1 Scattering of light by an array of atoms

In our experiment we observe the scattering of photons from atoms confined in an optical lattice, here we treat this situation by obtaining the the field scattered from a single atom and then summing the field contributions from all the atoms coherently at the location of our detector. The main goal of this document is to find the connection between the intensity that we measure in our cameras and the spin structure factor as it is calculated by the theorists in our collaboration.

1.1 Coherent and Incoherent scattering

To calculate the scattered field, one uses the source-field expression, which relates the radiated field to the emitting dipole moment, this is derived in the standard textbooks [1, 2]. The field at the position of the detector $\boldsymbol{r}_D$ is given by

$$E^{(+)}(\boldsymbol{r}_D, t) = \eta e^{-i\omega_L(t-r_D/c)} S_-\left(t - \frac{r_D}{c}\right) \tag{1}$$

where η is a proportionality factor that we will address later on.

The time-averaged intensity at the detector is

$$\begin{aligned}\langle I(t)\rangle =&\langle E^{(-)}(\boldsymbol{r}_D, t) E^{(+)}(\boldsymbol{r}_D, t)\rangle \\ =&|\eta|^2 \langle S_+(t - r_D/c) S_-(t - r_D/c)\rangle \\ =&|\eta|^2 \rho_{ee}(t - r_D/c) \\ =&|\eta|^2 \rho_{ee}\end{aligned} \tag{2}$$

Where in the last step the time dependence is dropped since we are interested in the steady state solution of ρ_{ee}.

We can elucidate the coherence properties of the scattered light if we rewrite the $S_\pm$ operators as

$$S_\pm(t - r_D/c) = \langle S_\pm(t - r_D/c)\rangle + \delta S_\pm(t - r_D/c) \tag{3}$$

at the same time defining the difference δ between $S_\pm$ and its average value. Writing S this way will allow us to distinguish between two components in the radiated light, the radiation of the average dipole $\langle S_\pm\rangle$ which is the radiation of a classical oscillating dipole with a phase that is well defined relative to the incident laser field, and the radiation form the $\delta S_\pm$ component which does not have a phase that is well defined relative to the incident field because this radiation comes form the fluctuating part of the atomic dipole. Dropping the time-dependencies (since we are interested in the steady-state solution only) we have

$$\langle I\rangle = \eta^2 \langle S_+\rangle\langle S_-\rangle + \eta^2 \langle \delta S_+ \delta S_-\rangle \tag{4}$$

where we have used the fact that by definition $\langle \delta S_\pm\rangle = 0$.The first and second terms of this equation are the coherent and incoherent intensity which can be calculated by using the steady-state solutions to the optical Bloch equations

$$\begin{aligned}\frac{1}{\eta^2}\langle I_{\text{coh}}\rangle =&\frac{1}{2}\frac{s}{(1+s)^2} = \rho_{ee}\frac{1}{1+s} \\ \frac{1}{\eta^2}\langle I_{\text{incoh}}\rangle =&\langle S_+ S_-\rangle - |\langle S_+\rangle|^2 \\ =&\frac{1}{2}\frac{s^2}{(1+s)^2} = \rho_{ee}\frac{s}{1+s}\end{aligned} \tag{5}$$

Here s is the saturation parameter

$$s = \frac{2I/I_{\text{sat}}}{1 + 4\Delta^2} \tag{6}$$

1.2 Resonant scattering cross-section

It is seen that coherent and incoherent scattering can be treated independently by thinking about it as an effective value of ρ_{ee} that results for coherent and incoherent scattered light. In our treatment this is what we will do and we will separate the coherent and incoherent part of the scattering. Now we will turn onto the evaluation of the proportionality factor η which will contain the angular dependence of the scattered intensity.

Using the source-field expression for the scattered field allowed us to separate the scattered light into the coherent and incoherent components. Now we are interested in calculating the angular dependence of the transition matrix element, between the following inital and final states

$$\begin{aligned} |\varphi_i\rangle =& |g; \boldsymbol{k}\boldsymbol{\varepsilon}\rangle \\ |\varphi_f\rangle =& |g; \boldsymbol{k}'\boldsymbol{\varepsilon}'\rangle \end{aligned} \tag{7}$$

The transition rate to from $i \to f$ is given by

$$w_{fi} = \frac{2\pi}{\hbar} |\mathcal{T}_{fi}|^2 \delta(E_f - E_i) \tag{8}$$

Where we use the notation in [2], and $\mathcal{T}_{fi}$ is given by

$$\mathcal{T}_{fi} = \frac{\langle g; \boldsymbol{k}'\boldsymbol{\varepsilon}' | H_I' | e; 0\rangle \langle b; 0 | H_I' | g; \boldsymbol{k}\boldsymbol{\varepsilon}\rangle}{\hbar\omega - \hbar\omega_0 + i\hbar(\Gamma/2)} \tag{9}$$

where H_I' is the interaction Hamiltonian

$$H_I' = -\boldsymbol{d} \cdot \boldsymbol{E}_\perp(\boldsymbol{r}) \tag{10}$$

and

$$\boldsymbol{E}_\perp(\boldsymbol{r}) = i \sum_j \left[\frac{\hbar\omega_j}{2\varepsilon_0 L^3}\right]^{1/2} \left(\hat{a}_j \boldsymbol{\varepsilon}_j e^{i\boldsymbol{k}_j\cdot\boldsymbol{r}} - \hat{a}_j^{+} \boldsymbol{\varepsilon}_j e^{-i\boldsymbol{k}_j\cdot\boldsymbol{r}}\right) \tag{11}$$

