Advanced Topics in Condensed Matter (ATCOMA): Lecture 2

for physics students for VF (Vertiefungsfächer)

- “Bio/Medical Physics“
- “Nanostructures“
- “Condensed Matter”

for NanoScience students

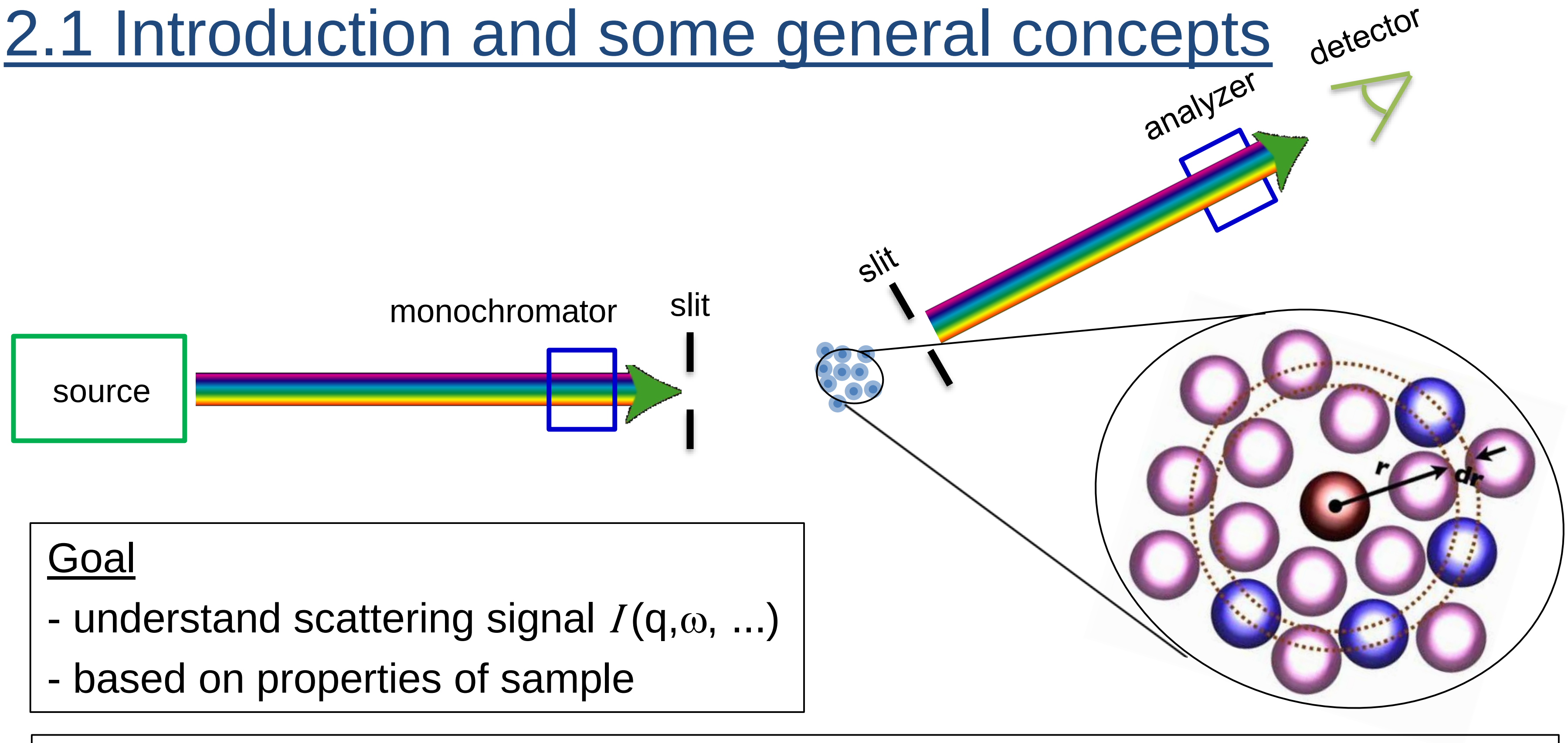
Today:

- Introduction and some general concepts
- Elementary scattering process

Later:

