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.

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

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

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:

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

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

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

$$\tag{31}$$

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

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

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

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

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

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

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

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

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

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 $\rho_{ee} = \frac{1}{2}\frac{s}{1+s}$.

2 Numerical calculation

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 $L_{\rm AFM} \times L_{\rm AFM} \times L_{\rm AFM}$ 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.

3 Calculation of scattering cross section

3.1 Coherent and Incoherent scattering

The differential scattering cross section has two componets, one which is due to elastic scattering of photons (the delta-function peak in the fluorescence spectrum) and the other one which is due to inelastic scattering. A single driven two-level atom scatters photons at a rate equal to

$$\Gamma_{\rm tot} = \Gamma \rho_{ee} = \frac{\Gamma}{2} \frac{S}{1+S} \tag{45}$$

where Γ is the natural linewidth of the transition, and ρ_{ee} is the excited state population and S is the saturation parameter given by

$$S = \frac{2I/I_{\rm sat}}{1+4\Delta^2} \tag{46}$$

where I is the intensity of the driving laser, and Δ is its detuning in units of the natural linewidth. Here $I_{\rm sat}$ is defined such that $I/I_{\rm sat} = (\Omega/\Gamma)^2$, where Ω is the Rabi frequency.

The formula for the scattering rate is familiar to all of us, but what is not always present in our minds are the coherence properties of the emitted radiation. I won't go into the details here, but the treatment starts by writing the electric field emitted by the two-level system using the source-field expression (this can be found in Loudon, or in the book called Atom-Photon Interactions by Cohen-Tannoudji). This expression links the emmited electric field to the raising and lowering operators of the two-level system. With this in hand the first order correlation function of the emmited light can be calculated in the steady-state. The bottom line is that the quantum fluctuations in the two-level system give rise to a component of the spectrum that is incoherent. It can be shown that the scattering rate for coherent photons is given by

$$\Gamma_{\rm coh} = \frac{\Gamma_{\rm tot}}{1+S} \tag{47}$$

and the incoherent part follows from $\Gamma_{\rm incoh} + \Gamma_{\rm coh} = \Gamma_{\rm tot}$.

The consideration of the coherent and incoherent fractions of the scattered light is important for our experiment since Bragg scattering is the result of the interference of the coherent photons. We operate in a range of detunings that is close enough to the atomic transitions such that the incoherent fraction plays a role in our observations. In some sense we want to be in this regime because this allows us to have a signal on our cameras on every shot, regardless of whether we have an ordered sample. In this way we can quantify Bragg by noticing how much does the signal on the cameras changes upon the appereance of order in the sample.

Later on we will use the scattering amplitude for a single atom to obtain the differential scatteirng cross-section for our array of N atoms (this is what is done in Ted's paper). The scattering amplitude for an atom in state σ is

$$f_\sigma = -\frac{3}{2k}(\boldsymbol{e}^*_{\boldsymbol{k}_f\lambda_f}\cdot\boldsymbol{e}_m)(\boldsymbol{e}^*_m\cdot\boldsymbol{e}^*_{\boldsymbol{k}_i\lambda_i})\frac{\Gamma/2}{\Delta_\sigma + i\Gamma/2} \tag{48}$$

Here we define the coherent and incoherent amplitudes as

$$\begin{aligned} f_{{\rm c},\sigma} =& f_\sigma\sqrt{\frac{1}{1+S_\sigma}} \\ f_{{\rm i},\sigma} =& f_\sigma\sqrt{\frac{S_\sigma}{1+S_\sigma}} \end{aligned} \tag{49}$$

such that if one were to caculate coherent and incoherent cross sections, then their sum would lead to the familiar result. This treatment is clearly incomplete because the coherent and incoherent photons can definitely interfere with each other to produce a certain intensity at a certain direction. In any case it would be very complicated to treat the problem exactly and this idea serves as a crude first approximation since the effects of this interference between coherent and incohernt photons are expected to average out given the randomness in the phase of the incoherent light.

