P555

May 6, 2021

SHOW ALL YOUR WORK TO GET FULL CREDIT!

Problem 1: In the periodic table we see that the P atom has an electronic structure given by [Ne]$3s^2 3p^3$.

a) Use Hund rules to obtain S, L, and J for the ground state of the P 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)

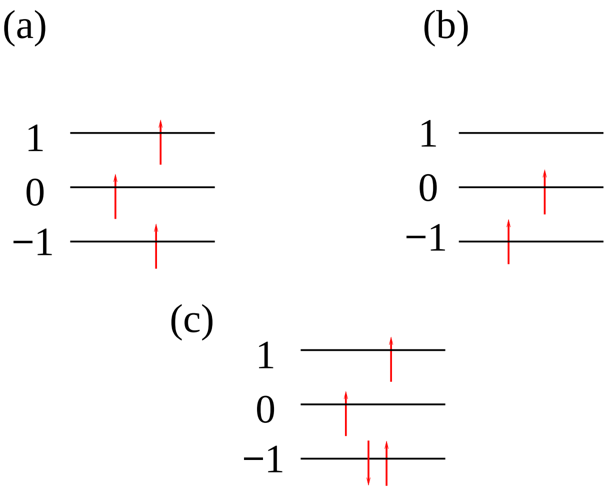

FIG. 1:

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 p-shell which is half-filled (see panel (a) of Fig. 1). We see that the total spin is $S = 3/2$, and $L = 0$, then $J = S = 3/2$ and the spectroscopic notation for the ground state of the atom is:${}^4S_{3/2}$.

b) Provide the electronic structure of the phosphorus ion P^+. (5 points)

In this case we need to remove 1 electron from the p-shell. Thus the electronic structure is [Ne]$3s^2 3p^2$.

c) Use Hund rules to obtain S, L, and J for the ground state of the P^+ 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 p-shell has 2 electrons and is less than half-filled (see panel (b) of Fig. 1). We see that the total spin is $S = 2/2 = 1$, and $L = 1$, then $J = |L - S| = 1 - 1 = 0$ and the spectroscopic notation for the ground state of the atom is:${}^3P_0$.

d) Now provide the electronic structure of the P ion P^-. (5 points)

In this case we need to add 1 electron in the p-shell. Thus the electronic structure is [Ne]$3s^2 3p^4$.

e) Use Hund rules to obtain S, L, and J for the ground state of the P^- 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 p-shell has 4 electrons and is more than half-filled (see panel (c) of Fig. 1). We see that the total spin is $S = 2/2 = 1$, and $L = 1$, then $J = |L + S| = 1 + 1 = 2$ and the spectroscopic notation for the ground state of the atom is:${}^3P_2$.

Problem 2: Consider a two-dimensional rectangular lattice of particles with mass M and lattice constants a and $b = a/2$. 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 there is a nearest neighbor harmonic potential between the atoms. The spring constant along a is K_a and along b is K_b with $K_b = K_a/4$.

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

$$\mathbf{a}_1 = a(1,0); \mathbf{a}_2 = b(0,1) = \frac{a}{2}(0,1). \tag{1}$$

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)

In the rectangular lattice each site has $n = 4$ nearest neighbors. The positions are given by $\mathbf{r}_{i1} = \mathbf{R}_i + \mathbf{a}_1 = (i_x + a, i_y)$, $\mathbf{r}_{i2} = \mathbf{R}_i + \mathbf{a}_2 = (i_x, i_y + a/2)$, $\mathbf{r}_{i3} = \mathbf{R}_i - \mathbf{a}_1 = (i_x - a, i_y)$, and $\mathbf{r}_{i4} = \mathbf{R}_i - \mathbf{a}_2 = (i_x, i_y - a/2)$.