- Scattering from crystals
- Scattering from disordered systems / liquids
- Scattering from surfaces and interfaces
- General scattering theory: Correlations in space and time
- Miscellaneous topics, applications, and examples

2.1 Introduction and some general concepts



Goal

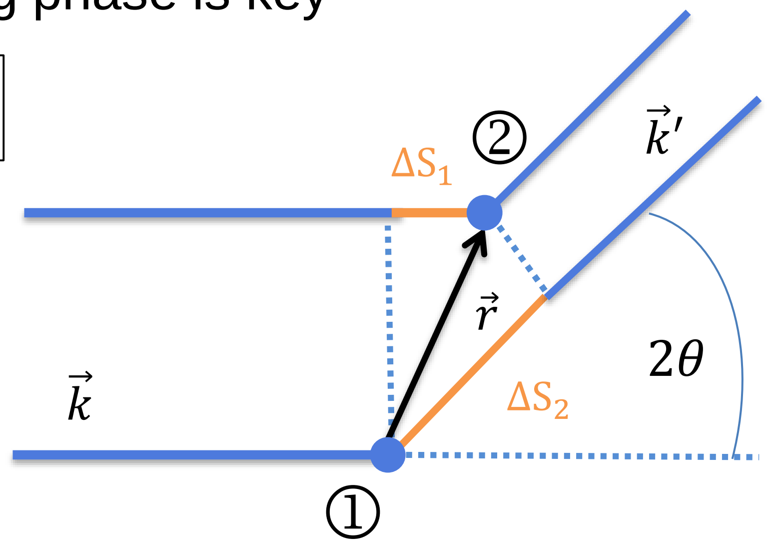
- understand scattering signal I(q,ω, ...)
- based on properties of sample

incident beam		sample	scattered beam
energy	$E = \hbar\omega_i$	N particles at positions $\overrightarrow{r_n}(t)$ with cross section σ_n	$E_f = \hbar\omega_f$
wavelength	λ_i		λ_f
wave vector	$\overrightarrow{k_i}$ (direction!)		$\overrightarrow{k_f}$
flux	$I_0 \quad \left[\frac{\text{quanta}}{\text{cm}^2\text{s}}\right]$		I

2.1 Introduction and some general concepts

Scattering phase is key

$$e^{i\vec{q}\cdot\vec{r}}$$



$$\vec{q} = \vec{k}' - \vec{k}$$

$$|\vec{q}| = \frac{4\pi}{\lambda}\sin\left(\frac{2\theta}{2}\right)$$

Roadmap

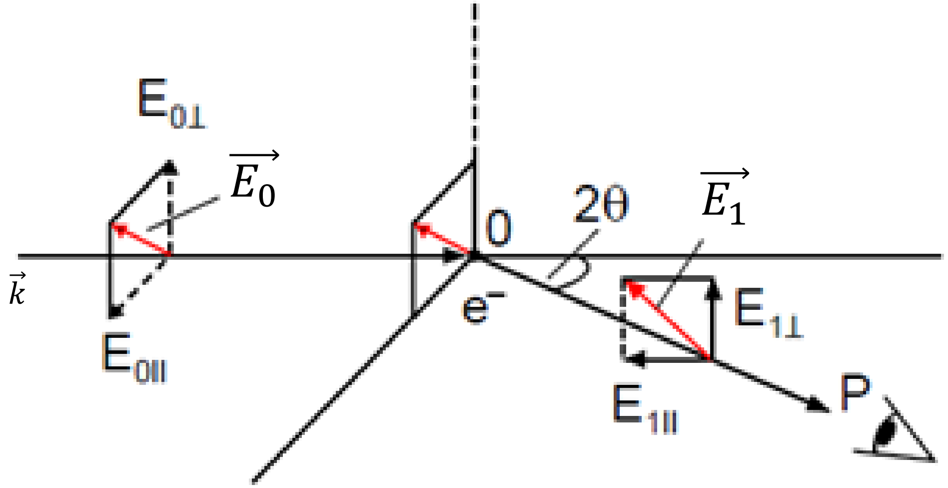
- understand elementary scattering process (individual atom)
- then “assemble“ atoms to a complete sample
- then resulting signal from scattering from all atoms with $e^{i\vec{q}\cdot\vec{r}}$

