The fundamental formulation that links up the theoretical description of the neutron scattering to the experimental measurement contains the following two equations:

$$C = \phi \Delta\Omega \eta \left(\frac{d\sigma}{d\Omega}\right)_{k_i,\sigma_i \to k_f,\sigma_f} \tag{1}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{k_i,\sigma_i \to k_f,\sigma_f} = \left(\frac{m}{2\pi\hbar^2}\right)^2 |\langle k_f, \sigma_f |V| k_i, \sigma_i \rangle|^2 \tag{2}$$

The Eqn. (1) links up the counting rate C of an experiment detector with the differential cross section. The Eqn. (2) then gives the formulation for calculating the differential cross section. A bit more detailed description will be given in next slide. The following is the information about the symbols used in Eqn. (1) and (2):

$C \rightarrow$ **The counting rate**

$\Delta\Omega \rightarrow$ **The corresponding solid angle that the detector subtends**

$\eta \rightarrow$ **Efficiency**

$\phi \rightarrow$ **The uniform flux of neutrons**

k_i, σ_i and k_f, σ_f refers to the initial (before the scattering) and final (after the scattering) wave vector and neutron spin, respectively.

The fundamental principle here is that we have the neutron beam coming in with some initial state $|i\rangle$ and scattered to a final state $|f\rangle$ by the interaction potential V. The differential cross section given in Eqn. (2) in last slide is based on the so-called Fermi's golden rule, which basically describes the probability of the scattering from a given initial state to a final state with the influence of the specified scattering potential.

Specifically for neutron scattering event, it is illustrated in the following diagram:
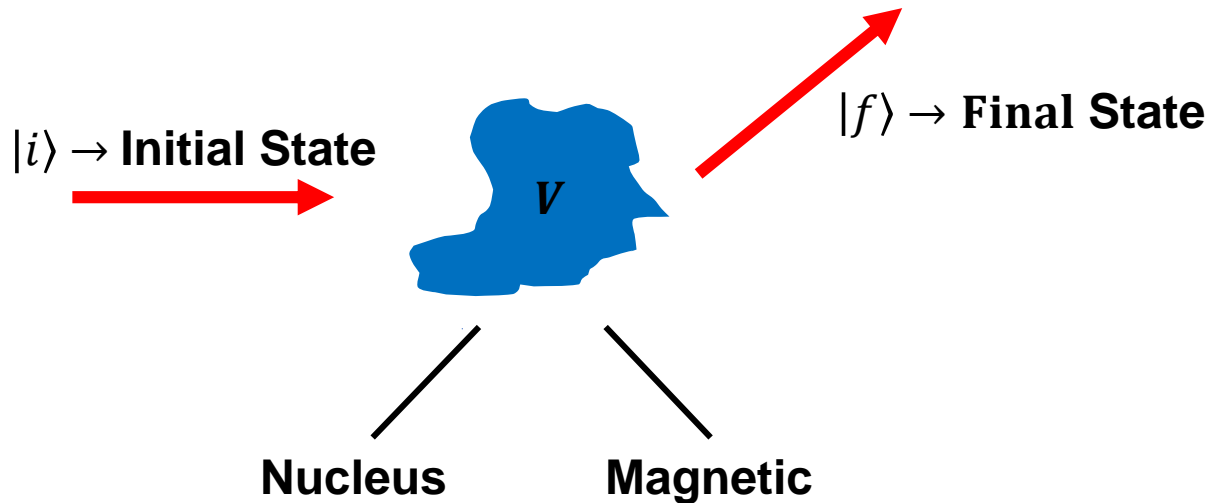
where we have the scattering potential composed of both the nucleus part and the magnetic part.

For the scattering from the nucleus part, if we are concerned with only the thermal neutron [1] (which is the case for common neutron scattering experiment), of which the energy is well below 1 eV, also if considering the short-range of the nuclear forces ($10^{-13} - 10^{-12}$ cm, between the incoming neutrons and the nucleus that we are detecting) as compared to the neutron wavelength (10^{-8} cm), the neutron scattering from a single nucleus can be described by a single parameter b, which is called the neutron scattering length. Otherwise if the nuclear interaction potential is going to be considered in details, as mentioned at the beginning of section 19.2.1.1 in the book *Methods of experimental physics*, Vol. 23 (Neutron scattering, Part-C), the so-called Breit-Wigner resonance formula should be taken into account (i.e. the nucleus scattering cross section can then be calculated using B-W formula [2]).

Nowadays, we have already got the neutron scattering length tabulated for most of the elements in the periodic table, and following is a link to the on-line available source for it: **https://www.ncnr.nist.gov/resources/n-lengths/**. Detailed description about how the neutron scattering length is calculated theoretically can be found in the Appendix-A in the book *Methods of experimental physics*, Vol. 23 (Neutron scattering, Part-A) [3].

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[1] Introduction about thermal neutron and several other types of neutrons with different level of energy can be found on Wikipedia: **Neutron Temperature**, or **here**.
[2] Refer to the following attachment: **Scattering Theory** for the formulation.
[3] In this appendix, not only the dependence of the neutron scattering length on each different isotope is described, but also the contribution from the nuclear spin is also discussed.

As mentioned in the third footnote in last slide, the scattering length not only is related to the type of the isotope, but also depends on the relative coupling between the neutron and nucleus spins of the isotope. By putting these two parts of contributions together, the appropriate formulation for the neutron scattering from the nucleus could be given.

