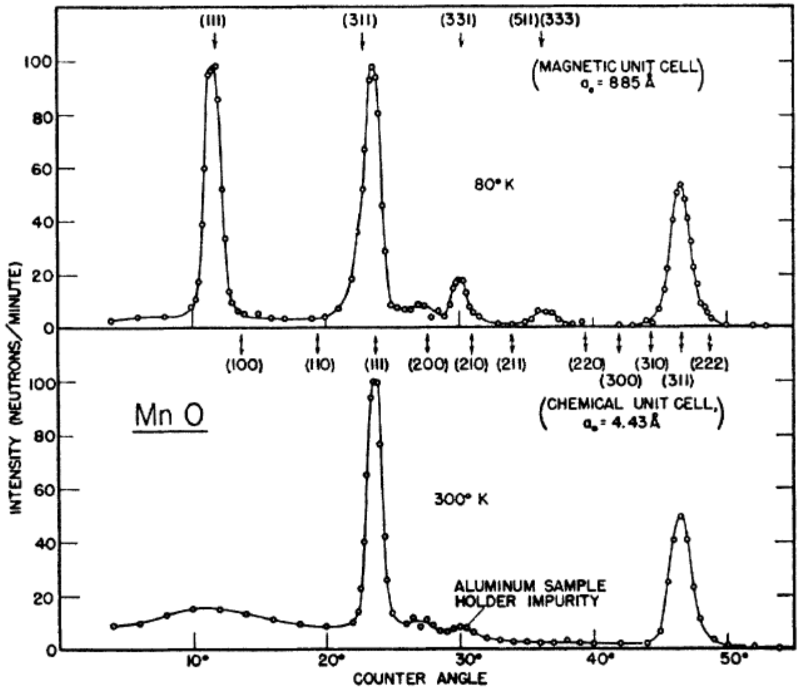
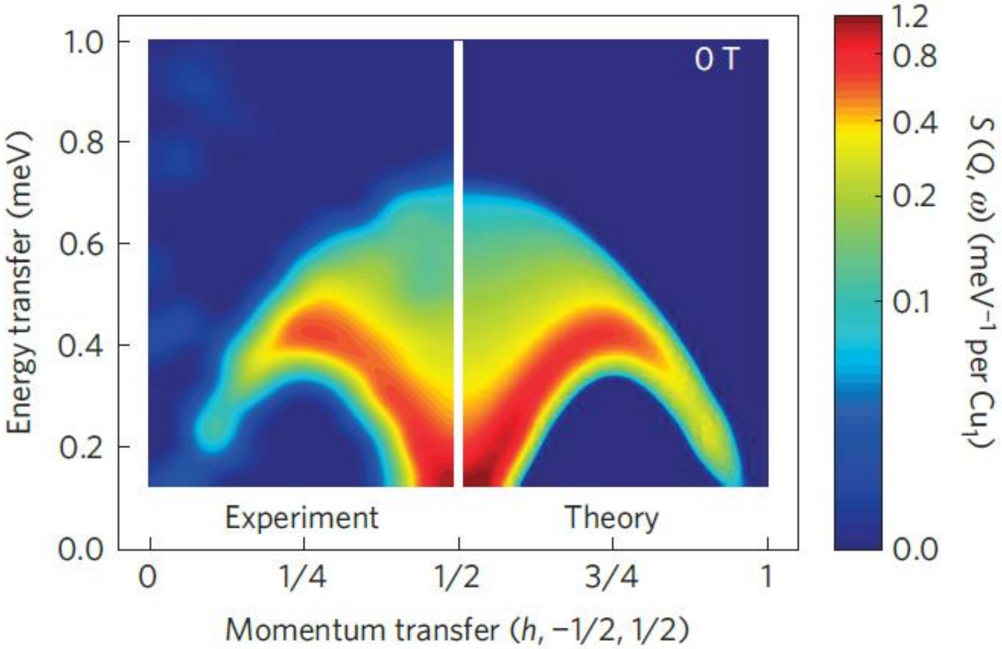




Røntgen og neutronspredning: Introduktion

Niels Bech Christensen

Lektor, DTU Fysik

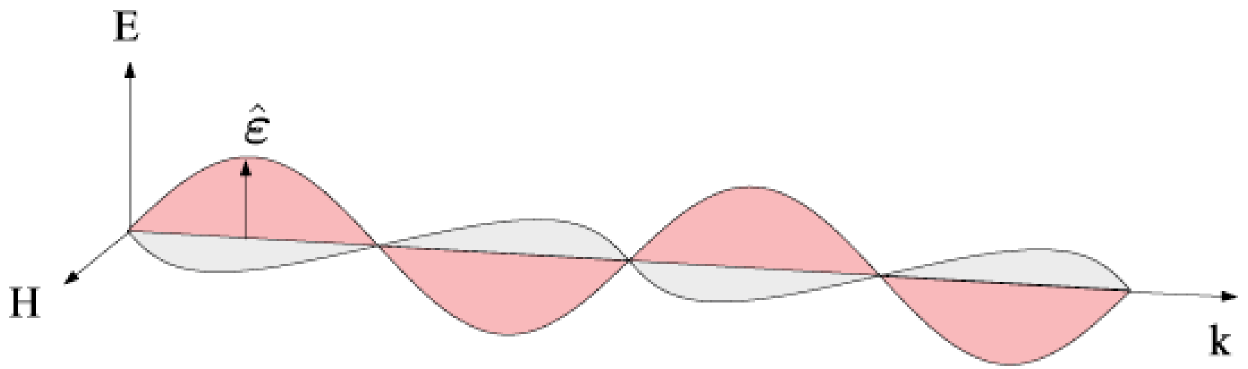
Røntgen

Opdagelse af Røntgenstråling (1895)

W. C. Röntgen
Røntgen-stråling, ”X-rays” (1895)
Nobelpris i Fysik 1901

Anna Berthe’s (Röntgen’s kone)
hånd og vielsesring

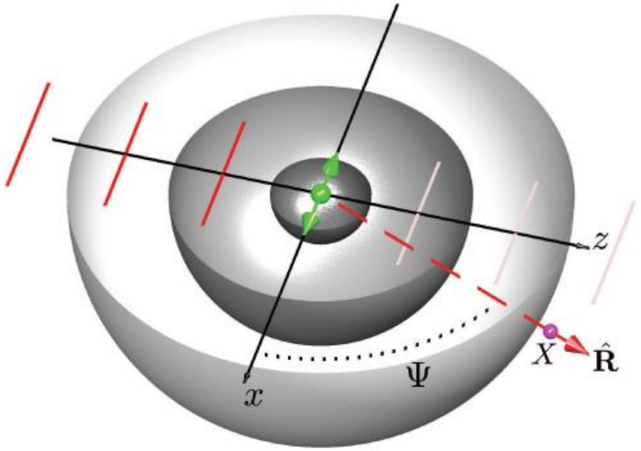
Røntgens vekselvirkning med materialer



Røntgenstråling er **elektromagnetiske bølger** med bølgelængder af størrelsesorden 10^{-10} m

Elements of Modern X-ray Physics, 2. udgave, J. Als-Nielsen & D. McMorrow, Wiley (2011)

Røntgens vekselvirkning med materialer



Det elektriske felt påvirker en elektron med en **Lorentz** kraft

$$\boldsymbol{F} = e\boldsymbol{E}$$

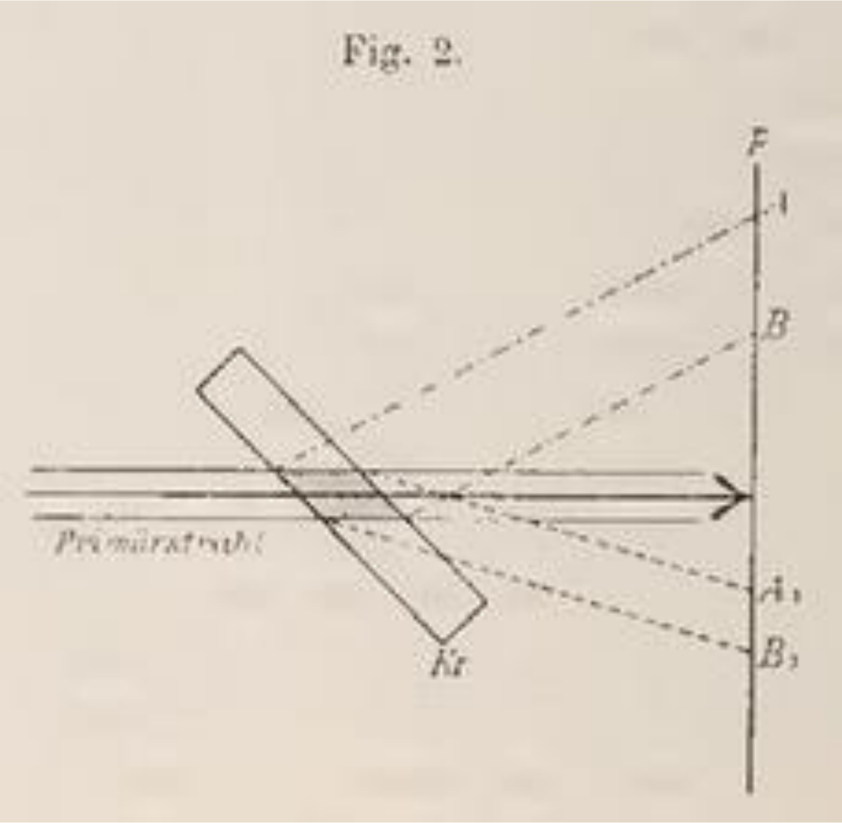
Kraften får elektronen til at accelerere.

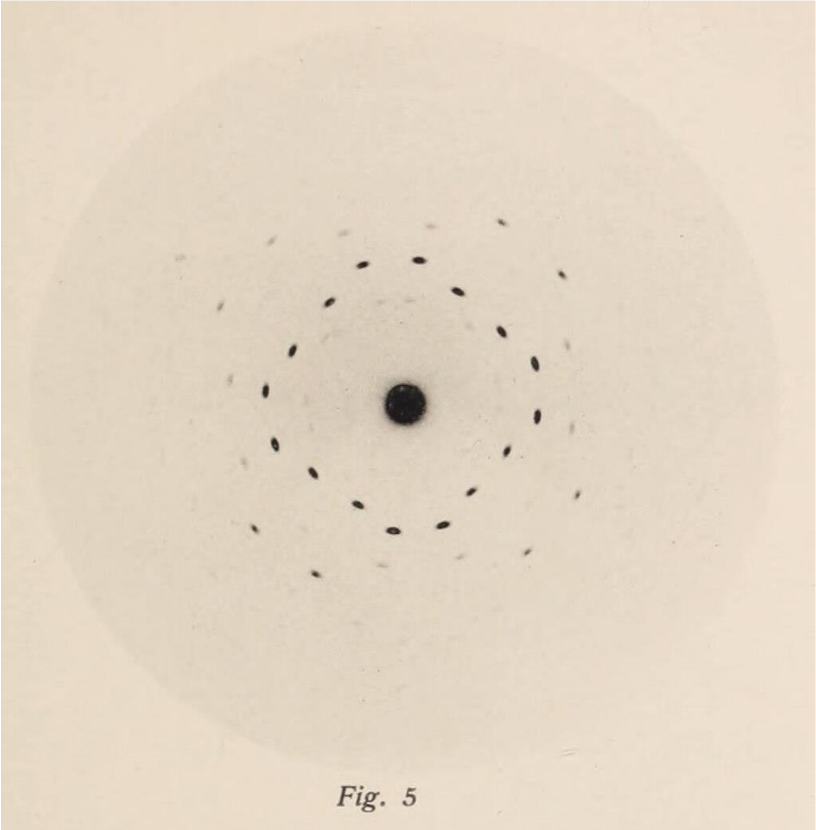
Accelererede elektriske ladninger udsender stråling (kuglebølger).

