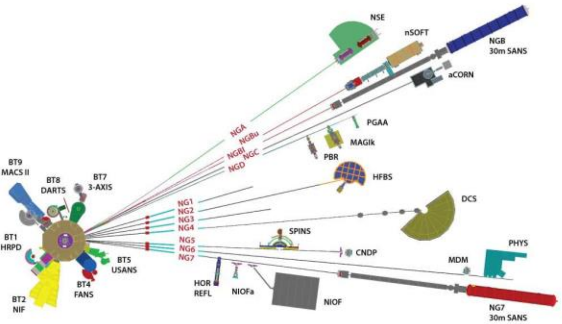
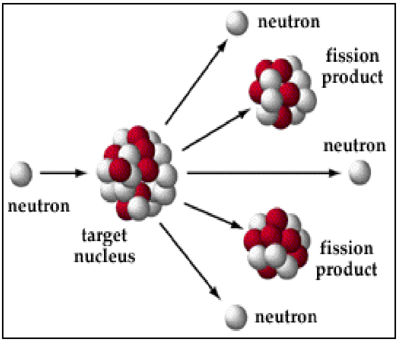
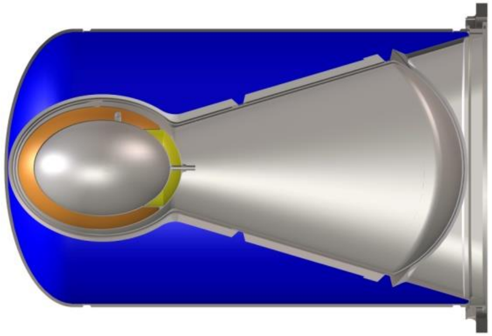


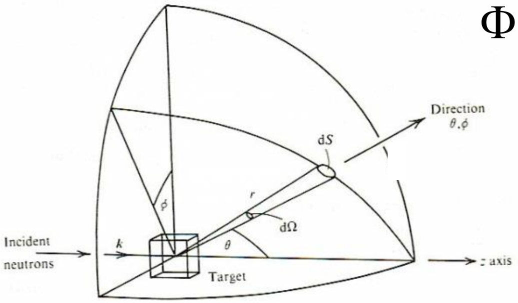
QuarkNet 2017
Johns Hopkins University

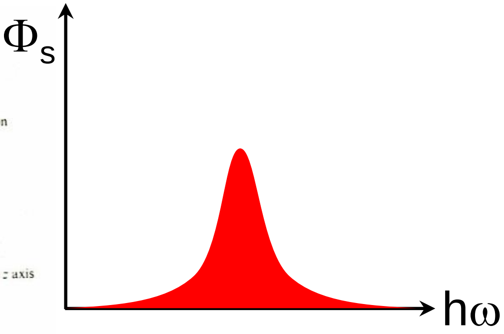
Using Neutrons to Study Quasiparticle Physics in Materials Science

Peter M. Gehring
National Institute of Standards and Technology
NIST Center for Neutron Research
Gaithersburg, MD USA





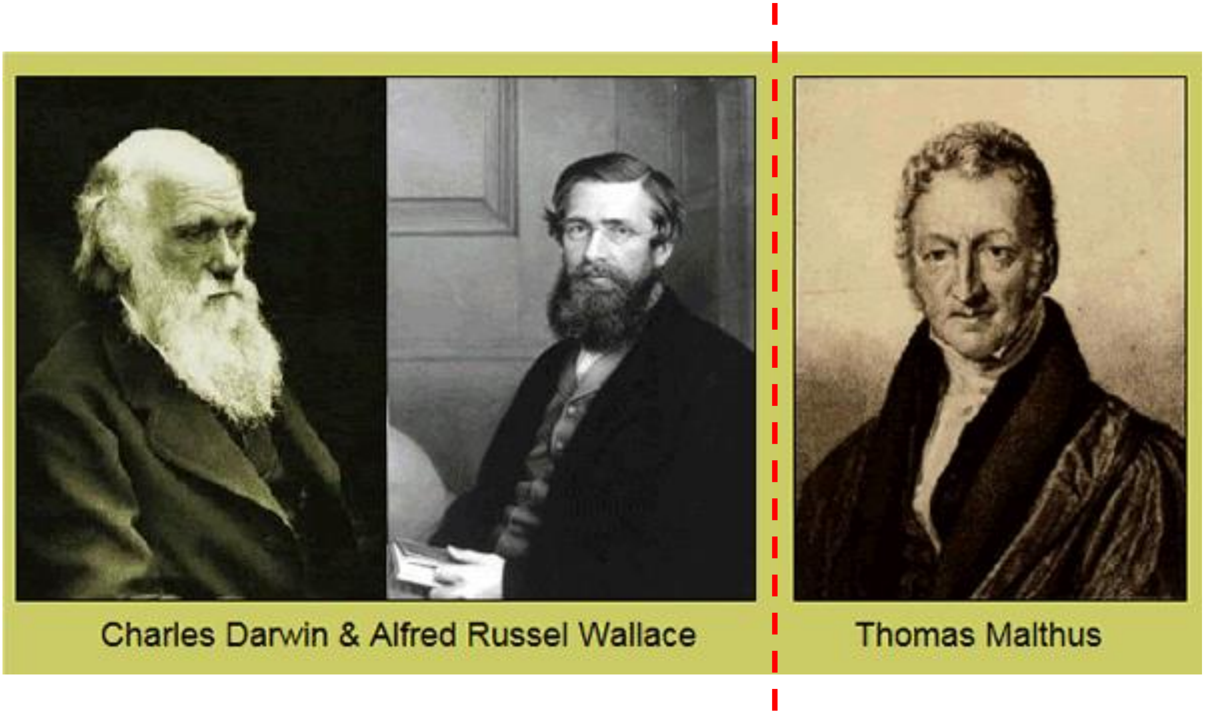




Seminal ideas in one field are often found/applied in others

Biology

Economics



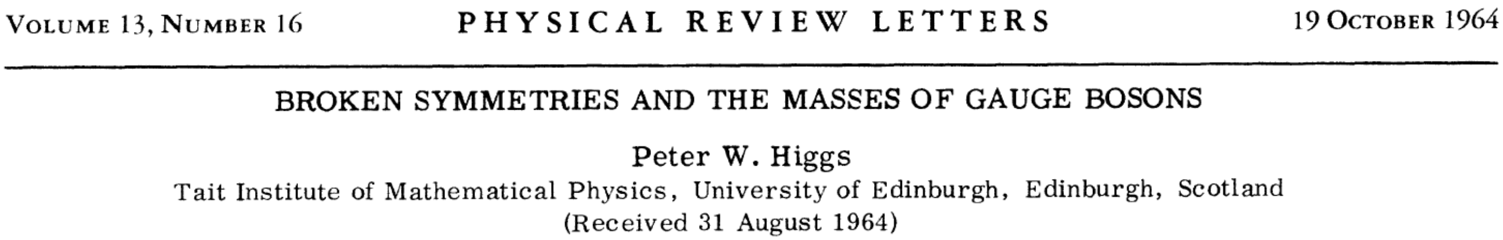
Charles Darwin & Alfred Russel Wallace

Thomas Malthus

Charles Darwin and Alfred Russel Wallace were influenced by British political economist Thomas Malthus (1766–1834). In his 1798 book “Essay on the Principle of Population,” Malthus argued that human reproduction grows geometrically, far out-pacing available resources. Individuals must compete for resources to survive.

Both Darwin and Wallace incorporated this idea as part of natural selection.

Higgs Boson: An idea from condensed matter physics!



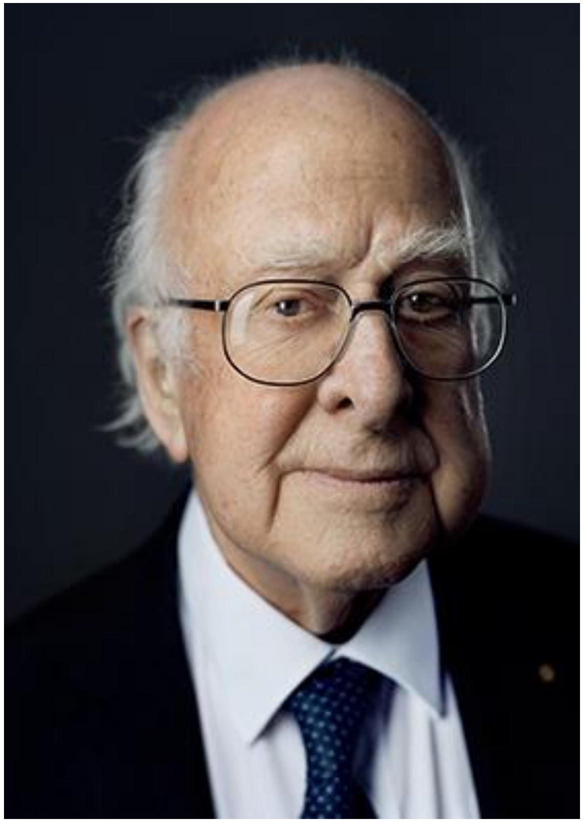
VOLUME 13, NUMBER 16 PHYSICAL REVIEW LETTERS 19 OCTOBER 1964

BROKEN SYMMETRIES AND THE MASSES OF GAUGE BOSONS

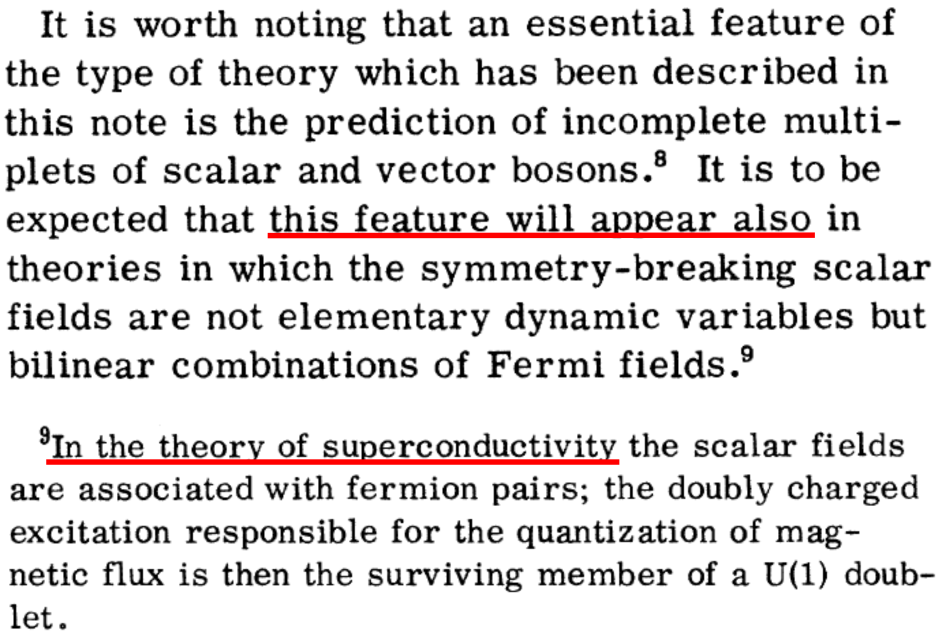
Peter W. Higgs
Tait Institute of Mathematical Physics, University of Edinburgh, Edinburgh, Scotland

(Received 31 August 1964)

2013 Nobel Laureate in Physics

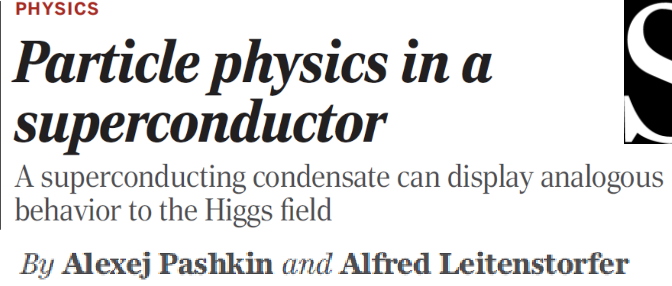


"... for the theoretical discovery of a mechanism that contributes to our understanding of the origin of mass of subatomic particles …"



It is worth noting that an essential feature of the type of theory which has been described in this note is the prediction of incomplete multiplets of scalar and vector bosons.[8] It is to be expected that this feature will appear also in theories in which the symmetry-breaking scalar fields are not elementary dynamic variables but bilinear combinations of Fermi fields.[9]

[9] In the theory of superconductivity the scalar fields are associated with fermion pairs; the doubly charged excitation responsible for the quantization of magnetic flux is then the surviving member of a U(1) doublet.



