

Neutron Scattering by Magnetic Crystals

I: About Neutrons

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Outline

I. About Neutrons

II. General Description

II.I Neutron Diffractometer and Spectrometer

II.II Neutron Scattering Theory

II.III Applications in Condensed Matter

III. Neutron Reflectometry

III.I Theory: specular && non-specular

III.II Neutron Reflectometer

III.III Data Analysis: Model and Fitting

I. About Neutrons

Standard Model: Fundamental Particles and Interactions

Standard Model of Elementary Particles $24 + 6 + 1 = 31$

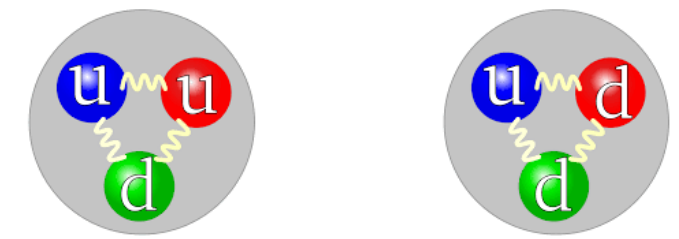
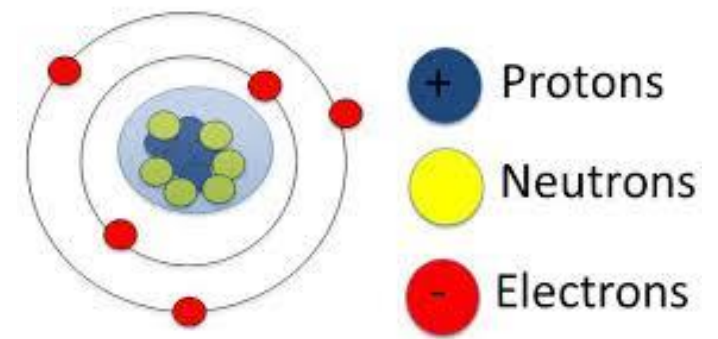
	three generations of matter (elementary fermions)			three generations of antimatter (elementary antifermions)			interactions / force carriers (elementary bosons)	
	I	II	III	I	II	III		
mass	$\approx 2.2 \text{ MeV}/c^2$	$\approx 1.28 \text{ GeV}/c^2$	$\approx 173.1 \text{ GeV}/c^2$	$\approx 2.2 \text{ MeV}/c^2$	$\approx 1.28 \text{ GeV}/c^2$	$\approx 173.1 \text{ GeV}/c^2$	0	$\approx 124.97 \text{ GeV}/c^2$
charge	$\frac{2}{3}$	$\frac{2}{3}$	$\frac{2}{3}$	$-\frac{2}{3}$	$-\frac{2}{3}$	$-\frac{2}{3}$	0	0
spin	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1	0
	u up	c charm	t top	ū antiup	c̄ anticharm	t̄ antitop	g gluon	H higgs
	d down	s strange	b bottom	d̄ antidown	s̄ antistrange	b̄ antibottom	γ photon	
	e electron	μ muon	τ tau	e⁺ positron	μ̄ antimuon	τ̄ antitau	Z⁰ Z ⁰ boson	
	ν_e electron neutrino	ν_μ muon neutrino	ν_τ tau neutrino	ν̄_e electron antineutrino	ν̄_μ muon antineutrino	ν̄_τ tau antineutrino	W⁺ W ⁺ boson	W⁻ W ⁻ boson