Kuglebølger fra forskellige elektroner kan **interferere konstruktivt og destruktivt** med hinanden, hvorfor den spredte stråling afhænger af hvilken vinkel vi beskuer prøven fra.

Elements of Modern X-ray Physics, 2. udgave, J. Als-Nielsen & D. McMorrow, Wiley (2011)

Spredning af røntgen fra krystaller (1912)

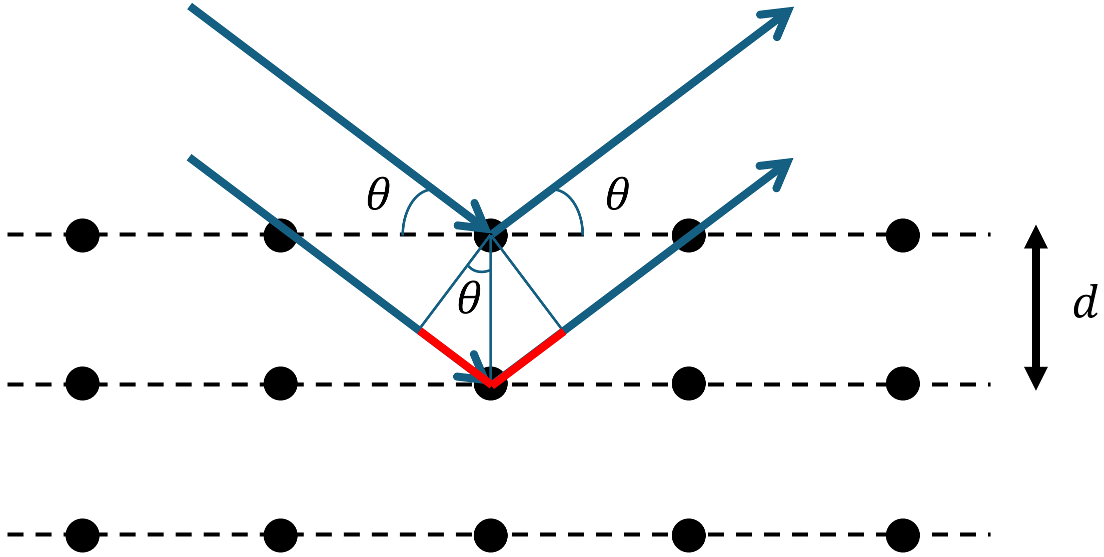


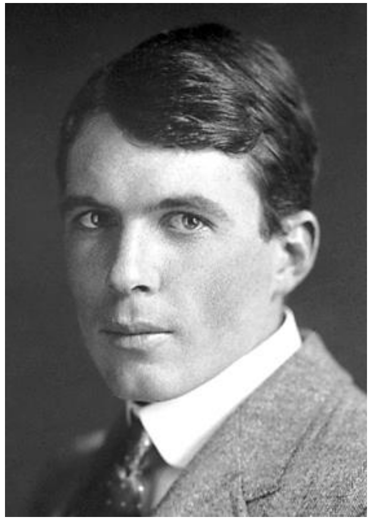


M. v. Laue
Spredning fra krystallinske materialer (1912)
Nobelpris i Fysik 1914

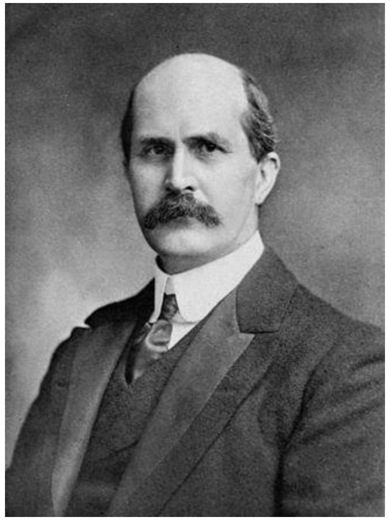
Laue-diffraktionsmønster af ZnS

Bragg’s lov (1913)





W. L. Bragg
Teori
Nobelpris i Fysik 1915



W. H. Bragg
Eksperimenter
Nobelpris i Fysik 1915

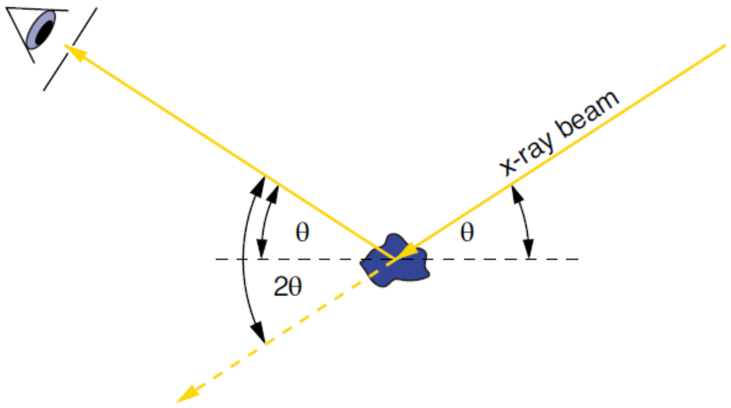
Betingelse for konstruktiv interferens af bølger spredt fra nabo-lag:
Forskel i vejlængde = heltalligt antal bølgelængder λ af strålingen

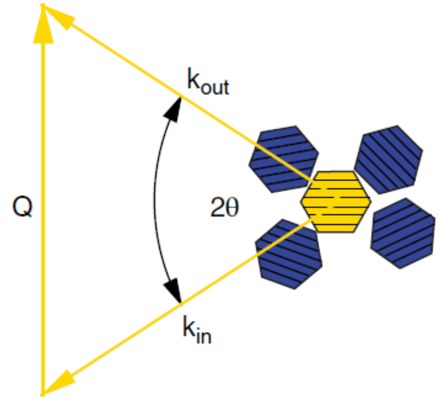
$$n\lambda = 2d\sin\theta$$

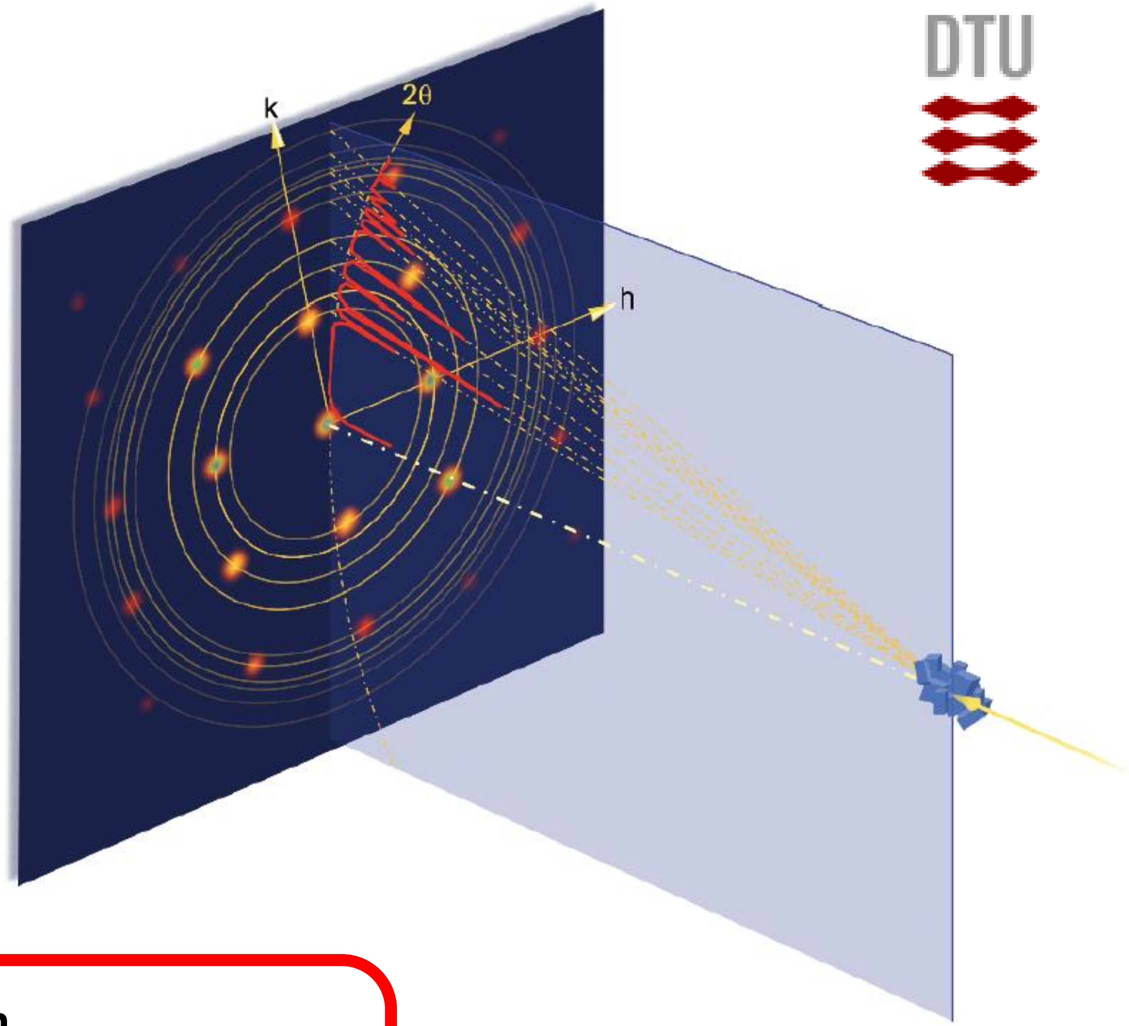
“W. H. Bragg reported their results at meetings and in a paper, giving credit to "his son" (unnamed) for the equation, but not as a co-author, which gave his son some heartaches, which he never overcame.”

