Homework 5 - Solutions

Problem 1 - Fraunhofer Pattern

To start, we note that we write $\gamma(x)$ as

$$\gamma(x) = \nabla\theta - \frac{2e}{\hbar}\int_1^2 \vec{A}\cdot d\vec{\ell} \tag{1}$$

In our case $\nabla\theta = \text{const}$ and $\vec{A} = -Bx\ \hat{z}$. Thus

$$\begin{aligned} \gamma(x) = \nabla\theta - \frac{2e}{\hbar}\int_0^d (-Bx)dz \quad &= \quad \nabla\theta - \frac{2Bed}{\hbar}x &(2)\\ &= \quad \nabla\theta - \frac{2\pi Bd}{\varphi_0}x &(3)\end{aligned}$$

Where $\varphi_0 = \frac{h}{2e}$

The total flux through the josephson junction is

$$\begin{aligned} \Phi \quad &= \quad \oint \vec{A}\cdot d\vec{\ell} &(4)\\ &= \quad \int_0^d A_z(x=L_x)dz \ + \ \int_d^0 A_z(x=0)dz &(5)\\ &= \quad -BL_x(d)\ +0 &(6)\\ \Rightarrow \quad \Phi \quad &= \quad -BL_xd &(7)\end{aligned}$$

Therefore

$$\gamma(x) = \Delta\theta + \frac{2\pi\,\Phi}{L_x\varphi_0}x \tag{8}$$

Now, we have that the total current is given by

$$\begin{aligned} I \quad &= \quad \int_0^{L_x} j_c \sin\big(\gamma(x)\big) &(9)\\ &= \quad \int_0^{L_x} j_c \sin\left(\Delta\theta \ + \ \frac{2\pi\Phi}{L_x\varphi}\,x\right)dx &(10)\\ &= \quad -j_c\frac{L_x\varphi_0}{2\pi\,\Phi}\left[\cos\left(\Delta\theta \ + \ \frac{2\pi\Phi}{L_x\varphi}\,x\right)\right]_0^{L_x} &(11)\\ &= \quad j_c\frac{L_x}{2\pi}\frac{\varphi_0}{\Phi}\left(\cos\big(\Delta\theta\big) - \cos\big(\Delta\theta + \frac{2\pi\Phi}{\varphi_0}\big)\right) &(12)\end{aligned}$$

Now we write:

$$\begin{aligned}
\cos(\Delta\theta) - \cos(\Delta\theta + a) &= \cos(\Delta\theta) - \cos(\Delta\theta)\cos(a) + \sin(\Delta\theta)\sin(a) && (13)\\
&= \cos(\Delta\theta)[1 - \cos(a)] + \sin(\Delta\theta)\sin(a) && (14)\\
&= \cos(\Delta\theta)[2\sin^2(a/2)] + 2\sin(\Delta\theta)\sin(a/2)\cos(a/2) && (15)\\
&= 2\sin(a/2)[\cos(\Delta\theta)\sin(a/2) + \sin(\Delta\theta)\cos(a/2)] && (16)\\
&= 2\sin(a/2)[\sin(\Delta\theta + a/2] && (17)
\end{aligned}$$

Therefore, using this identity in our equation for current gives

$$I = j_c \frac{L_x}{\pi} \frac{\varphi_0}{\Phi} \sin\left(\frac{\pi\Phi}{\varphi_0}\right) \sin\left(\Delta\theta + \frac{\pi\Phi}{\varphi_0}\right) \tag{18}$$

Therefore, clearly the max current is:

$$j_c \frac{L_x}{\pi} \frac{\varphi_0}{\Phi} \sin\left(\frac{\pi\Phi}{\varphi_0}\right) \tag{19}$$

Problem 2 - Hund's Rule

For an ion which has 4 electrons in its d shell, Hund's first rule tell's us that we want to maximize the total spin. Sine the d shell has orbital quantum number $\ell \in \{-2, 2\}$, there are five possible angular momentum state we can put the electron in. Then we can safely put all 4 electrons in the spin up $s = +1/2$ states so that total spin is $S = 2$.

Hund's second rule states that we want to maximize total angular momentum L_z. Each electron can have $m_\ell \in \{-2, \ldots, 2\}$. Pauli's exclusion principle states states that we can only have one spin up electron for each value of m_ℓ so that the maximum total L^z that we can assign to the group of 4 electrons $m_\ell = 2, 1, 0, -1$. Then the overall angular momentum is $L = 2 + 1 + 0 + (-1) = 2$. Finally, the d shell can hold 10 electrons, so it is less than half filled, so that Hund's third rule states that $J = |L - S| = |2 - 2| = 0$.

Therefore $S = 2$, $L = 2$ and $J = 0$. Or in spectroscopic notation

$$^{2S+1}L_J \;=\; ^5P_0$$

(Where P represents the $L = 2$ state in this notation).

Now, if we instead consider an ion with 2 f electrons in its outer shell, in this case each angular quantum number can take on any value from $\ell = \{-3, \ldots, 3\}$, so that the shell can hold 14 possible electrons. Then, Hund's first rule implies that all electrons are spin up $s = +1/2$ so that $S = 3/2$.

Hund's second rule says we want to assign the angular numbers $m_\ell = 3, 2$ and 1 to our three electrons so that the total angular momentum is $L = 3 + 2 + 1 = 6$.