QUARKS

LEPTONS

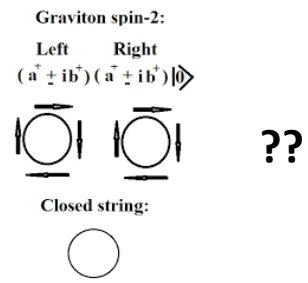
Gauge Bosons
Vector Bosons

Scalar Bosons



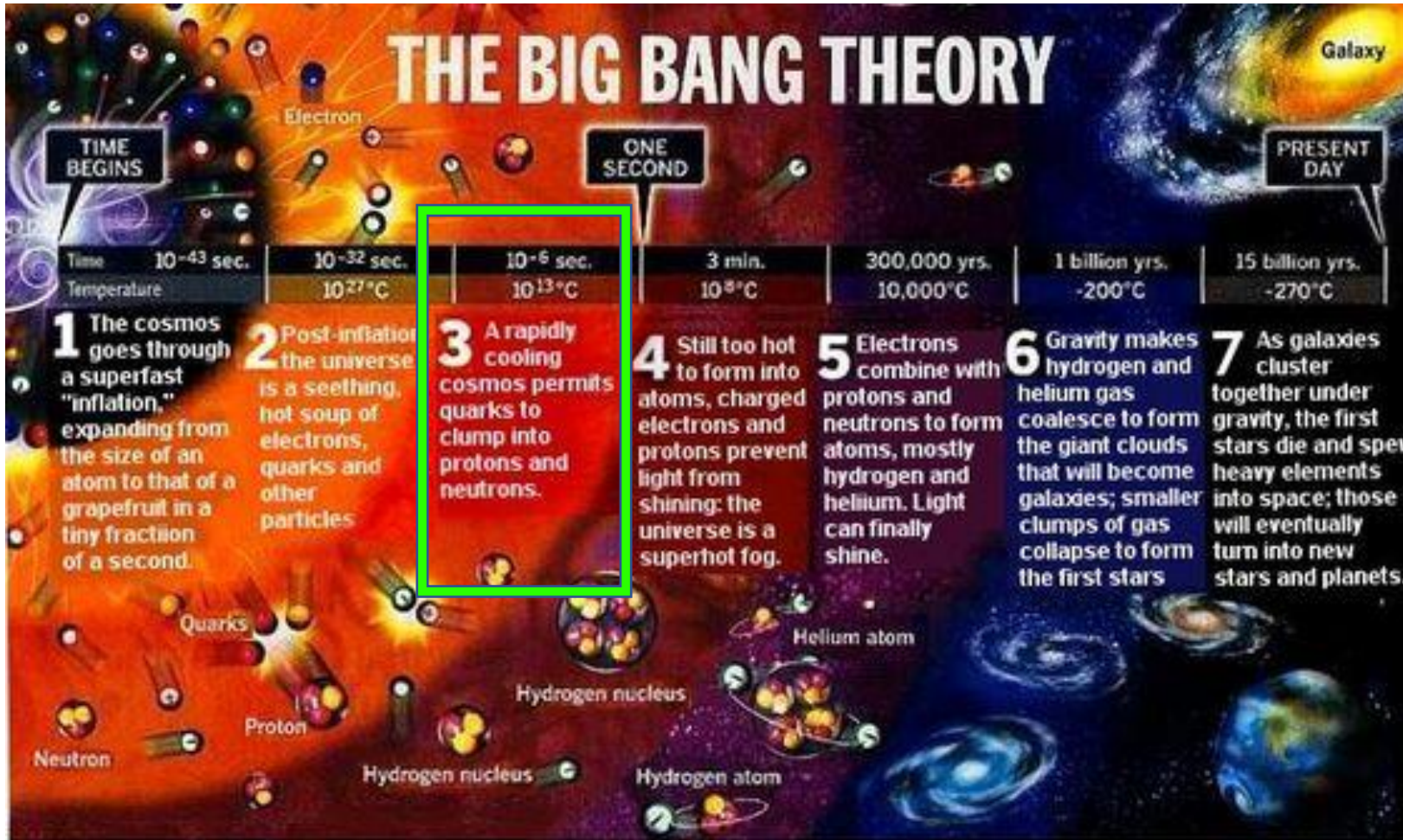
$$SU(3)_c \times SU(2)_L \times U(1)_Y \times SL(4, \mathbf{R})$$