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)

As we did in class we propose

$$\mathbf{u}_i = \epsilon e^{i(\mathbf{k}.\mathbf{R}_i - \omega t)}. \tag{2}$$

We know that $M\ddot{\mathbf{u}}_i = \mathbf{F}_i$ and for an harmonic potential $F_i^l = K_l \sum_j (u_j^l - u_i^l)$ where $l = a, b$ labels the component of the force and j is a nearest neighbor along l. We have chosen the x axis along a and the y axis along b. Then along x we obtain:

$$M\ddot{u}_i^x = K_a[(u_{i_1}^x - u_i^x) + (u_{i_3}^x - u_i^x)]. \tag{3}$$

Replacing Eq. 2 in Eq. 3:

$$-M\omega^2 u_i^x = K_a[(e^{ik_x a} - 1) + (e^{-ik_x a} - 1)]u_i^x. \tag{4}$$

Dividing by u_i^x we obtain:

$$-M\omega^2 = 2K_a[\cos(k_x a) - 1] = -4K_a \sin^2(k_x a/2). \tag{5}$$

Then

$$\omega_1 = \omega_x = 2\sqrt{\frac{K_a}{M}}|\sin(k_x a/2)|. \tag{6}$$

Now for the displacements along y we obtain:

$$M\ddot{u}_i^y = K_b[(u_{i_2}^y - u_i^y) + (u_{i_4}^y - u_i^y)]. \tag{7}$$

Replacing Eq. 2 in Eq. 7:

$$-M\omega^2 u_i^y = K_b[(e^{ik_y a/2} - 1) + (e^{-ik_y a/2} - 1)]u_i^y. \tag{8}$$

Dividing by u_i^y we obtain:

$$-M\omega^2 = 2K_b[\cos(k_y a/2) - 1] = -4K_b \sin^2(k_x a/4). \tag{9}$$

Then

$$\omega_2 = \omega_y = 2\sqrt{\frac{K_b}{M}}|\sin(k_y a/4)|. \tag{10}$$

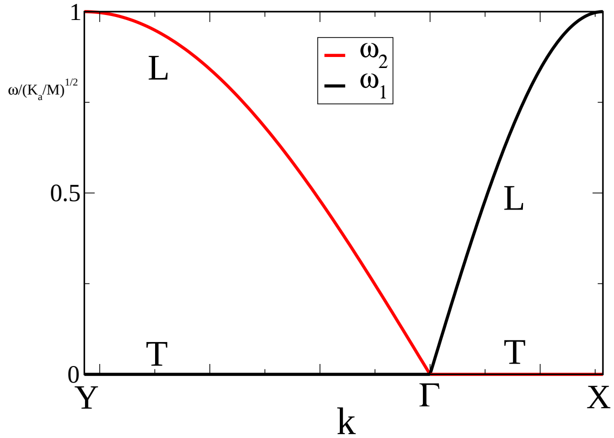

FIG. 2:

d) Plot the two solutions $\omega_{1\mathbf{k}}$ and $\omega_{2\mathbf{k}}$ versus $\mathbf{k}$ along the path in k-space $Y-\Gamma-X$ where $\Gamma=(k_x,k_y)=(0,0)$, $X=(k_x,k_y)=(\pi/a,0)$, and $Y=(k_x,k_y)=(0,\pi/b)$. 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 $\omega_1=2\sqrt{\frac{K_a}{M}}|\sin(k_xa/2)|$ and $\omega_2=\sqrt{\frac{K_a}{M}}|\sin(k_ya/4)|$, where we have used that $K_b=K_a/4$, along $Y-\Gamma-X$ as shown in the figure.

Notice that along $\Gamma-X$ the transversal mode is 2 because the ions oscillate along x which is the direction parallel to k_x, while along $Y-\Gamma$ the longitudinal mode is 2 because the ionic displacements are parallel to k_y.

e) Take the limit $k\to 0$ and find the speed of sound along a and along b in this system. Along what direction is the speed of sound larger? (5 points)

In the limit $k\to 0$ we obtain that $\omega_1\approx\sqrt{K_a/M}|k_x|a$ and $\omega_2\approx\sqrt{K_b/M}|k_y|a/2$. Then the speed of sound is

$$c_{s,1}=a\sqrt{K_a/M}, \tag{11}$$

$$c_{s,2}=\frac{a\sqrt{K_b/M}}{2}. \tag{12}$$

The speed of sound is larger along a as it can be seen in Fig.2 because the slope of the curve at Γ is larger along Γ-X than along Γ-Y.