2.2 The elementary scattering process

2.2.1 X-rays

2.2 The elementary scattering process

2.2.1 X-rays



an electromagnetic wave stimulates an electron to forced oscillations

force on charge $\vec{F} = e\overrightarrow{E_0}$

acceleration $\vec{a} = \frac{\vec{F}}{m} = \frac{e\overrightarrow{E_0}}{m}$

accelerated charge radiates $E_1 \sim a\frac{e}{r}$

more precisely

$$E_1 = \frac{eE_0}{m}\left(\frac{\mu_0}{4\pi}\right)\frac{e}{r}\, sin(\overrightarrow{OP}, \vec{a})$$

$$E_{1\perp} = \frac{\mu_0}{4\pi}\frac{e^2}{m}\frac{E_{0\perp}}{r}$$

$$E_{1\parallel} = \frac{\mu_0}{4\pi}\frac{e^2}{m}\frac{E_{0\parallel}}{r}\, cos(2\theta)$$

$(= 0 \text{ for } 2\theta = 90°)$

2.2 The elementary scattering process

2.2.1 X-rays

... with the classical electron radius

$$r_e = \frac{\mu_0}{4\pi}\frac{e^2}{m} = \frac{e^2}{mc^2}\frac{1}{4\pi\epsilon_0} = 2.814 \cdot 10^{-5}\ \text{Å}$$

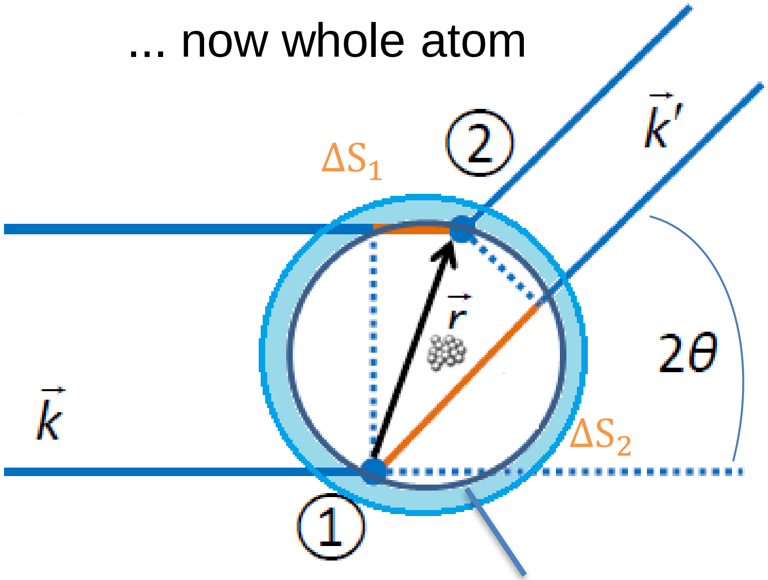
... and, after angular integration, the total scattering cross section

$$\boxed{\sigma_{total} = \frac{8\pi}{3} r_e^2 \approx 6 \cdot 10^{-9}\ \text{Å}^2}$$

2.2 The elementary scattering process

2.2.1 X-rays

... now whole atom



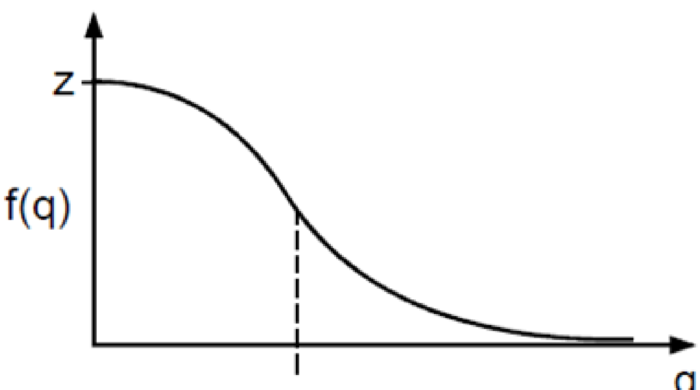
… sum of the scattering contributions from all volume elements of the electron cloud with their respective phase