$$SU(3)_c \times U(1)_{em} \times SL(4, \mathbf{R})$$

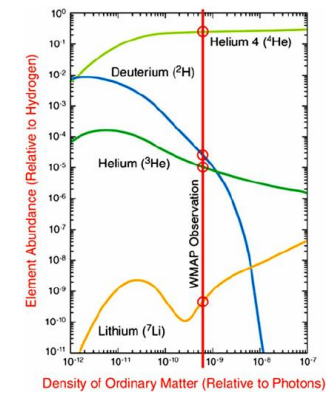


Force	Diagram	Strength	Range (m)	Particle
Strong		1	10^{-15} (diameter of a medium sized nucleus)	gluons, π (nucleons)
Electromagnetic		$\frac{1}{137}$	Infinite	photon mass = 0 spin = 1
Weak		10^{-6}	10^{-18} (0.1% of the diameter of a proton)	Intermediate vector bosons W ⁺ , W ⁻ , Z ₀ , mass > 80 GeV spin = 1
Gravity		6×10^{-39}	Infinite	graviton? mass = 0 spin = 2

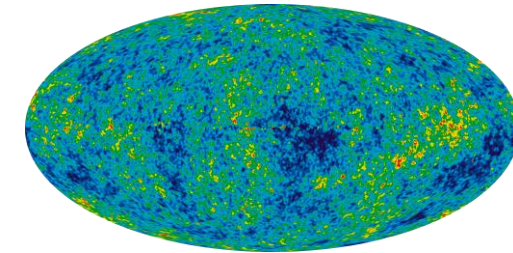
First Batch of Neutrons in the History of Universe



1) Abundance of light elements

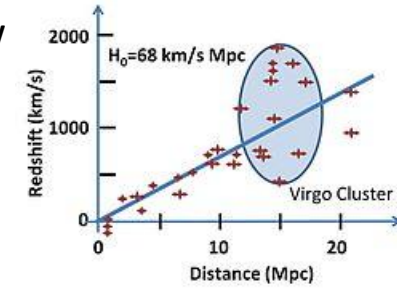


2) CMB



3) Large-scale structure

4) Hubble-Lemaître law



String Theory:
Membrane Collision

$$g + \gamma + (Z, W) + G$$

$$g + \gamma + (Z, W); G;$$

$$g; \gamma + (Z, W); G;$$

Baryogenesis: birth of matter



Steven Hawking :
Quantum Fluctuation

Cosmic Inflation: increased by a factor of 10⁷⁸

Properties of Neutron: Bond State of Quarks

$$I(J^P) = \frac{1}{2} \left(\frac{1}{2} \right)^+$$

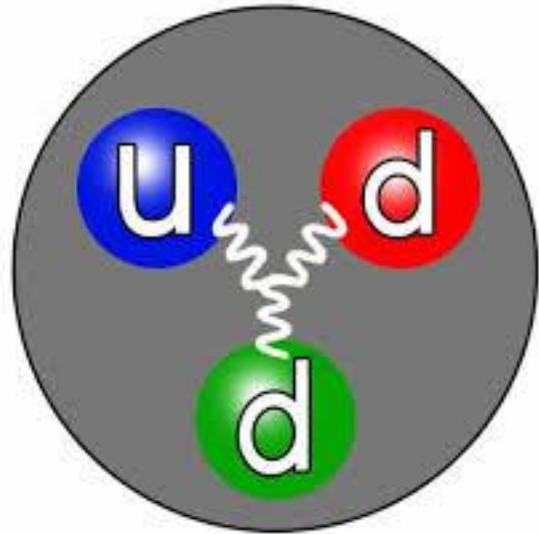


Table 1: Neutron Properties

Gravity	Mass
	Spin
Electromagnetic interaction	magnetic moment
Weak interaction	β -decay lifetime
	confinement radius
Strong interaction	quark structure