3.2 Summation for a collection of atoms

With the above in mind we can proceed to calculate the incoherent and coherent cross section for a collection of atoms and to calculate the total cross section we will add them up in the end. The procedure for the coherent part is derived in Ted's paper. Here we follow the same procedure, except that we use the coherent fraction of the scattering amplitude.

$$\begin{aligned} \frac{d\,\sigma_E}{d\,\Omega} =& \frac{9}{4k^2}\sum_{\lambda_f}|(\boldsymbol{e}^*_{\boldsymbol{k}_f\lambda_f}\cdot\boldsymbol{e}_m)(\boldsymbol{e}^*_m\cdot\boldsymbol{e}^*_{\boldsymbol{k}_i\lambda_i})|^2 \\ &\times\sum_{\sigma,\sigma',j,j'}[\langle\hat{n}_{j\sigma}\hat{n}_{j'\sigma'}e^{i\boldsymbol{K}\cdot(\hat{\boldsymbol{r}}_j-\hat{\boldsymbol{r}}_{j'})}\rangle\bar{f}_\sigma\bar{f}^*_{\sigma'}] \end{aligned} \tag{50}$$

The following notation is used:

k	Magnitude of k-vector for incoming photon, $\frac{2\pi}{671\,\mathrm{nm}}$
$\boldsymbol{e}_{\boldsymbol{k}_f\lambda_f}$	Polarization vector of outgoing photon
$\boldsymbol{e}_{\boldsymbol{k}_i\lambda_i}$	Polarization vector of incoming photon
$\boldsymbol{e}_m$	Polarization that couples to optical transition
$\hat{n}_{j\sigma}$	Number operator at site j for atoms in state σ
$\boldsymbol{K}$	Momentum transfer of light scattering, $\boldsymbol{k}_f - \boldsymbol{k}_i$
$\bar{f}_\sigma$	Detuning dependent portion of the scattering amplitude, $\frac{\Gamma/2}{\Delta_\sigma + i\Gamma/2}\sqrt{\frac{1}{1+S_\sigma}}$

In addition to the elastic part, the inelastic scattering cross section for the sample has to be considered. This can be obtained from the cross section of a single atom and and then multiplied by the number of atoms in the sample. Interference effects are not present for the inelastic component, and the incoherent fraction factor is included at the end of the expression.

$$\frac{d\,\sigma_I}{d\,\Omega} = \frac{9}{4k^2}\sum_{\lambda_f} |(\boldsymbol{e}^*_{\boldsymbol{k}_f\lambda_f}\cdot\boldsymbol{e}_m)(\boldsymbol{e}^*_m\cdot\boldsymbol{e}^*_{\boldsymbol{k}_i\lambda_i})|^2 \sum_{j\sigma}\frac{\langle\hat{n}_\sigma\rangle}{1+4\Delta_\sigma^2+2I/I_{\mathrm{sat}}}\frac{S_\sigma}{1+S_\sigma} \tag{51}$$

Finally we abbreviate the sum over final polarizations as

$$\Lambda = \sum_{\lambda_f} |(\boldsymbol{e}^*_{\boldsymbol{k}_f\lambda_f}\cdot\boldsymbol{e}_m)(\boldsymbol{e}^*_m\cdot\boldsymbol{e}^*_{\boldsymbol{k}_i\lambda_i})|^2 \tag{52}$$

to obtain

$$\begin{aligned}
\frac{d\,\sigma_E}{d\,\Omega} &= \frac{9\Lambda}{4k^2}\sum_{\sigma,\sigma',j,j'}[\langle\hat{n}_{j\sigma}\hat{n}_{j'\sigma'}e^{i\boldsymbol{K}\cdot(\hat{\boldsymbol{r}}_j-\hat{\boldsymbol{r}}_{j'})}\rangle\bar{f}_\sigma\bar{f}^*_{\sigma'}] \\
\frac{d\,\sigma_I}{d\,\Omega} &= \frac{9\Lambda}{4k^2}\sum_{j\sigma}\frac{\langle\hat{n}_\sigma\rangle}{1+4\Delta_\sigma^2+2I/I_{\mathrm{sat}}}\frac{S_\sigma}{1+S_\sigma}
\end{aligned} \tag{53}$$

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

$$\begin{aligned}
\langle\hat{n}_{j\sigma}\hat{n}_{j'\sigma'}\rangle &= \langle(\frac{1}{2}+\sigma\hat{S}_{zj})(\frac{1}{2}+\sigma'\hat{S}_{j'})\rangle \\
&= \frac{1}{4}+\frac{1}{2}\langle\sigma\hat{S}_{zj}\rangle+\frac{1}{2}\langle\sigma'\hat{S}_{zj'}\rangle+\langle\sigma\sigma'\hat{S}_{zj}\hat{S}_{zj'}\rangle
\end{aligned} \tag{54}$$

For this last step

$$\begin{gathered}
\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow}=1 \\
\sigma=\pm1 \\
\hat{S}_{zi}=\tfrac{1}{2}(\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow})
\end{gathered}$$