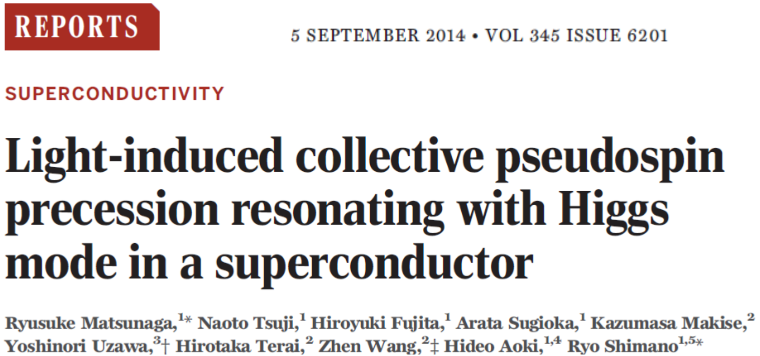
PHYSICS

Particle physics in a superconductor

A superconducting condensate can display analogous behavior to the Higgs field

By Alexej Pashkin and Alfred Leitenstorfer

Science



REPORTS

5 SEPTEMBER 2014 • VOL 345 ISSUE 6201

SUPERCONDUCTIVITY

Light-induced collective pseudospin precession resonating with Higgs mode in a superconductor

Ryusuke Matsunaga,[1*] Naoto Tsuji,[1] Hiroyuki Fujita,[1] Arata Sugioka,[1] Kazumasa Makise,[2] Yoshinori Uzawa,[3†] Hirotaka Terai,[2] Zhen Wang,[2‡] Hideo Aoki,[1,4] Ryo Shimano[1,5*]

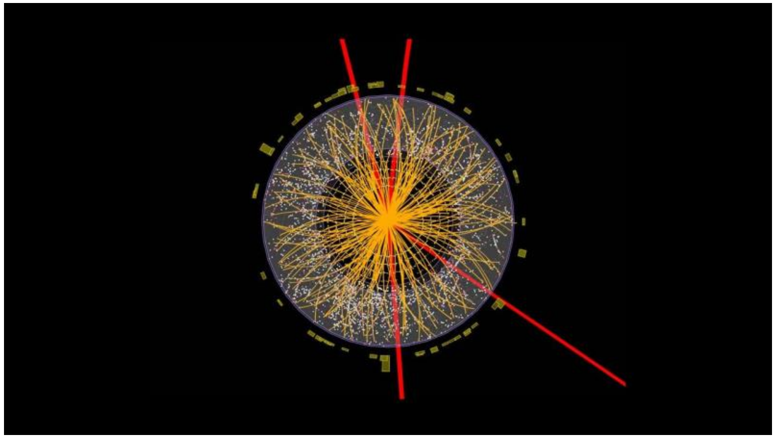
Daily News - 5 September 2014
Mother of Higgs boson found in superconductors
By Michael Slezak

“The Higgs field, which gives rise to its namesake boson, is credited with giving other particles mass by slowing their movement through the vacuum of space. First proposed in the 1960s, the particle finally appeared at the Large Hadron Collider at CERN near Geneva, Switzerland, in 2012, and some of the theorists behind it received the 2013 Nobel prize in physics.

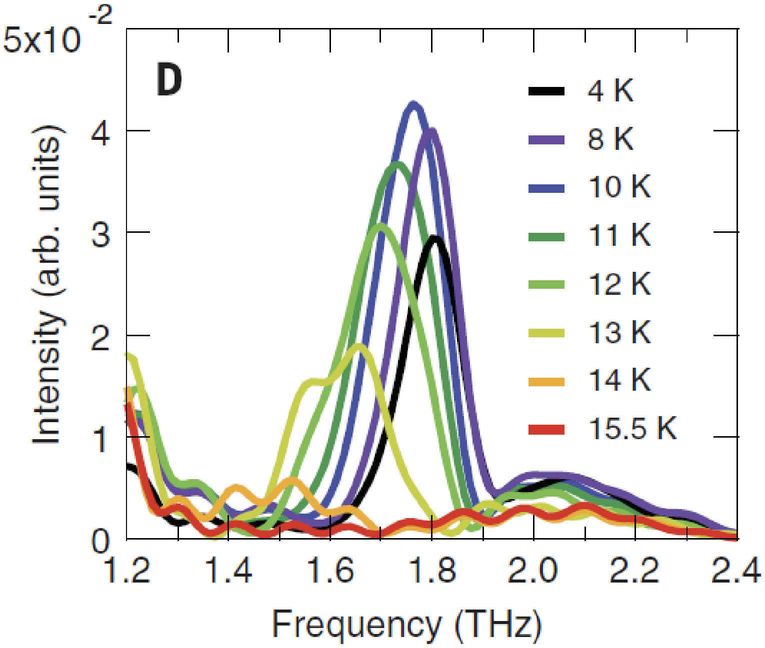
But the idea was actually borrowed from the behaviour of photons in superconductors, metals that, when cooled to very low temperatures, allow electrons to move without resistance. Near zero degrees kelvin, vibrations are set up in the superconducting material that slow down pairs of photons travelling through, making light act as though it has a mass.

‘Those vibrations are the mathematical equivalent of Higgs particles,’ says Ryo Shimano at the University of Tokyo, who led the team that made the new discovery. The superconductor version explains the virtual mass of light in a superconductor, while the particle physics Higgs field explains the mass of W and Z bosons in the vacuum.”(Matsunaga *et al*., Science Vol. 345, pp. 1145 (2014).)

One idea covers vastly different energy scales

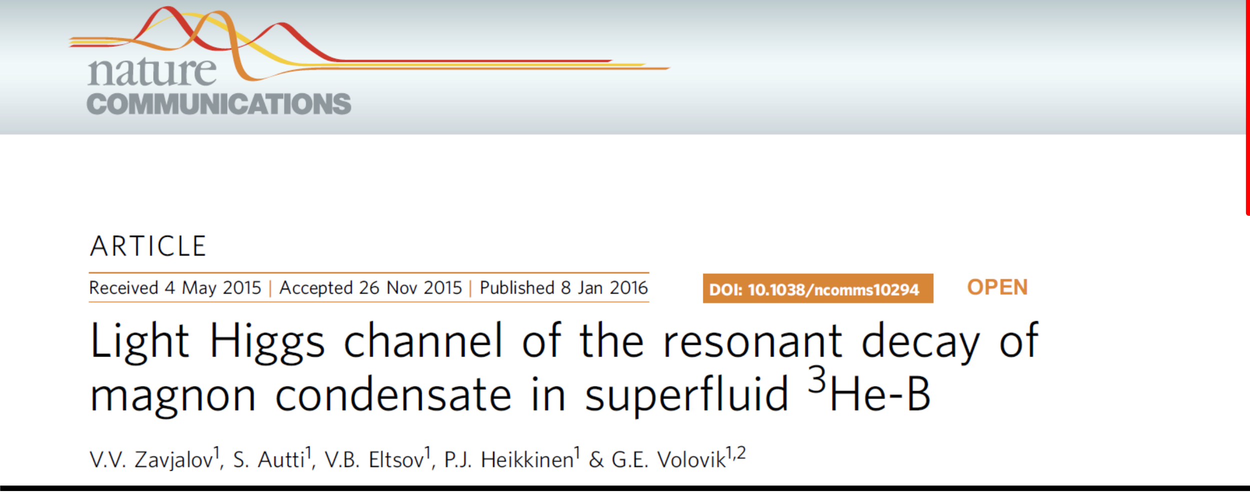


LHC:
Higgs Boson
E ≈ 10^{11} eV



Superconductor:
Higgs Boson
E ≈ 10^{-3} eV

Recent work on superfluid Helium-3 may guide future research on Higgs boson.



nature COMMUNICATIONS

ARTICLE

Received 4 May 2015 | Accepted 26 Nov 2015 | Published 8 Jan 2016 DOI: 10.1038/ncomms10294 OPEN

Light Higgs channel of the resonant decay of magnon condensate in superfluid ^{3}He-B

V.V. Zavjalov[1], S. Autti[1], V.B. Eltsov[1], P.J. Heikkinen[1] & G.E. Volovik[1,2]

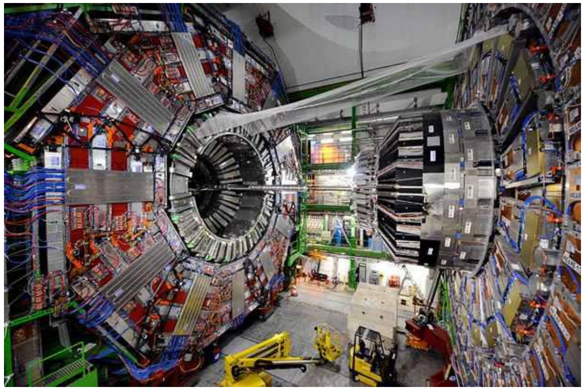
In 2012, a proposed observation of the Higgs boson was reported at the Large Hadron Collider in CERN. The observation has puzzled the physics community, as the mass of the observed particle, 125 GeV, looks lighter than the expected energy scale, about 1 TeV.

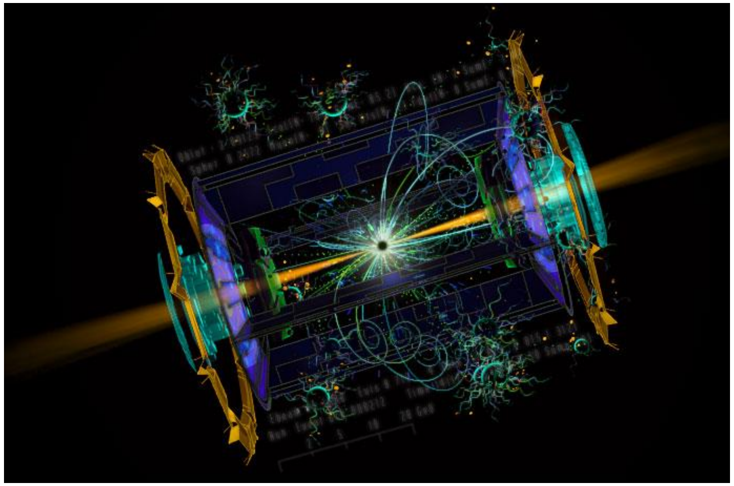
Researchers at Aalto University in Finland now propose that there is more than one Higgs boson, and they are much heavier than the 2012 observation.

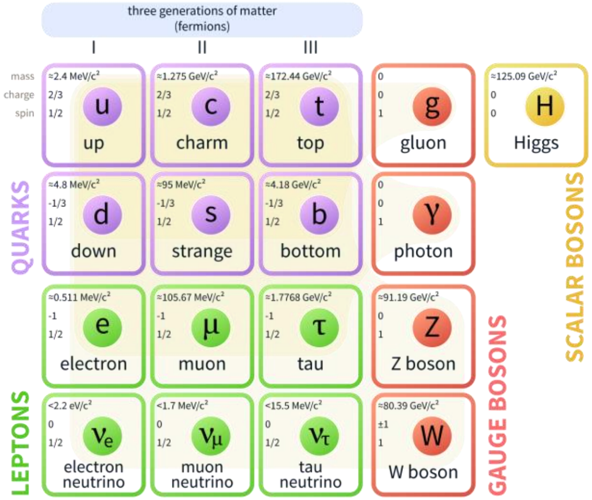
"Our recent ultra-low temperature experiments on superfluid helium (^{3}He) suggest an explanation why the Higgs boson observed at CERN appears to be too light. By using the superfluid helium analogy, we have predicted that there should be other Higgs bosons, which are much heavier (about 1 TeV) than previously observed," says Professor (emeritus) Volovik.

Understanding our universe in terms of particles

1 Determine the fundamental particles that form the Universe.





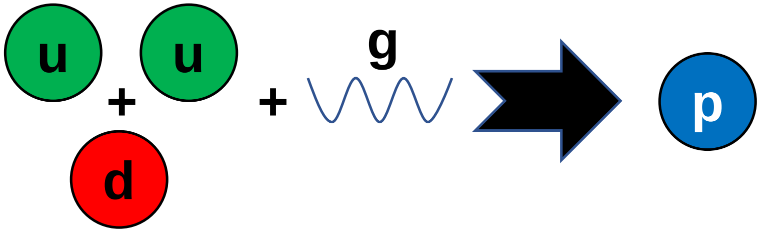


Standard Model of Elementary Particles

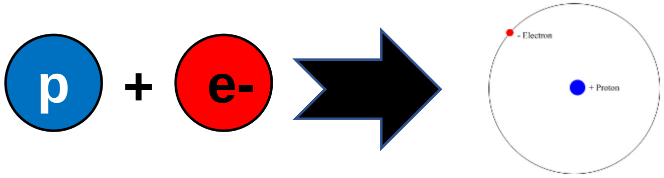
	three generations of matter (fermions)				
	I	II	III		
mass charge spin	≈2.4 MeV/c² 2/3 1/2 u up	≈1.275 GeV/c² 2/3 1/2 c charm	≈172.44 GeV/c² 2/3 1/2 t top	0 0 1 g gluon	≈125.09 GeV/c² 0 0 H Higgs
QUARKS	≈4.8 MeV/c² -1/3 1/2 d down	≈95 MeV/c² -1/3 1/2 s strange	≈4.18 GeV/c² -1/3 1/2 b bottom	0 0 1 γ photon	SCALAR BOSONS
	≈0.511 MeV/c² -1 1/2 e electron	≈105.67 MeV/c² -1 1/2 μ muon	≈1.7768 GeV/c² -1 1/2 τ tau	≈91.19 GeV/c² 0 1 Z Z boson	
LEPTONS	<2.2 eV/c² 0 1/2 ν_e electron neutrino	<1.7 MeV/c² 0 1/2 ν_μ muon neutrino	<15.5 MeV/c² 0 1/2 ν_τ tau neutrino	≈80.39 GeV/c² ±1 1 W W boson	GAUGE BOSONS

Understanding our universe in terms of particles

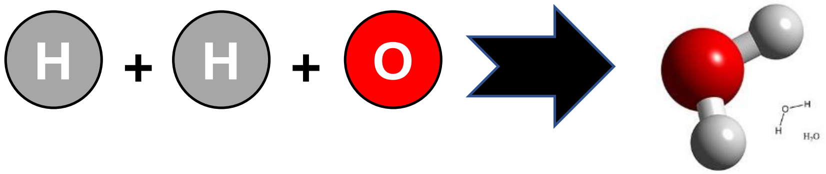
② Study the ways that particles can be “put together.”



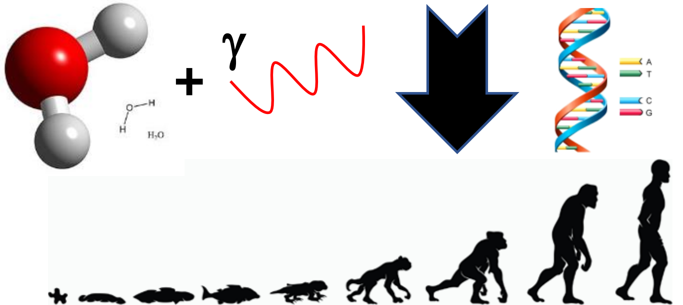
Nuclear Physics



Chemistry



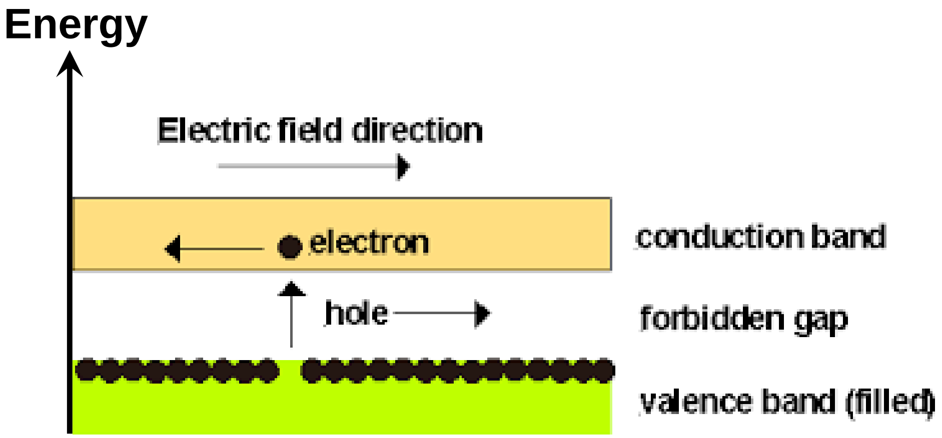
Biology



Particle Physics

Understanding our universe in terms of particles

3 Study how particles behave in new environments.

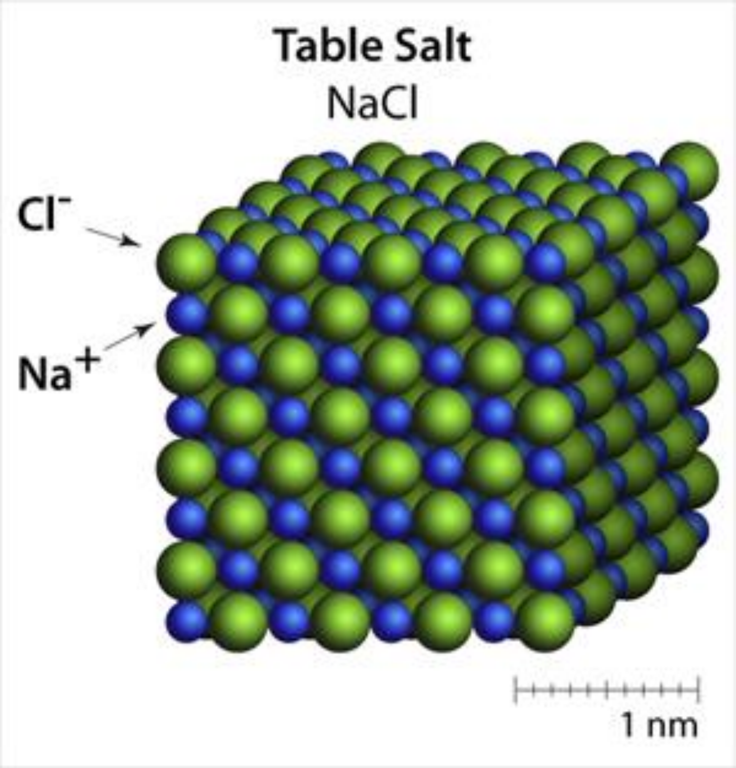


Conduction via electrons & holes in a semiconductor

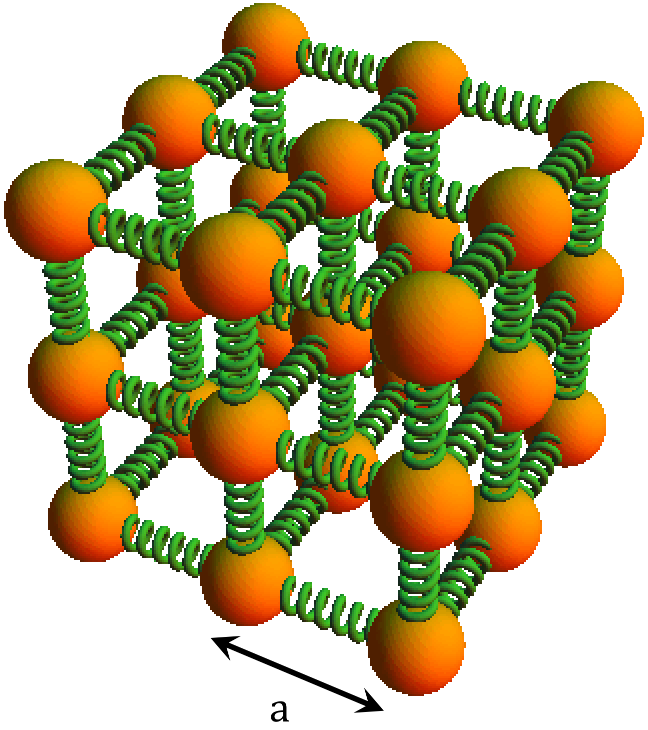
The aggregate motion of the electrons in the valence band of a semiconductor is the same *as if* the material instead contained positively charged quasiparticles called “holes.”

Concept of particles can be generalized to quasiparticles
to help us understand many properties of solids

Consider a crystal that contains
Avogadro's number of atoms (6 x 10^{23})

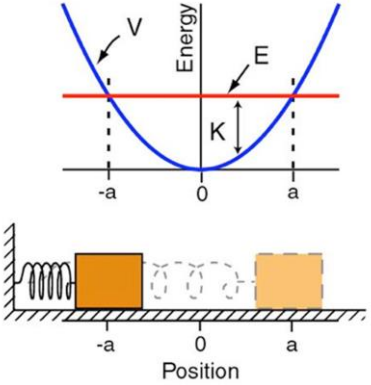


Atoms sit on a periodic lattice, forming
bonds represented below by springs



How can we keep track of so many atoms?

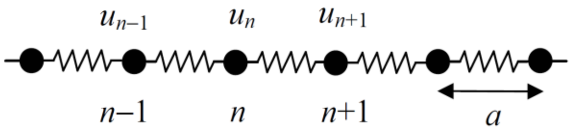
Classical Approach



Assume a simple interatomic potential: $V(x) = \frac{1}{2}Cx^2$

$$-\frac{dV}{dx} = F = Cx$$

Solve equations of motion in 1-dimension: $\sum F = Ma$



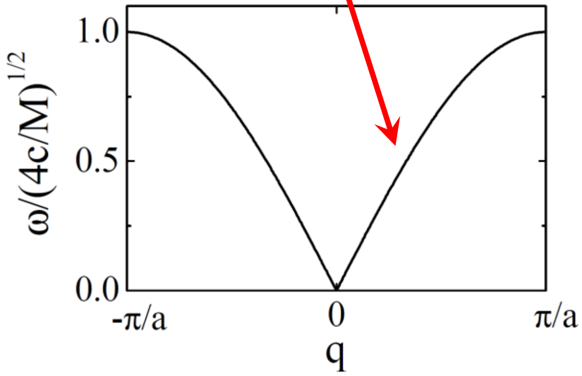
$$M\ddot{u}_n = C(u_{n+1} - u_n) - C(u_n - u_{n-1})$$

Traveling wave solutions: $u_n(t) = Ae^{-i(qna-\omega t)}$

$$\omega(q) = \sqrt{4C/M}|\sin qa/2|$$

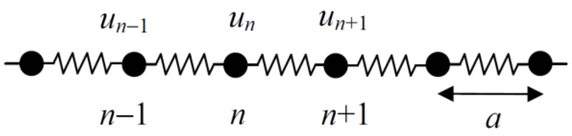
Dispersion relation

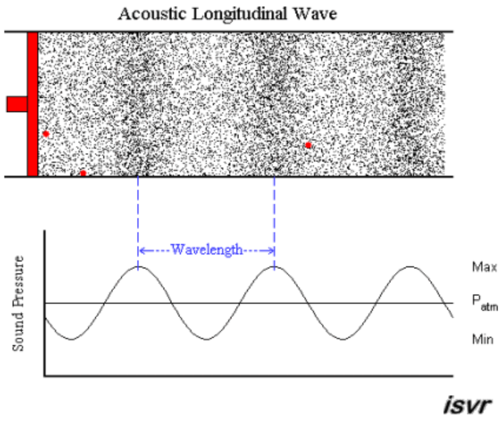
The Phonon Quasiparticle!



How can we keep track of so many atoms?

Solutions in 1-dimension are longitudinal waves (acoustic)



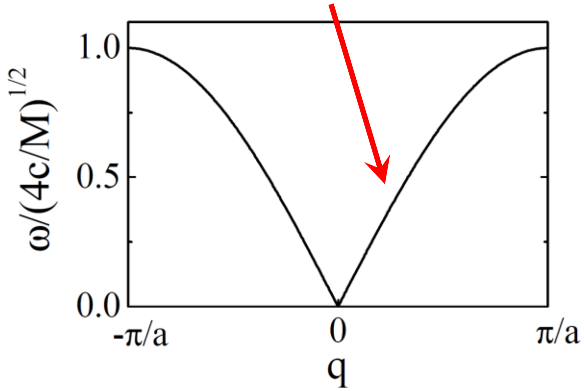


For large wavelengths:

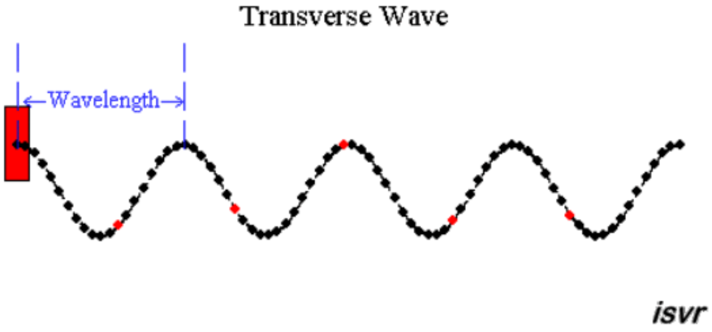
$$\omega(q) = a\sqrt{C/M}q$$

Limiting slope as $q \to 0$
gives the speed of sound.

Acoustic Phonon



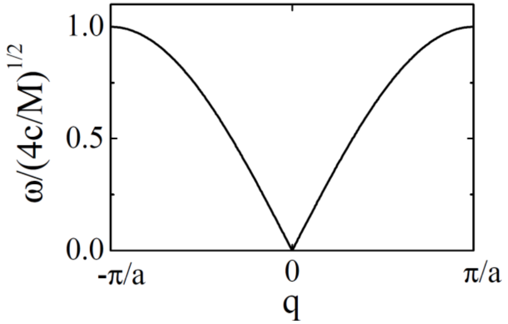
Solutions in > 1 dimensions also admit transversely polarized waves.



Beyond 1 dimension and one type of atom

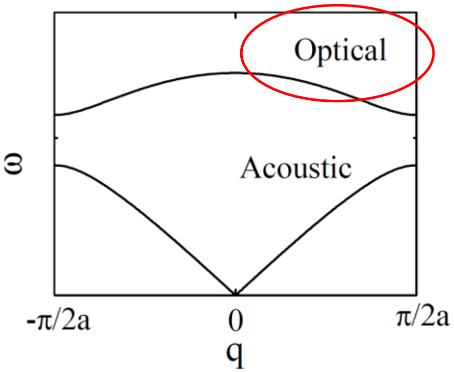
Identical atoms of mass M in 1 dimension:

$$\omega(q) = \sqrt{4C/M}\,|\sin qa/2|$$

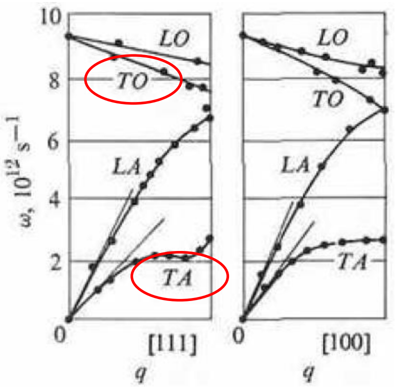


Two atoms (mass M_1 and M_2) in 1 dimension:

$$\omega^2 = C\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \pm C\sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4\sin^2 qa}{M_1 M_2}}$$

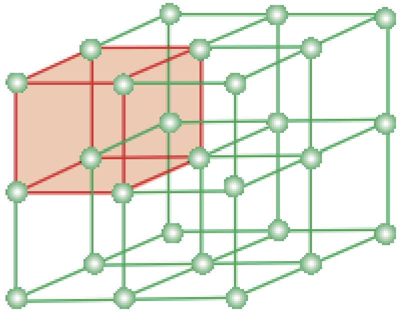


A real material – germanium (3 dimensions):



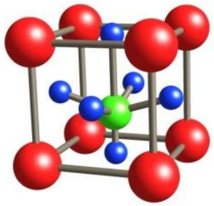
Beyond 1 dimension and one type of atom

Unit cell = smallest "building block" that can be used to generate a crystal lattice.



Given p distinct atoms in a unit cell of a crystal there will be 3 acoustic modes and 3p - 3 optical modes.

<u>Example</u>: PbTiO$_3$, a very famous perovskite material (a ferroelectric).
5 atoms / unit cell → 3 acoustic modes + 12 optical modes = 15 total.

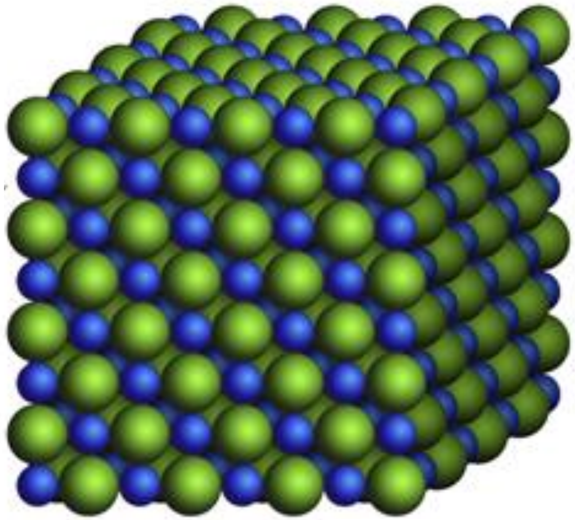


KEY POINT: The quasiparticle concept can be used to reduce a system with 6x10^{23} atoms to just a few non-interacting phonons.

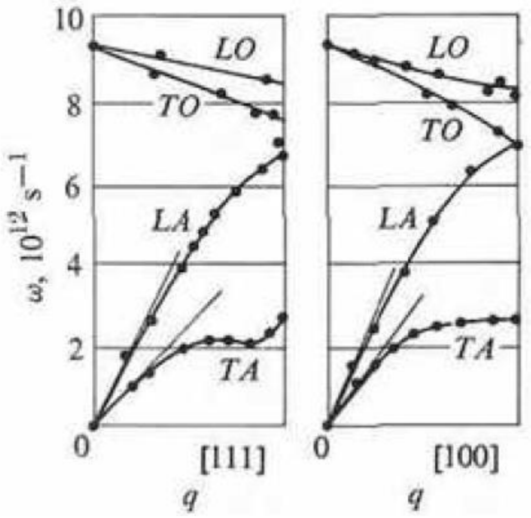
Mini-Summary

The quasiparticle concept is fundamental to condensed matter physics because it is one of the few known ways of simplifying the quantum mechanical many-body problem.

6×10^{23} atoms



A few phonons



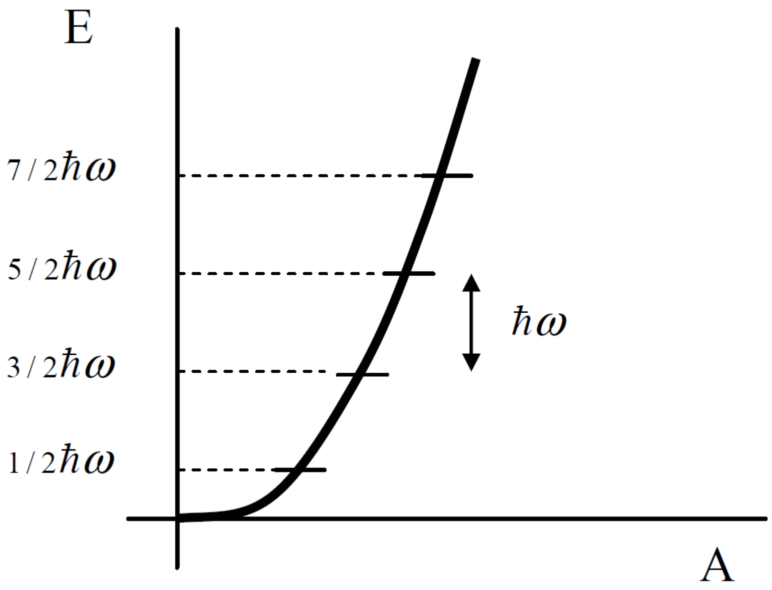
Quasiparticles are emergent phenomena that occur when a microscopically complicated system such as a solid behaves *as if* it contained different weakly interacting particles in free space.

Cannot exist in a vacuum.

So where is the quantum nature?

The energy levels of a quantum harmonic oscillator are quantized:

$$\boxed{E = \frac{1}{2}(n+1)h\omega}$$



If we equate this with the average energy of the phonon we obtain

$$\boxed{E = \frac{1}{2}MA^2\omega^2 = \frac{1}{2}(n+1)h\omega}$$

Classically any amplitude is allowed.
Here the phonon amplitude is quantized.

The Phonon Quasiparticle

Igor Tamm: 8 July 1895 – 12 April 1971. A Soviet physicist who received the 1958 Nobel Prize in Physics, jointly with Pavel Cherenkov and Ilya Frank, for their 1934 discovery of Cherenkov radiation.

A fascinating series of letters posted online by CERN, between Igor Tamm and Paul Dirac in the 1930's, indicate that Tamm "introduced the notion of quanta of elastic oscillations later called 'phonons'" in a 1930 letter to Dirac. This adds credibility to the 1929 date from the Russia stamp, as it's likely he would have mulled the concept over before discussing it with his European colleague.

Phonons are fundamental to many properties of materials

Velocity of sound

Conduction of heat

Heat capacity

Thermal expansion

Superconductivity (BCS)

Ferroelectricity

Structural phase transitions

But a harmonic potential leads to unphysical behavior

Velocity of sound – OK

Conduction of heat – Infinite

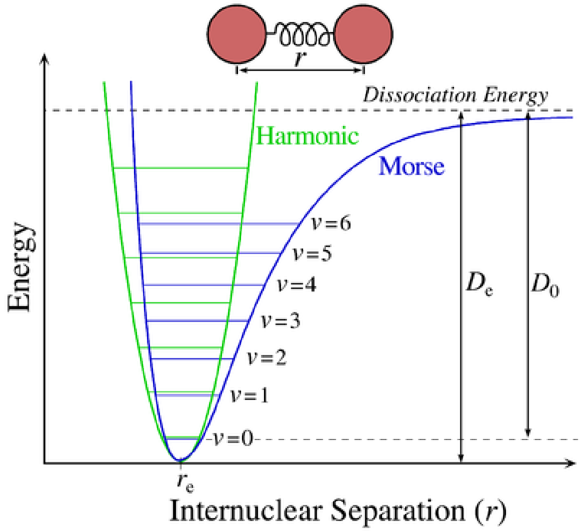
Heat capacity – OK

Thermal expansion – Zero

Superconductivity (BCS) – Not possible

Ferroelectricity – Not possible

Structural phase transitions – Not possible



$$V(x) = \frac{1}{2}Cx^2 + \underbrace{x^3 + \cdots}$$

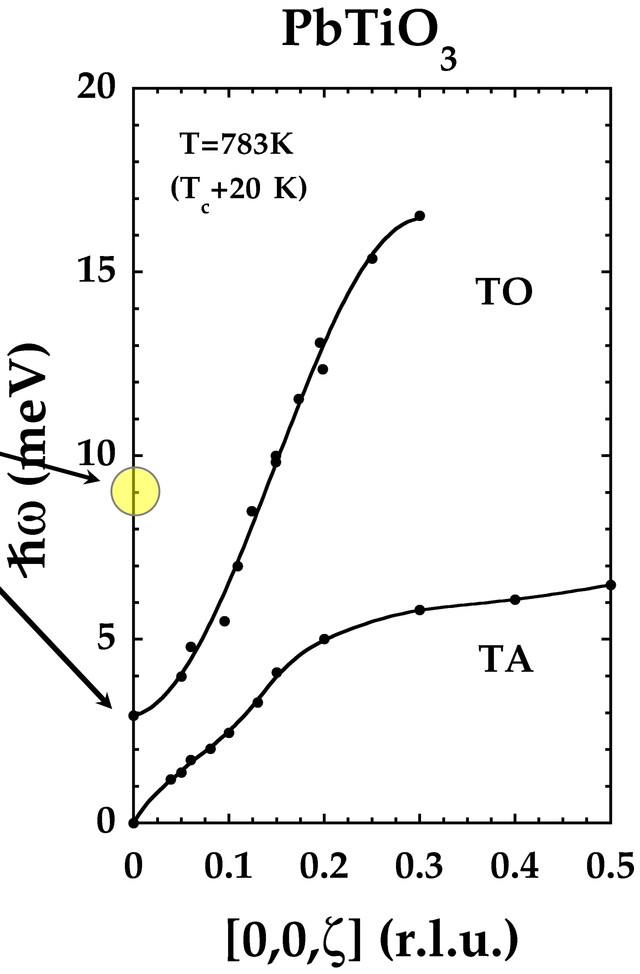
Need anharmonicity!

Most “famous” phonon: The soft mode

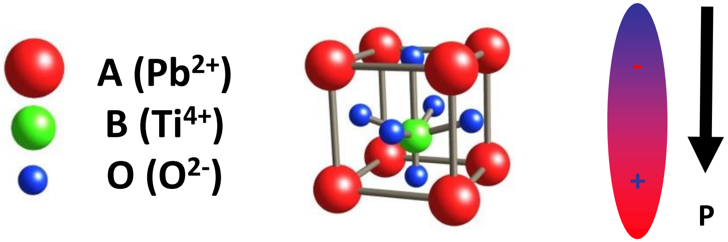
In $PbTiO_3$ a cubic to tetragonal structural phase transition takes place at T_c = 763K.

The lowest-lying TO phonon frequency $h\omega_{TO} \rightarrow 0$ as $T \rightarrow T_c$.

This is a phonon instability known as a “soft mode,” and is typical of displacive ferroelectrics.



Shirane *et al.*,
Phys. Rev. B **2**, 155 (1970)



What about other quasiparticles?

Magnon (aka spin waves) – magnetic analogue of a phonon

Hole – an electron vacancy

Polaron – an electron moving in a dielectric (larger effective mass)

Polariton – a photon moving in a material (e.g. superconductor)

Exciton – a bound electron hole pair

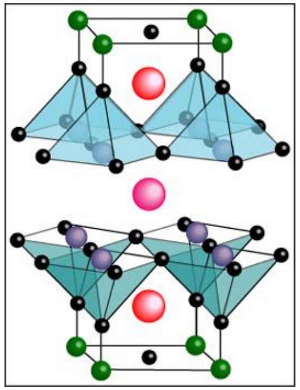
Plasmon – local oscillation of charge density

Many, many more … !

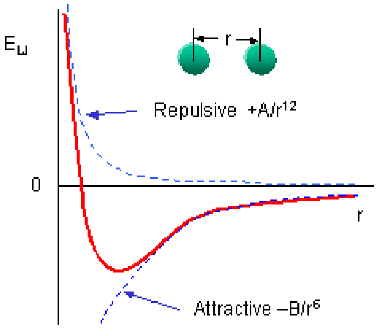
How do we measure quasiparticles?

Why do we / how can we study quasiparticles?

The most important property of any material is its underlying atomic / molecular structure (structure dictates function).



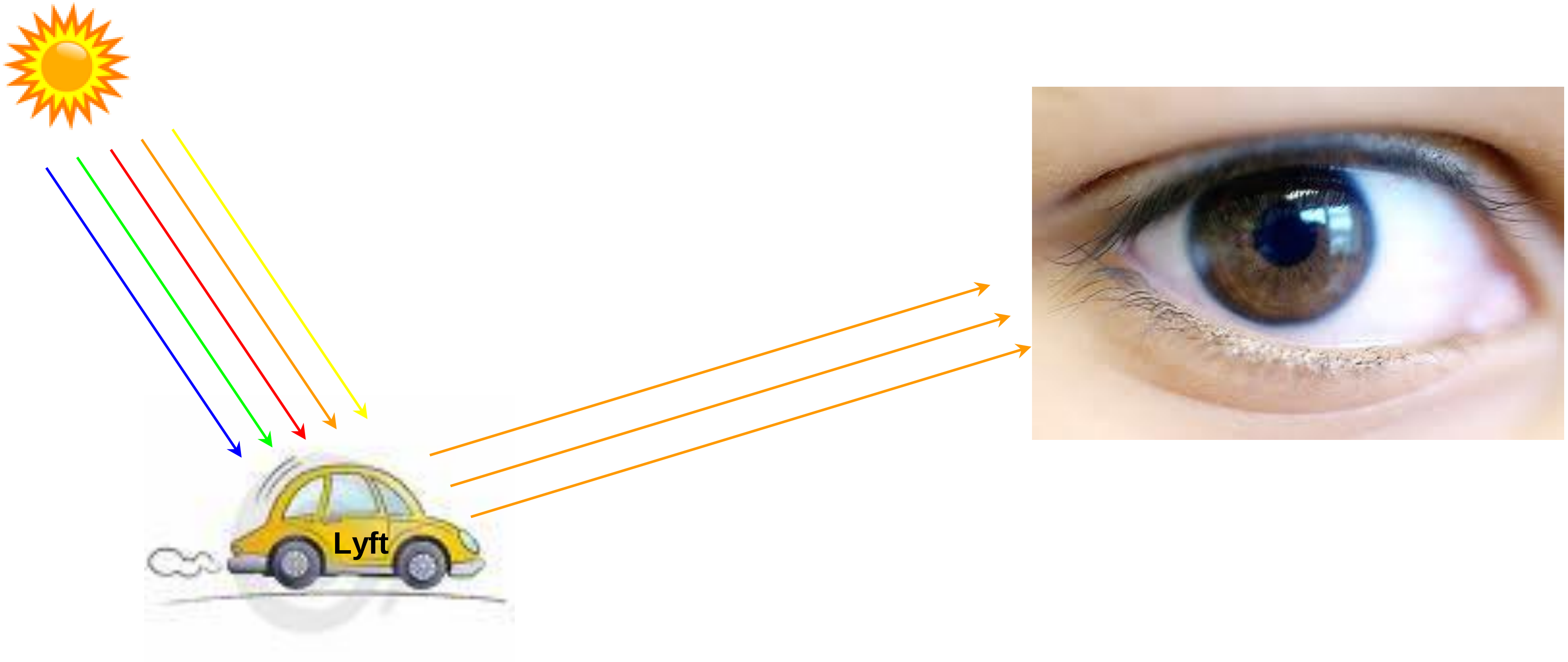
$Bi_2Sr_2CaCu_2O_{8+\delta}$



The motions of the atoms (dynamics) are extremely important because they provide information about the interatomic potentials.

An ideal method of characterization would provide detailed information about <u>both</u> structure and dynamics.

Why do we / how can we study quasiparticles?



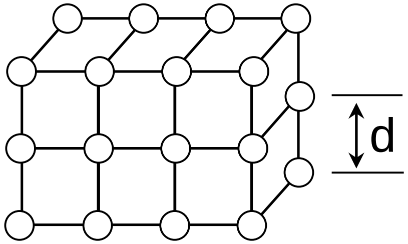
- We see something when light scatters from it. → Thus scattering conveys information!
- Light is composed of electromagnetic waves. → $\lambda \sim 4000$ A – 7000 A
- However, the details of what we can see are ultimately limited by the wavelength.

Why do we / how can we study quasiparticles?

The tracks of a compact disk act as a diffraction grating, producing a separation of the colors of white light when it scatters from the surface.

From this one can determine the nominal distance between tracks on a CD, which is 1.6×10^{-6} meters = 16,000 Angstroms.

To characterize materials we must determine the underlying structure. We do this by using the material as a diffraction grating.



Problem: Distances between atoms in materials are of order Angstroms → light is inadequate. Moreover, most materials are opaque to light.

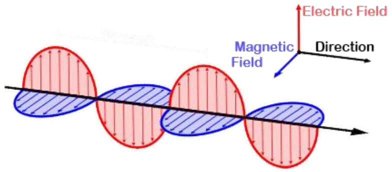
$\lambda_{\text{Light}} >> d \sim 4$ Å

Scattering Probes

Need a probe with λ≈ length scale of interest

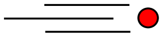
Some candidates …

X rays



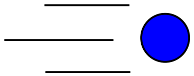
EM - wave

Electrons



Charged particle

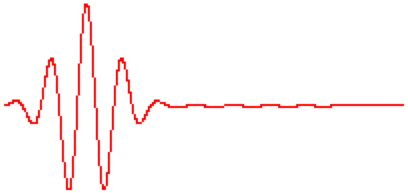
Neutrons



Neutral particle

1929 Nobel Laureate
in Physics

Remember de Broglie: $\lambda = h/p = h/mv$
Particles have wave properties too.



Scattering Probes

Pros and Cons …

Which one should we choose?

If we wish only to determine relative atomic positions, then we should choose x rays almost every time.

1. Relatively cheap

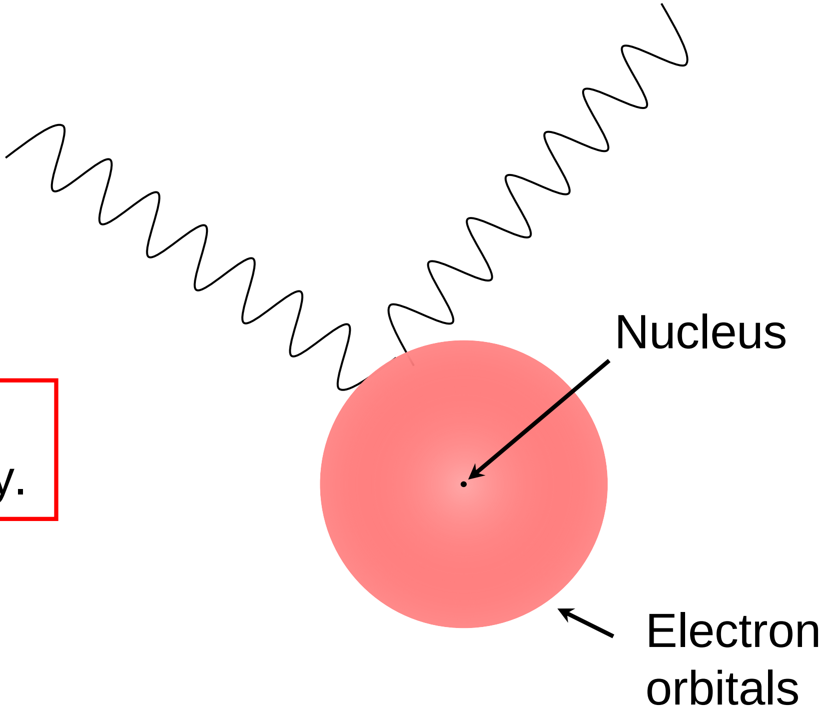
2. Sources are ubiquitous → easy access

3. High flux → can study small samples

However …

Scattering Probes

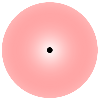
X rays are electromagnetic radiation.
Thus they scatter from the charge density.



Consequences:

Low-Z elements are hard to see.

Hydrogen



(Z = 1)

Elements with similar atomic numbers have very little contrast.

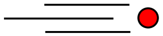
Cobalt Nickel

(Z = 27) (Z = 28)

X rays are strongly attenuated as they pass through the walls of furnaces, cryostats, etc.

Scattering Probes

What about electrons?



Electrons are charged particles → they see both the atomic electrons and nuclear protons at the same time.

1. Relatively cheap

2. Sources are not uncommon → easy access

3. Fluxes are extremely high → can study tiny crystals

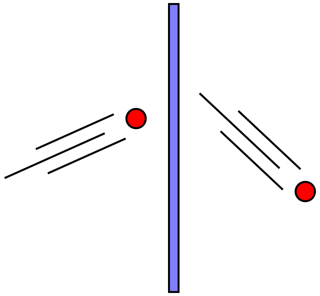
4. Very small wavelengths → more information

However …

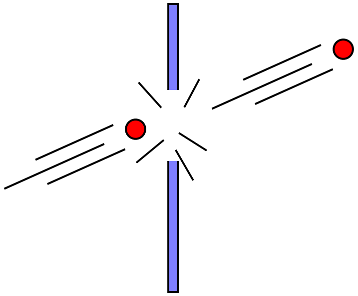
Scattering Probes

Electrons have some deficiencies too ...

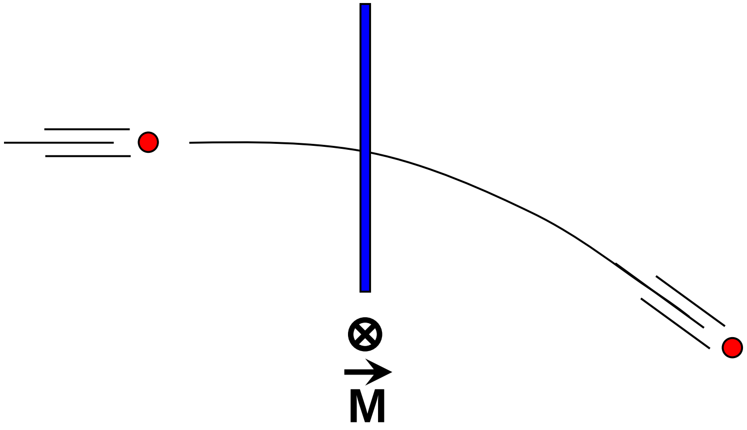
Requires very thin samples.



Radiation damage is a concern.

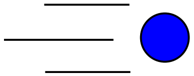


Magnetic structures are hard to determine because electrons are deflected by the internal magnetic fields.



Scattering Probes

What about neutrons?



Advantages

Wavelengths easily varied to match atomic spacings

Zero charge → not strongly attenuated by furnaces, etc.

Magnetic dipole moment → can study magnetic structures

Nuclear interaction → can see low-Z elements easily like H → good for the study of biomolecules and polymers.

Nuclear interaction is simple → scattering is easy to model

Low energies → Non-destructive probe

Disadvantages

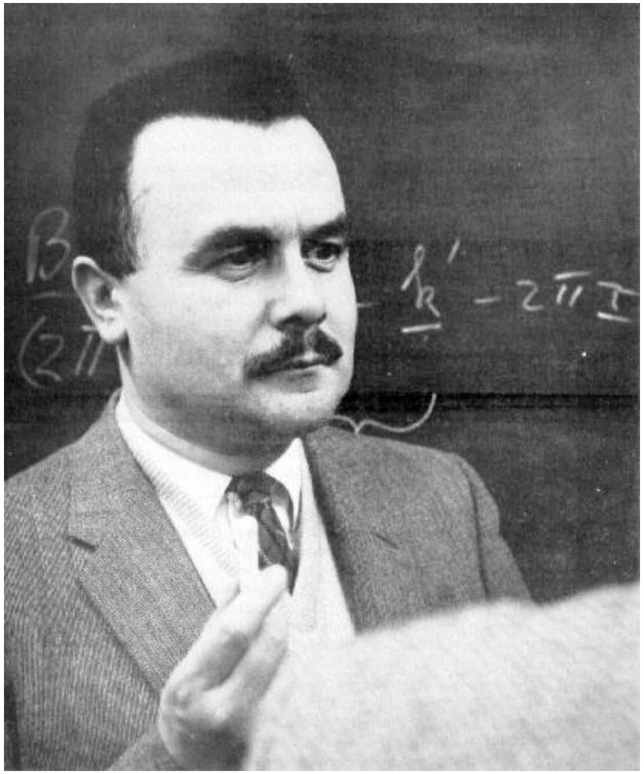
Neutrons expensive to produce → access not as easy

Interact weakly with matter → often require large samples

Available fluxes are low compared to those for x rays

Let’s consider neutrons …

The Neutron



“If the neutron did not exist, it would need to be invented.”

Bertram Brockhouse
1994 Nobel Laureate in Physics

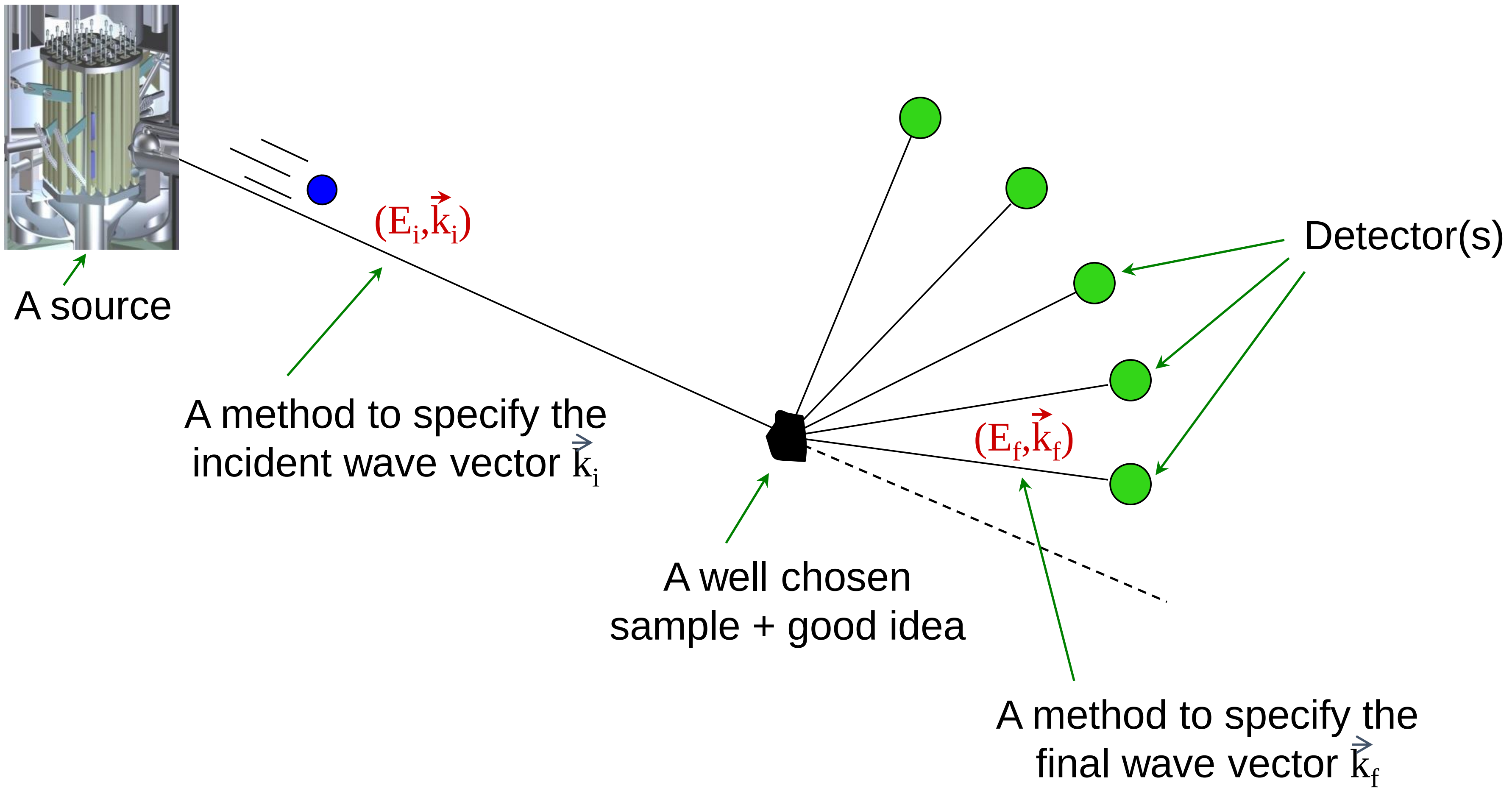
The Neutron

“… for the discovery of the neutron.”

Sir James Chadwick
1935 Nobel Laureate in Physics

Basics of Scattering

Elements of all scattering experiments



A source

$(E_i,\vec{k}_i)$

A method to specify the incident wave vector $\vec{k}_i$

A well chosen sample + good idea

Detector(s)

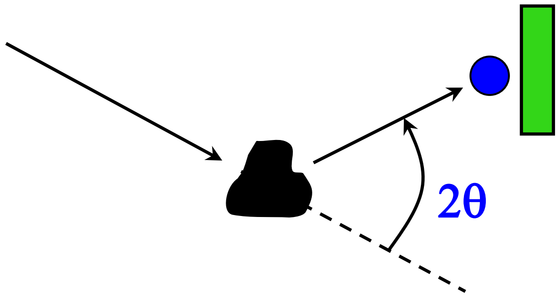
$(E_f,\vec{k}_f)$

A method to specify the final wave vector $\vec{k}_f$

Basics of Scattering

(1) Neutron scattering experiments measure the flux of neutrons scattered by a sample into a detector as a function of the change in neutron wave vector ($\vec{Q}$) and energy ($\hbar\omega$).

$$\Phi(Q,\hbar\omega) = \frac{\text{neutrons}}{\text{sec–cm}^2}$$



Momentum

$\hbar k = \hbar(2\pi/\lambda)$

$\hbar Q = \hbar\vec{k}_i - \hbar\vec{k}_f$

Energy

$\hbar\omega_n = \hbar^2 k_n{}^2/2m$

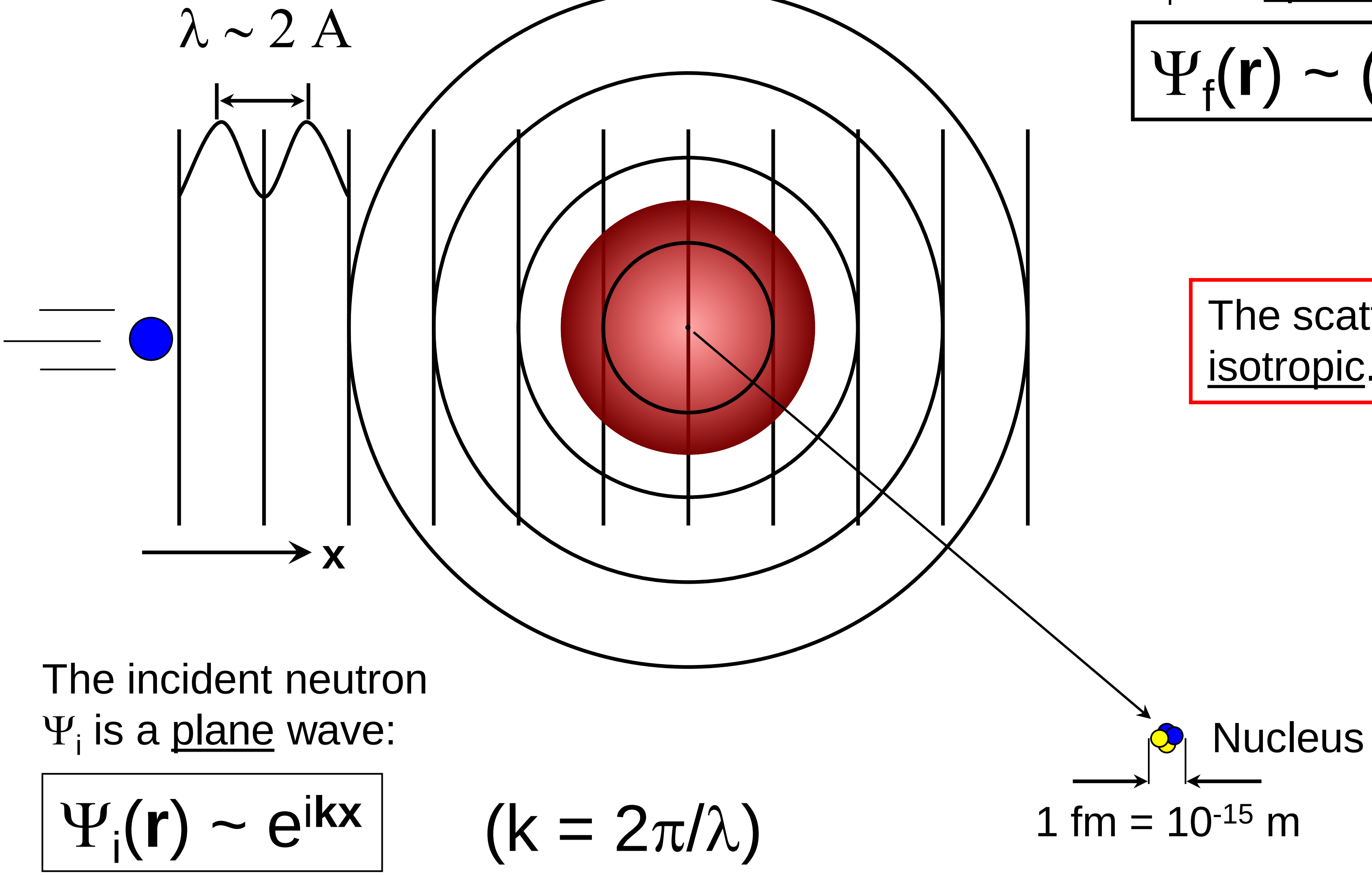
$\hbar\omega = \hbar\omega_i - \hbar\omega_f$

(2) The expressions for the scattered neutron flux Φ involve the positions and motions of atomic nuclei or unpaired electron spins.

Φ is important, as it provides information about <u>all</u> these quantities!

Nuclear Scattering

Consider the simplest case:
A fixed, isolated nucleus.



The scattered (final) neutron Ψ_f is a spherical wave:

$$\boxed{\Psi_f(\mathbf{r}) \sim (-b/r)e^{ikr}}$$

The scattering is isotropic. Why?

The incident neutron Ψ_i is a plane wave:

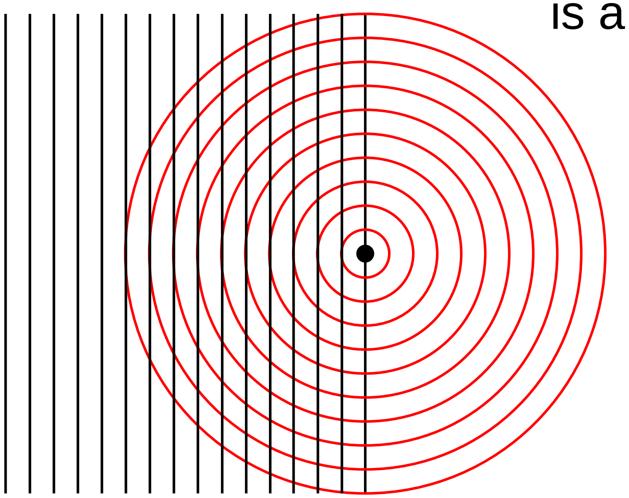
$$\boxed{\Psi_i(\mathbf{r}) \sim e^{ikx}}$$

$$(k = 2\pi/\lambda)$$

Nuclear Scattering

What if many atoms are present?

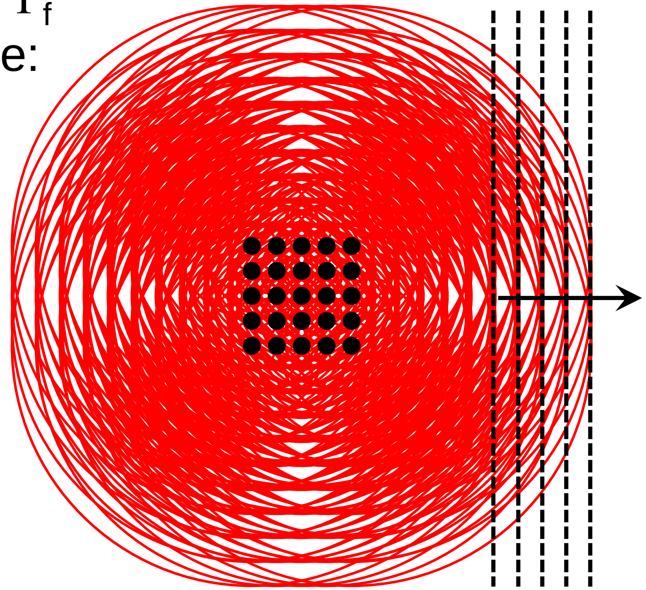
Scattering from one nucleus



Scattered neutron Ψ_f is a spherical wave:

The incident neutron Ψ_i is a plane wave:

Scattering from many nuclei



Get strong scattering in some directions, but not in others. Angular dependence yields information about how the nuclei are arranged or correlated.

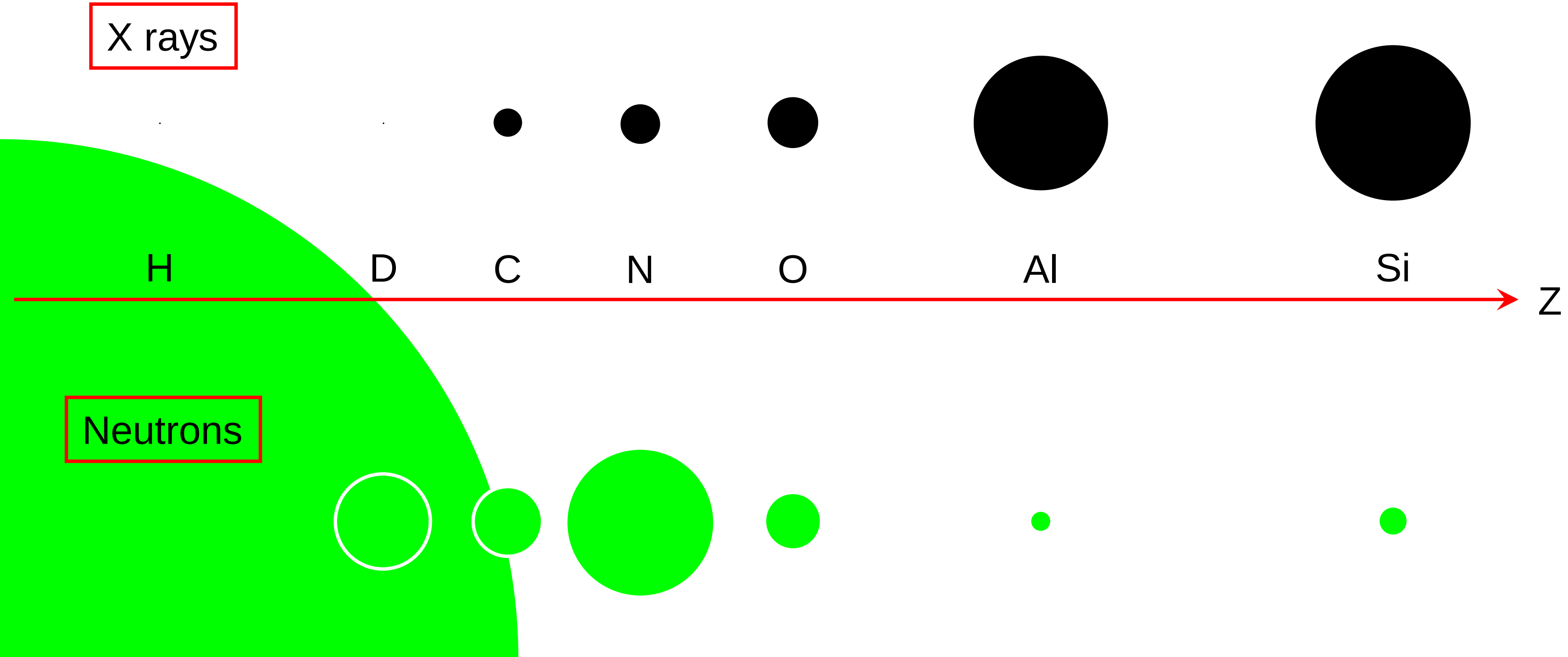
Nuclear Scattering

The Neutron Scattering Length - b

Units of length:
$b \sim 10^{-12}$ cm.

Varies randomly with Z and isotope
→ Neutrons "see" atoms x rays can't.

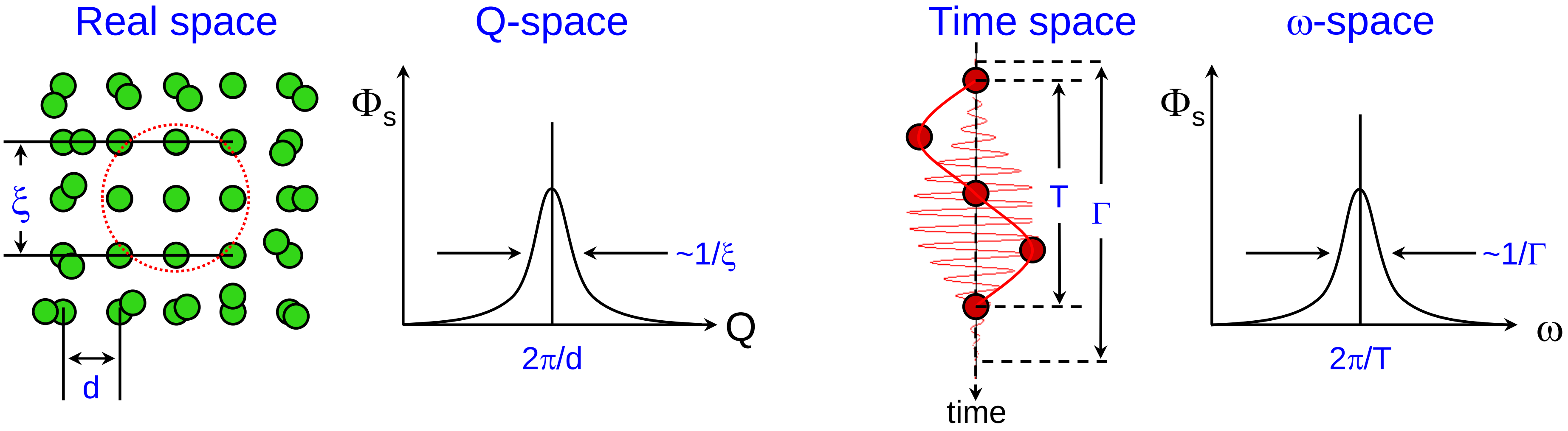
Total Scattering Cross Section: $\sigma = 4\pi b^2$



Correlation Functions

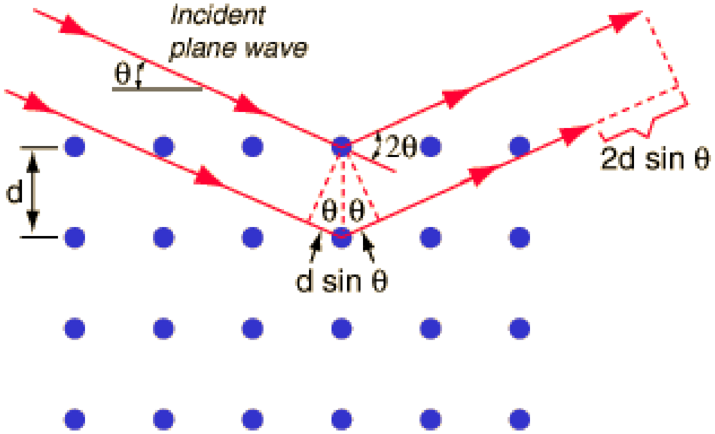
The scattered neutron flux $\Phi_s(\vec{Q},\hbar\omega)$ is proportional to the space ($\vec{r}$) and time (t) Fourier transform of the probability $G(\vec{r},t)$ of finding an atom at ($\vec{r}$,t) given that there is another atom at r = 0 at time t = 0.

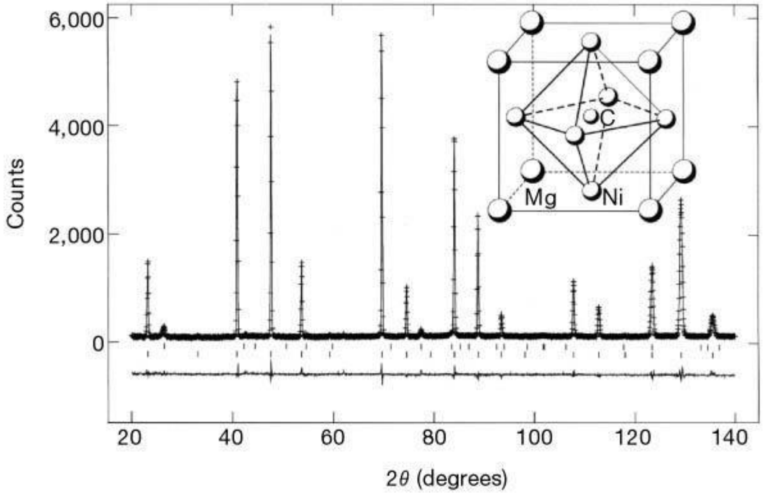
$$\Phi_s \propto \frac{\partial^2\sigma}{\partial\Omega\,\partial\omega} \propto \iint e^{i(\vec{Q}\cdot\vec{r}-\omega t)}\,G(\vec{r},t)\,d^3\vec{r}\,dt$$

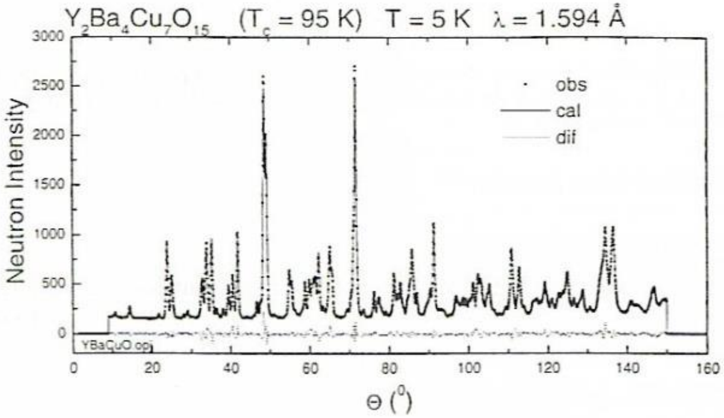


Nuclear Scattering

Neutron diffraction → Crystal structure





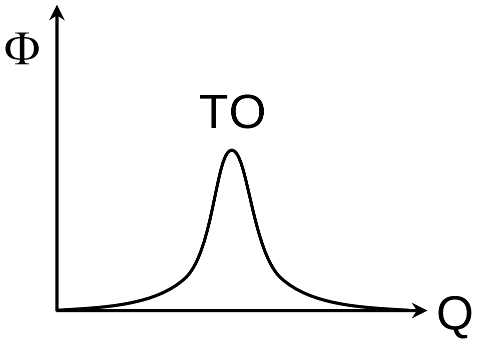


Nuclear Scattering

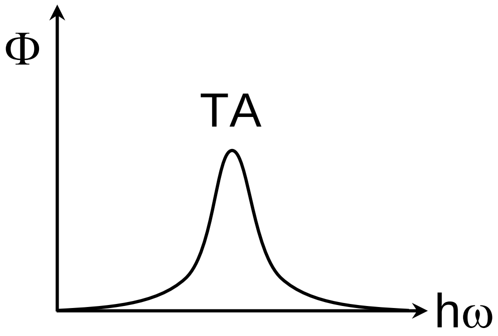
Neutron inelastic scattering → Dynamics (Quasiparticles)

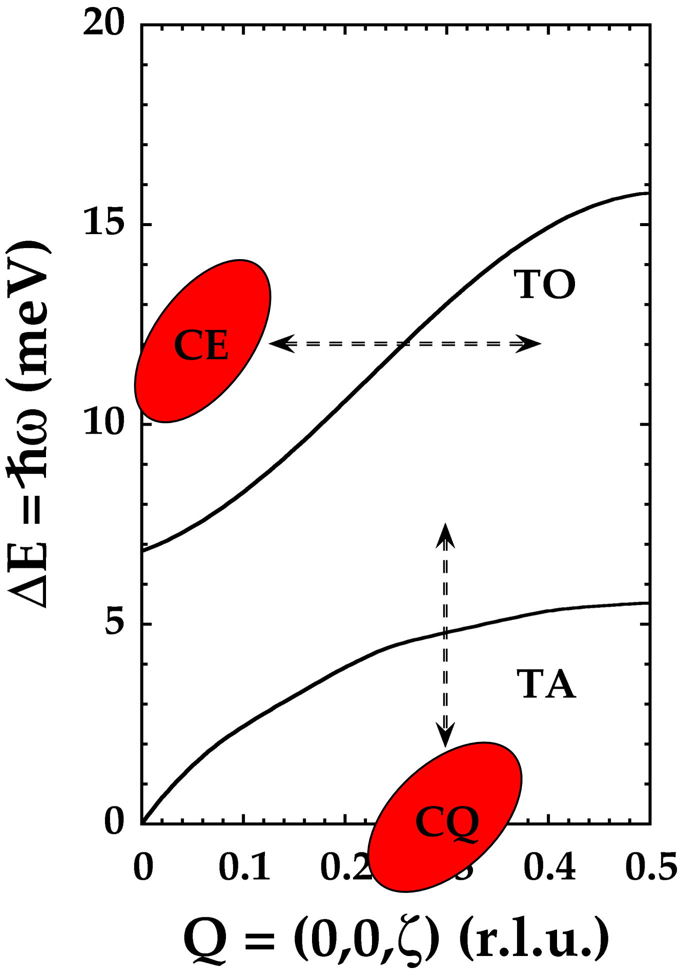
There are two main ways of measuring phonon dispersions.

Constant-E scans: vary Q at fixed hω.



Constant-Q scans: vary hω at fixed Q.





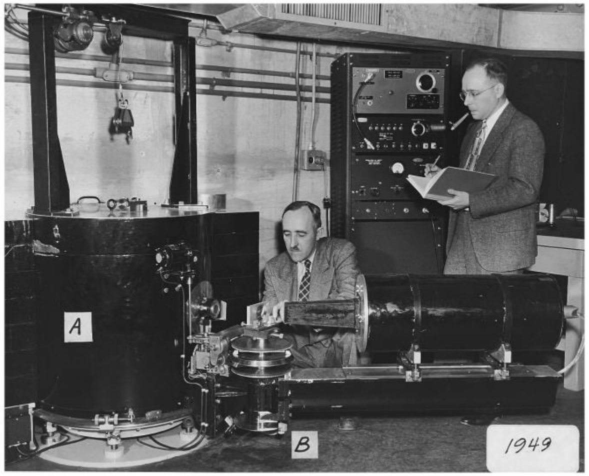
Nobel Prize
in Physics
1994

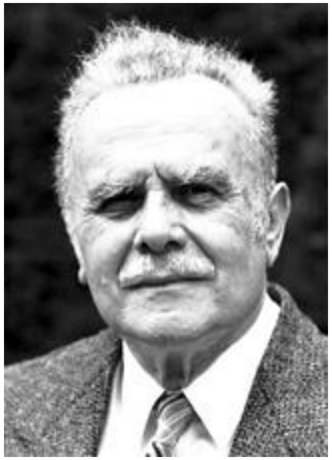
The Fathers of Neutron Scattering

“For pioneering contributions to the development of neutron scattering techniques for studies of condensed matter"

“For the development of the neutron diffraction technique"

“For the development of neutron spectroscopy"





Clifford G Shull
MIT, USA
(1915 – 2001)

Showed us where the atoms are …

Ernest O Wollan
ORNL, USA
(1910 – 1984)

Did first neutron diffraction expts …

Bertram N Brockhouse
McMaster University, Canada
(1918 – 2003)

Showed us how the atoms move …

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Thank-You for your Attention!