Before moving on, it should be mentioned that to make expression for the neutron scattering formulation convenient, the scattering amplitude operator was introduced, which is related to the scattering potential as given in Eqn. (2) in the following way [4]:

$$|\langle \boldsymbol{k}_f, \boldsymbol{\sigma}_f | \hat{a} | \boldsymbol{k}_i, \boldsymbol{\sigma}_i \rangle| = |\langle \boldsymbol{\sigma}_f | \hat{a}(\boldsymbol{Q}) | \boldsymbol{\sigma}_i \rangle| = \frac{m}{2\pi\hbar^2} |\langle \boldsymbol{k}_f, \boldsymbol{\sigma}_f | V | \boldsymbol{k}_i, \boldsymbol{\sigma}_i \rangle| \qquad \textbf{(3)}$$

Back to the dependence of the neutron scattering length on isotope type and the coupling between neutron and nucleus spins, that means the scattering of neutron from a single nucleus can no longer be described by a single parameter. Instead, we have the nuclear scattering amplitude operator given as:

$$a_N(\boldsymbol{Q}) = b_i + A_i \boldsymbol{\sigma} \cdot \boldsymbol{I}_i \qquad \textbf{(4)}$$

which will then go into Eqn. (3) for the calculation of the differential cross section. Here b_i is just the neutron scattering length of the isotope i, and A_i is another constant which is related to b_i and the nucleus spin I. Again, about how they are obtained theoretically, refer to Appendix-A in the book *Methods of experimental physics*, Vol. 23 (Neutron scattering, Part-A).

Furthermore, the fluctuation of either b_i (here this b_i means specifically the first term in Eqn. 4, attention to the difference from what we usually mean by scattering length, which is, actually, the effective scattering length considering its dependence on both the isotope and nucleus spin, as mentioned in last slide) or nucleus spin will then contribute incoherently to the scattering [5]. Assuming the unpolarized neutron beam scattered from nuclear without polarization (more reference materials will be given later), the differential cross section can be separated to two parts – coherent and incoherent part:

$$\frac{d\sigma_N}{d\Omega} = (d\sigma_N/d\Omega)_{coh} + (d\sigma_N/d\Omega)_{inc} \tag{5}$$

where

$$(d\sigma_N/d\Omega)_{coh} = |\bar{b}|^2 = \sigma_c/4\pi \tag{6}$$

and

$$(d\sigma_N/d\Omega)_{inc} = \overline{b_i^2} - \bar{b}_i^2 + \overline{A_i^2 I(I+1)} = \sigma_i/4\pi \tag{7}$$

---

[4] Here the elastic scattering is assumed so we have $Q = k_i - k_f$. For inelastic scattering, the picture here will change since then we have to consider the double differential cross section $d^2\sigma/d\Omega dE$. A bit more introduction will be given later in this document. Also, for a bit more discussion about Q, refer to [7].

[5] Explanation about the difference between coherent, incoherent, elastic and inelastic scattering can be found in the attached **Q&A on ResearchGate**. Basically, the incoherent scattering means that the scattered beam does not interfere with each other to modulate the phase and the total intensity is just the sum of the intensity for each.

Following is given an illustration for the decomposition of the scattering into coherent and incoherent parts [6]:

| Overall | Average | Deviation |

| Total Scattering | Coherent Scattering | Incoherent Scattering |
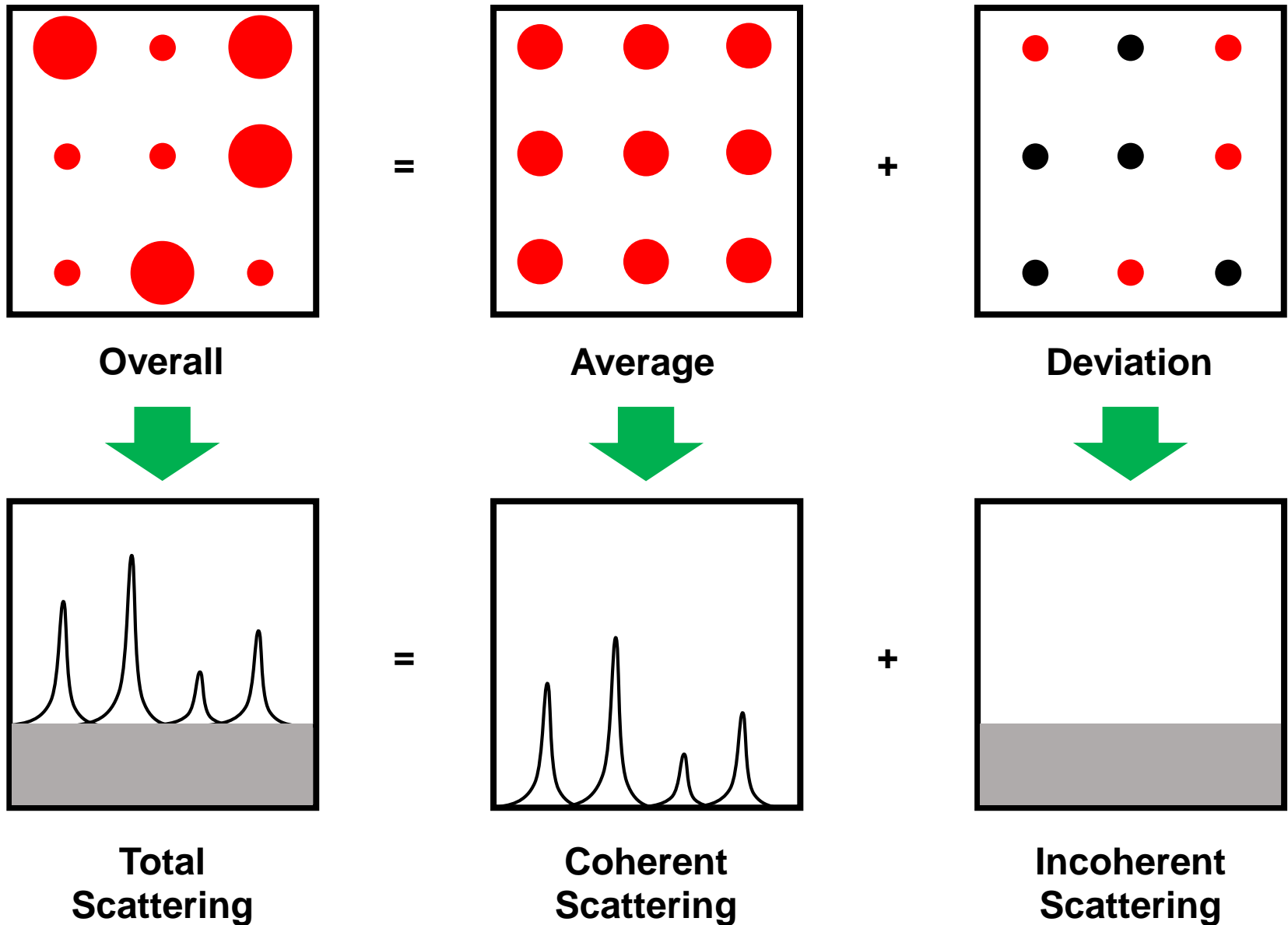
Next, we will move on to the magnetic part of the scattering. Back to the Eqn. (2), we know that the first step should be to build up the potential concerning the magnetic scattering. Without going into details, the potential form is given as following:

Neutron magnetic moment

$$\boldsymbol{\mu}_n = -\gamma \mu_N \boldsymbol{\sigma}$$

- $\gamma = 1.9132$
- $\mu_N \rightarrow Nuclear\ magneton$
- $\boldsymbol{\sigma} \rightarrow Neutron\ spin$

Electron spin moment

$$\boldsymbol{\mu}_i = -2\mu_B \boldsymbol{s}_i$$

- $\mu_B \rightarrow Electron\ magneton$
- $\boldsymbol{s}_i \rightarrow Electron\ spin$

Electron orbital moment $\rightarrow \boldsymbol{p}_i$

$$V_M(\boldsymbol{r}) = -\boldsymbol{\mu}_n \cdot \boldsymbol{H} = -\boldsymbol{\mu}_n \cdot (curl\frac{\boldsymbol{\mu}_i \times \hat{r}}{r^2} - \frac{2\mu_B \boldsymbol{p}_i \times \hat{r}}{\hbar r^2}) \qquad \textbf{(8)}$$

Considering Eqn. (3) for the definition of scattering amplitude operator, the one corresponding to potential given in Eqn. (8) is as following:

$$a_M(Q) = -p\boldsymbol{\sigma} \cdot \sum_i [\hat{\boldsymbol{Q}} \times 2\boldsymbol{s}_i \times \hat{\boldsymbol{Q}} + (2i/\hbar Q)(\boldsymbol{p}_i \times \hat{\boldsymbol{Q}})]e^{i\boldsymbol{Q} \cdot \boldsymbol{r}_i} \qquad \textbf{(9)}$$

where p is a constant. Also, the first cross product in the first term of Eqn. (9) comes from the curl operation in the first term of Eqn. (8)

In page-74 to 77 of the book *Methods of experimental physics*, Vol. 23 (Neutron scattering, Part-C), the two terms (in the bracket) in Eqn. (9) were worked out separately. Here the result is given as following:

$$Spin\ part \rightarrow -\widehat{Q} \times M_S(Q) \times \widehat{Q}$$

$$Orbital\ part \rightarrow -\widehat{Q} \times M_L(Q) \times \widehat{Q}$$

where $M_S(Q)$ and $M_L(Q)$ are the Fourier transform of the magnetization density for the spin ($M_S(r)$) and orbital ($M_L(r)$) part, respectively. For example:

$$M_S(r) = -\sum_i 2s_i \delta(r - r_i) \tag{10}$$

Together the two parts give:

$$M(r) = M_S(r) + M_L(r) \tag{11}$$

and accordingly

$$M(Q) = M_S(Q) + M_L(Q) = \int M(r)e^{iQ \cdot r} d^3r \tag{12}$$

---

[7] To understand Eqn. (3) in a more specific way, we need to go back to the quantum scattering theory, e.g. given in <u>Scattering Theory</u> (page-40). There it is presented how the Lippmann-Schwinger equation is embedded into the scattering function therefore giving the expression for the scattering amplitude (which is directly linked to the scattering cross section) at the bottom of page-40 of that document. Specifically for Eqn. (8) to (9), there are two things to point out: 1) first Born approximation is used (only the first term of the expansion is kept, refer to page-44 of the same doc mentioned above). 2) we are concerned about the single point scatterer here therefore the potential function becomes a function centered at the position r_i, and that's why we have r_i in the exponential term in Eqn. (9).

Collecting all together and going back to Eqn. (9) we have:

$$a_M(Q) = p\sigma \cdot [\widehat{Q} \times M(Q) \times \widehat{Q}] \tag{13}$$

Furthermore $\widehat{Q} \times M(Q) \times \widehat{Q}$ can be worked out as:

$$M_\perp(Q) = Q \times M(Q) \times Q = M(Q) - [\widehat{Q} \cdot M(Q)]\widehat{Q} \tag{14}$$

and

$$a_M(Q) = p\sigma \cdot M_\perp(Q) \tag{15}$$

where $M_\perp(Q)$ represents the magnetization component $M_\perp(Q)$ perpendicular to the scattering vector Q. Having the scattering amplitude operator, in principle we can then follow Eqn. (2) and (3) to calculate the differential cross section from a single magnetic ion. In fact, the steps are not so straightforward therefore it will not be covered in this document. Though, it's still worth mentioning that the book *Methods of experimental physics*, Vol. 23 (Neutron scattering, Part-C, page-75 & 76) gives the derivation with the so-called dipole approximation. It was also mentioned in the book that the general algebra is given in the book *Theory of thermal neutron scattering* by Marshall and Lovesey. One thing to point out is that during the derivation (following whichever way mentioned above), the magnetic form factor $f(Q)$ (analogue to, e.g. the X-ray scattering form factor or the aforementioned neutron scattering length) will be introduced, which makes the expression for the magnetic scattering quite similar in form with the nucleus scattering when considering the scattering from a lattice.

Based on the result here we have, there are two aspects to highlight: 1) the magnetic form factor is Q-dependent, which makes it only possible to observe the magnetic scattering peaks in the low-Q region in the neutron scattering experiment. 2) from Eqn. (15) we can tell that neutrons can only 'see' the magnetic moment components that are perpendicular to the scattering vector Q.