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

$$\begin{aligned}
\frac{1}{4}\sum_{\sigma\sigma'}\bar{f}_\sigma\bar{f}^*_{\sigma'} &= \frac{1}{4}(\bar{f}_\uparrow+\bar{f}_\downarrow)(\bar{f}^*_\uparrow+\bar{f}^*_\downarrow) \\
&= \frac{1}{4}|\bar{f}_\uparrow+\bar{f}_\downarrow|^2 \equiv \alpha
\end{aligned} \tag{55}$$

$$\frac{1}{2}\sum_{\sigma\sigma'}\sigma'\bar{f}_\sigma\bar{f}^*_{\sigma'} = \frac{1}{2}(-\bar{f}_\downarrow\bar{f}^*_\downarrow+\bar{f}_\downarrow\bar{f}^*_\uparrow-\bar{f}_\uparrow\bar{f}^*_\downarrow+\bar{f}_\uparrow\bar{f}^*_\uparrow) \equiv \kappa \tag{56}$$

$$\frac{1}{2}\sum_{\sigma\sigma'}\sigma\bar{f}_\sigma\bar{f}^*_{\sigma'} = \frac{1}{2}(-\bar{f}_\downarrow\bar{f}^*_\downarrow - \bar{f}_\downarrow\bar{f}^*_\uparrow + \bar{f}_\uparrow\bar{f}^*_\downarrow + \bar{f}_\uparrow\bar{f}^*_\uparrow) \equiv \kappa^* \tag{57}$$

$$\begin{aligned}\sum_{\sigma\sigma'}\sigma\sigma'\bar{f}_\sigma\bar{f}^*_{\sigma'} &= (\bar{f}_\uparrow + \bar{f}_\downarrow)(\bar{f}^*_\uparrow + \bar{f}^*_\downarrow)\\ &= |\bar{f}_\uparrow - \bar{f}_\downarrow|^2 \equiv \beta\end{aligned} \tag{58}$$

The elastic cross section is then

$$\frac{d\,\sigma_E}{d\,\Omega} = \frac{9\Lambda}{4k^2}\sum_{jj'}\langle e^{i\boldsymbol{K}\cdot(\hat{\boldsymbol{r}}_j - \hat{\boldsymbol{r}}_{j'})}\rangle\left(\alpha + \langle\hat{S}_{zj}\rangle\kappa + \langle\hat{S}_{zj'}\rangle\kappa^* + \langle\hat{S}_{zj}\hat{S}_{zj'}\rangle\beta\right) \tag{59}$$

3.3 Debye-Waller factor

The position operators $\hat{\boldsymbol{r}}_j$,$\hat{\boldsymbol{r}}_{j'}$ inside the exponential in the thermal average can be replaced by the position vector of the lattice sites plus a displacement operator with respect to the lattice site.

$$\begin{aligned}\langle e^{i\boldsymbol{K}\cdot(\hat{\boldsymbol{r}}_j - \hat{\boldsymbol{r}}_{j'})}\rangle &= e^{i\boldsymbol{K}\cdot(\boldsymbol{R}_j - \boldsymbol{R}_{j'})}\langle e^{i\boldsymbol{K}\cdot(\Delta\hat{\boldsymbol{r}}_j - \Delta\hat{\boldsymbol{r}}_{j'})}\rangle\\ &= e^{i\boldsymbol{K}\cdot(\boldsymbol{R}_j - \boldsymbol{R}_{j'})}\langle e^{i\boldsymbol{K}\cdot(\Delta\hat{\boldsymbol{r}}_j - \Delta\hat{\boldsymbol{r}}_{j'})}\rangle\\ &= e^{i\boldsymbol{K}\cdot(\boldsymbol{R}_j - \boldsymbol{R}_{j'})}\langle e^{i\boldsymbol{K}\cdot\Delta\hat{\boldsymbol{r}}_j}\rangle\langle e^{-i\boldsymbol{K}\cdot\Delta\hat{\boldsymbol{r}}_{j'}}\rangle\end{aligned} \tag{60}$$