Once again, our outer shell is less than half full so that Hund's third rule states that $J = |L - S| = |6 - \frac{3}{2}| = \frac{9}{2}$

Therefore our ground state would be the state with $S = \frac{3}{2}$, $L = 6$ and $J = \frac{9}{2}$

In spectroscopic notation (noting that $L = 6$ is represented by a capital I), this groundstate is denoted by

$$^{2S+1}L_J \;=\; ^4I_{9/2}$$

Problem 3 - Brillouin Function

Part (a)

The energy of a spin S moment in a magnetic feld H with g-factor g is given by

$$E = -\vec{\mu} \cdot \vec{H} = m_s g \mu_B H \tag{20}$$

where $m_s \in \{S, S-1, \ldots, -S\}$

Then, the probability that the spin will be in a state with $m_s = m$ is given by

$$P(m) = \frac{e^{-E(m)/k_B T}}{\sum_{m=-S}^{S} e^{-E(m)/k_B T}} \tag{21}$$

Then, the average magnetization of the moment is then given by the average of the magnetic moment along the field directions $\langle m \rangle$ time $g\mu_B$. That is $M = g\mu_B \langle m \rangle$

Now, note that

$$\begin{aligned}
\langle m \rangle &= \sum_{m=-S}^{S} m\ P(m) && (22)\\
&= \frac{e^{-E(m)/k_B T}}{\sum_{m=-S}^{S} e^{-E(m)/k_B T}} && (23)\\
&= \frac{\sum_{-S}^{S} m e^{-mg\mu H/k_B T}}{\sum_{-S}^{S} e^{-mg\mu H/k_B T}} && (24)\\
&= \frac{\sum_{-S}^{S} m e^{mx}}{\sum_{-S}^{S} e^{mx}} && (25)\\
&= \frac{d}{dx} \ln \left(\sum_{m=-S}^{S} e^{mx} \right) && (26)
\end{aligned}$$

where $x = -g\mu H / k_B T$.

Using mathematica we see that the sums in this expression are equal to

$$\begin{aligned}
\sum_{m=-S}^{S} a^m &= \frac{a^{-S}(a^{2S+1} - 1)}{a - 1} \\
\Rightarrow \sum_{m=-S}^{S} e^{mx} &= \frac{e^{-Sx}(e^{(2S+1)x} - 1)}{e^x - 1} = \frac{e^{(S+1)x} - e^{-Sx}}{e^x - 1} && (27)\\
&= \frac{e^{(S+\frac{1}{2})x} - e^{-(S+\frac{1}{2})x}}{e^{x/2} - e^{-x/2}} && (28)\\
&= \frac{\sinh[(S+\frac{1}{2})x]}{\sinh(x/2)} && (29)
\end{aligned}$$

Therefore

$$\begin{aligned}
\langle m \rangle &= \frac{d}{dx} \ln \left(\frac{\sinh[(S+\frac{1}{2})x]}{\sinh(x/2)} \right) && (30)\\
&= \frac{\sinh(x/2)}{\sinh[(S+\frac{1}{2})x]} \left[\frac{(S+\frac{1}{2})\cosh[(S+\frac{1}{2})x]}{\sinh(x/2)} - \frac{\sinh[(S+\frac{1}{2})x]}{2\sinh^2(x/2)} \cosh(x/2) \right] && (31)\\
&= (S + \frac{1}{2}) \coth[(S + \frac{1}{2})x] - \frac{1}{2} \coth(x/2) && (32)
\end{aligned}$$

Now, write our answer in terms of $x' = g\mu_B SH/k_B T \; = -Sx$, then

$$M = -g\mu_B S\langle m\rangle = g\mu_B S\left[\frac{2S+1}{2S}\coth\left(\frac{2S+1}{2S}x'\right) \; - \; \frac{1}{2S}\coth\left(\frac{x'}{2S}\right)\right] \tag{33}$$

Therefore

$$M = g\mu_B S \; B_s(g\mu_B SH/k_B T) \tag{34}$$

Part (b)

Let $a = (2S+1)$ and $b = 1/(2S)$. Then

$$B_S(x) = ab\coth(abx) - b\coth(bx) \quad \approx \quad 1 - 1 + \frac{(ab)^2 x}{3} - \frac{b^2 x}{3} \tag{35}$$

$$= \quad \frac{1}{3}b^2 x(a^2-1) \tag{36}$$

$$\Rightarrow \qquad \left.\frac{d\,B_s(x)}{dx}\right|_{x\to 0} \quad = \quad \frac{1}{3}(a^2-1)b^2 \; = \; \frac{1}{3}\frac{(2S+1)^2-1}{4S^2} \; = \frac{1}{3}\frac{S+1}{S} \tag{37}$$

Then,

$$\left.\frac{\partial M}{\partial H}\right| H\to 0 \qquad = \qquad g\mu_B S\left.\frac{\partial\,B_s(x)}{\partial x}\right|_{x\to 0}\frac{\partial x}{\partial H} \tag{38}$$

$$= \quad g\mu_B S\,\frac{S+1}{3S}\,\frac{g\mu_B S}{k_B T} \qquad\qquad \text{using} \quad x = g\mu_B SH/k_B T \tag{39}$$

Therefore

$$\chi = \left.\frac{\partial M}{\partial H}\right|_{H=0} \quad = \quad \frac{(g\mu_B)^2\,S(S+1)}{3k_B T} \tag{40}$$