Using the expressions for H_I' and $\boldsymbol{E}_\perp(\boldsymbol{r})$ we obtain for the matrix element

$$\langle e; 0 | H_I' | g; \boldsymbol{k}\boldsymbol{\varepsilon}\rangle = -i\sqrt{\frac{\hbar\omega}{2\varepsilon_0 L^3}} \langle e | (\boldsymbol{d}\cdot\boldsymbol{\varepsilon}) e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} | g\rangle \tag{12}$$

At this point the textbook treatment usually assumes that the atom is at the origin and so the exponential inside the matrix element tipically does not show up. In our case the atom is in a lattice site and it occupies one of the harmonic oscillator states of a lattice well. The center of mass and internal states of the atom can be separated, and still using the labels e and g for the internal state of the atom, and writing the center of mass initial and final states as $|u\rangle$ and $|u'\rangle$ respectively we have

$$\langle e; 0 | H_I' | g; \boldsymbol{k}\boldsymbol{\varepsilon}\rangle = -i\sqrt{\frac{\hbar\omega}{2\varepsilon_0 L^3}} \langle e | \boldsymbol{d}\cdot\boldsymbol{\varepsilon} | g\rangle \langle v | e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} | u\rangle \tag{13}$$

and similarly

$$\langle g; \boldsymbol{k}'\boldsymbol{\varepsilon}' | H_I' | e; 0\rangle = i\sqrt{\frac{\hbar\omega'}{2\varepsilon_0 L^3}} \langle g | \boldsymbol{d}\cdot\boldsymbol{\varepsilon}' | e\rangle \langle u' | e^{i\boldsymbol{k}'\cdot\boldsymbol{r}} | v\rangle \tag{14}$$

This gives for the matrix element

$$\mathcal{T}_{fi} = \sum_v \frac{\sqrt{\omega\omega'}}{2\varepsilon_0 L^3} \frac{\langle g | \boldsymbol{d}\cdot\boldsymbol{\varepsilon}' | e\rangle \langle e | \boldsymbol{d}\cdot\boldsymbol{\varepsilon} | g\rangle \langle u' | e^{i\boldsymbol{k}'\cdot\boldsymbol{r}} | v\rangle \langle v | e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} | u\rangle}{\omega - \omega_0 + i(\Gamma/2)} \tag{15}$$

where we have summed over all possible intermediate center of mass states. Note that the sum can be taken out using the closure relation $\sum_v |v\rangle\langle v| = \mathbb{1}$.

In our experiment we are driving a sigma-minus transition so we can consider only the projection of $\boldsymbol{d}$ onto $\boldsymbol{\varepsilon}_-$

$$\langle e|\boldsymbol{d}\cdot\boldsymbol{\varepsilon}|g\rangle \equiv d_-\boldsymbol{\varepsilon}_- \tag{16}$$

which leads to

$$\mathcal{T}_{fi} = \frac{\sqrt{\omega\omega'}}{2\varepsilon_0 L^3}\frac{|d_-|^2(\boldsymbol{\varepsilon}_-\cdot\boldsymbol{\varepsilon}')(\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon}_-)}{\omega-\omega_0+i(\Gamma/2)}\langle u'|e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}}|u\rangle \tag{17}$$

We use the relation between $|d_-|^2$ and the linewidth of the transition

$$|d_-|^2 = 3\pi\varepsilon_0\hbar\left(\frac{c}{\omega_0}\right)^3\Gamma \tag{18}$$

and also the approximation $\omega'\approx\omega\approx\omega_0$ (except careful not to use this in the term in the denominator) to obtain

$$\mathcal{T}_{fi} = \frac{3}{k^2}\frac{\pi\hbar c}{L^3}(\boldsymbol{\varepsilon}_-\cdot\boldsymbol{\varepsilon}')(\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon}_-)\frac{\Gamma/2}{\omega-\omega_0+i(\Gamma/2)}\langle u'|e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}}|u\rangle \tag{19}$$

The number of final states with energy between $\hbar ck'$ and $\hbar c(k'+\mathrm{d}k')$ whose wave vector points inside the solid angle $\mathrm{d}\Omega'$ equals

$$\rho(\hbar ck')\hbar c\mathrm{d}k'\mathrm{d}\Omega' = \frac{L^3}{8\pi^3}k'^2\mathrm{d}k'\mathrm{d}\Omega' \tag{20}$$

$$\begin{aligned}\sum_{fu'} w_{fi} =& \frac{2\pi}{\hbar}\mathrm{d}\Omega'\int_0^\infty \frac{k'^2\mathrm{d}k'}{(2\pi/L^3)^3}|\mathcal{T}_{fi}|^2\delta(\hbar ck'-\hbar ck)\\ =&\mathrm{d}\Omega'\frac{9}{4k^2}\frac{c}{L^3}|(\boldsymbol{\varepsilon}_-\cdot\boldsymbol{\varepsilon}')(\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon}_-)|^2\left|\frac{\Gamma/2}{\omega-\omega_0+i(\Gamma/2)}\langle u'|e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}}|u\rangle\right|^2\\ =&\mathrm{d}\Omega'\frac{9}{4k^2}\frac{c}{L^3}|(\boldsymbol{\varepsilon}_-\cdot\boldsymbol{\varepsilon}')(\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon}_-)|^2\frac{(\Gamma/2)^2}{\Delta^2+(\Gamma/2)^2}\left|\langle u'|e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}}|u\rangle\right|^2\end{aligned} \tag{21}$$