The last step follows since the operators $\Delta\hat{\boldsymbol{r}}_j$ and $\Delta\hat{\boldsymbol{r}_{j'}}$ act on different particles. The equality $\langle e^{\hat{A}}\rangle = e^{\frac{1}{2}\langle\hat{A}^2\rangle}$ is used here, 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

$$\begin{aligned}\langle e^{i\boldsymbol{K}\cdot(\hat{\boldsymbol{r}}_j - \hat{\boldsymbol{r}}_{j'})}\rangle &= e^{i\boldsymbol{K}\cdot(\boldsymbol{R}_j - \boldsymbol{R}_{j'})}e^{-\frac{1}{2}\langle(\boldsymbol{K}\cdot\Delta\hat{\boldsymbol{r}}_j)^2\rangle}e^{-\frac{1}{2}\langle(\boldsymbol{K}\cdot\Delta\hat{\boldsymbol{r}}_{j'})^2\rangle}\\ &= e^{i\boldsymbol{K}\cdot(\boldsymbol{R}_j - \boldsymbol{R}_{j'})}e^{-\langle(\boldsymbol{K}\cdot\Delta\hat{\boldsymbol{r}})^2\rangle}\\ &= e^{i\boldsymbol{K}\cdot(\boldsymbol{R}_j - \boldsymbol{R}_{j'})}e^{-2W}\end{aligned} \tag{61}$$

In the last step we made use of the fact that in our sample all the atoms are in the same harmonic oscillator state, so the expectation value is be independent of j. The second exponential with the expectation value is the Debye-Waller factor, generally written as e^{-2W}. Expanding the dot product inside the Debye-Waller exponential leaves us with

$$\langle e^{i\boldsymbol{K}\cdot(\hat{\boldsymbol{r}}_j - \hat{\boldsymbol{r}}_{j'})}\rangle = e^{i\boldsymbol{K}\cdot(\boldsymbol{R}_j - \boldsymbol{R}_{j'})}\prod_{i=x,y,z}e^{-K_i^2\langle\Delta r_i^2\rangle} \tag{62}$$

In an isotropic lattice all three expectation values are the same and equal to

$$\langle\Delta r_i^2\rangle = \frac{\hbar}{m\omega}\left(n + \frac{1}{2}\right) = \frac{\lambda^2}{8\pi^2\sqrt{V_0}}(1 + 2n) \tag{63}$$

so the Debye-Waller factor is

$$e^{-2W} = \exp\left[-K^2\frac{\lambda^2}{8\pi^2\sqrt{V_0}}(1 + 2n)\right] \tag{64}$$

In our case, where we only occupy the first band of the lattice then $n = 0$, and

$$e^{-2W} = \exp\left[-K^2\frac{\lambda^2}{8\pi^2\sqrt{V_0}}\right] \tag{65}$$

3.4 Crystal and Structure factors

Putting it all back together

$$\frac{d\,\sigma_E}{d\,\Omega} = \frac{9\Lambda}{4k^2}e^{-2W}\left(\alpha\sum_{jj'}e^{i\boldsymbol{K}\cdot(\boldsymbol{R}_j-\boldsymbol{R}_{j'})} + \kappa\sum_{jj'}\langle\hat{S}_{zj}\rangle e^{i\boldsymbol{K}\cdot(\boldsymbol{R}_j-\boldsymbol{R}_{j'})}\right.$$
$$\left. +\kappa^*\sum_{jj'}\langle\hat{S}_{zj'}\rangle e^{i\boldsymbol{K}\cdot(\boldsymbol{R}_j-\boldsymbol{R}_{j'})} + \beta\sum_{jj'}\langle\hat{S}_{zj}\hat{S}_{zj'}\rangle e^{i\boldsymbol{K}\cdot(\boldsymbol{R}_j-\boldsymbol{R}_{j'})}\right) \quad (66)$$

PAY ATTENTION TO WHAT IS GOING ON HERE:

The two terms in the center can be simplified by noting that as N gets larger one of the sums approaches a delta-function,

$$\sum_j e^{i\boldsymbol{K}\cdot\boldsymbol{R}_j} = \sum_{\boldsymbol{n}\in\mathbb{Z}^3}\delta\left(\boldsymbol{n}-\boldsymbol{K}\frac{a}{2\pi}\right) \quad (67)$$

so those two terms will be zero unless $\boldsymbol{K}$ is zero or equal to a reciprocal lattice vector. The second option is not a possibility in our setup since we cannot shine light in or image along a lattice vector. If $\boldsymbol{K}=0$ we would then be left with a sum over $\langle\hat{S}_{zj}\rangle$, which is zero in our case since we have a sample without spin imbalance. This leaves us with

$$\begin{aligned}\frac{d\,\sigma_E}{d\,\Omega} =& \frac{9\Lambda}{4k^2}e^{-2W}\left(\alpha\sum_{jj'}e^{i\boldsymbol{K}\cdot(\boldsymbol{R}_j-\boldsymbol{R}_{j'})} + \beta\sum_{jj'}\langle\hat{S}_{zj}\hat{S}_{zj'}\rangle e^{i\boldsymbol{K}\cdot(\boldsymbol{R}_j-\boldsymbol{R}_{j'})}\right)\\ =& \frac{9\Lambda}{4k^2}e^{-2W}\left(\alpha C(\boldsymbol{K})+\beta S(\boldsymbol{K})\right)\end{aligned} \quad (68)$$

In the last step we have the defined the crystal and magnetic structure factors.

