1 Relationship between $I/I_{\mathbf{TOF}}$ and $S(\boldsymbol{Q})$

The expression for the scattered intensity in the direction $\boldsymbol{k}'$ by a collection of atoms is given by

$$I = \left(\frac{\hbar c k \Gamma}{r_D^2}\frac{9}{24\pi}\Lambda\right)\frac{I_{\mathrm{p}}/I_{\mathrm{sat}}}{4\Delta^2 + 2I_{\mathrm{p}}/I_{\mathrm{sat}}}\left[\frac{e^{-2W}4\Delta^2}{(4\Delta^2+2I_{\mathrm{p}}/I_{\mathrm{sat}})}\left(4\sum_{mn} e^{i\boldsymbol{Q}(\boldsymbol{R}_m-\boldsymbol{R}_n)}S_{zm}S_{zn} - N\right) + N\right] \tag{1}$$

Here, the momentum transfer is $\boldsymbol{Q} = \boldsymbol{k}' - \boldsymbol{k}$, where $\boldsymbol{k}$ is the wave vector of the probe light. The probe light has intensity I_{p}, and I_{sat} is the saturation intensity of the optical transition. This expression is obtained for a mixture of atoms in states $|1\rangle$ and $|2\rangle$, for light with a detuning $\Delta_1 = -\Delta_2$, in the limit $|\Delta_{1,2}| \gg 1$ (the detuning is in units of the linewidth of the transition). No approximations have been made regarding the relative magnitude of $|\Delta_{1,2}|$ and $I_{\mathrm{p}}/I_{\mathrm{sat}}$. The Debye-Waller factor is e^{-2W}, and the letter Λ denotes a sum over output polarizations

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

The two states satisfy

$$\hat{S}_z|1\rangle = +\frac{1}{2}|1\rangle \quad \hat{S}_z|2\rangle = -\frac{1}{2}|2\rangle \tag{3}$$

The indices m, n denote different atoms, we identify the sum with the spin structure factor at momentum $\boldsymbol{Q}$:

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

We consider a measurement of the intensity after some time-of-flight (TOF). After TOF, the Debye-Waller factor goes to zero due to the expanding size of the atomic wavefunction, so we have

$$I_{\mathrm{TOF}} = \left(\frac{\hbar c k \Gamma}{r_D^2}\frac{9}{24\pi}\Lambda\right)\frac{I_{\mathrm{p}}/I_{\mathrm{sat}}}{4\Delta^2 + 2I_{\mathrm{p}}/I_{\mathrm{sat}}}N \tag{5}$$

$$\frac{I}{I_{\mathrm{TOF}}} = \frac{e^{-2W}4\Delta^2}{(4\Delta^2+2I_{\mathrm{p}}/I_{\mathrm{sat}})}\left(S(\boldsymbol{Q}) - 1\right) + 1 \tag{6}$$

We note that doublons do not contribute to $S(\boldsymbol{Q})$. This can be easily seen from

$$S(\boldsymbol{Q}) = \frac{4}{N}\sum_{m} e^{i\boldsymbol{Q}\boldsymbol{R}_m}S_{zm}\sum_{n} e^{-i\boldsymbol{Q}\boldsymbol{R}_n}S_{zn} \tag{7}$$

A doublon pair contributes $e^{i\boldsymbol{Q}\boldsymbol{R}_D}(+1/2 - 1/2) = 0$ to each sum. If we think about a sample with only doublons, according to the equation above for I/I_{TOF} we have

$$\frac{I_D}{I_{\mathrm{TOF}}} = 1 - \frac{e^{-2W}4\Delta^2}{(4\Delta^2+2I_{\mathrm{p}}/I_{\mathrm{sat}})} \tag{8}$$

Lately we have been performing scattered intensity measurements where we magneto-associate doublons into molecules. The molecules do not scatter the probe light, so they do not contribute at all to the scattered intensity. Under this protocol, for a sample with only doublons we would have

$$\frac{I_D}{I_{\mathrm{TOF}}} = 0 \tag{9}$$

which is consistent with scattering in the limit of an infinitely deep lattice ($e^{-2W} \to 1$) and for a weak probe ($\Delta^2 \gg I_{\rm p}/I_{\rm sat}$), where we have the simple equivalence

$$\frac{I}{I_{\rm TOF}} = S(\boldsymbol{Q}) \tag{10}$$

The magneto-association protocol thus makes the doublons contribute to the scattering in an ideal manner, whereas the atoms in singly occupied sites still suffer from Debye-Waller and saturation effects. This suggests an expression like the following

$$\frac{I}{I_{\rm TOF}} = [c(1-D) + D]\,(S(\boldsymbol{Q}) - 1) + 1 \tag{11}$$

Where D is the fraction of atoms in doubly occupied sites, and the correction factor (Debye-Waller plus saturation corrections) for a sample with only singly occupied sites is

$$c = \frac{e^{-2W} 4\Delta^2}{4\Delta^2 + 2I_{\rm p}/I_{\rm sat}} \tag{12}$$

The fraction of atoms in doubly occupied sites can be obtain from TOF measurements with and without magneto-association as

$$D = 1 - I_{\rm TOFAssoc}/I_{\rm TOF} \tag{13}$$

2 Latest data at 5.5 E_R

Lately we have been taking data with three shots:

1. In-situ with magneto-association, I
2. TOF without magneto-association, $I_{\rm TOF}$
3. TOF with magneto-association, $I_{\rm TOFAssoc}$

The data is shown at the end of this document. For this data we have calculated $S(\boldsymbol{Q})$ using the two different TOF measurements:

$$S_{\rm Assoc}(\boldsymbol{Q}) = \frac{1}{c}\left(\frac{I}{I_{\rm TOFAssoc}} - 1\right) + 1 \tag{14}$$

$$S(\boldsymbol{Q}) = \frac{1}{c}\left(\frac{I}{I_{\rm TOF}} - 1\right) + 1 \tag{15}$$

where, again

$$c = \frac{e^{-2W} 4\Delta^2}{4\Delta^2 + 2I_{\rm p}/I_{\rm sat}} \tag{16}$$

We perform in-situ measurements in a $50E_R$ lattice and for $I_{\rm p}/I_{\rm sat} \approx 15$. In units of the transition linewidth, $\Delta = 6.5$ for our case. With this values we have

$$\begin{aligned} e^{-2W} &= 0.81 \\ 1 + \frac{I_{\rm p}/I_{\rm sat}}{2\Delta^2} &= 1.18 \end{aligned} \tag{17}$$

As usual the data has measurements at two values of $\boldsymbol{Q}$, the one labeled 2 corresponds to the $(1/2, 1/2, 1/2)$ direction, and the other one, labeled 1, corresponds to the intensity measured with our other camera.

We still have not applied a correction such as the one suggested in Eq. 11 because we have not yet reached consensus on the validity of this equation. In fact I am just suggesting it in this pdf to see what everybody's opinions are on this matter.

An interesting feature of this data is that, with the magneto-association, we get better agreement with $S(\boldsymbol{Q}_1)$ as calculated by Thereza. In the data that we took at $7E_R$ we did not have much agreement with $S(\boldsymbol{Q_1})$.

The corrected value of $S(\boldsymbol{Q_2})$ is 1.4, which would be consistent with a temperature T/t of around 1.1.

We have also ploted $S(\boldsymbol{Q_1})/S(\boldsymbol{Q_2})$ for this data. In the abscense of antiferromagnetic correlations this should go to 1.