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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)

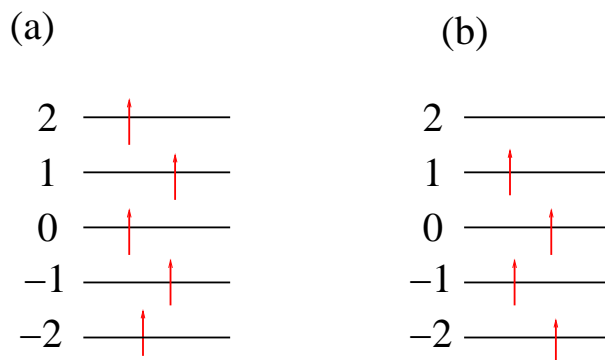


FIG. 1:

Notice that the s-shell is filled and thus, its electrons do not contribute to the magnetic quantum numbers. Thus we need to look at the d-shell which is half-filled (see panel (a) of Fig. 1). We see that the total spin is $S = 5/2$, and $L = 0$, then $J = S = 5/2$ and the spectroscopic notation for the ground state of the atom is: $^6S_{5/2}$.

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)

The result is the same as in (a) because now the s-shell is empty and thus, it still does not contribute to the magnetic quantum numbers. The electronic structure of the d-shell is the same as in the previous case shown in panel (a) of Fig. 1. Then the result is $^6S_{5/2}$.

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

In this case we need to remove 1 electron and the only available shell to remove it is the d-shell. Thus the electronic structure is $3d^4$.

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)

Now the d-shell has 4 electrons and is less than half-filled (see panel (b) of Fig. 1). We see that the total spin is $S = 4/2 = 2$, and $L = 2$, then $J = |L - S| = 2 - 2 = 0$ and the spectroscopic notation for the ground state of the atom is: 5D_0 .

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; $k = 1.38 \times 10^{-23} J/K = 8.617 \times 10^{-5} eV/K$; $\hbar = 1.054 \times 10^{-34} Js = 6.582 \times 10^{-16} eVs$.

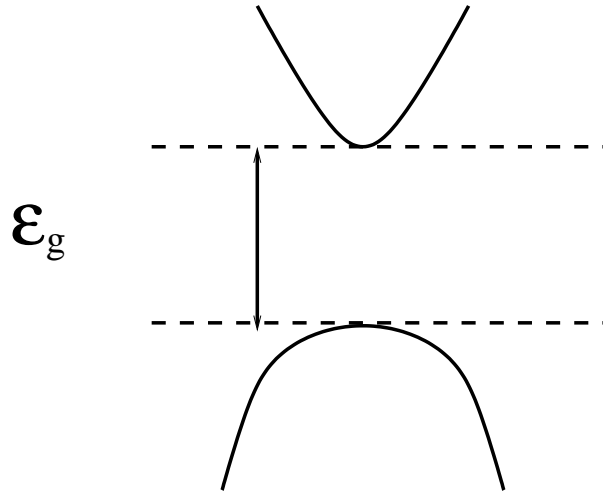


FIG. 2:

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)

We know that the concavity of the bands is related to the effective mass of the fermions. If the band is flat the electrons are localized and thus, have a very large effective mass, while a large concavity or convexity indicate a light particle with very small effective mass. Since in the figure the valence band is much flatter than the conduction band it is clear that electrons in the conduction band have a smaller effective mass than holes in the valence band.

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)

From Eq.(19.24a) we know that

$$N_c = \frac{1}{4} \left(\frac{2m_n^* kT}{\pi \hbar^2} \right)^{3/2}. \quad (1)$$

Replacing with the corresponding numerical values we obtain $N_c(T = 4K) = 6.4 \times 10^{19} m^{-3}$ and $N_c(T = 300K) = 4.16 \times 10^{22} m^{-3}$.

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)

From Eq.(19.17) we know that

$$n = N_c e^{-\beta(\epsilon_c - \mu)} = N_c e^{-\beta \epsilon_g / 2}, \quad (2)$$

where we have used that, since the chemical potential is in the middle of the gap, $\epsilon_c - \mu = \epsilon_g/2$. Then replacing in the equation using N_c and β for the corresponding values of T (from part (b)). We obtain: $n_{4K} = 0$ and $n_{300K} = 1.2796 \times 10^{21} m^{-3}$.

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)

Since the semiconductor is undoped we know that any electrons that go to the conduction band need to leave the corresponding number of holes in the valence band. This means that $n = p$ then $p_{4K} = 0$ and $p_{300K} = 1.2796 \times 10^{21} m^{-3}$.

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)

From (18.23) we know that

$$\epsilon_b = \frac{e^2}{2\epsilon a} = \frac{e^4 m^*}{2\epsilon^2 \hbar^2} = \frac{m^*}{m_e} \frac{1}{\epsilon^2} 13.6 eV = 6.58 \times 10^{-4} eV. \quad (3)$$

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)

Now

$$n - p = N_d \quad (4)$$

and

$$np = n_i^2. \quad (5)$$

Combining the two previous equations we obtain:

$$n^2 - nN_d - n_i^2 = 0, \quad (6)$$

and

$$p^2 + pN_d - n_i^2 = 0. \quad (7)$$

Solving the quadratics we obtain:

$$n = \frac{N_d}{2} + \frac{1}{2}(N_d^2 + 4n_i^2)^{1/2}, \quad (8)$$

and

$$p = -\frac{N_d}{2} + \frac{1}{2}(N_d^2 + 4n_i^2)^{1/2}. \quad (9)$$

Then, at $T = 4K$ we obtain $n = N_d = 10^{20} m^{-3}$ and $p = 0$. We see that the electrons in the conduction band come from the ionized impurities.

