Final Exam

P555

May 17, 2022

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Problem 1: In the periodic table we see that the Te atom has an electronic structure given by $4d^{10}5s^25p^4$.

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

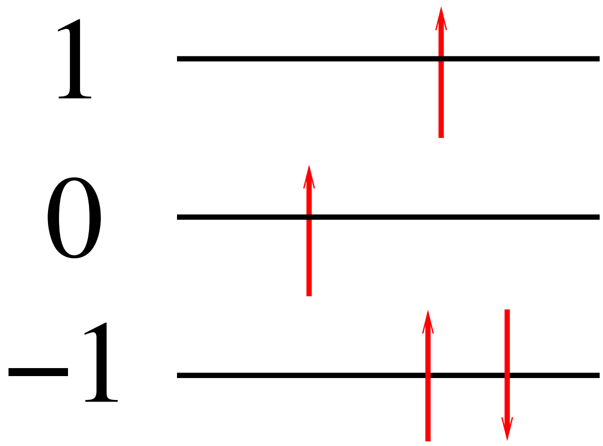

FIG. 1:

Notice that the s-shell and d-shell are filled and thus, its electrons do not contribute to the magnetic quantum numbers. Thus, we need to look at the p-shell which is more than half-filled (see Fig. 1). We see that the total spin is $S = 1$, and $L = 1$, then $J = S + L = 2$ since the shell is more than half-filled and the spectroscopic notation for the ground state of the atom is:$^3P_2$.

b) What is the degeneracy of the ground state of Te? (5 points)

The degeneracy of the ground state is $2J + 1$. Since $J = 2$ we see that the degeneracy is 5.

c) Calculate the Landé factor g for the Te atom. (5 points)

The Landé factor is given by

$$
\begin{aligned}
g = \frac{1}{2}\frac{[3J(J+1) - L(L+1) + S(S+1)]}{J(J+1)} &= \\
\frac{1}{2}\frac{[6(2+1) - 1(1+1) + 1(1+1)]}{2(2+1)} &= \\
\frac{1}{2}\frac{[18 - 2 + 2)]}{6)} = \frac{3}{2}&.
\end{aligned}
\tag{1}
$$

d) What is the energy splitting ΔE linear in the magnetic field B for the ground state of a Te atom placed in a magnetic field B? Provide the energy of each energy level as a function of B. (5 points)

The energy splitting is given by

$$\Delta E = g\mu_B B = \frac{3}{2}\mu_B B. \tag{2}$$

The degeneracy 5 is now split and each level will have energy

$$E = E_0 + J_z g\mu_B B = E_0 + J_z\frac{3}{2}\mu_B B, \tag{3}$$

where E_0 is the energy of the degenerate level and $J_z = \pm 2, \pm 1, 0$. Thus, $E_{-2} = E_0 - 3\mu_B B$, $E_{-1} = E_0 - \frac{3}{2}\mu_B B$, $E_0 = E_0$, $E_1 = E_0 + \frac{3}{2}\mu_B B$, and $E_2 = E_0 + 3\mu_B B$.

e) What is the magnetization **M** of a sample of Te that contains N atoms in a volume V? (5 points)

The magnetization is given by

$$M = n\mu_B gJ\mathcal{B}_J(\beta\mu_B gJB) = \frac{N}{V}\mu_B\frac{3}{2}(2)\mathcal{B}_2(\beta\mu_B 3B) = 3\frac{N}{V}\mu_B\mathcal{B}_2(\beta\mu_B 3B). \tag{4}$$

f) Provide the value of the magnetization M calculated in (e) when $kT \gg \mu_B B$ and when $kT \ll \mu_B B$. (5 points)

Let define $x = \mu_B gJB/kT = \mu_B 3B/kT$. We know that if $kT \gg \mu_B B$

$$\mathcal{B}_J(x) \approx \frac{1}{3}\frac{J+1}{J}x. \tag{5}$$

In our case

$$\mathcal{B}_2(x) \approx \frac{1}{3}\frac{2+1}{2}\frac{\mu_B 3B}{kT} = \frac{1}{3}\frac{3}{2}\frac{\mu_B 3B}{kT} = \frac{3}{2}\frac{\mu_B B}{kT}. \tag{6}$$

Replacing in Eq. 4 we obtain:

$$M \approx 3\frac{N}{V}\mu_B\frac{3}{2}\frac{\mu_B B}{kT} = \frac{9}{2}\frac{N}{V}\frac{\mu_B^2 B}{kT}. \tag{7}$$

We see that the magnetization at high temperature goes like $1/T$, i.e., as expected, decreasing as T increases and following Curie's law.

If $kT \ll \mu_B B$ then $x = \mu_B 3B/kT$ becomes very large. Since

$$\mathcal{B}_2(x) = \frac{5}{4}\coth(5x/4) - \frac{1}{4}\coth(x/4), \tag{8}$$

We know that

$$\lim_{x\to\infty}\coth(x) = \lim_{x\to\infty}\frac{\cosh(x)}{\sinh(x)} = 1. \tag{9}$$

Then

$$\lim_{x\to\infty}\mathcal{B}_2(x) = \frac{5}{4} - \frac{1}{4} = 1. \tag{10}$$

Replacing in Eq. 4 we obtain:

$$M = 3\frac{N}{V}\mu_B\mathcal{B}_2(\beta\mu_B 3B) \approx 3\frac{N}{V}\mu_B, \tag{11}$$

which is the maximum value that the magnetization can have, as expected at very low temperature.

Problem 2: In the second midterm you found that in a two-dimensional solid made of N atoms with one atom at each point of the Bravais lattice, the phonon density of states in the Einstein approximation is given by

$$D_E(\omega) = \frac{2N}{A}\delta(\omega - \omega_E), \tag{12}$$

where ω_E is the Einstein frequency and A is the area of the sample, while in the Debye approximation the phonon density of states is given by

$$D_D(\omega) = \frac{\omega}{\pi c^2}\Theta(\omega - \omega_D), \tag{13}$$

where c is the angular average of the speed of sound in the material and Θ is the Heaviside function.

a) Calculate the heat capacity C_E of the material in the Einstein approximation. (5 points)

We know that the heat capacity is given by

$$C = A\int_0^\infty d\omega D(\omega)\frac{\partial}{\partial T}\frac{\hbar\omega}{e^{\beta\hbar\omega}-1} = A\int_0^\infty d\omega D(\omega)\frac{\hbar^2\omega^2 e^{\beta\hbar\omega}}{kT^2(e^{\beta\hbar\omega}-1)^2}, \tag{14}$$

where $\beta = 1/(kT)$. Then in the Einstein approximation we obtain:

$$\begin{aligned} C_E = A\int_0^\infty d\omega D_E(\omega)\frac{\hbar^2\omega^2 e^{\beta\hbar\omega}}{kT^2(e^{\beta\hbar\omega}-1)^2} &= \\ A\int_0^\infty d\omega \frac{2N}{A}\delta(\omega-\omega_E)\frac{\hbar^2\omega^2 e^{\beta\hbar\omega}}{kT^2(e^{\beta\hbar\omega}-1)^2} &= \\ 2N\frac{\hbar^2\omega_E^2 e^{\beta\hbar\omega_E}}{kT^2(e^{\beta\hbar\omega_E}-1)^2}&. \end{aligned} \tag{15}$$

b) Provide an expression for C_E when $T \to \infty$ and when $T \to 0$. (5 points)

$$\begin{aligned} \lim_{T\to\infty} C_E = 2N\frac{\hbar^2\omega_E^2}{kT^2(1-\beta\hbar\omega_E-1)^2} &= \\ 2N\frac{\hbar^2\omega_E^2 k^2T^2}{kT^2\hbar^2\omega_E^2} &= \\ 2Nk&, \end{aligned} \tag{16}$$

as expected since at high T we obtain the Dulong and Petit result equating the heat capacity to $k/2$ times the number of degrees of freedom.

Now let's obtain the low temperature limit:

$$\begin{aligned} \lim_{T\to 0} C_E = 2N\frac{\hbar^2\omega_E^2 e^{\beta\hbar\omega_E}}{kT^2 e^{2\beta\hbar\omega_E}} &= \\ 2N\frac{\hbar^2\omega_E^2 e^{-\beta\hbar\omega_E}}{kT^2}&, \end{aligned} \tag{17}$$

which goes to zero exponentially with the temperature as expected in the Einstein approximation.

c) Calculate the heat capacity C_D of the material in the Debye approximation. (5 points)

$$
\begin{aligned}
C_D = A\int_0^\infty d\omega D_D(\omega)\frac{\hbar^2\omega^2 e^{\beta\hbar\omega}}{kT^2(e^{\beta\hbar\omega}-1)^2} &= \\
A\int_0^\infty d\omega\frac{\omega}{\pi c^2}\Theta(\omega-\omega_D)\frac{\hbar^2\omega^2 e^{\beta\hbar\omega}}{kT^2(e^{\beta\hbar\omega}-1)^2} &= \\
A\int_0^{\omega_D} d\omega\frac{\omega}{\pi c^2}\frac{\hbar^2\omega^2 e^{\beta\hbar\omega}}{kT^2(e^{\beta\hbar\omega}-1)^2} &= \\
A\int_0^{\Theta_D/T} dx\frac{xkT}{\hbar\pi c^2}\frac{\hbar^2 x^2 k^2 T^2 e^x}{\hbar kT^2(e^x-1)^2} &= \\
A\frac{k^3T^2}{\hbar^2\pi c^2}\int_0^{\Theta_D/T} dx\frac{x^3e^x}{(e^x-1)^2}&,
\end{aligned} \tag{18}
$$

where we used the change of variables $x = \beta\hbar\omega$ and $\Theta_D = \hbar\omega_D/k$ is the Debye temperature.

d) Provide an expression for C_D when $T \to \infty$ and when $T \to 0$. (5 points)

Let's obtain the high temperature behavior. In this case $x \ll 1$ then

$$
\begin{aligned}
\lim_{T\to\infty} C_D = A\frac{k^3T^2}{\hbar^2\pi c^2}\int_0^{\Theta_D/T} dx\frac{x^3}{(1+x-1)^2} &= \\
A\frac{k^3T^2}{\hbar^2\pi c^2}\int_0^{\Theta_D/T} xdx &= \\
A\frac{k^3T^2}{\hbar^2\pi c^2}\frac{x^2}{2}|_0^{\Theta_D/T} &= \\
A\frac{k^3T^2}{\hbar^2\pi c^2}\frac{\Theta_D^2}{2T^2} &= \\
A\frac{k^3T^2}{\hbar^2\pi c^2}\frac{\Theta_D^2}{2T^2} &= \\
A\frac{k^3T^2}{\hbar^2\pi c^2}\frac{4\hbar^2c^2N\pi}{2T^2k^2A} &= \\
2Nk
\end{aligned} \tag{19}
$$

where we used that $\omega_D = 2c\sqrt{n\pi}$ and $n = N/A$. The result is as expected since at high T we obtain the Dulong and Petit result equating the heat capacity to $k/2$ times the number of degrees of freedom.

Now let's obtain the low temperature behavior. In this case $x \gg 1$ then

$$
\begin{aligned}
\lim_{T\to 0} C_D = A\frac{k^3T^2}{\hbar^2\pi c^2}\int_0^\infty dx\frac{x^3e^x}{e^{2x}} &= \\
A\frac{k^3T^2}{\hbar^2\pi c^2}\int_0^\infty dx x^3 e^{-x}&,
\end{aligned} \tag{20}
$$

where the integral is just a number. Thus, we see that the heat capacity goes to zero like T^2 following a power law behavior as expected in Debye's approximation.