If we consider the flux correspoding to the state of the initial photon $\phi = c/L^3$ then we can define the differential cross section

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega'} = \frac{\sum_f w_{fi}}{\mathrm{d}\Omega'\phi} = \frac{9}{4k^2}|(\boldsymbol{\varepsilon}_-\cdot\boldsymbol{\varepsilon}')(\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon}_-)|^2\frac{(\Gamma/2)^2}{\Delta^2+(\Gamma/2)^2}\left|\langle u'|e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}}|u\rangle\right|^2 \tag{22}$$

From here we can write down the intensity at a detector located at $\boldsymbol{r}_D$ in the direction of $\mathrm{d}\Omega'$ as

$$\begin{aligned}I =& \frac{1}{r_D^2}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega'}I_{\text{probe}} = \frac{1}{r_D^2}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega'}\frac{\hbar ck^3\Gamma}{6\pi}\frac{I_{\text{probe}}}{I_{\text{sat}}}\\ =&\frac{\hbar ck\Gamma}{r_D^2}\frac{9}{4(6\pi)}|(\boldsymbol{\varepsilon}_-\cdot\boldsymbol{\varepsilon}')(\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon}_-)|^2\left|\langle u'|e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}}|u\rangle\right|^2\frac{I_{\text{probe}}/I_{\text{sat}}}{4(\Delta/\Gamma)^2+1}\end{aligned} \tag{23}$$

and if we identify the last term as ρ_{ee} (in the limit of low intensity) we can write down an expression for η which was defined back in Eq. (2),

$$\eta = \left[\frac{\hbar ck\Gamma}{r_D^2}\frac{9}{24\pi}\right]^{1/2}(\boldsymbol{\varepsilon}_-\cdot\boldsymbol{\varepsilon}')(\boldsymbol{\varepsilon}\cdot\boldsymbol{\varepsilon}_-)\langle u'|e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}}|u\rangle \tag{24}$$

Notice that we used the limit of low intensity to identify ρ_{ee}. The factor η which contains the angular part of the scattered photon distribution should not be affected if we use the expression for ρ_{ee} that can be obtained from the optical Bloch equations, which is valid for any intensity since the Bloch equations are not a perturbative treatment.

1.3 Summation for a collection of atoms

For a collection of atoms, the resulting fied is the sum of the field produced by each individual atom, so we have

$$\langle I(t)\rangle = \left\langle \left(\sum_m E_m^{(-)}(\boldsymbol{r}_D, t)\right)\left(\sum_n E_n^{(+)}(\boldsymbol{r}_D, t)\right)\right\rangle \tag{25}$$

where we have labeled the atoms with the indices m and n. Dropping the time dependence

$$\langle I\rangle = \sum_{mn} \eta_m \eta_n^* \langle S_{m+} S_{n-}\rangle \tag{26}$$

Using $S = \langle S\rangle + \delta$, as we did above to obtain the coherent and icoherent parts of the intensity, we obtain

$$\begin{aligned}\langle I\rangle &= \sum_{mn} \eta_m \eta_n^* \left(\langle S_{m+}\rangle\langle S_{n-}\rangle + \langle \delta S_{m+}\delta S_{n-}\rangle\right) \\ &= \sum_{mn} \eta_m \eta_n^* \langle S_{m+}\rangle\langle S_{n-}\rangle + \sum_n |\eta_n|^2 \langle \delta S_{n+}\delta S_{n-}\rangle\end{aligned} \tag{27}$$

The steady state solutions of the optical Bloch equations will be used to evaluate the expectation values and we state them here:

$$\langle S_\pm\rangle = u \pm iv \tag{28}$$

$$u = \frac{\Delta}{\Gamma\sqrt{I/I_{\text{sat}}}}\frac{s}{1+s} \tag{29}$$

$$v = \frac{1}{2\sqrt{I/I_{\text{sat}}}}\frac{s}{1+s} \tag{30}$$

$$\tag{31}$$

Putting this back in the equation for $\langle I\rangle$

$$\begin{aligned}\langle I\rangle = \sum_{mn} \eta_m \eta_n^* &\left(\frac{\Delta_m}{\Gamma\sqrt{I/I_{\text{sat}}}}\frac{s_m}{1+s_m} + i\frac{1}{2\sqrt{I/I_{\text{sat}}}}\frac{s_m}{1+s_m}\right)\left(\frac{\Delta_n}{\Gamma\sqrt{I/I_{\text{sat}}}}\frac{s_n}{1+s_n} - i\frac{1}{2\sqrt{I/I_{\text{sat}}}}\frac{s_n}{1+s_n}\right) \\ &+ \sum_n |\eta_n|^2 \frac{1}{2}\frac{s_n^2}{(1+s_n)^2}\end{aligned} \tag{32}$$

$$\langle I\rangle = \sum_{mn} \eta_m \eta_n^* \frac{s_m s_n}{(I/I_{\text{sat}})(1+s_m)(1+s_n)}\left(\frac{\Delta_m\Delta_n}{\Gamma^2} + i\frac{\Delta_n}{2\Gamma} - i\frac{\Delta_m}{2\Gamma} + \frac{1}{4}\right) + \sum_n |\eta_n|^2 \frac{1}{2}\frac{s_n^2}{(1+s_n)^2} \tag{33}$$