At $T = 300K$ we obtain $n = 1.33 \times 10^{21} m^{-3}$ and $p = 1.23 \times 10^{21} m^{-3}$. Now we see that the electrons in the conduction band come from the ionized impurities and from the valence band.

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

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

where j indexes nearest neighbors of i .

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

$$\mathbf{a}_1 = a(1, 0); \mathbf{a}_2 = a(0, 1). \quad (10)$$

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 $j = 1, \dots, n$) in terms of the primitive vectors that you provided in (a). (5 points)

In the square lattice each site has $n = 4$ nearest neighbors. The positions are given by $\mathbf{r}_{i1} = \mathbf{a}_1$, $\mathbf{r}_{i2} = \mathbf{a}_2$, $\mathbf{r}_{i3} = -\mathbf{a}_1$, and $\mathbf{r}_{i4} = -\mathbf{a}_2$.

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)

Following (13.23) we propose

$$\mathbf{u}_i = \epsilon e^{i(\mathbf{k} \cdot \mathbf{R}_i - \omega t)}. \quad (11)$$

We know that $M\ddot{\mathbf{u}}_i = \mathbf{F}_i$ then we obtain:

$$\begin{aligned} -M\omega^2 \epsilon e^{i(\mathbf{k} \cdot \mathbf{R}_i - \omega t)} &= M\omega_0^2 \sum_j^4 \hat{r}_{ij} [\hat{r}_{ij} \cdot \epsilon (e^{i(\mathbf{k} \cdot \mathbf{R}_j - \omega t)} - e^{i(\mathbf{k} \cdot \mathbf{R}_i - \omega t)})] = \\ &M\omega_0^2 \sum_j^4 \hat{r}_{ij} [\hat{r}_{ij} \cdot \epsilon (e^{i(\mathbf{k} \cdot (\mathbf{R}_j - \mathbf{R}_i))} - 1)] e^{i(\mathbf{k} \cdot (\mathbf{R}_i - \omega t))}. \end{aligned} \quad (12)$$

Simplifying we obtain:

$$\begin{aligned} -\omega^2 \epsilon &= \omega_0^2 \sum_j^4 \hat{r}_{ij} [\hat{r}_{ij} \cdot \epsilon (e^{i\mathbf{k} \cdot \mathbf{r}_{ij}} - 1)] = \\ &\omega_0^2 (2\epsilon_x (\cos k_x a - 1), 2\epsilon_y (\cos k_y a - 1)). \end{aligned} \quad (13)$$

Then, the two equations are:

$$\omega_1^2 = -2\omega_0^2 (\cos k_x a - 1), \quad (14)$$

and

$$\omega_2^2 = -2\omega_0^2 (\cos k_y a - 1). \quad (15)$$

d) Plot the two solutions $\omega_{1\mathbf{k}}$ and $\omega_{2\mathbf{k}}$ versus \mathbf{k} along the path in \mathbf{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)

We need to plot $\omega_1 = [-2\omega_0^2 (\cos k_x a - 1)]^{1/2}$ and $\omega_2 = [-2\omega_0^2 (\cos k_y a - 1)]^{1/2}$ along $\Gamma - X - M - \Gamma$ as shown in the figure.

Notice that along $\Gamma - X$ the transversal mode is 1 because the ions oscillate along x which the direction parallel to k_x , while along $X - M$ the longitudinal mode is 2 because the ionic displacements are parallel to k_y . Finally, along $M - \Gamma$ the longitudinal and transverse modes have the same dispersion (they are actually linear combinations of the modes 1 and 2).

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

In the limit $k \rightarrow 0$ we obtain that $\omega_1 \approx \omega_0 k_x a$ and $\omega_2 \approx \omega_0 k_y a$. Then the speed of sound in both cases is

$$c_s = \omega_0 a. \quad (16)$$

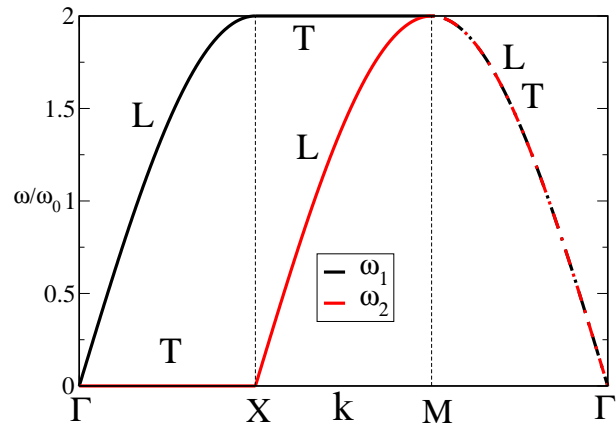


FIG. 3: