Basic Principles of Scattering and Diffraction

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1. Going between real space and reciprocal space: Waves and Fourier transforms.

2. Hitting the target: The differential scattering cross section.

Acknowledgements
Going between real space and reciprocal space

Waves and Fourier transforms
What do we want to ‘see’? Namely, structure


Crystal structure of the receptor binding domain (in green) in SARS-CoV2. Model from synchrotron x-ray data (Nature, Li et al, 2020)
What do we observe? Structure in reciprocal space

In reciprocal space you measure the Bragg peaks known as reflections, but also more than that.

- **Powder diffraction rings from synchrotron X-ray beamline 17-BM, Advanced Photon Source**
- **X-ray single crystal of Bi_{1.7}V_{8}O_{16} showing an incommensurate satellite reflections.**
- **Diffuse neutron scattering from instrument CORELLI (Spallation Neutron Source) on a plastically deformed crystal of SrTiO_{3}.**
How do we get back from the images in reciprocal space?

Fast powder diffraction ( < 5 sec) allows for in situ materials studies


**Chemical Looping Cycle**

 oxidation in air

\[ \text{ABO}_3 \]

A reduction by fuel

\[ \text{ABO}_3 - \delta \]

Understanding nature of metal-insulator transition through analysis of incommensurate charge order

Plastic deformation of SrTiO$_3$ single crystal with enhanced superconductivity revealed by diffuse scattering

Larson et al. EER, *J. Mater. Chem. C* 2017, 5 4967

Hameed et al., *Nature Mat.* 2022, 21 54-61
Add time or energy to the map

We directly visualize excitations in condensed matter. Example: Phonon dispersion curves of silicon taken. Data taken on ARCS spectrometer at SNS (PNAS, Fultz et al, 2018)

Energy, or $\hbar \omega$

Reciprocal space, or $Q$
Diffraction at the beach!

interference of waves
What is diffraction?

• Scattering of a wave from an object, so that it becomes like a point source of a radial wave.
• Example a slit diffracts a plane wave.
• Circular waves emerge from the slit.
• Key is that slit size must be similar in scale to wavelength of wave!

GIFs of plane wave arriving at a slit
Young’s double slit experiment

\[ k_i = k_f = \frac{2\pi}{\lambda} \]

The scattered waves are radial waves and destructively and constructively interfere to make a diffraction grating.

The scattering is described as *elastic*, since no energy transfer leads to the same wavelength.

\[ |k_i| = |k_f| = \frac{2\pi}{\lambda} \]

Incoming plane wave

monochromatic planar wave (e.g. a laser)

screen with two slits

optical screen (front view)
We define a plane wave:
Amplitude in the $z$-direction,
Propagates in $y$- and $x$-directions.

$r' = $ direction of propagation

$k = $ wavevector

$|\vec{k}| = \frac{2\pi}{\lambda}$

$\psi = A \sin(\vec{k} \cdot \vec{r} + \varphi)$
Momentum transfer or $Q$

- $k_i$ is the incident wavevector and $k_f$ is the scattered wavevector
- Useful to work with another vector besides $k_i$ or $k_f$
- We define $\vec{Q}$, as our momentum transfer

$$\vec{Q} = \vec{k}_i - \vec{k}_f$$
Momentum transfer, or Q-space

\[ \mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f \quad \text{or} \quad \mathbf{Q} = \mathbf{k}_f - \mathbf{k}_i \]

\[ |\mathbf{k}| = \frac{2\pi}{\lambda} \]

For elastic scattering, no energy transfer

\[ |\mathbf{k}_i| = |\mathbf{k}_f| \]

\[ \frac{|\mathbf{Q}|}{2} = |\mathbf{k}| \sin \theta \]
Scattering from an ensemble of atoms

\[ \mathbf{Q} = \mathbf{k}_f - \mathbf{k}_i \]

Waves scattered can add up in phase

\[ |\mathbf{Q}| = \frac{4\pi \sin \theta}{\lambda} \]
The Fourier transform

• We call $F(k)$ the Fourier transform of $f(x)$, and vice versa
• We can toggle between real space ($x$) and reciprocal space ($k$)

Real space function as Fourier transform of function $F(k)$

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{ikx} dk$$

$k$-space function as an inverse Fourier transform of real space function $f(x)$

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$$
The phase problem in scattering experiments

- The Fourier transform includes information on the amplitude and phase (or argument) of the function.
- Pictures of (a) Big Ben and (b) Lil’ Ben.
- In (c) the amplitude from Lil’ Ben is mixed with the phase information of Big Ben. The resulting inverse Fourier transform looks like Big Ben.
- In (d) the amplitude from Big Ben is mixed with the phase information of Lil’ Ben, resulting inverse Fourier transform is Lil’ Ben.

From D. S. Sivia, Elementary Scattering Theory¹⁷