Total scattered wave

$$A = r_e \int \rho(\vec{r})\, e^{i\vec{q}\vec{r}}\, d\vec{r}$$

'atomic form factor'
(Fourier transform of the electron cloud)

$$f(\vec{q}) = \int \rho(\vec{r})\, e^{i\vec{q}\vec{r}}\, d\vec{r}$$



$$\sim \frac{2\pi}{\text{`atomic radius'}}$$

$$f(q=0) = \sum_{n=1}^{z} f_e^{(n)}(q=0) = \sum_{n=1}^{z} 1 = Z$$

valency

2.2 The elementary scattering process

2.2.2 Neutrons

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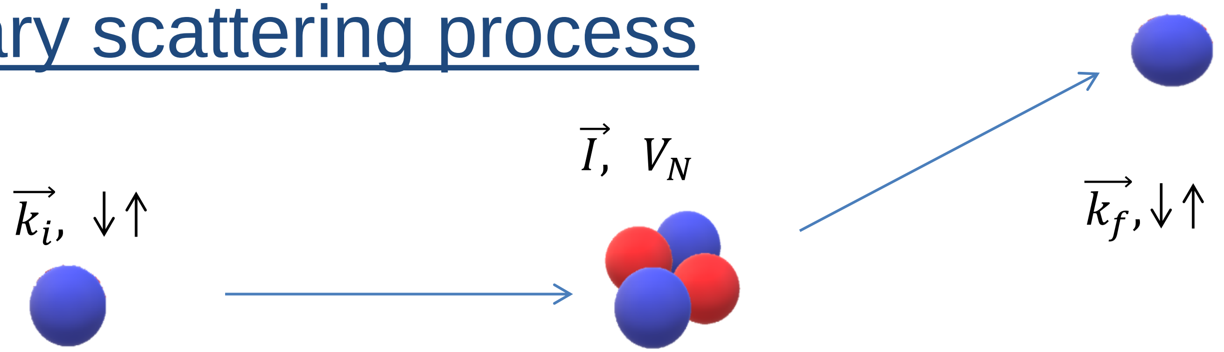
2.2.2 Neutrons



Scattering due to nuclear interaction using Fermi's Golden Rule:

$$a = -\frac{m}{2\pi\hbar^2}\langle\Psi_f|V_N(\vec{r})|\Psi_i\rangle = -\frac{m}{2\pi\hbar^2}\int V_N(\vec{r})\, e^{i\vec{q}\cdot\vec{r}}\, d\vec{r}$$

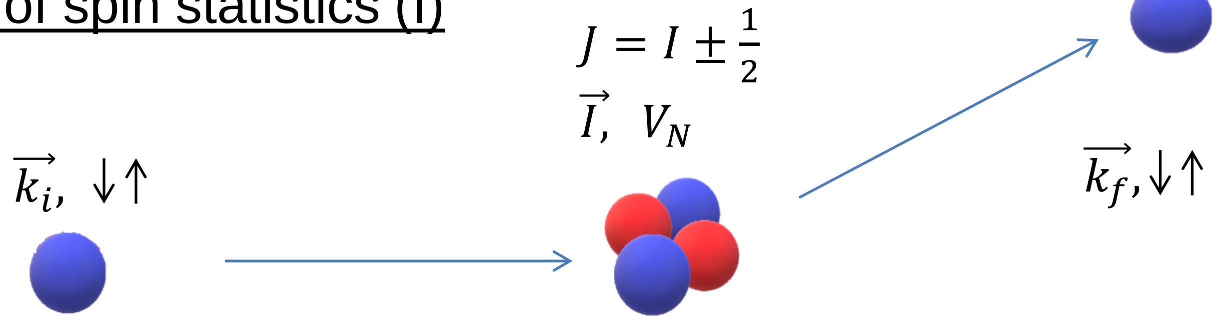
Potential V_N of nucleus is negligible for distance $r > 10^{-5}$Å;
with $q = 2\pi$Å^{-1} we have qr << 1 and thus

$$e^{i\vec{q}\cdot\vec{r}} \approx 1.$$

The scattering amplitude then becomes q independent, i.e. constant

$$b \equiv -a = \frac{m}{2\pi\hbar^2}\int V_N(\vec{r})\, d\vec{r}$$

Neutrons --- Influence of spin statistics (I)



spin of a neutron $s = \frac{1}{2}$

spin of nucleus I with ($2I$ +1) orientations

spin of total system (temporary compound = neutron + nucleus) $J = I \pm \frac{1}{2}$