Finally, considering the scattering from collections of atoms, the formulation for the contribution from nucleus and magnetic scattering can be given, respectively [8]. First the nucleus part, the structure factor is given as:

$$F_N(\boldsymbol{Q}) = \sum_{j,s} \bar{b}_j e^{i\boldsymbol{Q}\cdot r_j^s} e^{-W_j^s} \tag{16}$$

where s represents the crystallographic sites in the unit cell and j labels different atoms sitting on the site. W_j^s refers to the Debye-Waller factor. As for the magnetic part, we need to Fourier expand the magnetic moments as following:

$$\boldsymbol{m}_{lj} = \sum_k \boldsymbol{m}_{k,j} e^{-i k \cdot R_l} \tag{17}$$

where $m_{k,j}$ refers to the magnetic moment in the zeroth unit cell.

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[8] Here the unpolarized neutron is considered, for which the nucleus and magnetic contribution can be separated without problem. As for the polarized neutron scattering, since the neutrons doe not interact with the magnetic moment from the magnetic structure but also they will interact with the nucleus spins (coherently this time, not like the interaction mentioned previously which only contributes incoherently), which makes it difficult to separate them.

The Fourier expansion given by Eqn. (17) seems like describing the magnetic moment in the zeroth unit cell propagating following certain pattern of Cos and Sin combinations, and the pattern that it is following is determined by the vector k. This is why k is called the propagation vector, which is a crucial and convenient notation for describing the magnetic structure of the system. Having the definition of the propagation vector, the differential cross section for the magnetic part is given as following:

$$\frac{d\sigma_M}{d\Omega}(\boldsymbol{Q}) = N \frac{(2\pi)^3}{v_0} \sum_{\tau} \sum_{k} \left| F_{M_\perp}(\boldsymbol{Q}) \right|^2 \delta(\boldsymbol{Q} - \boldsymbol{k} - \boldsymbol{\tau}) \tag{18}$$

where

$$F_M(\boldsymbol{Q} = \boldsymbol{\tau} + \boldsymbol{k}) = p f(\boldsymbol{Q}) \sum_{j} m_{\boldsymbol{k},j} e^{i\boldsymbol{Q}\cdot\boldsymbol{r}_j} e^{-W_j} \tag{19}$$

Here the reason for why the magnetic scattering happens at the position $\boldsymbol{Q} = \boldsymbol{\tau} + \boldsymbol{k}$ in the reciprocal space, refer to the notes given in the following document: **Reminder: Magnetic structures description and determination by neutron diffraction**. Also, it should be mentioned that Eqn. (17) only applies for the situation of crystalline structure, which is actually just a special case of the general scattering.

Finally, still one thing to mention, since we still haven't taken care of the spin part in Eqn. (2). The thing is, for a non-polarized neutron experiment, the flipped and non-flipped neutrons are randomly distributed therefore it does not contribute to the scattering actually.

At last, some important references and a bit more supplementary (and probably, extending) discussion will be given, which is presented as diagram with links to files shown as below:
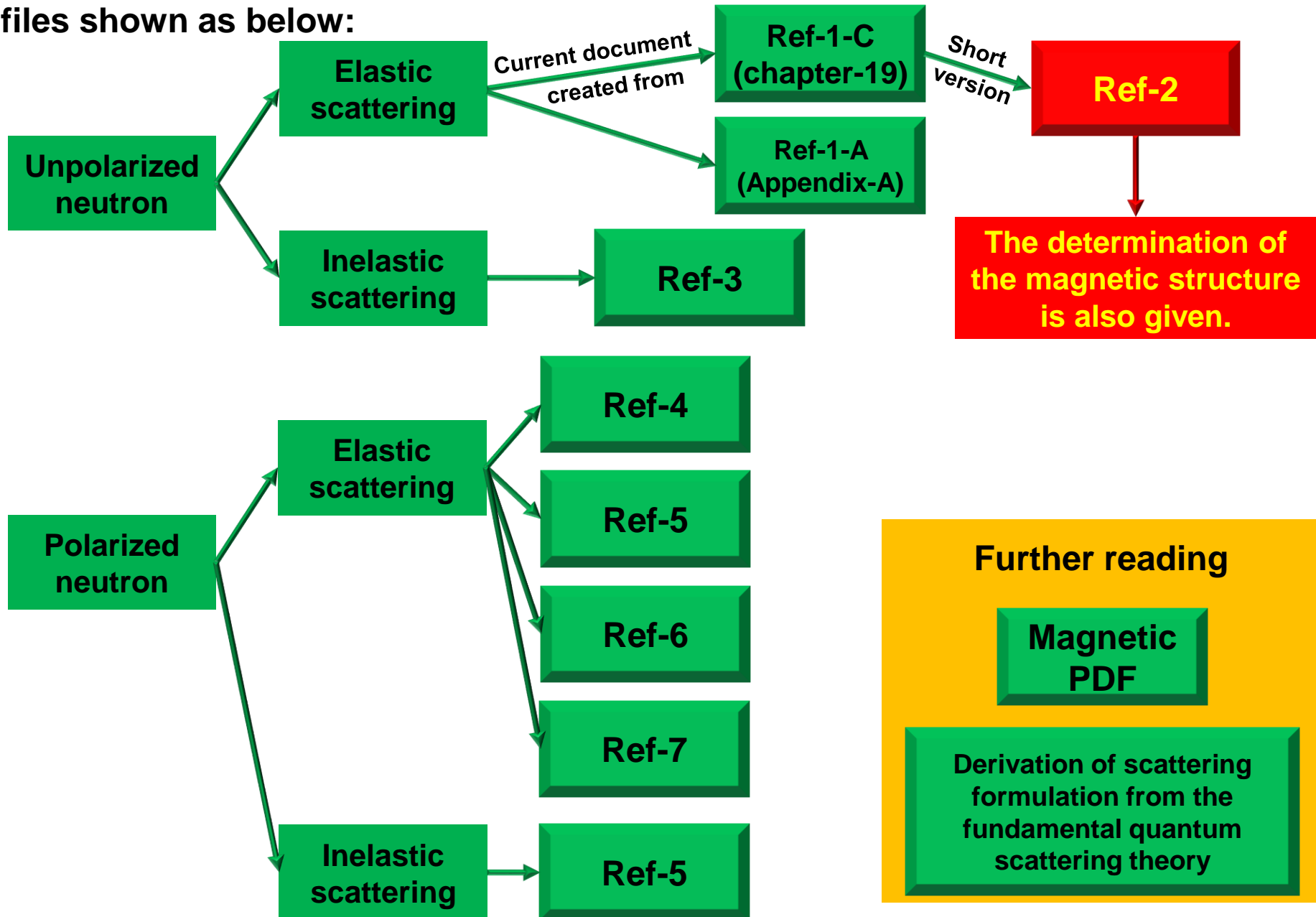
Furthermore, focusing on the nucleus scattering and in real experiment we are not measuring the structure factor as given by Eqn. (16). Instead, we are measuring the intensity, i.e. the modulus of Eqn. (16):