https://en.wikipedia.org/wiki/Lawrence_Bragg

Pulverspredning







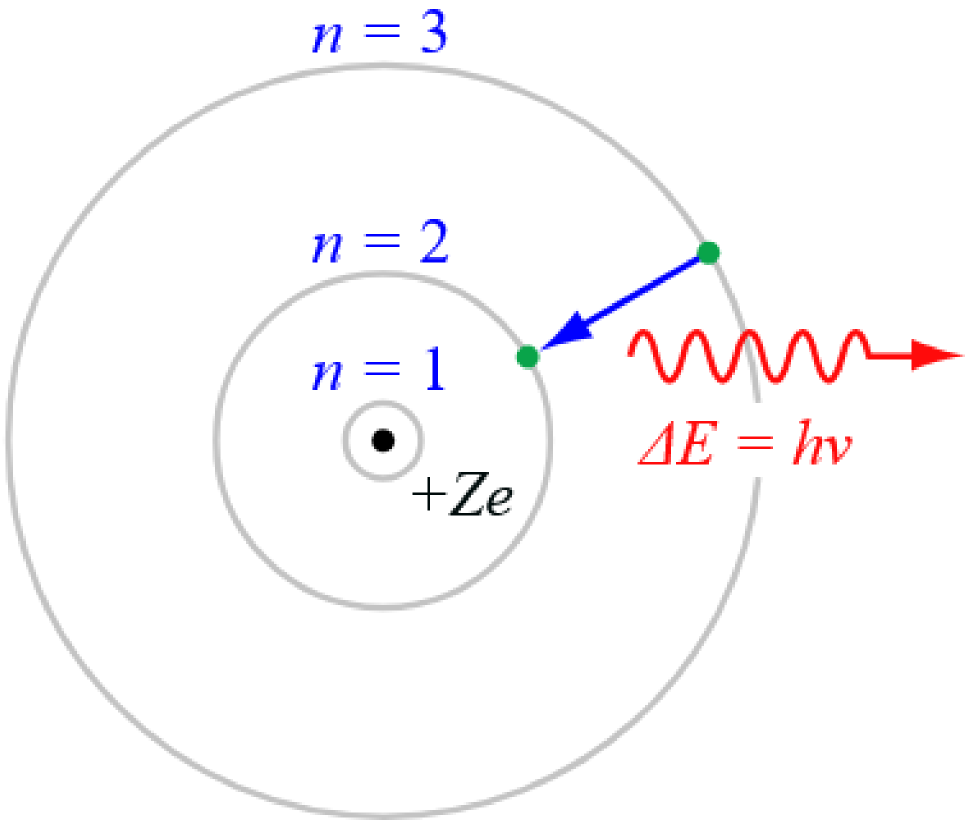
Spredningsmønsteret er et **finger-aftryk af krystal-strukturen**

- **Peak positioner** (vinkler 2θ) giver information om gitter-afstande d
- **Peak Intensiteter** giver information om relative atomare positioner

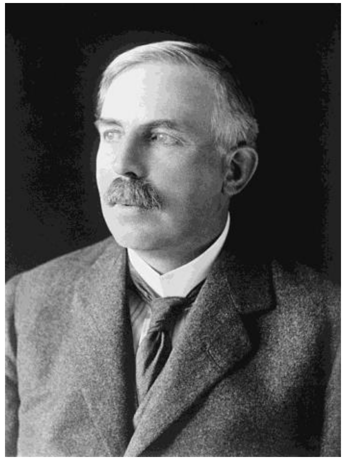
Philip Willmott, *An Introduction to Synchrotron Radiation: Techniques and Applications*, Wiley 2019

Neutroner

Elektroner, protoner og Bohr's atom-model



J. J. Thomson
Elektroner (1897)
Nobelpris i Fysik 1906

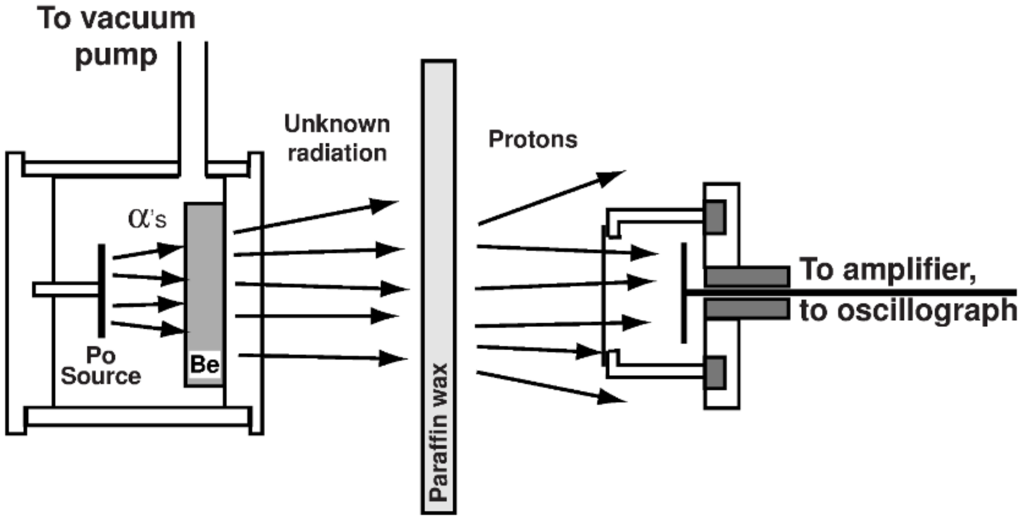


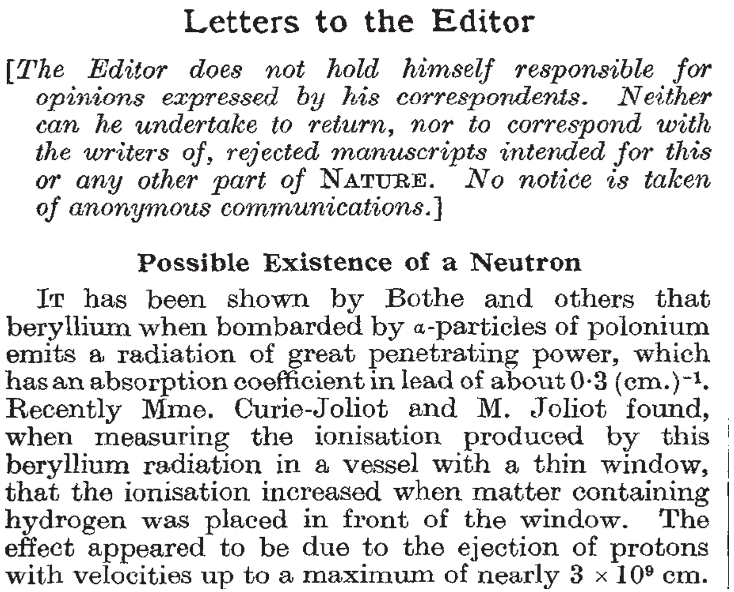
E. Rutherford
Atomkerner (1911)
Protoner (1919)
Nobelpris i Kemi 1908

N. H. D. Bohr
Atom-model
Nobelpris i Fysik 1922

Opdagelse af neutroner (1932)

J. Chadwick
Neutroner (1932)
Nobelpris I Fysik 1935





Letters to the Editor

[The Editor does not hold himself responsible for opinions expressed by his correspondents. Neither can he undertake to return, nor to correspond with the writers of, rejected manuscripts intended for this or any other part of NATURE. *No notice is taken of anonymous communications.]*

Possible Existence of a Neutron

IT has been shown by Bothe and others that beryllium when bombarded by α-particles of polonium emits a radiation of great penetrating power, which has an absorption coefficient in lead of about 0·3 (cm.)$^{-1}$. Recently Mme. Curie-Joliot and M. Joliot found, when measuring the ionisation produced by this beryllium radiation in a vessel with a thin window, that the ionisation increased when matter containing hydrogen was placed in front of the window. The effect appeared to be due to the ejection of protons with velocities up to a maximum of nearly 3×10^9 cm.

Nature (27/2 1932)

Neutronens egenskaber

“I am afraid neutrons will not be of any use to anyone”

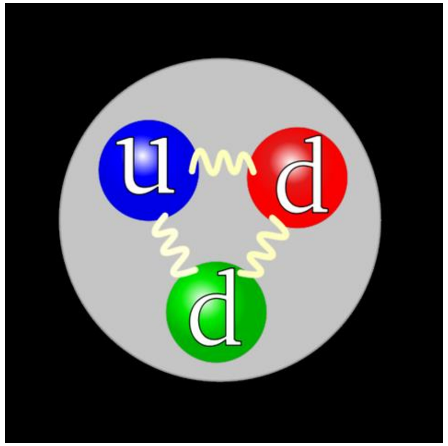
James Chadwick

Masse : $1.675\ 10^{-27}$ kg

Ladning : 0 (Ingen Coulomb kræfter)

${}^{1}_{0}n \rightarrow {}^{1}_{0}p + e^{-} + \overline{\mu}_{e}$

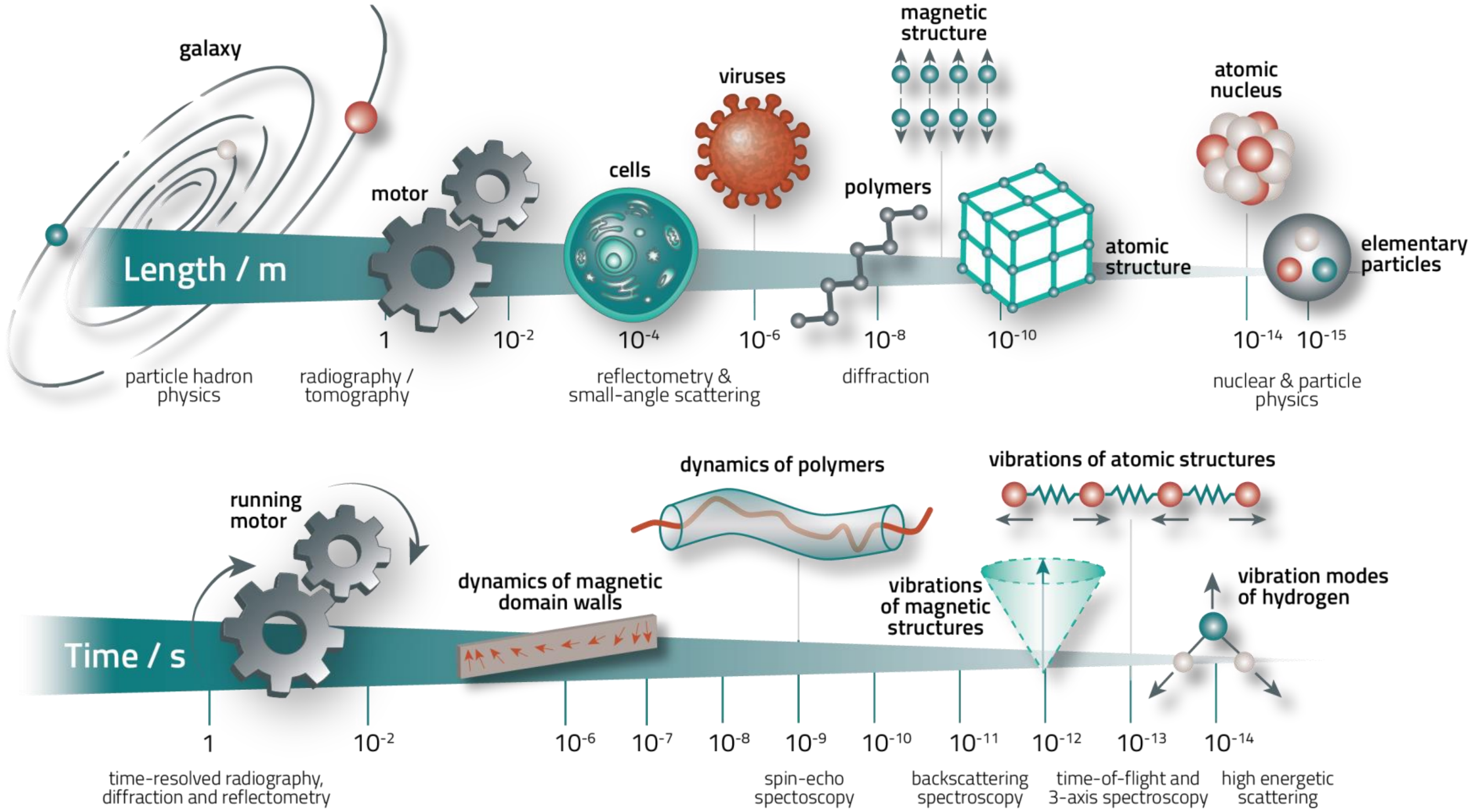
Levetid: 886(1) sekunder



Spin : ½ (magnetisk)

