Solution to Problem Set 3

First we will consider the scattering of a neutron by a single spin. If the spin is due to an electron, the magnetic dipole moment is $\vec{m} = 2\mu_B \vec{S}$, where $\vec{S}$ is the spin operator and can be represented by Pauli matrices as $\vec{S} = \vec{\sigma}/2$. The vector potential due to a magnetic dipole moment $\vec{m}$ is,

$$\vec{A}(\vec{r}) = -\frac{\mu_0}{4\pi}\left[\vec{m} \times \vec{\nabla}\left(\frac{1}{r}\right)\right], \quad (1)$$

from which the magnetic field can be calculated as,

$$\begin{aligned}\vec{B}(\vec{r}) &= \vec{\nabla} \times \vec{A}(\vec{r}) \\ &= \frac{\mu_0}{4\pi}\left[\frac{3\left(\hat{r}\cdot\vec{m}\right)\hat{r} - \vec{m}}{r^3} + 4\pi\vec{m}\delta^3(\vec{r})\right]. \quad (2)\end{aligned}$$

The magnetic moment of the neutron is $\vec{m}_N = \gamma_N \mu_N \vec{S}_N$, and the magnetic interaction between the two is given by the Hamiltonian,

$$\begin{aligned}\mathcal{H} &= -\vec{m}_N \cdot \vec{B} \\ &= \lambda \vec{S}_N \cdot \left[\vec{\nabla} \times \left\{\vec{S}_e \times \vec{\nabla}\left(\frac{1}{r}\right)\right\}\right] \\ &= \lambda \left(S_N\right)_i \epsilon_{imk}\partial_m \epsilon_{kjl}\left(S_e\right)_j \partial_l\left(\frac{1}{r}\right), \quad (3)\end{aligned}$$

where $\lambda = 2\mu_B\gamma_N\mu_N\mu_0/4\pi$.

To calculate the scattering cross-section for the neutron with incident wave-vector $\vec{k}$ and final wave-vector $\vec{k}'$, we have to evaluate the matrix element $\langle\, k|\epsilon_{imk}\epsilon_{kjl}\partial_m\partial_l\left(\frac{1}{r}\right)|k'\,\rangle$. This is the Fourier transform of the potential that the neutron experiences. The calculation is done using the trick (thanks to Chaikin & Lubensky),

$$\frac{1}{r} = \int \frac{d^3q}{(2\pi)^3}\frac{4\pi}{q^2}e^{-i\vec{q}\cdot\vec{r}}. \quad (4)$$

Then,

$$\begin{aligned}\langle\, k|\epsilon_{imk}\epsilon_{kjl}\partial_m\partial_l\left(\frac{1}{r}\right)|k'\,\rangle &= \epsilon_{imk}\epsilon_{kjl}\int d^3r e^{i\vec{q}\cdot\vec{r}}\partial_m\partial_l\left(\frac{1}{r}\right) \\ &= \epsilon_{imk}\epsilon_{kjl}\int d^3r e^{i\vec{q}\cdot\vec{r}}\partial_m\partial_l\int\frac{d^3k}{(2\pi)^3}\frac{4\pi}{k^2}e^{-i\vec{k}\cdot\vec{r}} \\ &= -4\pi\epsilon_{imk}\epsilon_{kjl}\int\frac{d^3k}{(2\pi)^3}\frac{k_m k_l}{k^2}\int d^3r e^{i(\vec{q}-\vec{k})\cdot\vec{r}} \\ &= 4\pi\left(q_i q_j - q^2\delta_{ij}\right)\frac{1}{q^2}, \quad (5)\end{aligned}$$

where $\vec{q} = \vec{k} - \vec{k}'$.