Interaction V_N depends on relative spin orientation,
resulting in different scattering lengths with different probability

b_+	with probability	$w_+ = \dfrac{I+1}{2I+1}$
b_-		$w_- = \dfrac{I}{2I+1}$

Example: Scattering of a neutron on a proton (hydrogen nucleus)

$$b_+ = 10.4 \text{ fm} \quad \mathrm{n}\uparrow\mathrm{p}\uparrow$$

$$b_- = -47.4 \text{ fm} \quad \mathrm{n}\uparrow\mathrm{p}\downarrow$$

Neutrons --- Influence of spin statistics (II)

Considering a beam of unpolarized neutrons and nuclei

$$\text{n}\ (\vec{k}_i\ \uparrow\downarrow) \longrightarrow (\ldots, b_i, \ldots, b_j, \ldots) \nearrow \text{n}\ (\vec{k}_f)$$

The intensity will be given by the weighted mean of every spin configuration

$$I = \langle AA^* \rangle = \sum_{i,j} \langle b_i b_j \rangle\, e^{i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)}$$

With unpolarized nuclear spins we obtain:

$$i \neq j: \quad \langle b_i b_j \rangle = \langle b_i \rangle \langle b_j \rangle = \langle b \rangle^2$$

$$i = j: \quad \langle b_i b_i \rangle = \langle b^2 \rangle$$

Rewriting

$$\langle b_i b_j \rangle = \langle b \rangle^2 + \delta_{ij}\,(\,\langle b^2 \rangle - \langle b \rangle^2\,)$$

gives

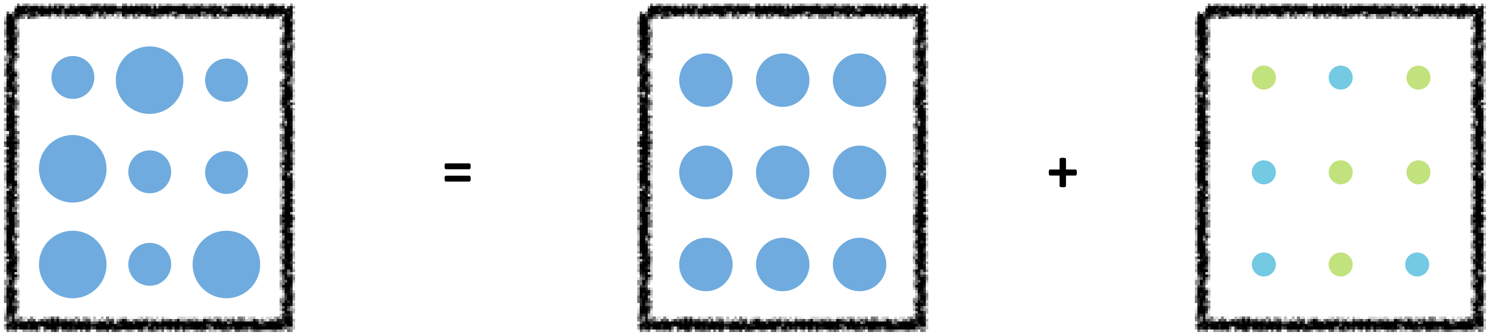
$$I = \langle b \rangle^2 \sum_{i,j} e^{i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)} + (\,\langle b^2 \rangle - \langle b \rangle^2\,)\,N$$

Coherent scattering — Incoherent scattering

$$\sigma_{coh} = 4\pi \langle b \rangle^2 \qquad \sigma_{inc} = 4\pi(\langle b^2 \rangle - \langle b \rangle^2)$$

Neutrons --- Illustration of coherent and incoherent scattering

nuclear scattering ... decompose into two contributions:



b_1 b_2

$$b = \frac{b_1 + b_2}{2}$$

$$\Delta b$$

Coherent	Incoherent
→ Pair-correlation	→ Self-correlation

similarity to X-ray scattering from disordered alloy:

“Bragg” + “diffuse scattering”

(“coherent”) (“incoherent”)

Figure courtesy of Michihiro Nagao

Neutrons --- Remarks on the scattering cross sections

1. Every isotope has both coherent and incoherent scattering (σ_{coh} and σ_{inc}) except when $I = 0$ (e.g. $^{58}\mathrm{Ni}$)
2. The most famous example for the difference between two isotopes is hydrogen ($I = 1/2$) and deuterium ($I = 1$)

	σ_{coh} (barn)	σ_{inc} (barn)
H	2.0	80
D	5.6	2.0

1 barn = 10^{-28} m^2

The incoherent cross section of hydrogen is highest.

The big difference between H and D is used in organic matter for a high contrast (H/D substitution, deuteration of selected components)

Neutrons --- Remarks on the scattering cross sections

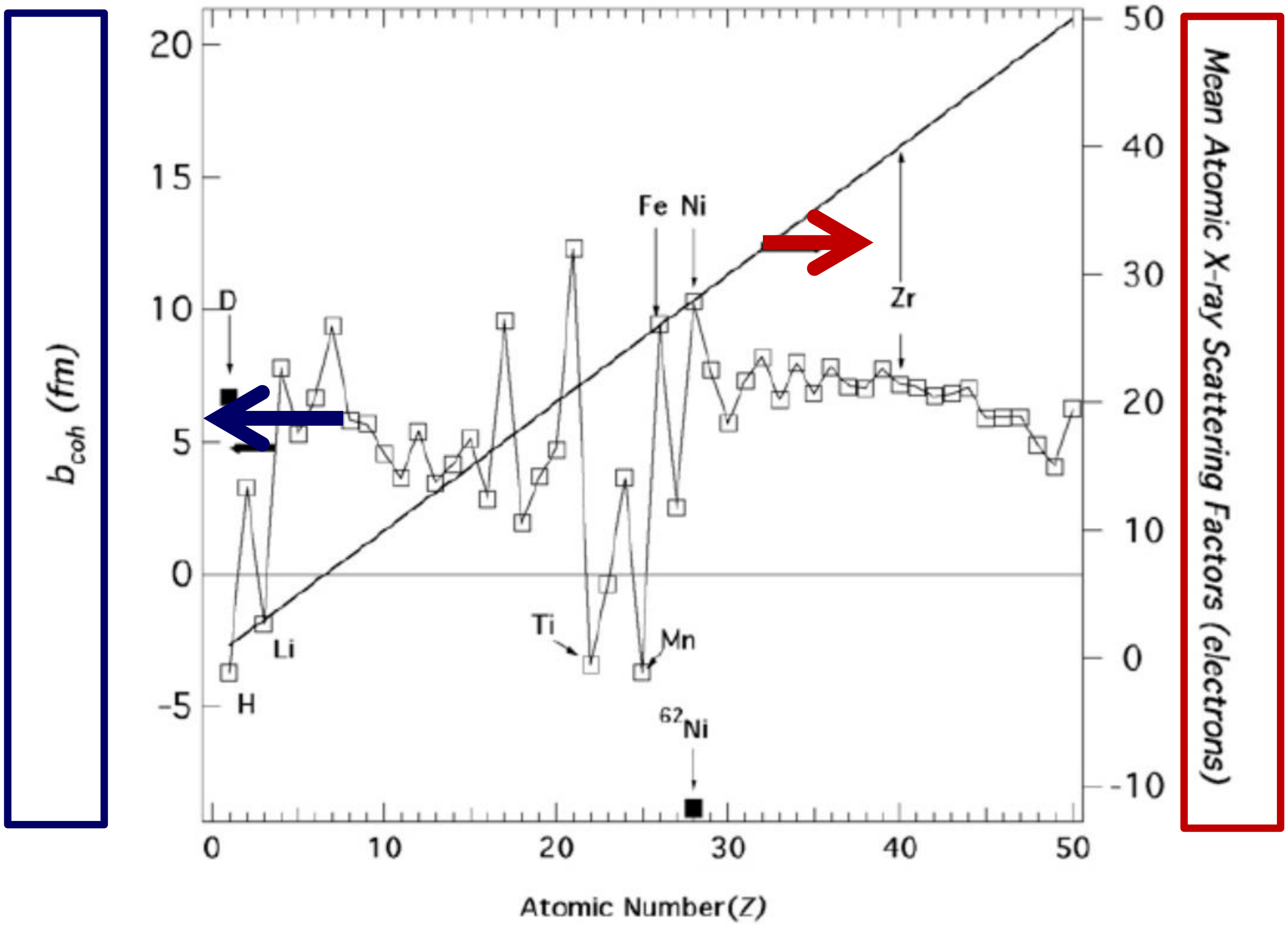
Column	Symbol	Unit	Quantity
1			element
2	Z		atomic number
3	A		mass number
4	$I(p)$		spin (parity) of the nuclear ground state
5	c	%	natural abundance (For radioisotopes the half-life is given instead.)
6	b_c	fm	bound coherent scattering length
7	b_i	fm	bound incoherent scattering length
8	s_c	barn[1]	bound coherent scattering cross section
9	s_i	barn	bound incoherent scattering cross section
10	s_s	barn	total bound scattering cross section
11	s_a	barn	absorption cross section for 2200 m/s neutrons[2]

(1) 1 barn = 100 fm^2
(2) E = 25.30 meV, k = 3.494 $Å^{-1}$, l = 1.798 Å

	Z	A	$I(\pi)$	c	b_c	b_i	σ_c	σ_i	σ_s	σ_a
H	1				−3.7390(11)		1.7568(10)	80.26(6)	82.02(6)	0.3326(7)
		1	1/2(+)	99.985	−3.7406(11)	25.274(9)	1.7583(10)	80.27(6)	82.03(6)	0.3326(7)
		2	1(+)	0.015	6.671(4)	4.04(3)	5.592(7)	2.05(3)	7.64(3)	0.000519(7)
		3	1/2(+)	(12.32 a)	4.792(27)	−1.04(17)	2.89(3)	0.14(4)	3.03(5)	0
He	2				3.26(3)		1.34(2)	0	1.34(2)	0.00747(1)
		3	1/2(+)	0.00014	5.74(7) −1.483(2)i	−2.5(6) +2.568(3)i	4.42(10)	1.6(4)	6.0(4)	5333.(7.)
		4	0(+)	99.99986	3.26(3)	0	1.34(2)	0	1.34(2)	0
Li	3				−1.90(2)		0.454(10)	0.92(3)	1.37(3)	70.5(3)
		6	1(+)	7.5	2.00(11) −0.261(1)i	−1.89(10) +0.26(1)i	0.51(5)	0.46(5)	0.97(7)	940.(4.)
		7	3/2(−)	92.5	−2.22(2)	−2.49(5)	0.619(11)	0.78(3)	1.40(3)	0.0454(3)
Be	4	9	3/2(−)	100	7.79(1)	0.12(3)	7.63(2)	0.0018(9)	7.63(2)	0.0076(8)

2.2.3 Comparison of neutrons and X-rays

For neutrons no monotonic dependence on Z as for X-rays



John B. Parise “Introduction to neutron science“

2.2.4 Comparison of neutrons and X-rays

Interactions different on the fundamental level, cross sections similarly weak.

Thus, many aspects of the scattering theory are similar for X-rays and neutrons, including kinematic theory, i.e. no multiple scattering, which is good.

This makes a common summer school particularly suitable!

It also makes it easier to cover both in this lecture and to use both in one's research.

Nevertheless, some differences neutrons vs.	X-rays
e.g.	
- penetration depth typically still higher	slightly less for X-rays
- stronger interaction with light elements	---------------
- contrast variation by isotopic substitution	absorption edges
- incoherent cross section (used for QENS)	---------------
- high energy resolution	possible, but less common
- magnetic scattering	different mechanism for X-rays
- flux lower for neutrons	higher for synchrotrons