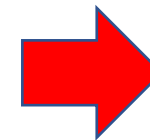
m	$= 1.674928(1) \cdot 10^{-27} \text{ kg}$
s	$= -\hbar/2$
μ	$= -9.6491783(18) \cdot 10^{-27} \text{ JT}^{-1}$
τ	$= 885.9 \pm 0.9 \text{ s}$
R	$= 0.7 \text{ fm}$
quark structure	udd

We Know
Its Structure
?

$$\mathcal{L}_{QCD} = \bar{\psi}_{qi} [i(\gamma^\mu D_\mu)_{ij} - \delta_{ij} m_q] \psi_{qj} - \frac{1}{4} G_{\mu\nu}^\alpha G_{\mu\nu}^\alpha$$

$$D_\mu \equiv \partial_\mu + ig A_\mu^\alpha t_\alpha \quad G_{\mu\nu}^\alpha \equiv \partial_\mu A_\nu^\alpha - \partial_\nu A_\mu^\alpha + gf_{\alpha\beta\gamma} A_\mu^\beta A_\nu^\gamma$$

Lattice
QCD



Mass
Moments
Spin

“Spin Crisis”
We Do Not Know
Its Structure !

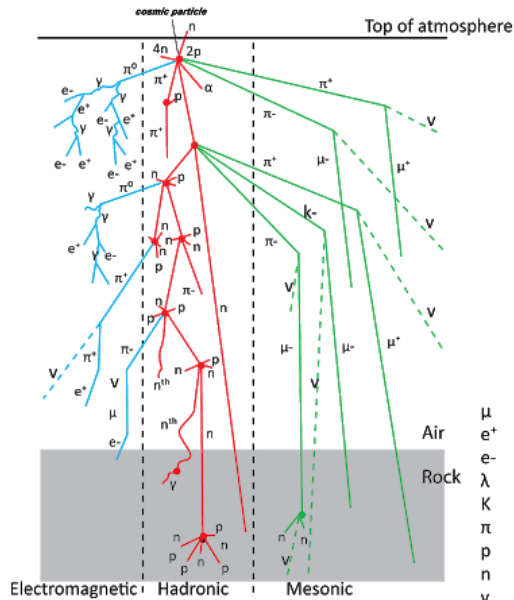
<https://www.reactor-physics.com/what-is-neutron-definition/>
Neutron data booklet: <https://www.ill.eu/about-the-ill/documentation/>

Gell, Y.; Lichtenberg, D. B. (1969). *Il Nuovo Cimento A*. Series 10. **61** (1):

Perkins, Donald H. (1982). *Introduction to High Energy Physics*. Reading, Massachusetts: Addison Wesley. pp. [201–202](#)

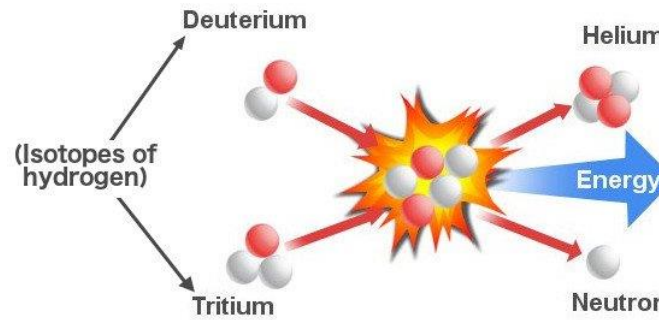
How to Get Neutrons: Sources and Mechanisms

Cosmic Ray Spallation Process



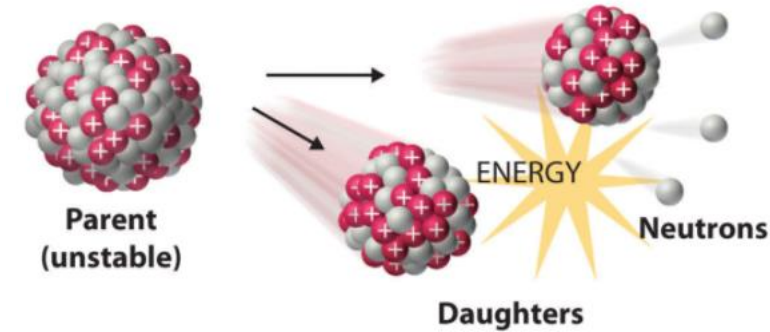
- μ muons
- e^+ positron
- e^- electron
- λ photons (gamma rays)
- K kaons
- π pions
- p protons
- n neutrons
- v neutrino

Fusion Process in Stars



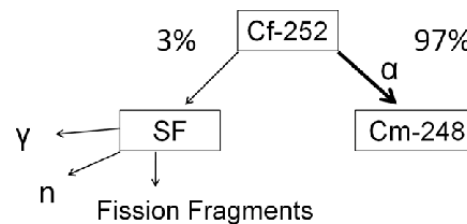
Fusion

Spontaneous Fission Process

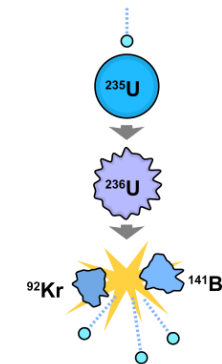


Natural

Spontaneous Fission

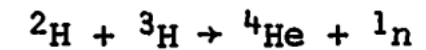
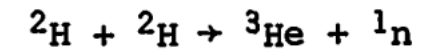


Fission reactor

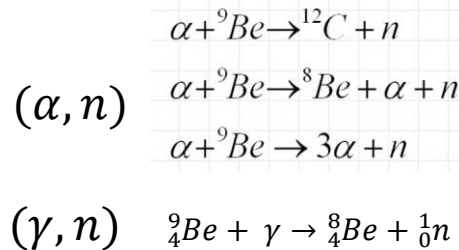


HFIR

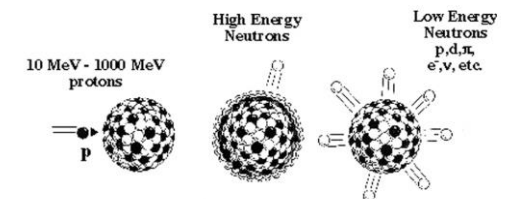
Fusion generator



Artificial



Spallation energetic protons



SNS

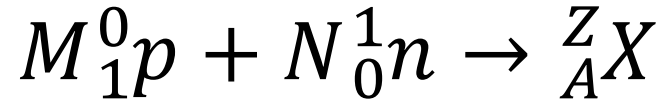
<http://cosmicray.com.au/what-is-a-cosmic-ray>

<https://www.scienceabc.com/nature/universe/how-were-the-elements-created.html>

Table of Isotopes, 8th ed., edited by R. B. Firestone and V. S. Shirley (Wiley, New York, 1996).

How to Get Neutrons: Stability of Nuclei and Elements

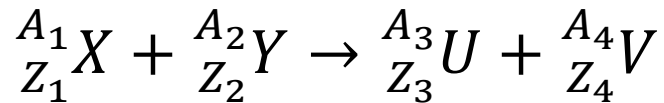
Strong interaction v.s. **Electromagnetic Interaction** Elements: Bonded States of Nucleons