$$|F_N(\boldsymbol{Q})|^2 = \sum_{j_1,s_1} \sum_{j_2,s_2} \overline{b_{j_1}} \cdot \overline{b_{j_2}} e^{i\boldsymbol{Q}\cdot(r_{s_2}^{s_1} - r_{j_2}^{s_2})} e^{-W_{j_1}^{s_1}} e^{-W_{j_2}^{s_2}} \tag{20}$$

Here we notice that what we are measuring experimentally is the correlation distance in between atoms in the system. In real life, as we will mention later, no matter what technique we use for the scattering experiment, we are just scanning through the Q. With a given Q, a certain distance between atoms will give the corresponding phase factor according to Eqn. (20), and effectively we are adding up all the phase factors (corresponding to all the possible distances in the system) to give us the modulus of the structure factor, which then corresponds to the experimentally measured scattering intensity with respect to that given Q. In fact, we could have a lot of different distances in the system, and if assuming they are distributed randomly, then when we adding all the phase factors up we will get nothing from the average perspective. The reason for this is simple, since Eqn. (20) is nothing but mixing up a series of *Cos* and *Sin* functions, and if the phases of those *Cos* and *Sin* functions are randomly distributed then on average the intensity of all those functions will cancel each other out, as illustrated following:
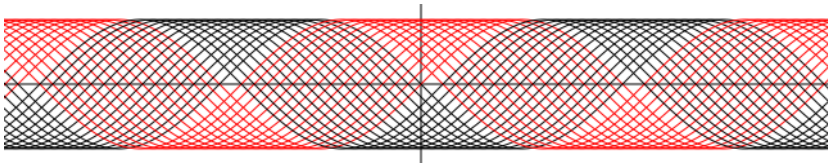
In this graph, for simplicity, all *Sin* functions has its counterparts with negative phase thus canceling each other out. In real situation, this is indeed a good approximation since we have huge amount of random phase factors therefore each of them could find its own negative counterpart.

However, if we have certain amount of atom pairs with the same distances in the system, the corresponding components in Eqn. (20) will then be in phase, which will make the corresponding observed intensity larger than that corresponding to the randomly distributed distances. The more atom pairs with the same distance we have, the larger the corresponding intensity as compared to the random components. In ideal crystalline materials, all atoms are aligned in a perfectly ordered way therefore we then have a lot of discrete distance values and each of them is repeated huge amount of times. When proper Q value is visited, a strong scattering peak will pop up corresponding to certain distance value, and the condition for such a strong peak to happen is just the Bragg law. The corresponding scattering is just the Bragg scattering. Furthermore, if the material is not a perfect crystal (or it may even not be a crystal) which means we cannot have those huge amount repetitions of the same atomic distances (i.e. we don't have the so-called long-range order), we then will not have the intensity contrast as mentioned above. However losing the long-range order does not mean we lose the order totally (which means the atomic distances are really randomly distributed), since we could have atoms in the system arranged locally following a certain pattern (e.g. the local Si-O tetrahedron in the SiO_2 system). This is just the so-called short-range order, which then means we do have certain amount of repeated distances but just the amount is not that huge as compared to that in the crystalline system. Accordingly we do have the contrast, though not that large as compared to the Bragg scattering, between the scattering intensity for the short-range order (those distances repeated by limited amount) and that for the randomly distributed distances.

This is just the so-called diffuse scattering. Here it should be mentioned that what we mean by diffuse scattering here is actually just one aspect of its real meaning. In fact, the diffuse scattering may arise from multiple sources, including the contribution from, e.g. the vibration of atoms in the system (which will then cause the inelastic scattering). Details about the diffuse scattering could refer to the book *Diffuse neutron scattering from crystalline materials* by V. M. Nield and D. A. Keen, and it will not be covered in this document. However, it's worth mentioning that in a diffuse scattering experiment where we do not discriminate the elastic and inelastic scattering (i.e. we do not discern the energy of the scattered beam), we are effectively integrating over all the inelastic scattering energy components. Since the inelastic scattering corresponds to the dynamic structure of the system and effectively it will give a snapshot for the structure of the system. Therefore by not discerning the energy, we are actually measuring the average of all the possible snapshots for the dynamic structure. Also it should be highlighted that the diffuse scattering experiment is totally different from the normal Bragg scattering measurement since for the data analysis we need a large Q-range (since we need to Fourier transform Eqn. (20) to real space (the pair correlation function) to find the hidden short-range order) and more careful background subtraction (since the diffuse scattering is not so strong as compared to the Bragg scattering as we discussed earlier, therefore it's more difficult to discern them from the background signal). More introduction about the diffuse scattering experiment requirements and subtleties, e.g. the compromising between the Q-range and Q-space resolution, etc., could be found in the aforementioned book on diffuse scattering (chapter-4).

Several other subtleties will be given here following, which may or may not be related directly to what we have discussed so far but is indeed worth taking a note of. First, the advantage of neutron scattering as compared to X-ray, especially with respect to the diffuse scattering measurement:

1) *Q*-independent scattering length, which means we can go to high *Q* easily (as compared to X-ray) which is necessary for diffuse scattering data analysis, since the large *Q* range will diminish the Fourier truncation problem when transforming from the reciprocal space to the real space.
2) Atomic number independent scattering length, which is suitable for 'seeing' light atoms which will not scatter X-ray due to the tiny X-ray form factor for the light atomic species.
3) The energy magnitude of the thermal neutron (about what thermal neutron means, refer to slide-3 of current document) is similar to that of the lattice vibrations, which makes neutron suitable for looking at the dynamics of the system.
4) Since neutron carries spin and it will be scattered not only by the nucleus but also by the magnetic moments as we have discussed earlier. Therefore neutron is more suitable for looking at the magnetic structure.