We proceed to split up the first sum into same-atom ($n = m$) and different atom ($n < m$) parts

$$\begin{aligned}\langle I\rangle = \sum_{m<n} \frac{s_m s_n}{(I/I_{\text{sat}})(1+s_m)(1+s_n)} &\left(\eta_m \eta_n^* \left(\frac{\Delta_m\Delta_n}{\Gamma^2} + i\frac{\Delta_n}{2\Gamma} - i\frac{\Delta_m}{2\Gamma} + \frac{1}{4}\right)\right. \\ &\left. + \eta_n \eta_m^* \left(\frac{\Delta_n\Delta_m}{\Gamma^2} + i\frac{\Delta_m}{2\Gamma} - i\frac{\Delta_n}{2\Gamma} + \frac{1}{4}\right)\right) \\ &+ \sum_n |\eta_n|^2 \frac{s_n s_n}{(I/I_{\text{sat}})(1+s_n)(1+s_n)}\left(\frac{\Delta_n\Delta_n}{\Gamma^2} + \frac{1}{4}\right) \\ &+ \sum_n |\eta_n|^2 \frac{1}{2}\frac{s_n^2}{(1+s_n)^2}\end{aligned} \tag{34}$$

$$\langle I \rangle = \sum_{m<n} \frac{s_m s_n}{(I/I_{\rm sat})(1+s_m)(1+s_n)} 2\Re\left[\eta_n \eta_m^* \left(\frac{\Delta_m \Delta_n}{\Gamma^2} + i\frac{\Delta_m}{2\Gamma} - i\frac{\Delta_n}{2\Gamma} + \frac{1}{4}\right)\right] + \sum_n |\eta_n|^2 \frac{1}{2}\frac{s_n}{(1+s_n)^2} + \sum_n |\eta_n|^2 \frac{1}{2}\frac{s_n^2}{(1+s_n)^2} \quad (35)$$

With this expression in hand we focus our attention on the terms $\eta_m \eta_n^*$ and $|\eta_n|^2$. We start with the latter

$$|\eta_n|^2 = \frac{\hbar c k \Gamma}{r_D^2} \frac{9}{24\pi} |(\boldsymbol{\varepsilon}_- \cdot \boldsymbol{\varepsilon}')(\boldsymbol{\varepsilon} \cdot \boldsymbol{\varepsilon}_-)|^2 \langle u| e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot \boldsymbol{r}_n} |u'\rangle \langle u'| e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot \boldsymbol{r}_n} |u\rangle \quad (36)$$

and notice that we have to sum over output polarizations λ and final center of mass states u', since our detector does not care about either. We obtain

$$\begin{aligned}
\sum_{\lambda u'} |\eta_n|^2 &= \sum_{\lambda u'} \frac{\hbar c k \Gamma}{r_D^2} \frac{9}{24\pi} |(\boldsymbol{\varepsilon}_- \cdot \boldsymbol{\varepsilon}'_\lambda)(\boldsymbol{\varepsilon} \cdot \boldsymbol{\varepsilon}_-)|^2 \langle u| e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot \boldsymbol{r}_n} |u'\rangle \langle u'| e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot \boldsymbol{r}_n} |u\rangle \\
&= \sum_{\lambda} \frac{\hbar c k \Gamma}{r_D^2} \frac{9}{24\pi} |(\boldsymbol{\varepsilon}_- \cdot \boldsymbol{\varepsilon}'_\lambda)(\boldsymbol{\varepsilon} \cdot \boldsymbol{\varepsilon}_-)|^2 \langle u| e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot \boldsymbol{r}_n} e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot \boldsymbol{r}_n} |u\rangle \\
&= \sum_{\lambda} \frac{\hbar c k \Gamma}{r_D^2} \frac{9}{24\pi} |(\boldsymbol{\varepsilon}_- \cdot \boldsymbol{\varepsilon}'_\lambda)(\boldsymbol{\varepsilon} \cdot \boldsymbol{\varepsilon}_-)|^2
\end{aligned} \quad (37)$$

where we have used the closure relation $\sum u' |u'\rangle\langle u'| = \mathbb{1}$. Similarly for $\eta_m \eta_n^*$

$$\sum_{\lambda u'_m u'_n} \eta_m \eta_n^* = \sum_{\lambda u'_m u'_n} \frac{\hbar c k \Gamma}{r_D^2} \frac{9}{24\pi} |(\boldsymbol{\varepsilon}_- \cdot \boldsymbol{\varepsilon}'_\lambda)(\boldsymbol{\varepsilon} \cdot \boldsymbol{\varepsilon}_-)|^2 \langle u_n| e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot \boldsymbol{r}_n} |u'_n\rangle \langle u'_m| e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot \boldsymbol{r}_m} |u_m\rangle \quad (38)$$