$$Z = M + N \quad A = M + N$$

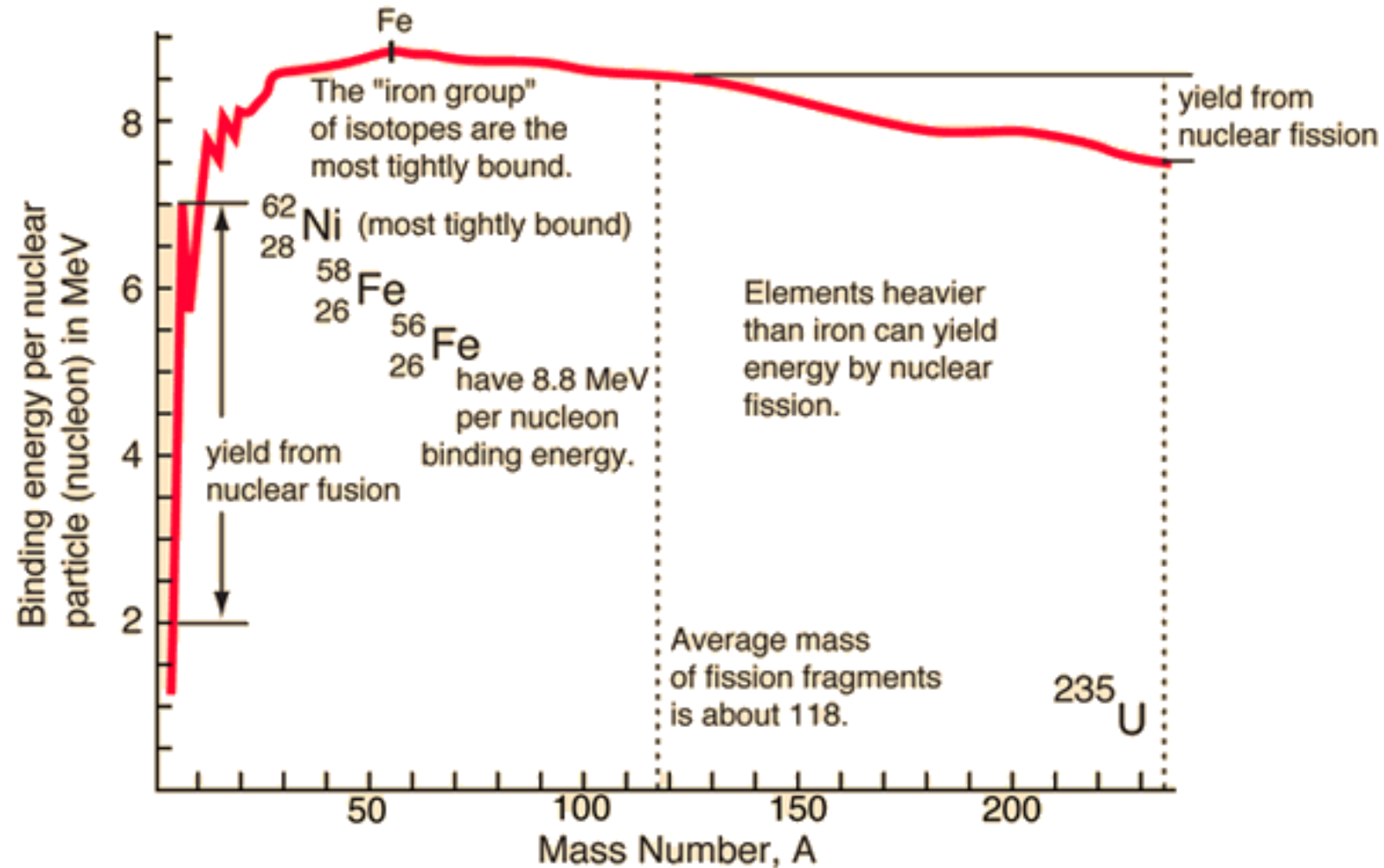
Binding Energy

$$:= \frac{(Mm_p + Nm_n - m_X)c^2}{M+N}$$



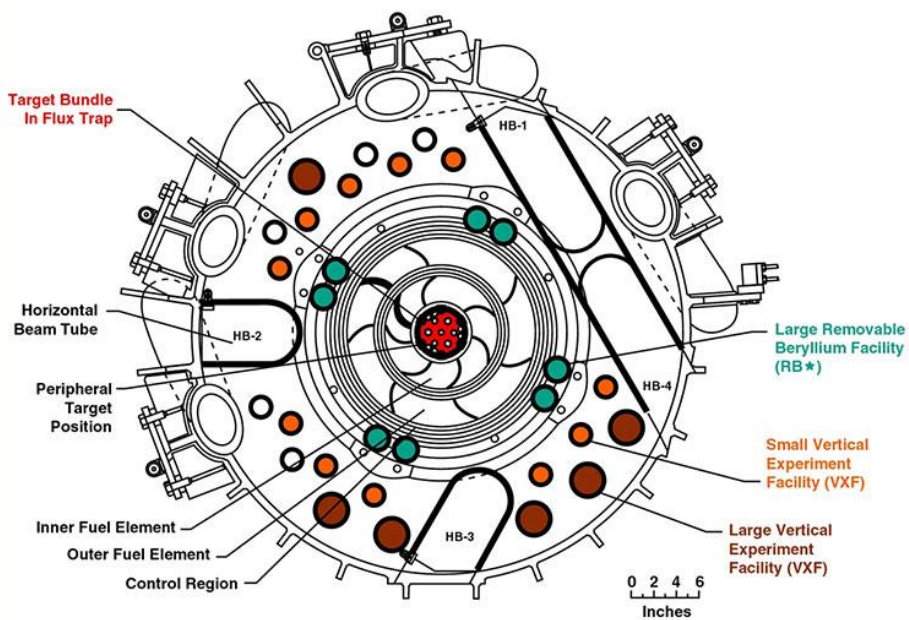
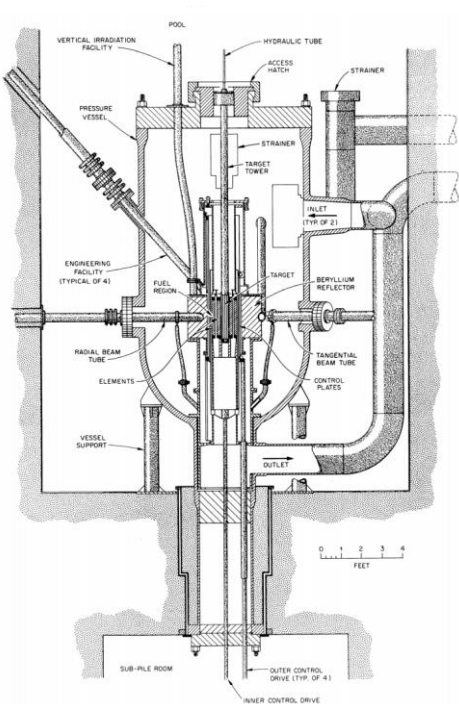