Talking about neutron scattering experiment, definitely we need large facilities to generate neutrons with flux high enough (to get an idea about the magnitude of the flux, refer to page-44 of the following document: [Neutron scattering](#)) for the scattering measurements.

For the generation of neutrons, we have two main approaches – the nuclear reaction (fission) and the spallation (hitting the target material with high energy protons and kick the neutrons out). Each of them has its own advantages, and a detailed comparison is given in the following document: **Neutron scattering** (page-42). For example, the reactor source could produce higher flux of neutrons, and it is easy to control the resolution (e.g. to improve the resolution, we could select to use a long neutron wavelength, but at the same time. We lose the ability to achieve high Q). As for the spallation source, owing to its pulse structure (determined by the proton accelerator, either linac- or synchrotron-based), it could produce high flux of high energy neutron (refer to the document mentioned above in current slide), which is suitable for the diffuse scattering experiment as discussed earlier in current document. However, the determination for using which one of them in history may not depend on the actual need. Instead, there were some political reason for it, since the Uranium source was (is, and probably will always be) under control of the international nuclear non-proliferation treaty prohibits civilian use of highly enriched uranium U^{235}. Indeed, historically the original proposal of a reactor-based Advanced Neutron Source at the Oak Ridge National Laboratory in the U.S. was rejected, and it was replaced by the accelerator-based Spallation Neutron Source, or SNS, project (although finally the proposal for the reactor-based source was approved, which, now becomes the High Flux Isotope Reactor, or HFIR at ORNL). More details about the introduction into spallation- and reactor- based neutron source can also be found in the following document: **Spallation neutron source and other high intensity proton sources**.

Also, due to the pulse structure of the spallation neutron source, it has lower time-averaged flux as compared to the reactor with constant flux, as illustrated in the following picture (regenerated from the picture shown in page-15 of the following document: **Basic elements of neutron inelastic scattering**):
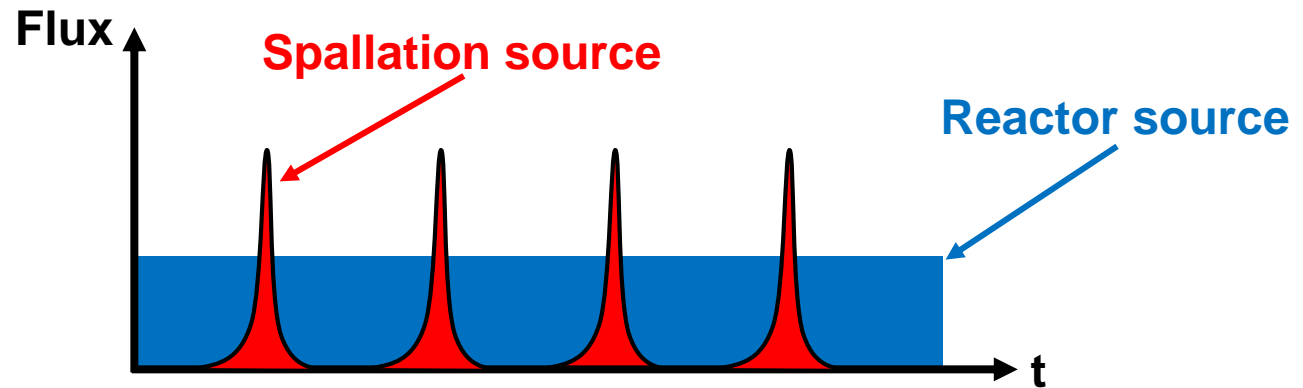
As mentioned earlier, the scattering measurement is just to scan the scattering intensity through the Q-space. To do that, we have two ways: 1) scanning the scattering angle with the wavelength fixed. 2) scanning the wavelength with the scattering angle fixed. For the first approach, we need the monochromator to filter out the single wavelength that we are going to use for the experiment. For reactor-based neutron source, this is not a problem since we have high time-averaged flux. But for the spallation source, since we have low time-averaged flux, we have to stay at one scanning angle for rather long time as compared to the reactor source to collect data with high enough signal-to-noise level (in principle, the longer we collect the data at one angle point, the more the difference between the scattering signal (which comes from the correlation in the material as discussed earlier) and the noise (which could come from multiple sources, e.g. the instrument) is accumulated).

Therefore for the spallation source, it's better to use the second approach to scan the wavelength. In practice, the so-called time-of-flight technique is always used. The principle here is quite simple, since the speed of neutron depends on its wavelength according to the de Broglie formula. Therefore by scanning the time-of-flight of neutrons, effectively we are scanning through the Q-space. In practice, we could easily know the distance that neutrons fly through and the time when they arrive the detector. Therefore the problem is how to control the starting time. Owing to the pulse structure of the spallation source, we could control the pulse rate (e.g. 50 Hz used at ISIS neutron source in the UK, or 60 Hz used at SNS in US) and know exactly the staring time. Again, with the pulse structure of at the spallation source, the incoming beam is polychromatic, and each single wavelength component will arrive the position-fixed detector at different time. Meanwhile, if employing the multiple detectors, then each detector will record a TOF pattern of its own and by composing the data from multiple detectors together we could improve the counting rate (i.e. the time needed to collect data with high enough signal-to-noise level shrinks, since by adding up various TOF patterns from multiple detectors, we increase the contrast between the signal and noise, as similarly for the improving of the signal-to-noise level by the increasing of the recording time). For the reactor source, the TOF technique could also be used (although, not often), and to do that we need to introduce the chopper (which is a rotating disk for block neutrons from passing through but with slits on it letting neutron through) to control the starting time. Finally, even for reactor source, multiple detectors are now in use for increasing the counting rate, e.g. the multiple detector used at HB2A beamline at HFIR, ORNL in US.