In this case we cannot use the closure relation. We simplify the treatment by considering only final states for the atom that are the same as the initial state $u' = u$ (these are going to have the largest matrix elements), so the sum is discarded. Furthermore we take the center of mass state of the atoms to be the ground state of the single lattice site harmonic oscilator. This leaves us with

$$\sum_{\lambda} \eta_m \eta_n^* = \sum_{\lambda} \frac{\hbar c k \Gamma}{r_D^2} \frac{9}{24\pi} |(\boldsymbol{\varepsilon}_- \cdot \boldsymbol{\varepsilon}'_\lambda)(\boldsymbol{\varepsilon} \cdot \boldsymbol{\varepsilon}_-)|^2 \langle 0_n| e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot \boldsymbol{r}_n} |0_n\rangle \langle 0_m| e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot \boldsymbol{r}_m} |0_m\rangle \quad (39)$$

1.3.1 Debye-Waller factor

For the center of mass expectation values we perform a translation of the vector $\boldsymbol{r}_n$ such that the position of the atom has a zero expectation value $\langle \boldsymbol{r}_n \rangle = 0$. A phase factor comes out that depends on the position $\boldsymbol{R}_n$ of the lattice site in which the atom is located:

$$\langle 0_n| e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot \boldsymbol{r}_n} |0_n\rangle = e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot \boldsymbol{R}_n} \langle 0_n| e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot \boldsymbol{r}_n} |0_n\rangle \quad (40)$$

We then use the equality $\langle e^{\hat{A}} \rangle = e^{\frac{1}{2}\langle \hat{A}^2 \rangle}$, which is valid for a simple harmonic osscilator where $\hat{A}$ is any linear combination of displacement and momentum operators of the oscillator. This leaves us with

$$\begin{aligned}
\langle 0_n| e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot \boldsymbol{r}_n} |0_n\rangle &= e^{-i(\boldsymbol{k}'-\boldsymbol{k})\cdot \boldsymbol{R}_n} e^{-\frac{1}{2}\left\langle [(\boldsymbol{k}'-\boldsymbol{k})\cdot \boldsymbol{r}_n]^2 \right\rangle} \\
&= e^{-i\boldsymbol{Q}\cdot \boldsymbol{R}_n} e^{-\frac{1}{2}\left\langle [\boldsymbol{Q}\cdot \boldsymbol{r}_n]^2 \right\rangle} \\
&= e^{-i\boldsymbol{Q}\cdot \boldsymbol{R}_n} \prod_{i=x,y,z} e^{-\frac{1}{2} Q_i^2 \langle r_{ni}^2 \rangle} \\
&= e^{-i\boldsymbol{Q}\cdot \boldsymbol{R}_n} e^{-W}
\end{aligned} \quad (41)$$

where we have defined the momentum transfer $\boldsymbol{Q} = \boldsymbol{k}' - \boldsymbol{k}$, and the Debye-Waller factor e^{-2W}.

Putting this back in the expression for $\eta_m \eta_n^*$ we get

$$\sum_\lambda \eta_m \eta_n^* = \sum_\lambda \frac{\hbar c k \Gamma}{r_D^2} \frac{9}{24\pi} |(\boldsymbol{\varepsilon}_- \cdot \boldsymbol{\varepsilon}'_\lambda)(\boldsymbol{\varepsilon} \cdot \boldsymbol{\varepsilon}_-)|^2 e^{i\boldsymbol{Q}(\boldsymbol{R}_m - \boldsymbol{R}_n)} e^{-2W} \tag{42}$$

And if we now return to the expression for the intensity at the detector we have

$$\begin{aligned}\langle I \rangle = \sum_{m<n} \frac{s_m s_n}{(I/I_{\text{sat}})(1+s_m)(1+s_n)} 2\Re \Bigg[\sum_\lambda \frac{\hbar c k \Gamma}{r_D^2} \frac{9}{24\pi} |(\boldsymbol{\varepsilon}_- \cdot \boldsymbol{\varepsilon}'_\lambda)(\boldsymbol{\varepsilon} \cdot \boldsymbol{\varepsilon}_-)|^2 e^{i\boldsymbol{Q}(\boldsymbol{R}_m - \boldsymbol{R}_n)} e^{-2W} \\ \left(\frac{\Delta_m \Delta_n}{\Gamma^2} + i\frac{\Delta_m}{2\Gamma} - i\frac{\Delta_n}{2\Gamma} + \frac{1}{4} \right) \Bigg] \\ + \sum_n \frac{1}{2} \sum_\lambda \frac{\hbar c k \Gamma}{r_D^2} \frac{9}{24\pi} |(\boldsymbol{\varepsilon}_- \cdot \boldsymbol{\varepsilon}'_\lambda)(\boldsymbol{\varepsilon} \cdot \boldsymbol{\varepsilon}_-)|^2 \frac{s_n}{1+s_n}\end{aligned} \tag{43}$$