Summing the elastic and inelastic cross sections we obtain:

$$\begin{aligned}\frac{d\,\sigma}{d\,\Omega} =& \frac{d\,\sigma_E}{d\,\Omega} + \frac{d\,\sigma_I}{d\,\Omega}\\ =& \frac{9\Lambda}{4k^2}\left(\alpha C(\boldsymbol{K})+\beta S(\boldsymbol{K}) + \sum_{j\sigma}\frac{\langle\hat{n}_\sigma\rangle}{1+4\Delta_\sigma^2+2I/I_{\text{sat}}}\frac{S_\sigma}{1+S_\sigma}\right)\end{aligned} \quad (69)$$

From here one, if one specifies a certain state of the atoms without entanglement (i.e. just a product of single site eigenstates of $\hat{S}_z$) then the summations can be performed using a computer. It is at this point that I have written a computer program that generates configurations with and AFM core in the center and a random distribution of the remaining spins in the center. For a given AFM core size many realizations of the ramdom distribution outside the core are averaged to obtain an estimate for the differential cross section.

3.5 Analytical dependence of crystal and magnetic structure factors on $\boldsymbol{Q}$

3.5.1 Crystal

$$C(\boldsymbol{Q}) = \sum_{jk} e^{i\boldsymbol{Q}\cdot(\boldsymbol{R}_j-\boldsymbol{R}_k)} \quad (70)$$

We can make the substitution $\boldsymbol{r}_k = \boldsymbol{R}_j - \boldsymbol{R}_k$. For an infinite crystal, the sum over all pairs jk may be replaced by the sum over all sites j and then sum over all $\boldsymbol{r}_k$.

$$C(\boldsymbol{Q}) = N\sum_k e^{i\boldsymbol{Q}\cdot\boldsymbol{r}_k} \quad (71)$$

3.5.2 Magnetic

$$S(\boldsymbol{Q}) = \sum_{jk} e^{i\boldsymbol{Q}\cdot(\boldsymbol{R}_j - \boldsymbol{R}_k)} \langle S_{zj} S_{zk} \rangle \tag{72}$$

In the zero temperature AFM state there is a staggered magnetization, such that

$$\langle S_{zj} S_{zk} \rangle = e^{i\boldsymbol{q}\cdot(\boldsymbol{R}_j - \boldsymbol{R}_k)} \quad \text{where} \quad \boldsymbol{q} = \frac{2\pi}{a}\left(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}\right) \tag{73}$$

At finite temperature, the staggered magnetization will have a finite correlation length L_c, which results in

$$\langle S_{zj} S_{zk} \rangle = e^{i\boldsymbol{q}\cdot(\boldsymbol{R}_j - \boldsymbol{R}_k)} e^{-|\boldsymbol{R}_j - \boldsymbol{R}_k|/L_\mathrm{c}} \quad \text{where} \quad \boldsymbol{q} = \frac{2\pi}{a}\left(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}\right) \tag{74}$$

$$S(\boldsymbol{Q}) = \sum_{jk} e^{i(\boldsymbol{Q}+\boldsymbol{q})\cdot(\boldsymbol{R}_j - \boldsymbol{R}_k)} e^{-|\boldsymbol{R}_j - \boldsymbol{R}_k|/L_\mathrm{c}} \tag{75}$$

At this point we can make the substitution $\boldsymbol{r}_k = \boldsymbol{R}_j - \boldsymbol{R}_k$. For an infinite crystal, the sum over all pairs jk may be replaced by the sum over all sites j and then sum over all $\boldsymbol{r}_k$.

$$S(\boldsymbol{Q}) = \sum_{jk} e^{i(\boldsymbol{Q}+\boldsymbol{q})\cdot\boldsymbol{r}_k} e^{-r_k/L_\mathrm{c}} = N \sum_{k} e^{i(\boldsymbol{Q}+\boldsymbol{q})\cdot\boldsymbol{r}_k} e^{-r_k/L_\mathrm{c}} \tag{76}$$

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