Finally, we have several points to remark about the scattering experiment. The first one is about the compromising between the flux and resolution for the TOF measurements. To discuss that, we need to know by what the resolution of TOF measurement is determined. Here following is shown a picture (taken from the following paper: [Texture investigation by neutron time-of-flight diffraction](#)) demonstrating the basics about the resolution in TOF measurement :
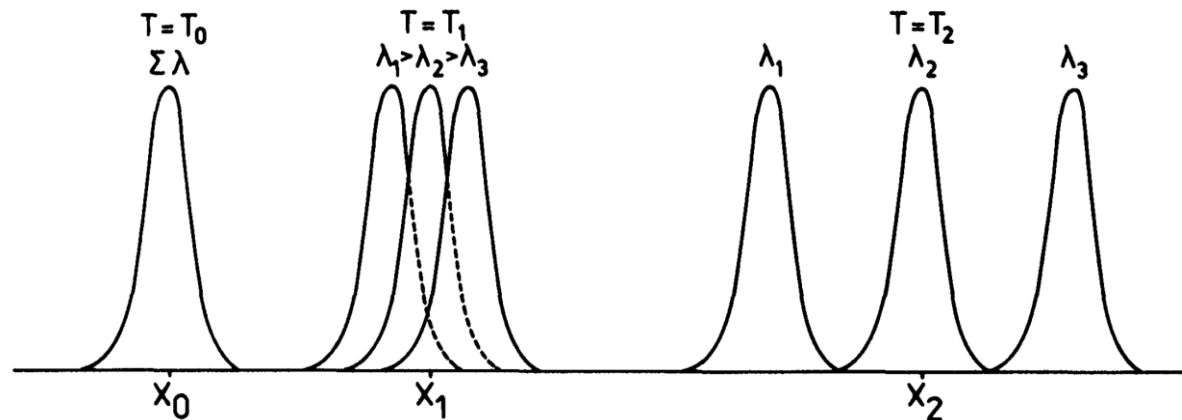
As mentioned earlier, the speed of neutron depends on its wavelength, and each wavelength has its corresponding distribution around the central value (e.g. following the Gaussian shape). At the beginning, all the wavelength components stay at the staring point x_0 overlapping with each other. As the neutrons propagate, since the speed of each wavelength component is different from each other therefore they start to separate an the overlapping reduces gradually (e.g. as illustrated by point x_1 in the picture above) until they separate completely. Therefore we know that the further neutrons propagate from the starting point before hitting the sample, the better resolution we will get (e.g. the POWGEN beamline at SNS, ORNL).

However, the further neutrons travels, the less collimated (i.e. the beam flux becomes more decentralized and less focusing), which means we will lose flux if we want to improve the resolution. In the same way, if we want high flux then we have to sacrifice the resolution (e.g. NOMAD beamline at SNS, ORNL for diffuse scattering experiments). Furthermore, on the detector side, the same principle applies as well. For each single one of the multiple detectors, we want to record the TOF pattern as the function of flying time therefore we want to discriminate different wavelength as best as we possibly can. That's why we always need a big tank for arranging the detectors – for the purpose of increasing the flying distance between the sample and the detector to increase the resolution.

The second point we want to mention is that to discriminate the energy for inelastic scattering measurement, we need to know the energy and wave vector of both the incoming and outgoing scattered neutrons to obtain the wave vector and energy transfer between neutron and the sample. For such a purpose, the so-called triple-axis diffractometer could be used, which is available both at reactor- and spallation- based neutron sources (refer to chapter-4 of the book *Diffuse neutron scattering from crystalline materials* for more details).

The last point to highlight is the scattering peak broadening. As we know, when the scattering vector **Q** satisfies the Bragg condition, a corresponding Bragg peak will pop up. Considering Eqn. (20), this means we will get an intensity maximum when $Qd = 2\pi$ where d is distance that repeatedly appears for large amount of times, which is just the so-called distance between lattice planes.

However, when the scattering vector Q is slightly away from the Bragg position, we still have the scattering intensity and it's just the value that is lower than that for the central Bragg position (where Bragg law is exactly satisfied). The further we go away from the central position, the lower the intensity according to Eqn. (20). Also the larger the crystal size is (i.e. the more repeated distances we have), the more obvious contrast we will get between the central Bragg position and those non-central Q points (since we get more and more accumulation of the intensity differences between the central and non-central Q points). Ideally if the crystal is infinitely big, we will get a δ function in the Q-space, which means the contrast now is infinitely large. In real life, we will never get an infinitely large crystal therefore we have to have a peak width around the central Bragg position. Such a peak width is definitely related to the real crystal size we have. The larger the crystal (or more exactly speaking, the larger the crystalline domain size), the closer we will get to the δ function. The mathematical relationship between the crystalline domain size and the Bragg peak width is given by the well-known Scherrer equation, for which the derivation can be found in the following summary: [About Scherrer Equation](). Understanding such a point from pure mathematical perspective, the broadening of the Bragg peak is the result of the convolution between the δ function and the *Sinc* function (which is the Fourier transform of the box function with limited size. The box function may become complicated considering complex sample shape, for which the Fourier transform may not be just a *Sinc* function). Furthermore, it should be mentioned that the limited sample size is not the only source of the peak broadening. In real life, the facility that we measure the Bragg scattering with