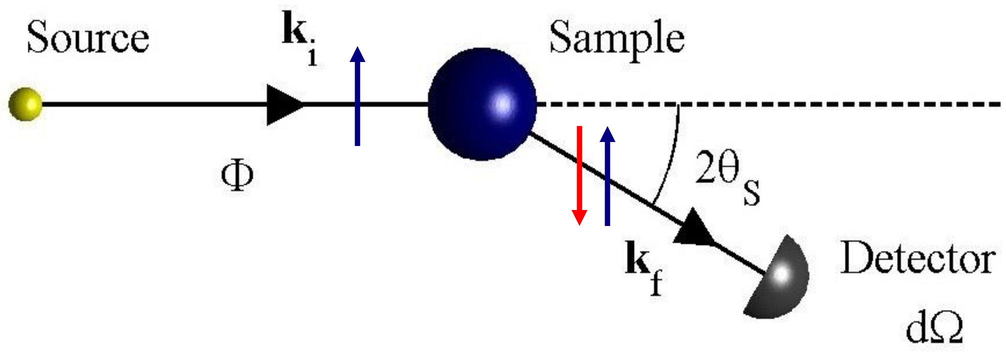
Magnetisk dipol-moment: $\mu = -1.913\ \mu_N$

De var nu nyttige alligevel
Hvad kan man studere med neutroner i 2025?

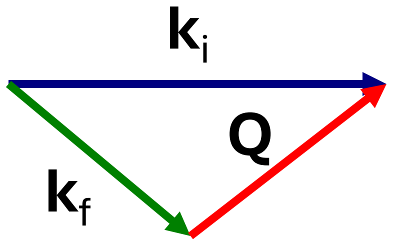


https://lens-initiative.org/lens-position-papers/

Sprednings-eksperimenter



Spredningstrekant



Impuls bevarelse

Energi bevarelse

$$\boldsymbol{Q} = \boldsymbol{k}_i - \boldsymbol{k}_f$$

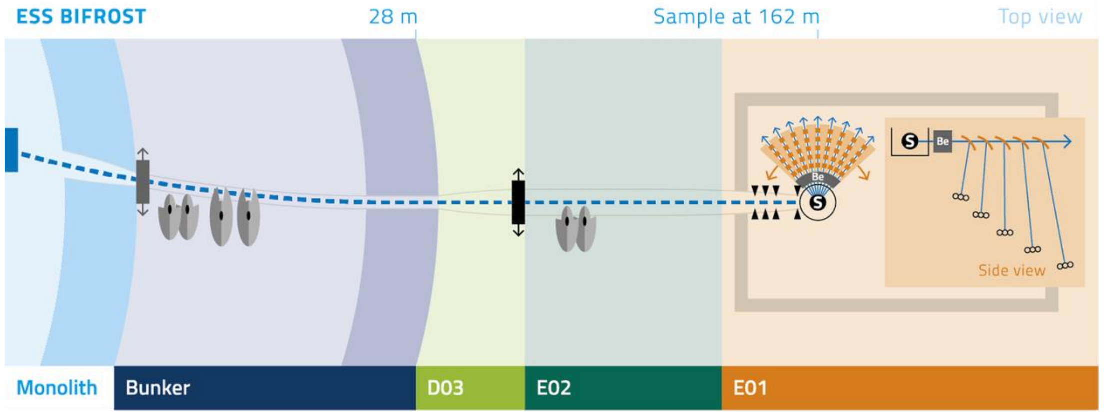
$$\hbar\omega = E_i - E_f$$

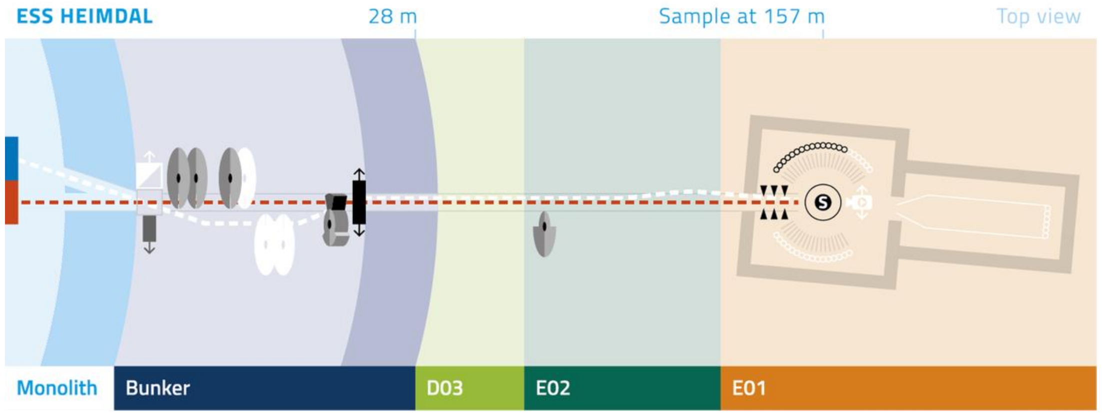
Neutroners to vekselvirkninger med materialer

1. Vekselvirkning med kerner
2. Vekselvirkning med elektroners magnetiske momenter

De to vekselvirkninger tillader eksperimentel bestemmelse af

- Materialers atomare og magnetiske struktur
- Materialers atomare og magnetiske dynamik

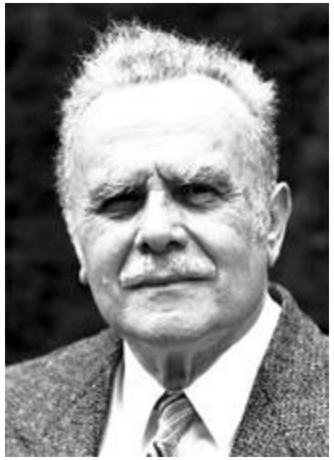




Nobelpris i Fysik (1994)

"for pionerarbejde med udviklingen af neutronspredningns-teknikker til studiet af faste stoffer"

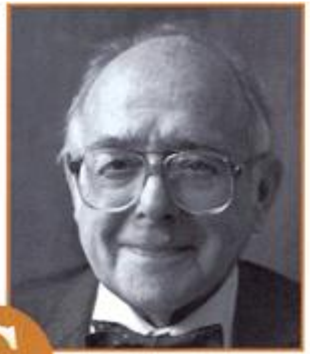
Clifford G. Shull (1915-2001), USA
"for udviklingen af neutron diffraktionsteknikker"



Bertram N. Brockhouse (1918-2003), Canada
"for udviklingen af neutron spektroscopi"

”Neutrons tell us where atoms are and what atoms do”

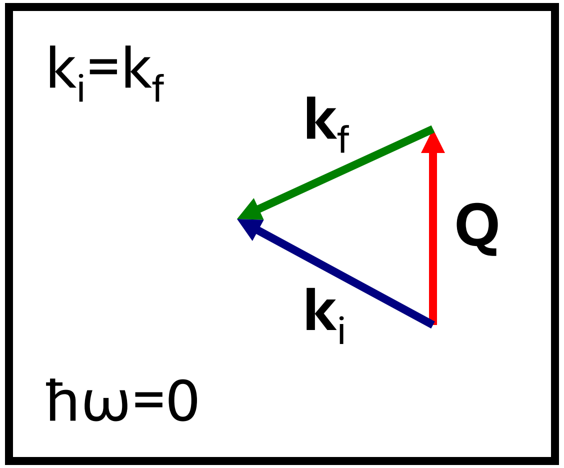
Elastisk spredning (diffraktion)



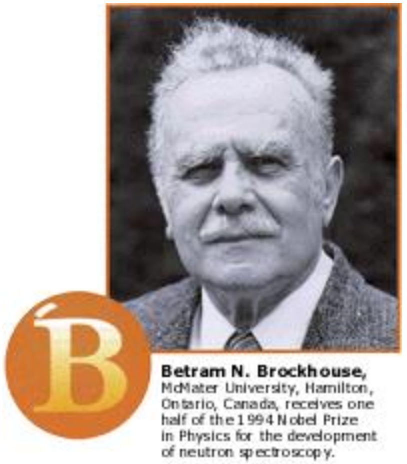
Clifford G. Shull, MIT, Camebridge, Massachusetts, USA, receives one half of the 1994 Nobel Prize in Physics for development of the neutron diffraction technique.

"...hvor atomer er..."

- Krystalstrukturer, polymerer, biologiske systemer, ...
- Magnetiske strukturer, ...
- Som funktion af tryk, elektrisk/magnetisk felt, temperature, fugtighed osv.

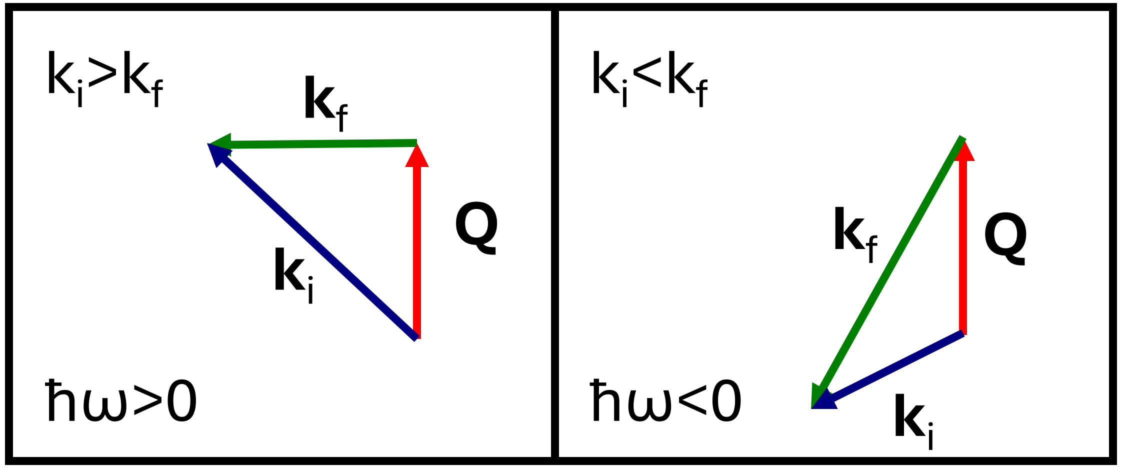


Uelastisk spredning (spektroskopi)



"...hvad atomer gør..."

- Gittervibrationer i krystallinske materialer
- Magnetiske eksitationer
- Som funktion af tryk, elektrisk/magnetisk felt, temperature, fugtighed osv.

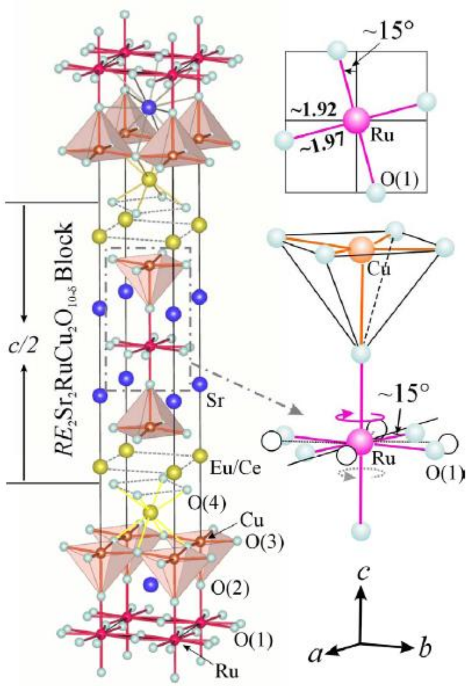


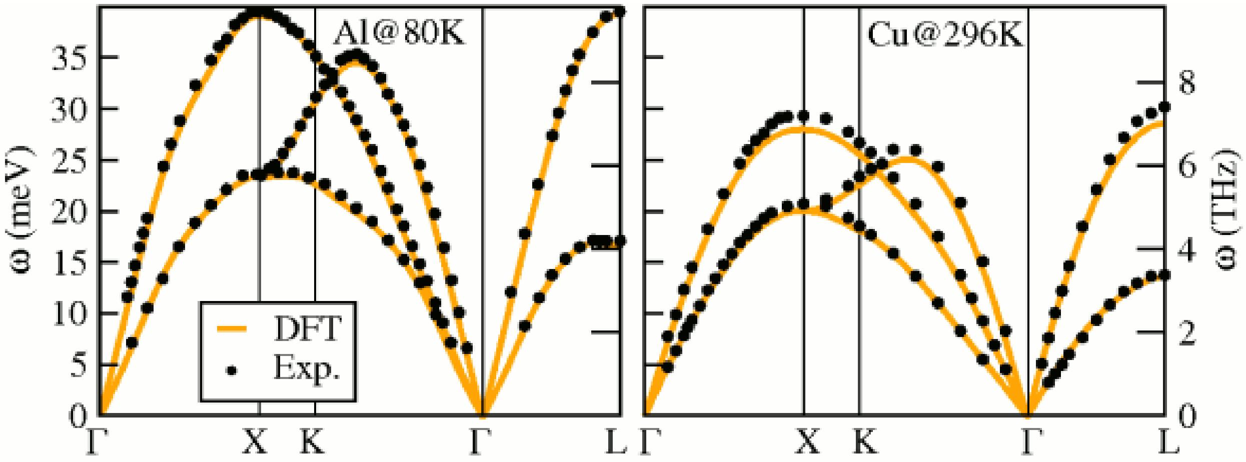
Fem gode grunde til at bruge neutroner

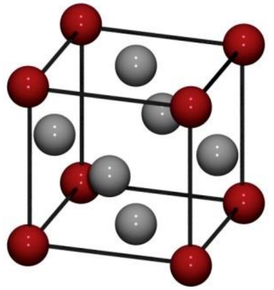
Fem gode grunde til at bruge neutroner

1. Bølgelængder og energier

Sammenlignelige med typiske gitterafstande og eksitations-energier i materialer → Vi kan få information om struktur og dynamik







Fem gode grunde til at bruge neutroner

2. Følsomhed over for isotoper og lette grundstoffer

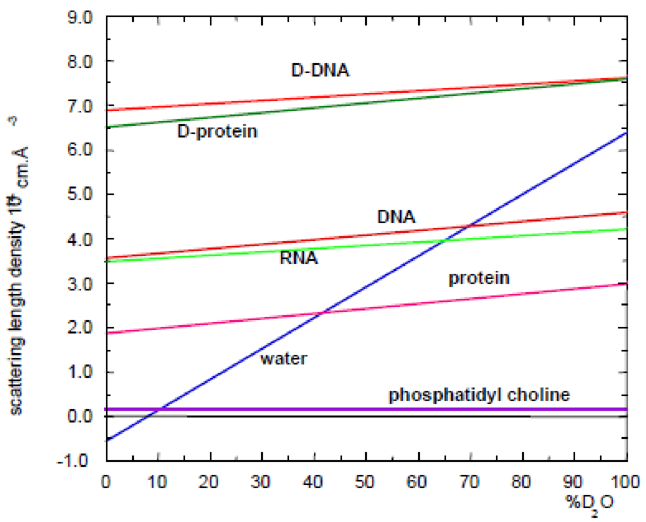
Tillader at finde positioner af lette grundstoffer, og at skelne imellem nabo-grundstoffer.

Kontrast-variation i studier af bløde materialer, f.eks. proteiner

Fig. a: Neutron radiography of a camera

Fig. b: Radiographic image of a camera made X-rays

Contrast variation

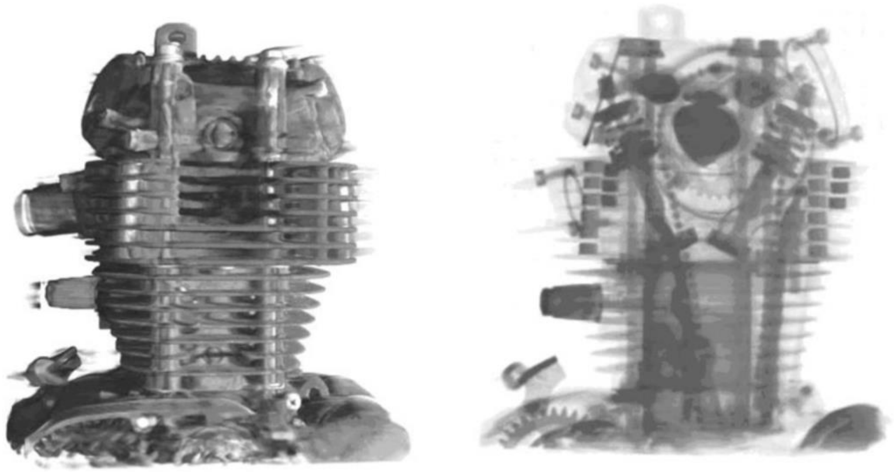


Fem gode grunde til at bruge neutroner

3. Gennemtrængnings-evne

Neutronens elektrisk neutralitet tillader at undersøge materialers indre (ikke kun strukturer nær overfladen)

Tillader forsøg ved høje magnetfelter/tryk og ekstreme temperaturer



Imaging billed af en motorblok
www.psi.ch

15T magnet ved ILL Grenoble

Fem gode grunde til at bruge neutroner

4. Magnetisme

Neutronens magnetiske moment vekselvirker med felter genereret af elektroner i prøven. Dette tillader detaljerede studier af magnetisk struktur og dynamik

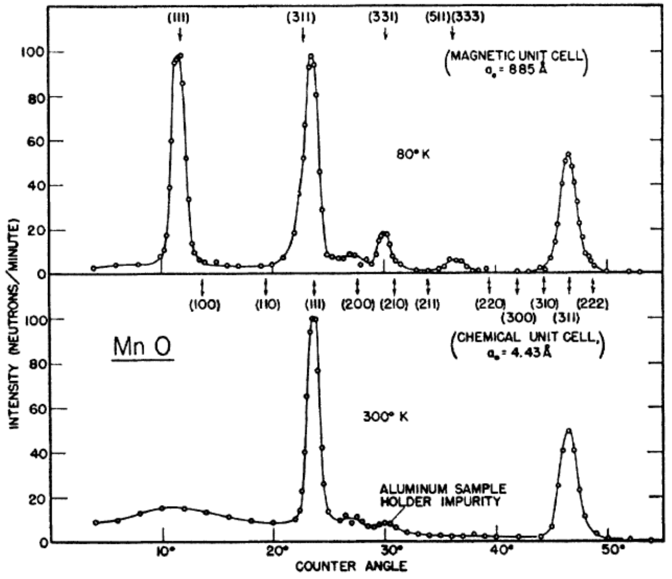
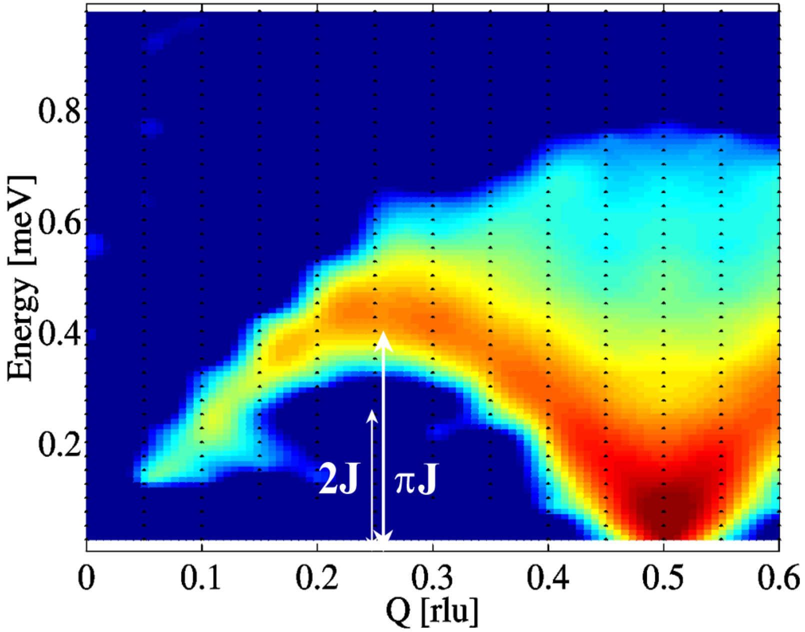


FIG. 1. Neutron diffraction patterns for MnO at room temperature and at 80°K.



Fem gode grunde til at bruge neutroner

5. Kvantitative eksperimenter

Vekselvirkningerne er svage og velkendte

Teorien for neutronspredning er derfor relativt simpel

$$\left(\frac{d\sigma}{d\Omega}\right)_N \propto \sum_{\boldsymbol{G}} |S_N(\boldsymbol{Q})|^2 \delta(\boldsymbol{Q} - \boldsymbol{G})$$

$$\left(\frac{d\sigma}{d\Omega}\right)_M \propto \sum_{\boldsymbol{G_M}} \left|\hat{\boldsymbol{Q}} \times S_M(\boldsymbol{Q}) \times \hat{\boldsymbol{Q}}\right|^2 \delta(\boldsymbol{Q} - \boldsymbol{G}_M)$$

Eksempler

Eksempel 1
Laue diffraktion med neutroner

Laue Photography of Neutron Diffraction

E. O. Wollan, C. G. Shull, and M. C. Marney
Clinton National Laboratory, Oak Ridge, Tennessee
January 19, 1948

THE photographic technique has played so important a role in the field of x-ray diffraction that it is of interest to develop this technique for use in neutron diffraction problems. With this idea in mind, we have obtained the Laue photograph, shown in Fig. 1, of the diffraction of neutrons by a NaCl crystal.