The matrix element for the transition of the neutron from an initial state of wave-vector $\vec{k}$ and spin state $|s\rangle$ and the elctron in the initial spin state $|\sigma\rangle$ to corresponding final states $\vec{k}'$ and $|s'\rangle$ for the neutron and $|\sigma'\rangle$ for the electron is,

$$\langle ks;\sigma|\mathcal{H}|k's';\sigma'\rangle = 4\pi\lambda\langle s|(\hat{S}_N)_i|s'\rangle\langle\sigma|(\hat{S}_e)_j|\sigma'\rangle(q_iq_j - q^2\delta_{ij})\frac{1}{q^2}. \tag{6}$$

In Born approximation the differential scattering cross-section for the neutron is given by,

$$\left(\frac{d\sigma}{d\Omega}\right)_{\vec{k},s\rightarrow\vec{k}',s'} = \left(\frac{m_N}{2\pi\hbar^2}\right)^2 \sum_{\sigma,\sigma'} P(\sigma)\left|\langle ks;\sigma|\mathcal{H}|k's';\sigma'\rangle\right|^2. \tag{7}$$

Here $P(\sigma)$ is the probability of the electron to be in the spin state $|\sigma\rangle$. The summation over the electron spins can be done easily and we have,

$$\sum_{\sigma,\sigma'} P(\sigma)\langle\sigma|(\hat{S}_e)_j|\sigma'\rangle\langle\sigma'|(\hat{S}_e)_k|\sigma\rangle = (\frac{1}{4})\delta_{jk}, \tag{8}$$

if the electron has an equal probability to be in up and down states. Then, combining equations (6), (7) and (8) we have,

$$\left(\frac{d\sigma}{d\Omega}\right)_{\vec{k},s\rightarrow\vec{k}',s'} = \left(\frac{m_N}{2\pi\hbar^2}\right)^2 (4\pi\lambda)^2(\frac{1}{4})\left(q^2\delta_{ij} - q_iq_j\right)\frac{1}{q^2}\langle s|(\hat{S}_N)_i|s'\rangle\langle s'|(\hat{S}_N)_j|s\rangle. \tag{9}$$

If the neutron is initially in the state $|\uparrow\rangle$ and finally in $|\downarrow\rangle$, then the scattering cross-section is,

$$\begin{aligned}
\left(\frac{d\sigma}{d\Omega}\right)_{\vec{k},\uparrow\rightarrow\vec{k}',\downarrow} &= \left(\frac{m_N}{2\pi\hbar^2}\right)^2 (4\pi\lambda)^2\frac{1}{q^2}\Big\{\langle\uparrow|(\hat{S}_N)_x|\downarrow\rangle\langle\downarrow|(\hat{S}_N)_x|\uparrow\rangle(q^2 - q_x^2) \\
&+ \langle\uparrow|(\hat{S}_N)_x|\downarrow\rangle\langle\downarrow|(\hat{S}_N)_y|\uparrow\rangle(-q_xq_y) + \langle\uparrow|(\hat{S}_N)_y|\downarrow\rangle\langle\downarrow|(\hat{S}_N)_x|\uparrow\rangle(-q_yq_x) \\
&+ \langle\uparrow|(\hat{S}_N)_y|\downarrow\rangle\langle\downarrow|(\hat{S}_N)_y|\uparrow\rangle(q^2 - q_y^2)\Big\} \\
&= \left(\frac{m_N}{2\pi\hbar^2}\right)^2 (4\pi\lambda)^2(\frac{1}{4})^2\left(1 + \cos^2\theta\right).
\end{aligned} \tag{10}$$

Similarly, we can show that,

$$\left(\frac{d\sigma}{d\Omega}\right)_{\vec{k},\uparrow\rightarrow\vec{k}',\uparrow} = \left(\frac{m_N}{2\pi\hbar^2}\right)^2 (4\pi\lambda)^2(\frac{1}{4})^2\sin^2\theta. \tag{11}$$

