which are labeled as ψ_{p^+} , ψ_{p^-} and ψ_{p_z} . These wavefunctions can be read off from the Table provided in class.
- (a) Construct real superpositions of ψ_{p^+} and ψ_{p^-} and label them as ψ_{p_x} and ψ_{p_y} as appropriate.
 - (b) Use the definitions of the angular momentum operators, e.g. $\hat{L}_x = -i\hbar(y\partial/\partial z - z\partial/\partial y)$ and determine the expectation values of the three components of the angular momentum in each of states ψ_{p_x} , ψ_{p_y} and ψ_{p_z} . **Is the orbital angular momentum quenched?**
 - (c) What is the expectation value of \hat{L}^2 ?
 - (d) Argue that if we have a real wave function then each component of the angular momentum operator averages to zero.
 - (e) In an isolated ion, the p orbitals are degenerate. What are the energies when the ion is placed inside an octahedral crystal field with (a) cubic symmetry ($a = b = c$) and (b) a distorted octahedron with tetragonal symmetry ($a = b \neq c$)? A sample

code from Mathematica is uploaded on the website that will help you define potentials and express them as series ([HW3assist.nb]).

4. The Cu^{2+} exhibits the Jahn-Teller effect similar to Mn^{3+} . Describe why this is true? To answer this question, write down the configuration of the ion inside an octahedral environment.
5. Attempt Blundell Q. 3.3. (This question will only be coarsely graded.)