$$\begin{aligned}\langle I \rangle = \left(\frac{\hbar c k \Gamma}{r_D^2} \frac{9}{24\pi} \Lambda \right) \times \\ \sum_{m<n} \frac{s_m s_n}{(I/I_{\text{sat}})(1+s_m)(1+s_n)} 2\Re \left[e^{i\boldsymbol{Q}(\boldsymbol{R}_m - \boldsymbol{R}_n)} e^{-2W} \left(\frac{\Delta_m \Delta_n}{\Gamma^2} + i\frac{\Delta_m}{2\Gamma} - i\frac{\Delta_n}{2\Gamma} + \frac{1}{4} \right) \right] + \sum_n \frac{1}{2} \frac{s_n}{1+s_n}\end{aligned} \tag{44}$$

where we have defined for brevity

$$\Lambda = \sum_\lambda |(\boldsymbol{\varepsilon}_- \cdot \boldsymbol{\varepsilon}'_\lambda)(\boldsymbol{\varepsilon} \cdot \boldsymbol{\varepsilon}_-)|^2 \tag{45}$$

It is good to see that for time-of-flight, where the Debye-Waller goes to zero due to large extent of the expanding atom wavefunctions, this formula reduces to the the standard uncorrelated scattering for N atoms with $\rho_{ee} = \frac{1}{2} \frac{s}{1+s}$.

1.4 Low intensity and large detuning limit

We start from Eq. (44) and concentrate on the two sums, the first of which is

$$\frac{e^{-2W}}{2I/I_{\text{sat}}} \Re \sum_{m<n} e^{i\boldsymbol{Q}(\boldsymbol{R}_m - \boldsymbol{R}_n)} \frac{s_m s_n}{(1+s_m)(1+s_n)} (4\Delta_m \Delta_n + 2i\Delta_m - 2i\Delta_n + 1) \tag{46}$$

where for simplicity we have now written the detunings in units of Γ. We will split this up further into four terms

$$\frac{e^{-2W}}{2I/I_{\text{sat}}} \Re \sum_{m<n} e^{i\boldsymbol{Q}(\boldsymbol{R}_m - \boldsymbol{R}_n)} \frac{s_m s_n}{(1+s_m)(1+s_n)} 4\Delta_m \Delta_n \tag{47}$$

$$\frac{e^{-2W}}{2I/I_{\text{sat}}} \Re \sum_{m<n} e^{i\boldsymbol{Q}(\boldsymbol{R}_m - \boldsymbol{R}_n)} \frac{s_m s_n}{(1+s_m)(1+s_n)} 2i\Delta_m \tag{48}$$

$$-\frac{e^{-2W}}{2I/I_{\text{sat}}} \Re \sum_{m<n} e^{i\boldsymbol{Q}(\boldsymbol{R}_m - \boldsymbol{R}_n)} \frac{s_m s_n}{(1+s_m)(1+s_n)} 2i\Delta_n \tag{49}$$

$$\frac{e^{-2W}}{2I/I_{\text{sat}}} \Re \sum_{m<n} e^{i\boldsymbol{Q}(\boldsymbol{R}_m - \boldsymbol{R}_n)} \frac{s_m s_n}{(1+s_m)(1+s_n)} \tag{50}$$

In the low intensity limit, and for a detuning such that $4\Delta_m^2, 4\Delta_n^2 \gg 1$ these four tend respectively to

$$e^{-2W}2(I/I_{\rm sat})\Re\sum_{m<n}e^{i\boldsymbol{Q}(\boldsymbol{R}_m-\boldsymbol{R}_n)}\frac{1}{4\Delta_m\Delta_n} \tag{51}$$

$$e^{-2W}2(I/I_{\rm sat})\Re\sum_{m<n}e^{i\boldsymbol{Q}(\boldsymbol{R}_m-\boldsymbol{R}_n)}\frac{i}{8\Delta_m\Delta_n^2} \tag{52}$$

$$-e^{-2W}2(I/I_{\rm sat})\Re\sum_{m<n}e^{i\boldsymbol{Q}(\boldsymbol{R}_m-\boldsymbol{R}_n)}\frac{i}{8\Delta_m^2\Delta_n} \tag{53}$$

$$e^{-2W}2(I/I_{\rm sat})\Re\sum_{m<n}e^{i\boldsymbol{Q}(\boldsymbol{R}_m-\boldsymbol{R}_n)}\frac{1}{16\Delta_m^2\Delta_n^2} \tag{54}$$

Furthermore, if we detune the light in between the two spin states then we can use $\frac{1}{2\Delta_m} = \frac{1}{|\Delta|}S_{zm}$, where $S_{zm} = \pm\frac{1}{2}$ is the spin state of the atom in site m, to obtain

$$e^{-2W}\frac{2I/I_{\rm sat}}{|\Delta|^2}\Re\sum_{m<n}e^{i\boldsymbol{Q}(\boldsymbol{R}_m-\boldsymbol{R}_n)}S_{zm}S_{zn} \tag{55}$$

$$e^{-2W}\frac{2I/I_{\rm sat}}{4|\Delta|^3}\Re\sum_{m<n}e^{i\boldsymbol{Q}(\boldsymbol{R}_m-\boldsymbol{R}_n)}iS_{zm} \tag{56}$$

$$-e^{-2W}\frac{2I/I_{\rm sat}}{4|\Delta|^3}\Re\sum_{m<n}e^{i\boldsymbol{Q}(\boldsymbol{R}_m-\boldsymbol{R}_n)}iS_{zn} \tag{57}$$

$$e^{-2W}\frac{2I/I_{\rm sat}}{16|\Delta|^4}\Re\sum_{m<n}e^{i\boldsymbol{Q}(\boldsymbol{R}_m-\boldsymbol{R}_n)} \tag{58}$$