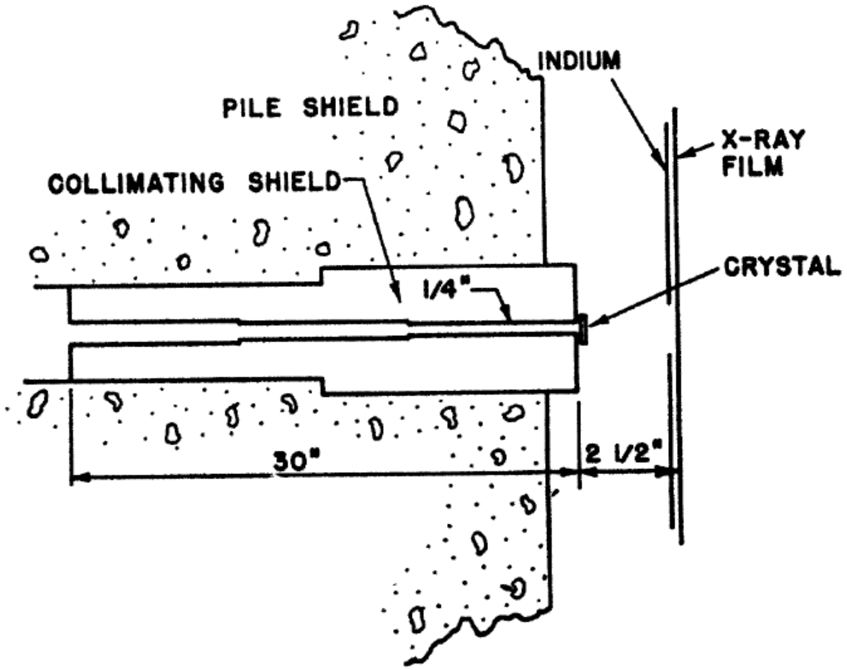


Fig. 2. Schematic diagram of Laue camera for obtaining neutron diffraction patterns.

Fig. 1. Laue photograph showing neutron diffraction by NaCl.

Pulver-diffraktion anno 1948-49

Wollan & Shull (1949)

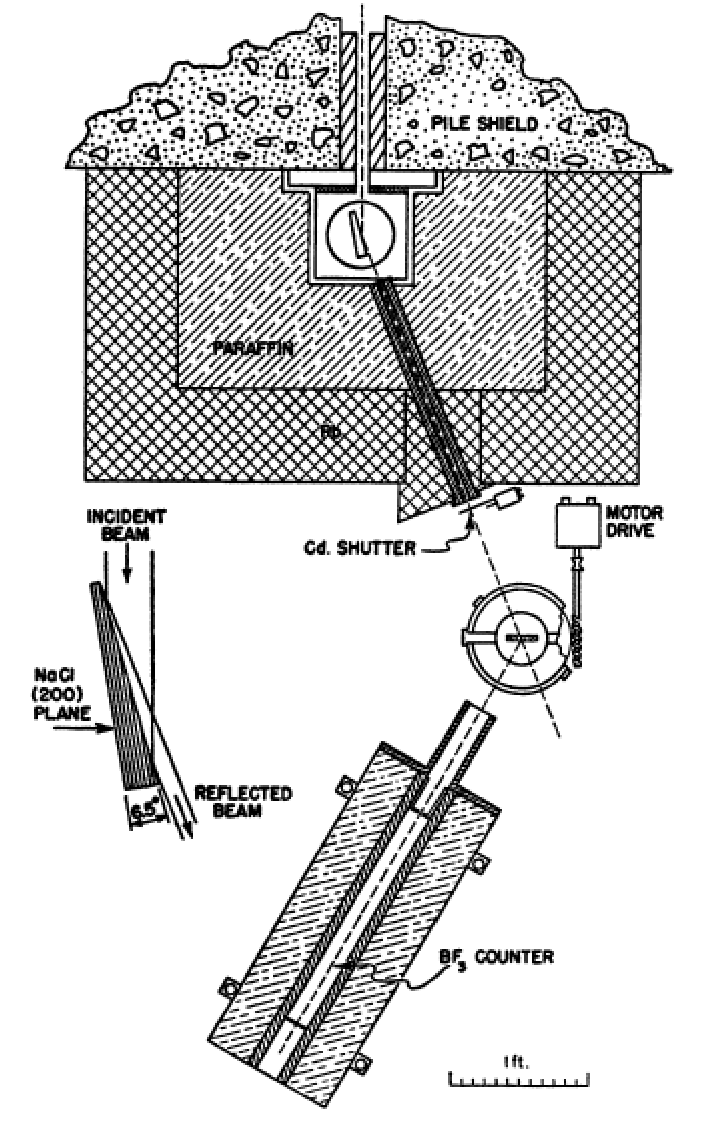
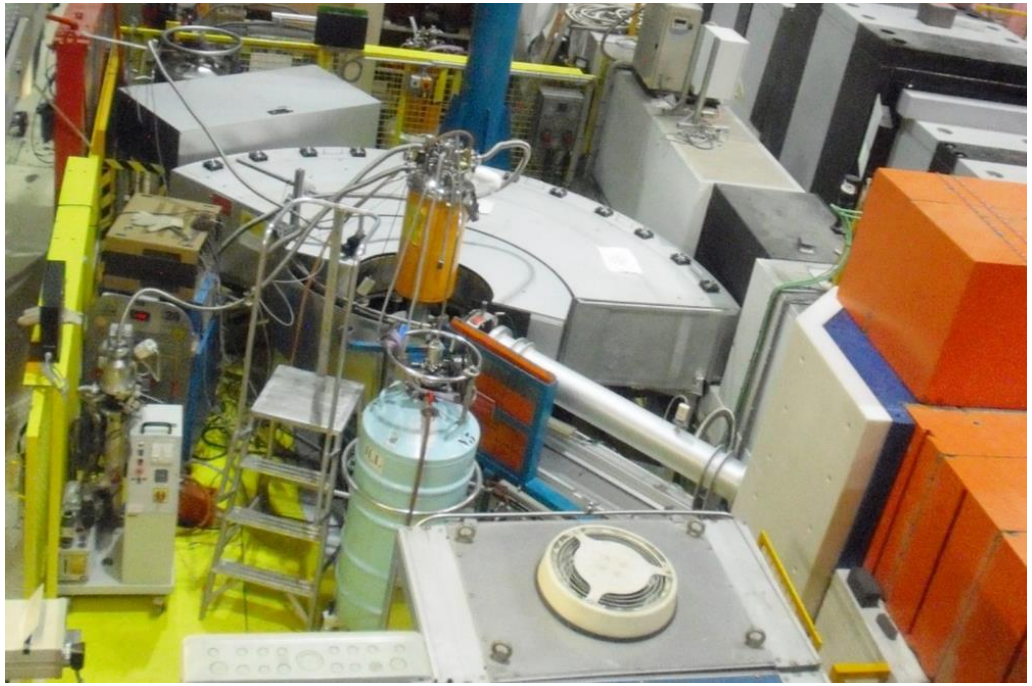
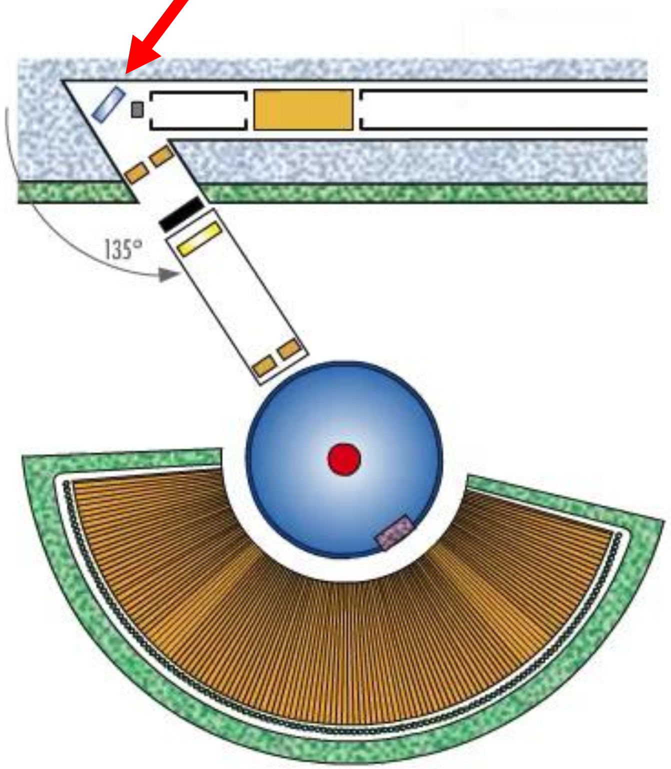


FIG. 1. Arrangement of apparatus, showing the monochromating crystal (detailed in left center) collimating slits, shielding, second spectrometer with location of powder specimen and counter.

Pulver-diffraktion anno 2025

Kendt (monokromator)-krystal bruges til at udvælge bølgelængden af de indkommende neutroner via Bragg’s lov





https://www.ill.eu/for-ill-users/instruments/instruments-list/d1b/description/instrument-layout

Eksempel 2
Krystalstrukturen af is D_2O

Baggrund:
Oxygen-atomerne position var velkendte fra røntgen-spredningsforsøg udført i 1920’erne.

Fordi Røntgen-diffraktion har meget svært ved at identificere ”lette” atomers (Hydrogen) positioner, hvis der også er ”tunge” atomer (Oxygen) til stede, var hydrogen atomernes positioner ukendte.

Eksempel 2
Krystalstrukturen af is D_2O

PHYSICAL REVIEW VOLUME 75, NUMBER 9 MAY 1, 1949

Neutron Diffraction Study of the Structure of Ice*

E. O. WOLLAN, W. L. DAVIDSON** AND C. G. SHULL
Oak Ridge National Laboratory, Oak Ridge, Tennessee
(Received January 24, 1949)

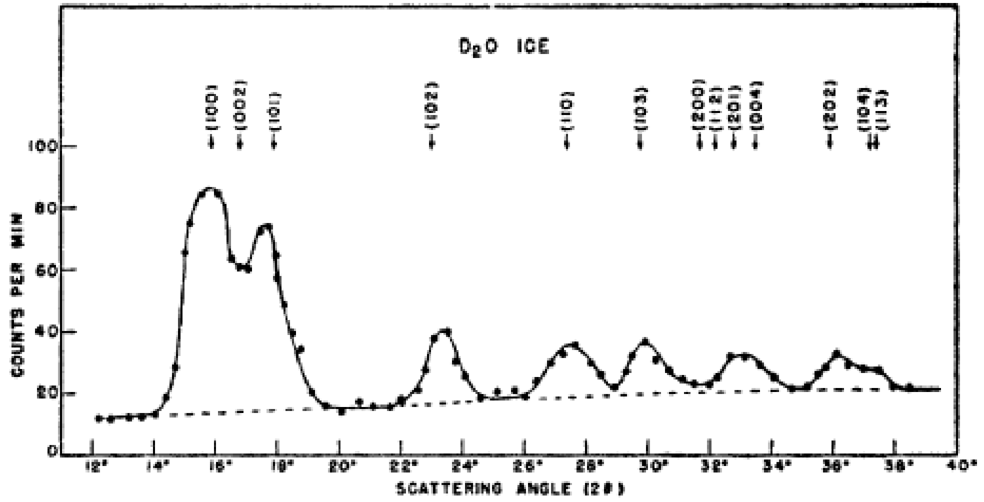


FIG. 1. Neutron diffraction powder pattern of heavy ice (D_2O) taken at −90°C with neutrons of wave-length 1.06A.