Now we consider, instead of a single spin, a regular array of spins in a lattice. Let the position of the spins be $\vec{R}_\alpha$. The magnetic moment per unit volume of the sample is defined as,

$$\vec{m}(\vec{r}') = \sum_\alpha \vec{m}_\alpha\delta(\vec{r}' - \vec{R}_\alpha), \tag{12}$$

where $\vec{m}_\alpha$ is the magnetic moment of the spin at $\vec{R}_\alpha$. The magnetic field created by the array of spins is,

$$\begin{aligned}\vec{B}(\vec{r}) &= -\left(\frac{\mu_0}{4\pi}\right)\vec{\nabla}\times\left[\vec{m}_\alpha\times\vec{\nabla}\left(\frac{1}{\left|\vec{r}-\vec{R}_\alpha\right|}\right)\right] \\ &= -\left(\frac{\mu_0}{4\pi}\right)\int d^3r'\;\vec{\nabla}\times\left[\vec{m}(\vec{r}')\times\vec{\nabla}\left(\frac{1}{|\vec{r}-\vec{r}'|}\right)\right], \qquad (13)\end{aligned}$$

where we have used equation (12) in the last step. The magnetic interaction between the neutron and the spins is given by,

$$\begin{aligned}\mathcal{H} &= \lambda\vec{S}_N\cdot\left[\int d^3r'\;\vec{\nabla}\times\vec{S}(\vec{r}')\times\vec{\nabla}\left(\frac{1}{|\vec{r}-\vec{r}'|}\right)\right] \\ &= \lambda\int d^3r'(\hat{S}_N)_i\epsilon_{imk}\partial_m\epsilon_{kjl}\hat{S}_j(\vec{r}')\;\partial_l\left(\frac{1}{|\vec{r}-\vec{r}'|}\right), \qquad (14)\end{aligned}$$

where $\vec{S}(\vec{r})$ is the total spin per unit volume of the array. The Fourier transform of the potential is similar to what we did before, and we have,

$$\langle\, k|\epsilon_{imk}\epsilon_{kjl}\partial_m\partial_l\left(\frac{1}{|\vec{r}-\vec{r}'|}\right)|k'\,\rangle = 4\pi\left(q_iq_j - q^2\delta_{ij}\right)\frac{1}{q^2}e^{i\vec{q}\cdot\vec{r}'}. \qquad (15)$$

The relevant matrix element is,

$$\langle\, ks;S|\mathcal{H}|k's';S'\,\rangle = 4\pi\lambda\langle\, s|(\hat{S}_N)_i|s'\,\rangle\langle\, S|\hat{S}_j(\vec{q})|S'\,\rangle(q_iq_j - q^2\delta_{ij})\frac{1}{q^2}. \qquad (16)$$

Here $|S\,\rangle$ and $|S'\,\rangle$ are the initial and final spin states of the array. $\vec{S}(\vec{q})$ is the Fourier transform of the spin of the array and is defined as,

$$\vec{S}(\vec{q}) = \int d^3r\vec{S}(\vec{r})e^{i\vec{r}\cdot\vec{q}}.$$

In the previous case, where there was a single spin, we considered elastic scattering of the neutron. This is usually the case, unless the spin has other degrees of freedom that the neutron can excite. However, now the neutron can exchange energy with the array. This is what happens in inelastic neutron scattering experiments. The scattering cross-section per unit energy, called the partial scattering cross-section is defined as,

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{\vec{k},s,E\to\vec{k}',s',E'} = \frac{k}{k'}\left(\frac{m_N}{2\pi\hbar^2}\right)^2\sum_{S,S'}P(S)\left|\langle\, ks;S|\mathcal{H}|k's';S'\,\rangle\right|^2\delta(E_S - E_{S'} + \hbar\omega), \qquad (17)$$

where E_S is the energy of the array in the spin state $|S\,\rangle$ and $\hbar\omega = E - E'$, is the energy transferred from the neutron to the array. The delta function, which ensures total energy conservation during the scattering, can be represented as,

$$\delta(E_S - E_{S'} + \hbar\omega) = \int\frac{dt}{2\pi\hbar}e^{(i/\hbar)(E_S - E_{S'} + \hbar\omega)t}. \qquad (18)$$