could also introduce the broadening effect to the Bragg peak, which is demonstrated as below:
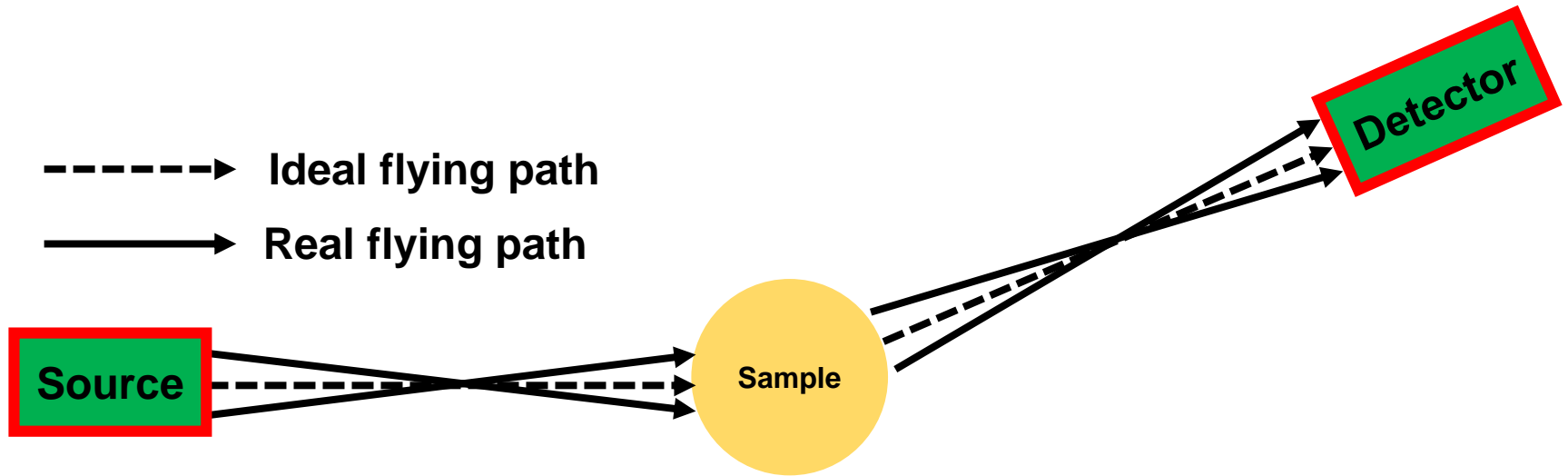
As demonstrated in the picture, the dashed line indicates the flying path that we expect it to be and the scattering vector Q is calculated based on such an assumption. However in the real situation, the incoming and outgoing beam may or may not be collimated just along the expected flying path. This means that in reality what we mean by the scattering vector Q may be a bit away from its real value. For example, for an ideal crystal with infinite size, when the expected Q position will give zero scattering intensity (for non Bragg Q positions), the measured value may not be zero since what we really are measuring may be some other Q point where the intensity is not supposed to be zero. Since the flying path may be wandering around the expected position in real situation, we then get a broadened peak even with a perfect crystal with infinite size. Therefore in real experiment, we need a bulk crystalline material (which we take

as the ideal crystal with infinite crystalline domain size) to be measured at the same instrument where measure our own samples. Then we can reduce the peak broadening effect of the bulk material from that of the our own sample to get an accurate estimation about the crystalline domain size.

Apart from the beam collimation variation, in real experiment, the sample also may not be exactly located at the position where the ideal incoming and outgoing beam intersects, as shown in the following figure:
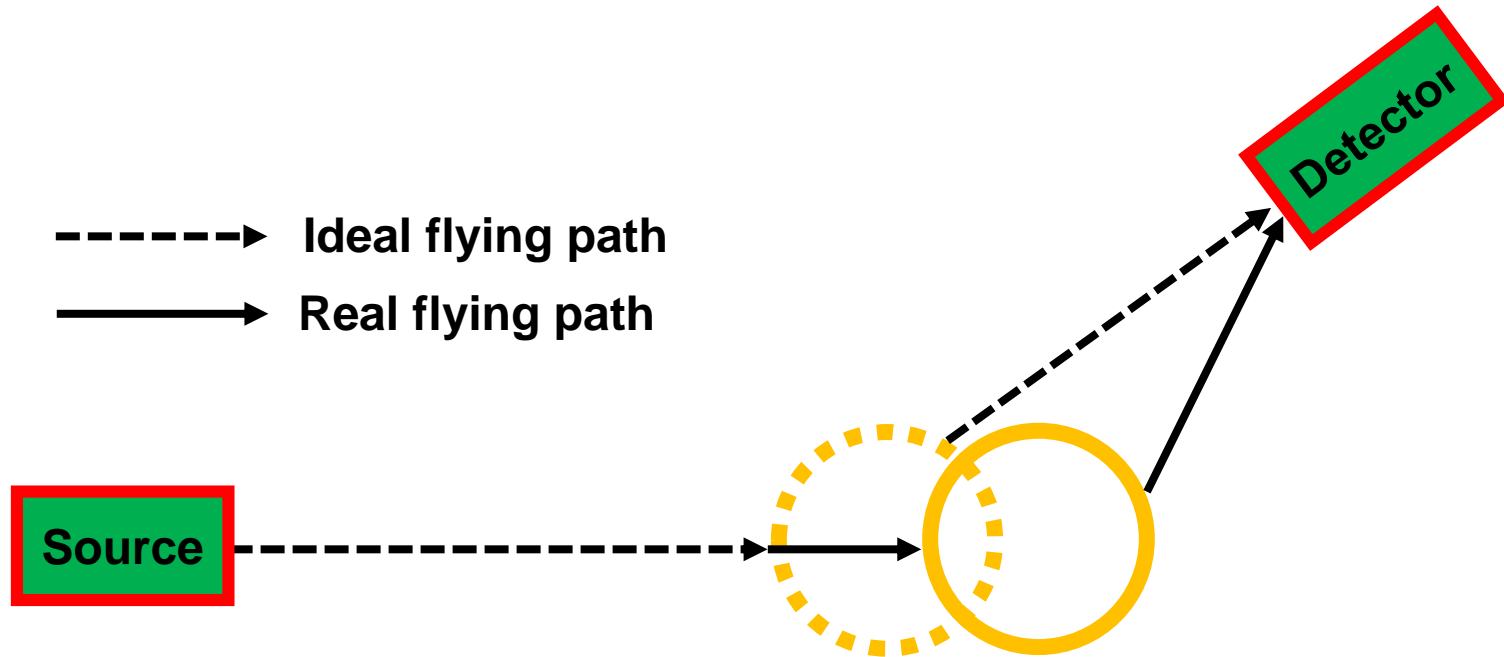
Therefore in practice when we measure our samples, it's always necessary to have the measurement of the standard sample (e.g. Si, may not be measured every time) for which we know exactly where the Bragg peaks are located so we can then correct the Q value accordingly for our sample measurements.