P555
April 29, 2020

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Submit a pdf file with your work not later that April 29 at 8PM.

Problem 1: In the periodic table we see that the Mn ion has an electronic structure given by $3d^5 4s^2$.

a) Use Hund rules to obtain S, L, and J for the ground state of the Mn atom. Draw the energy levels in the relevant shells and indicate the electronic placement. Provide your final result using spectroscopic notation: ${}^{2S+1}L_J$. (5 points)

b) The manganese ion Mn^{2+} has an electronic structure given by $3d^5$. Use Hund rules to obtain S, L, and J for the ground state of the Mn atom. Draw the energy levels in the relevant shells and indicate the electronic placement. Provide your final result using spectroscopic notation: ${}^{2S+1}L_J$. Compare your result with the result you obtained in part (a). (5 points)

c) Now provide the electronic structure of the Mn ion Mn^{3+}. (5 points)

d) Use Hund rules to obtain S, L, and J for the ground state of the Mn^{3+} ion. Draw the energy levels in the relevant shells and indicate the electronic placement. Provide your final result using spectroscopic notation: ${}^{2S+1}L_J$. (5 points)

Problem 2: Consider a semiconductor with the band structure shown in the figure. Its energy gap is $\epsilon_g = 0.18eV$, the effective electron mass in the conduction band is $m_c^* = 0.014m_e$, where m_e is the mass of a free electron, and $\epsilon = 17$ is the dielectric constant of the semiconductor. Useful constants: $m_e = 9.1093 \times 10^{-31}$ kg; $k = 1.38 \times 10^{-23} J/K = 8.617 \times 10^{-5} eV/K$; $\hbar = 1.054 \times 10^{-34} Js = 6.582 \times 10^{-16} eVs$.

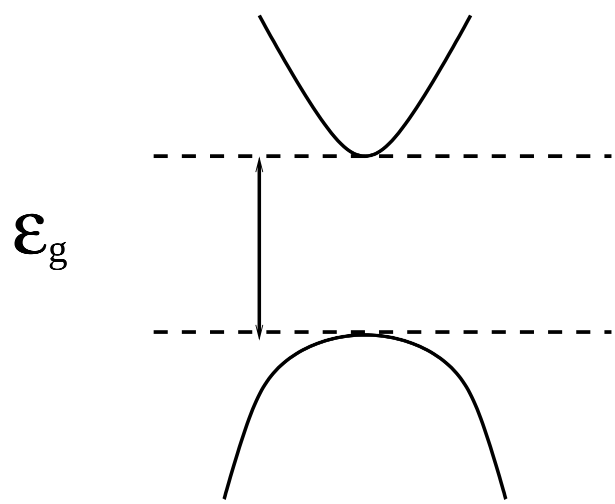

FIG. 1:

a) Just by looking at the figure say if the effective mass of the holes in the valence band is larger or smaller than the effective mass of the electrons in the conduction band. Justify your answer. (5 points)

b) Calculate N_c, the density of states per volume available to electrons in the conduction band. Provide its numerical value at $T = 4K$ and $T = 300K$. (5 points)

c) Calculate n, the density of electrons in the conduction band, at $T = 4K$ and $T = 300K$. Assume that the chemical potential μ is at the center of the gap. (5 points)

d) Calculate p, the density of holes in the valence band, at $T = 4K$ and $T = 300K$. Assume that the chemical potential μ is at the center of the gap. (5 points)

e) Now donor impurities will be added to the semiconductor:

i) Evaluate the binding energy of a donor electron. Provide the result in eV. (5 points)

ii) If the density of added donor impurities is $N_d = 10^{20}$ per m^3, calculate n, the density of electrons in the conduction band at 4K and 300K. (5 points)

Problem 3: Consider a two-dimensional square lattice of particles with mass M and lattice constant a. Let $\hat{r}_{ij}$ be a unit vector pointing from the equilibrium location $\mathbf{R}_i$ of particle i to the equilibrium location $\mathbf{R}_j$ of particle j. Let $\mathbf{u}_i$ give the two dimensional displacement of particle i from its equilibrium location. Suppose that the force on particle i is

$$\mathbf{F}_i = M\omega_0^2 \sum_j \hat{r}_{ij}[\hat{r}_{ij}.(\mathbf{u}_j - \mathbf{u}_i)],$$

where j indexes nearest neighbors of i.

a) Provide a set of primitive vectors for the lattice. (5 points)

b) Provide the number n of nearest neighbors for an atom located at site $\mathbf{R}_i$ and provide the location $\mathbf{r}_{i,j}$ of each of the neighbors (with $j = 1, ..., n$) in terms of the primitive vectors that you provided in (a). (5 points)

c) Find the two equations in two unknowns whose solution would give the dispersion relation $\omega_{\nu\mathbf{k}}$ for vibrations of the lattice. (5 points)

d) Plot the two solutions $\omega_{1\mathbf{k}}$ and $\omega_{2\mathbf{k}}$ versus $\mathbf{k}$ along the path in k-space $\Gamma - X - M - \Gamma$ where $\Gamma = (k_x, k_y) = (0, 0)$, $X = (k_x, k_y) = (\pi/a, 0)$, and $M = (k_x, k_y) = (\pi/a, \pi/a)$. Use a different color for $\omega_{1\mathbf{k}}$ and $\omega_{2\mathbf{k}}$ and in each panel of the plot identify which of the two is the longitudinal mode and which one is the transverse mode. (5 points)

e) Take the limit $k \to 0$ and find the speed of sound along the (1,0) and (0,1) directions in this system. (5 points)