We identify the first term and the last term as related to the spin structure factor and crystal structure factor that appear in Ted's paper. We have also two other terms show up here, which Ted discards in his derivation, see more details on Sec. 1.5. As was stated at the beginning of this document, our main goal here is to connect the intensity measured with our CCD to the spin-structure factor that is calculated by the theorists. In this last equation we see that the spin structure factor is going to have the main contribution to the intensity, as it goes as $|\Delta|^{-2}$, whereas the other terms go as larger powers of $1/|\Delta|$.

If we neglect terms other than the spin structure factor then in the low intensity and large detuning limit (with the detuning set in between the two spin states) we obtain

$$\langle I\rangle = \left(\frac{\hbar ck\Gamma}{r_D^2}\frac{9}{24\pi}\Lambda\right)\times\left(e^{-2W}\frac{2I/I_{\rm sat}}{|\Delta|^2}\Re\sum_{m<n}e^{i\boldsymbol{Q}(\boldsymbol{R}_m-\boldsymbol{R}_n)}S_{zm}S_{zn} + \frac{I/I_{sat}}{4\Delta^2}N\right) \tag{59}$$

where we have made use of $s_n/(1+s_n) \approx (I/I_{\rm sat})/\Delta_n^2$ to carry out the sum over n in Eq. (44). We then manipulate the $n < m$ sum and the real part to obtain

$$\langle I\rangle = \left(\frac{\hbar ck\Gamma}{r_D^2}\frac{9}{24\pi}\Lambda\right)\times\left(e^{-2W}\frac{I/I_{\rm sat}}{|\Delta|^2}\sum_{mn}e^{i\boldsymbol{Q}(\boldsymbol{R}_m-\boldsymbol{R}_n)}S_{zm}S_{zn} + (1-e^{-2W})\frac{I/I_{\rm sat}}{4|\Delta|^2}N\right) \tag{60}$$

In this formula the spin structure factor appears explicitly, we pull out some factors and get

$$\langle I\rangle = \frac{\hbar ck\Gamma}{r_D^2}\frac{9}{24\pi}\Lambda\frac{I/I_{\rm sat}}{4|\Delta|^2}N\left(1+e^{-2W}\left(\frac{4}{N}\sum_{mn}e^{i\boldsymbol{Q}(\boldsymbol{R}_m-\boldsymbol{R}_n)}S_{zm}S_{zn}-1\right)\right) \tag{61}$$

After time-of-flight the Debye-Waller factor goes to zero due to the expanding size of the atomic wave-functions and so

$$\langle I\rangle_{\mathrm{TOF}} = \frac{\hbar ck\Gamma}{r_D^2}\frac{9}{24\pi}\Lambda\frac{I/I_{\mathrm{sat}}}{4|\Delta|^2}N \tag{62}$$

giving finally

$$\frac{I}{I_{\mathrm{TOF}}} = 1 + e^{-2W}(S(\boldsymbol{Q}) - 1) \tag{63}$$

This has the expected form (we got this from David Huse), and it defines the spin structure factor as

$$S(\boldsymbol{Q}) = \frac{4}{N}\sum_{mn} e^{i\boldsymbol{Q}(\boldsymbol{R}_m - \boldsymbol{R}_n)} S_{zm}S_{zn} \tag{64}$$

IMPORTANT REMARK: We note here that this derivation which relates the observed intensity to the spin structure factor relies on the saturation parameter being much less than 1. In our case we have $I/I_{\mathrm{sat}} \approx 25$ and $\Delta \approx 6.5$ which gives a saturation parameter of $s = 0.3$ which is less than 1 but maybe not entirely negligible. In the near future we will attempt to use the exact expression for the intensity at the detector which considers saturation effects to determine what kind of corrections do we need to make to connect between our measurement and the exact spin structure factor.

1.5 Walk through Ted's derivation to find missing terms

We start with Ted's formula for the differential cross section

$$\begin{aligned}\frac{d\,\sigma}{d\,\Omega} =& \frac{9}{4k^2}\sum_{\lambda_f} |(\boldsymbol{e}^*_{\boldsymbol{k}_f\lambda_f}\cdot\boldsymbol{e}_m)(\boldsymbol{e}^*_m\cdot\boldsymbol{e}^*_{\boldsymbol{k}_i\lambda_i})|^2\\ &\times \sum_{\sigma,\sigma',j,j'} [\langle \hat{n}_{j\sigma}\hat{n}_{j'\sigma'} e^{i\boldsymbol{K}\cdot(\hat{\boldsymbol{r}}_j - \hat{\boldsymbol{r}}_{j'})}\rangle \bar{f}_\sigma \bar{f}^*_{\sigma'}]\end{aligned} \tag{65}$$