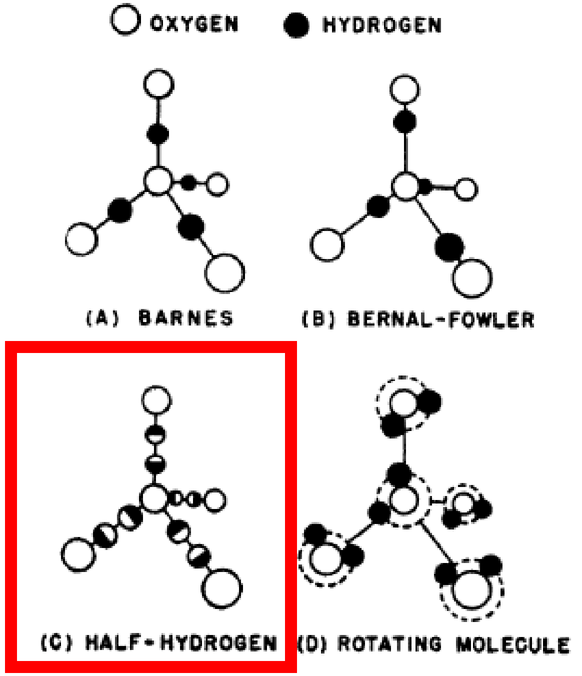


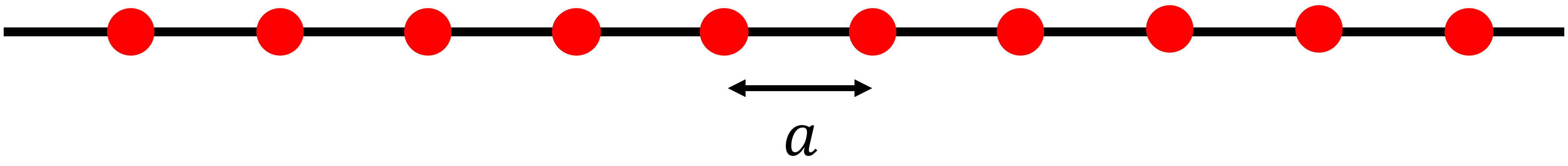
FIG. 2. Schematic diagram of four structural models which are used in calculating pattern intensities for various proposed structures of ice.

Resultat: Hydrogen-atomerne positioner er uordnede på en kompleks manér: Der er altid to H/D atomer tæt ved hvert Oxygen atom og to længere borte. Hver position er i gennemsnit besat af ét halvt H/D atom.

Magnetisk struktur og dynamik

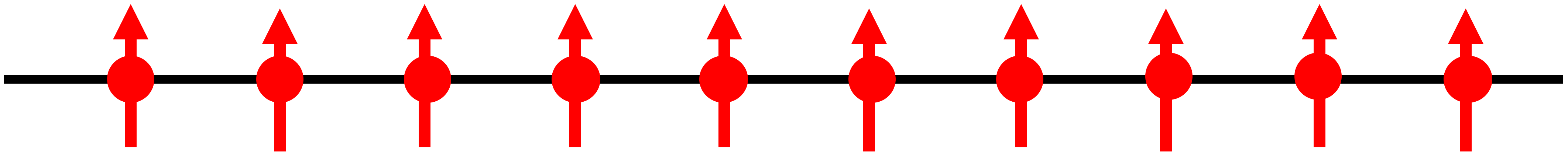
Atomar struktur

Krytalstrukturen gentager sig hvis den forskydes med **gitterafstanden** a
Krystalstrukturen har **diskret translations-symmetri**



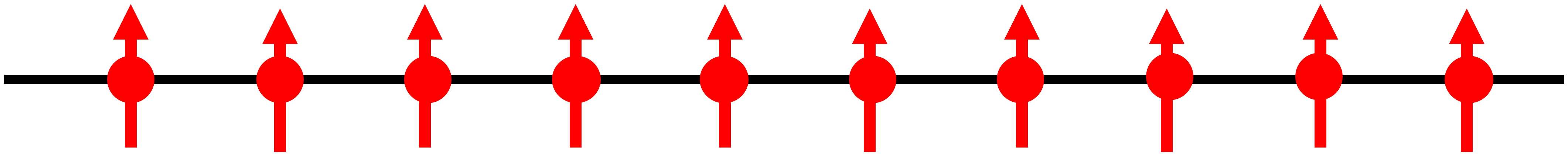
Magnetiske struktur

Ferromagnetisme: Alle elektroniske magnetiske momenter er parallelle
Den magnetiske struktur har **samme translations-symmetri** som krystalstrukturen

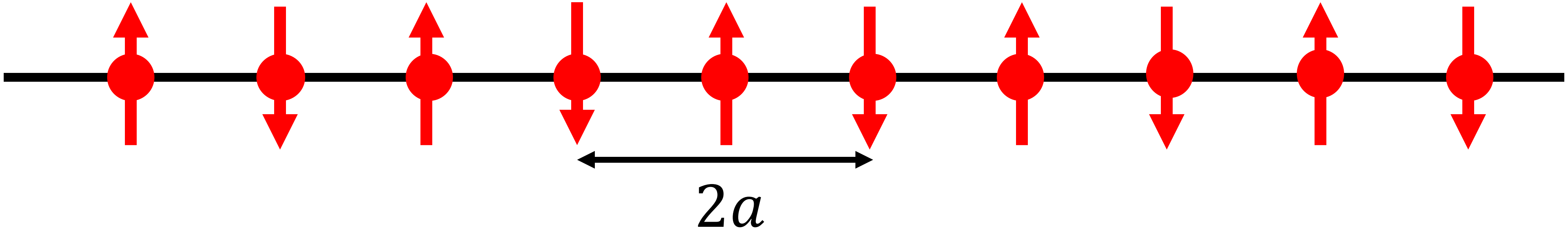


Magnetiske struktur

Ferromagnetisme: Alle elektroniske magnetiske momenter er parallelle
Den magnetiske struktur har **samme translations-symmetri** som krystalstrukturen

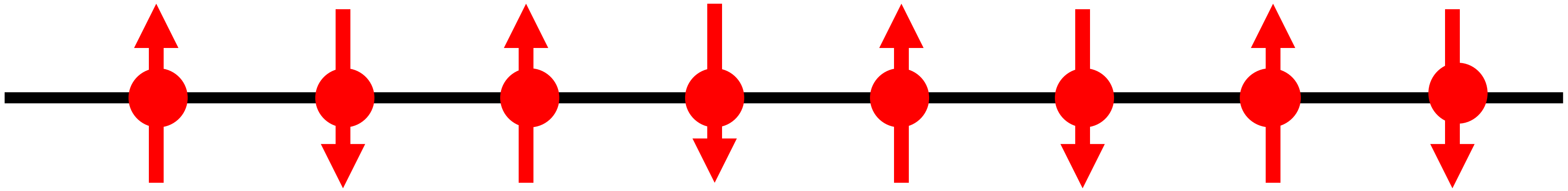


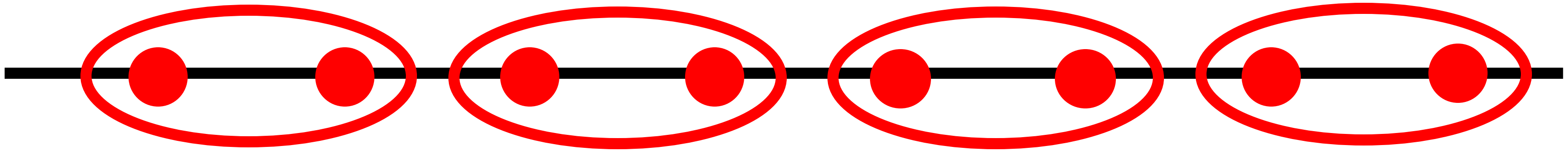
Anti-ferromagnetisme: Momenter af nabo-atomer er antiparallelle
Den **magnetiske gitterafstand** er nu $2a$. Der er en **ny translations-symmetri** i spil

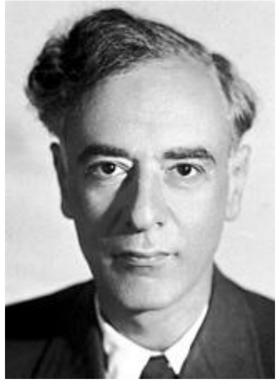


Magnetisk struktur

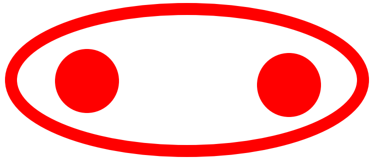
L. E. F. Néel
Nobelpris i Fysik 1970







L. D. Landau
Nobelpris i Fysik 1961



$$= \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$$

Entanglement

Eksempel 3: Opdagelse af antiferromagnetisme
Magnetisk struktur af MnO

Detection of Antiferromagnetism by Neutron Diffraction*

C. G. SHULL
Oak Ridge National Laboratory, Oak Ridge, Tennessee
AND
J. SAMUEL SMART
Naval Ordnance Laboratory, White Oak, Silver Spring, Maryland
August 29, 1949

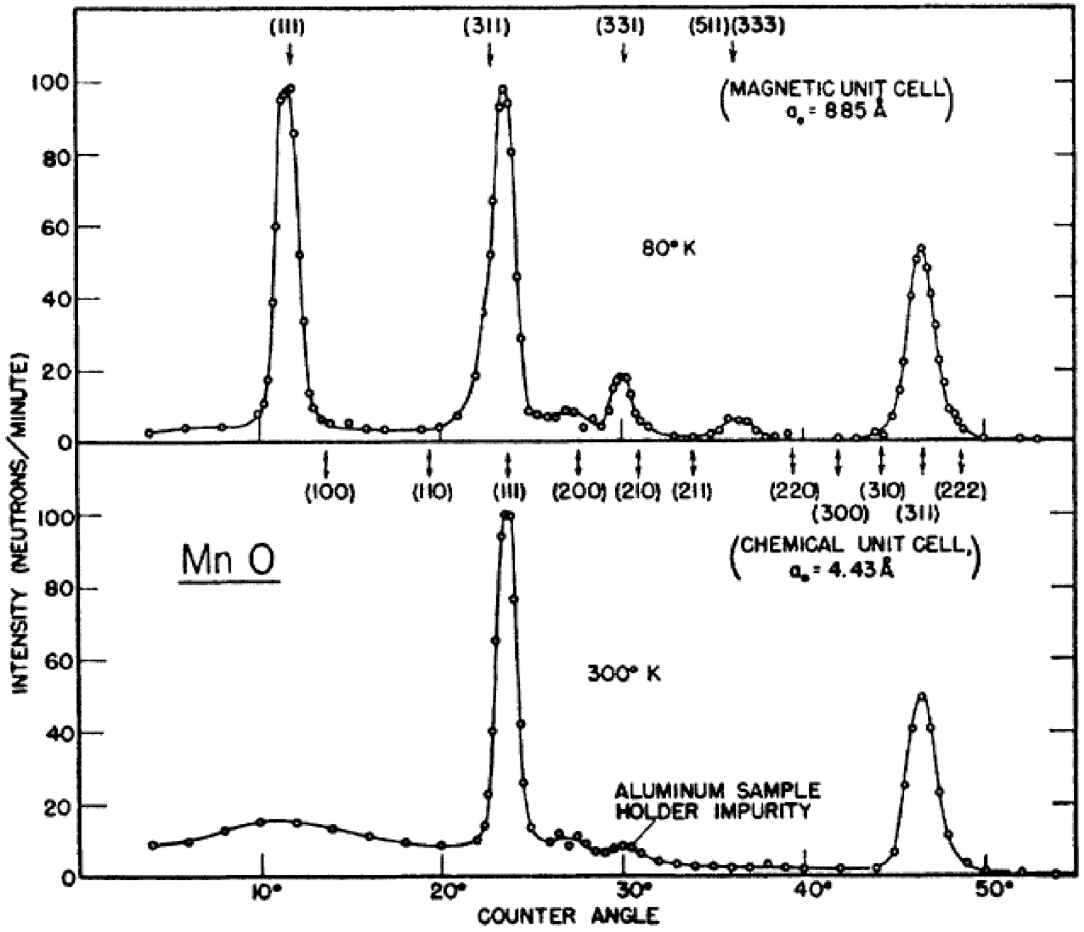


FIG. 1. Neutron diffraction patterns for MnO at room temperature and at 80°K.