The summation over the spin of the array gives,

$$\begin{aligned}\sum_{S,S'} P(S)\langle S|\hat{S}_j(\vec{q})|S'\rangle\langle S'|\hat{S}_l(-\vec{q})|S\rangle e^{(i/\hbar)(E_S-E_{S'})t} &= \sum_{S} P(S)\langle S|\hat{S}_j(\vec{q},t)\hat{S}_l(-\vec{q},0)|S\rangle \\ &= \chi_{jl}(\vec{q},t), \qquad (19)\end{aligned}$$

where $\chi_{jl}(\vec{q},t)$ is the dynamic spin-spin correlation function. The time integral from (18) Fourier transforms the correlation function,

$$\int dt\chi_{jl}(\vec{q},t)e^{i\omega t} = \chi_{jl}(\vec{q},\omega). \qquad (20)$$

Using equations (16), (17), (19) and (20) we can write a general expression for the partial differential scattering cross-section as,

$$\begin{aligned}\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{\vec{k},s,E\to\vec{k}',s',E'} &= \frac{k}{k'}\left(\frac{m_N}{2\pi\hbar^2}\right)^2\frac{(4\pi\lambda)^2}{2\pi\hbar}\frac{1}{q^4}\left(q_iq_j-q^2\delta_{i,j}\right)\left(q_kq_l-q^2\delta_{k,l}\right) \\ &\times\langle s|(\hat{S}_N)_i|s'\rangle\langle s'|(\hat{S}_N)_k|s\rangle\chi_{jl}(\vec{q},\omega). \qquad (21)\end{aligned}$$

Suppose the neutron is initially in the spin up state, and the detector can detect only down spins. Then, $|s\rangle = |\uparrow\rangle$, and $|s'\rangle = |\downarrow\rangle$.In this case it is easy to see that in equation (21) indices $i,k \neq z$. Doing a summation over the appropriate indices in equation (21), and after a bit of algebra we get the result,

$$\begin{aligned}\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{\vec{k},\uparrow,E\to\vec{k}',\downarrow,E'} &= \frac{k}{k'}\left(\frac{m_N}{2\pi\hbar^2}\right)^2\frac{(4\pi\lambda)^2}{2\pi\hbar}(\frac{1}{4})\frac{1}{q^4}\Big(q^4\chi_{-+}(\vec{q},\omega)+q_-q_+q_jq_l\chi_{jl}(\vec{q},\omega) \\ &-q^2q_+q_l\chi_{-l}(\vec{q},\omega)-q^2q_-q_j\chi_{j+}(\vec{q},\omega)\Big), \qquad (22)\end{aligned}$$

where, $q_+ = q_x + iq_y$ and $q_- = q_x - iq_y$.

If the neutron is in spin up state both initially and finally after the scattering, then $|s\rangle = |s'\rangle = |\uparrow\rangle$. In this case, we have $i = k = \hat{z}$ in equation (21).

If both the initial and final neutron beam are unpolarized, then we have to do a sum over the neutron spins. Since,

$$\sum_{s,s'} P(s)\langle s|(\hat{S}_N)_i|s'\rangle\langle s'|(\hat{S}_N)_k|s\rangle = (\frac{1}{4})\delta_{ik},$$

now equation (21) can be simplified as,

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{\vec{k},E\to\vec{k}',E'} = \frac{k}{k'}\left(\frac{m_N}{2\pi\hbar^2}\right)^2\frac{(4\pi\lambda)^2}{2\pi\hbar}(\frac{1}{4})\frac{1}{q^2}\left(q^2\delta_{jl}-q_jq_l\right)\chi_{jl}(\vec{q},\omega). \qquad (23)$$

Suppose the spins are ordered in the $\hat{z}$ direction, with an ordering wavevector $\vec{Q}$ (for ferromagnetic ordering $\vec{Q} = 0$, while $\vec{Q}$ is finite for antiferromagnetic ordering). Then $\chi_{zz}(\vec{Q})$ is peaked and the corresponding elastic scattering cross-section is large.