and we abbreviate the sum over final polarizations as

$$\Lambda = \sum_{\lambda_f} |(\boldsymbol{e}^*_{\boldsymbol{k}_f\lambda_f}\cdot\boldsymbol{e}_m)(\boldsymbol{e}^*_m\cdot\boldsymbol{e}^*_{\boldsymbol{k}_i\lambda_i})|^2 \tag{66}$$

to obtain

$$\frac{d\,\sigma}{d\,\Omega} = \frac{9\Lambda}{4k^2}\sum_{\sigma,\sigma',j,j'} [\langle \hat{n}_{j\sigma}\hat{n}_{j'\sigma'} e^{i\boldsymbol{K}\cdot(\hat{\boldsymbol{r}}_j - \hat{\boldsymbol{r}}_{j'})}\rangle \bar{f}_\sigma \bar{f}^*_{\sigma'}] \tag{67}$$

We will begin by disecting the sum that appears in the elastic cross section. The thermal average factorizes and

$$\begin{aligned}\langle \hat{n}_{j\sigma}\hat{n}_{j'\sigma'}\rangle =& \langle(\frac{1}{2} + \sigma\hat{S}_{zj})(\frac{1}{2} + \sigma'\hat{S}_{j'})\rangle\\ =& \frac{1}{4} + \frac{1}{2}\langle\sigma\hat{S}_{zj}\rangle + \frac{1}{2}\langle\sigma'\hat{S}_{zj'}\rangle + \langle\sigma\sigma'\hat{S}_{zj}\hat{S}_{zj'}\rangle\end{aligned} \tag{68}$$

For this last step

$$\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} = 1$$
$$\sigma = \pm 1$$
$$\hat{S}_{zi} = \tfrac{1}{2}(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})$$

We can manually perform the sums over $\sigma\sigma'$ for each of this four terms and define α, β, and κ,

$$\begin{aligned}\frac{1}{4}\sum_{\sigma\sigma'}\bar{f}_\sigma\bar{f}^*_{\sigma'} &= \frac{1}{4}(\bar{f}_\uparrow+\bar{f}_\downarrow)(\bar{f}^*_\uparrow+\bar{f}^*_\downarrow)\\ &= \frac{1}{4}|\bar{f}_\uparrow+\bar{f}_\downarrow|^2 \equiv \alpha\end{aligned} \tag{69}$$

$$\frac{1}{2}\sum_{\sigma\sigma'}\sigma'\bar{f}_\sigma\bar{f}^*_{\sigma'} = \frac{1}{2}(-\bar{f}_\downarrow\bar{f}^*_\downarrow+\bar{f}_\downarrow\bar{f}^*_\uparrow-\bar{f}_\uparrow\bar{f}^*_\downarrow+\bar{f}_\uparrow\bar{f}^*_\uparrow)\equiv\kappa \tag{70}$$

$$\frac{1}{2}\sum_{\sigma\sigma'}\sigma\bar{f}_\sigma\bar{f}^*_{\sigma'} = \frac{1}{2}(-\bar{f}_\downarrow\bar{f}^*_\downarrow-\bar{f}_\downarrow\bar{f}^*_\uparrow+\bar{f}_\uparrow\bar{f}^*_\downarrow+\bar{f}_\uparrow\bar{f}^*_\uparrow)\equiv\kappa^* \tag{71}$$

$$\begin{aligned}\sum_{\sigma\sigma'}\sigma\sigma'\bar{f}_\sigma\bar{f}^*_{\sigma'} &= (\bar{f}_\uparrow+\bar{f}_\downarrow)(\bar{f}^*_\uparrow+\bar{f}^*_\downarrow)\\ &= |\bar{f}_\uparrow-\bar{f}_\downarrow|^2\equiv\beta\end{aligned} \tag{72}$$

The elastic cross section is then

$$\frac{d\,\sigma_E}{d\,\Omega} = \frac{9\Lambda}{4k^2}\sum_{jj'}\langle e^{i\boldsymbol{K}\cdot(\hat{\boldsymbol{r}}_j-\hat{\boldsymbol{r}}_{j'})}\rangle\left(\alpha+\langle\hat{S}_{zj}\rangle\kappa+\langle\hat{S}_{zj'}\rangle\kappa^*+\langle\hat{S}_{zj}\hat{S}_{zj'}\rangle\beta\right) \tag{73}$$

In the Bragg scattering paper by Ted, the two central terms are ignored, but there is no mention of why they are ignored. As we saw above they also appear in the treatement of scattering that we have undertaken here.

2 Numerical calculations

For the numerical calculation of the scattered intensity we will consider a lattice with $L\times L\times L$ sites in which there is a core of size $L_{\mathrm{AFM}}\times L_{\mathrm{AFM}}\times L_{\mathrm{AFM}}$ in which the atoms have antiferromagnetically ordered spins. The distribution of the spins outside the core is random, but the spin imbalance is constrained to be zero, that is there is an equal number of atoms in state $|1\rangle$ and state $|2\rangle$ occupying the L^3 sites in the lattice.

The reults of the numerical calculation will be presented in a later version of this document as the implementation has not been finished yet.

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