Høje temperaturer
Kun Bragg toppe fra krystal-strukturen

Lave temperaturer
Der opstår nye Bragg toppe, som reflekterer en ny symmetri i systemet.

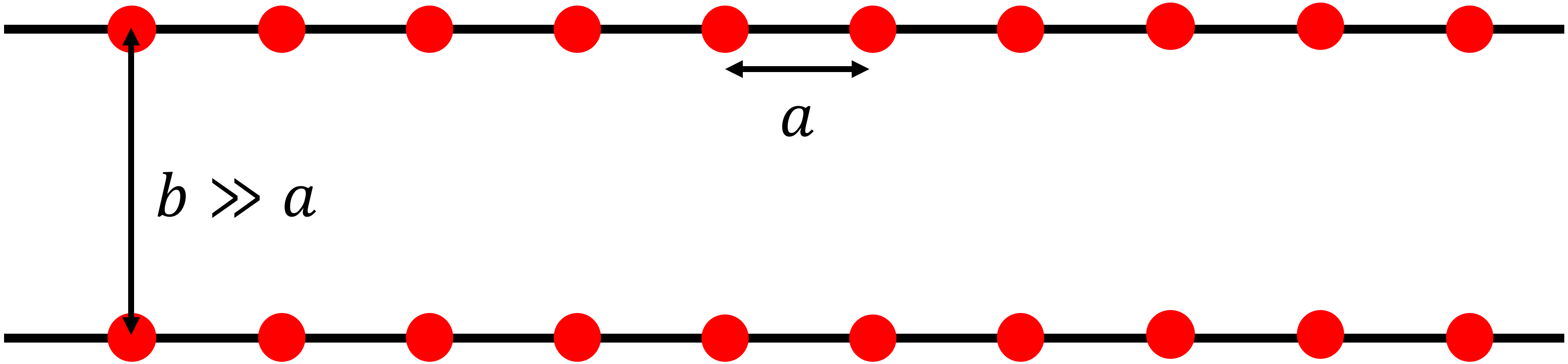
Konklusion: Lous Néel havde ret!
Antiferromagnetisme eksisterer

Eksempel 4
Kobber-sulfat: $CuSO_4 \cdot 5D_2O$

Eksempel 4
Kobber-sulfat: $CuSO_4 \cdot 5D_2O$

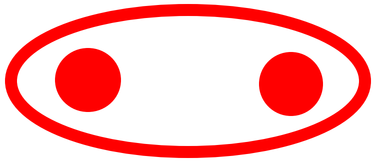
Krystal-strukturen indeholder kæder af kobber atomer.

Kæderne er effektivt magnetisk afkoblede fra hinanden.
De magnetiske egenskaber er derfor 1-dimensionelle

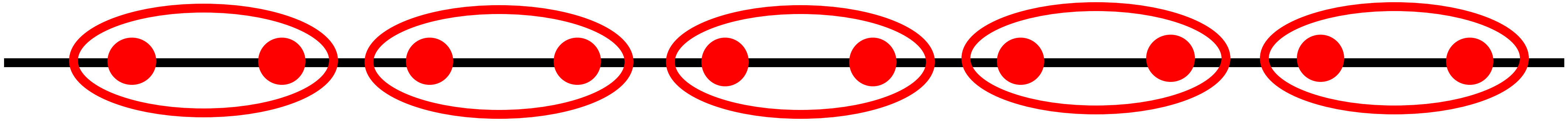


Eksempel 4
Kobber-sulfat: $CuSO_4 \cdot 5D_2O$

Magnet-felt = 0T



$$= \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$$

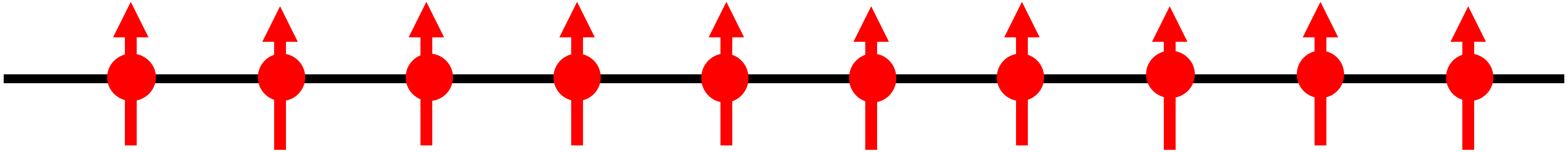


Eksperimentelt: Ingen magnetisk orden for T>40 mK.

Vi kan i stedet bevise at grundtilstanden er "entangled" ved at studere de magnetiske eksitationer og sammenligne med teorien

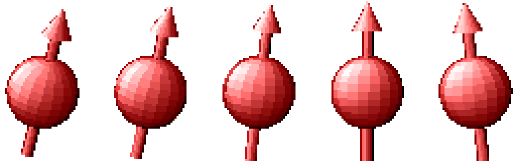
Eksempel 4
Kobber-sulfat: $CuSO_4 \cdot 5D_2O$

Magnet-felt = 5T



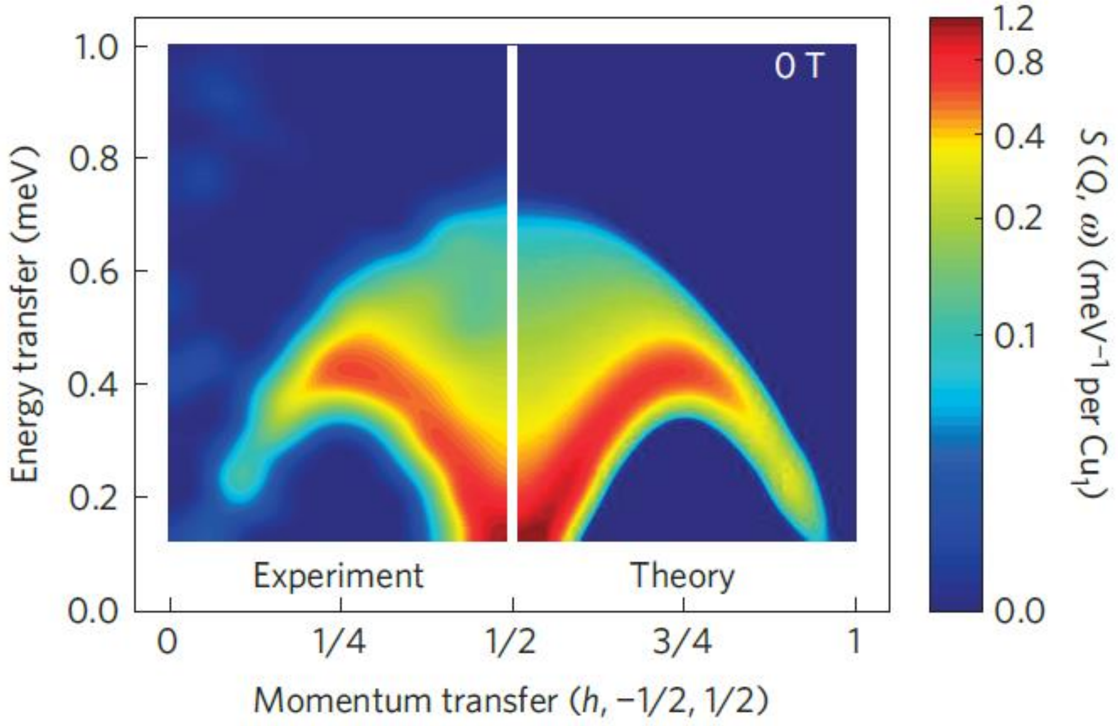
Eksperimentelt: Systemet er polariseret og ligner en ferromagnet

Nu forventer vi at de magnetiske eksitationer er spinbølger

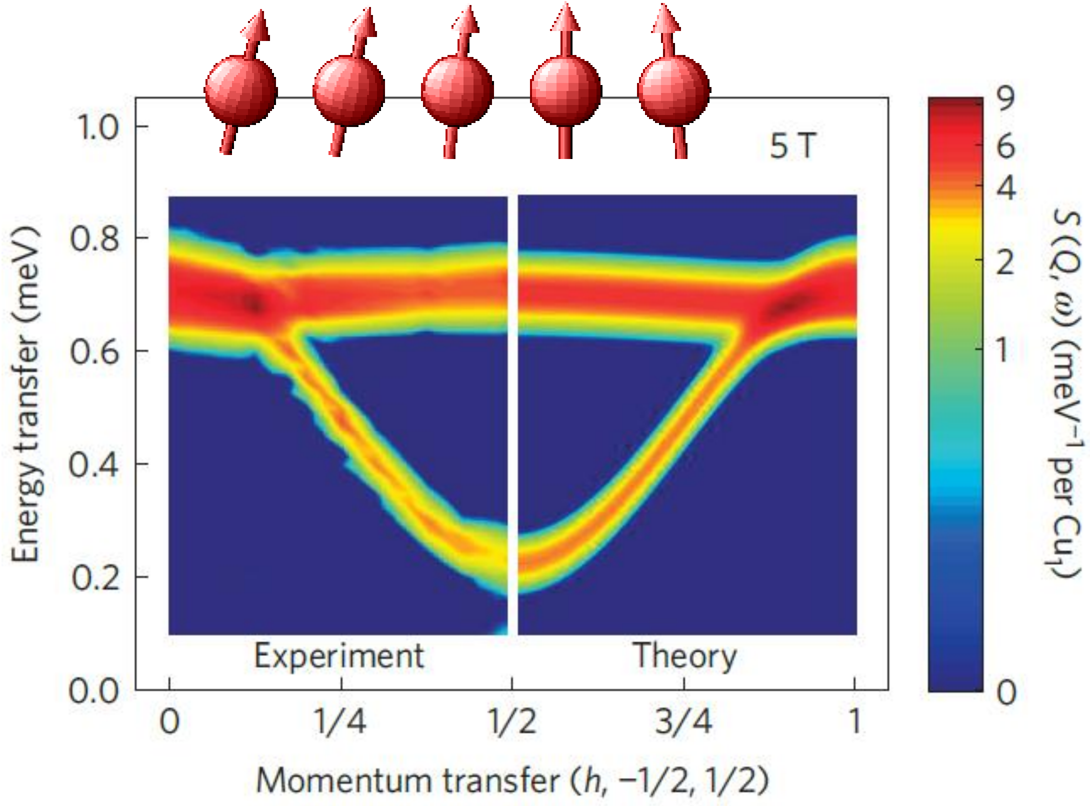


Eksempel 4
Magnetisk dynamik ved 50 milli-Kelvin

”Entanglement spektrum” - kontinuum



Klassiske eksitationer (spinbølger)



M. Mourigal et al, Nature Physics (2015)