Symmetry-induced selection rule:

Conservation of energy, momentum, charge, baryon number.....

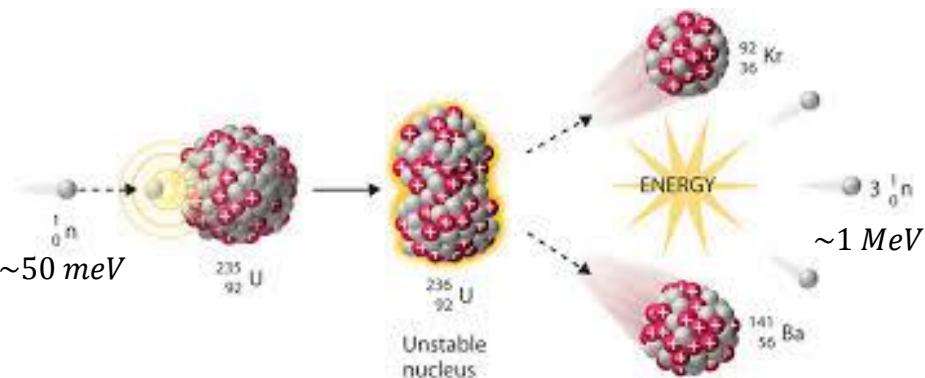


Two Neutron Sources in Oak Ridge National Lab: HFIR & SNS

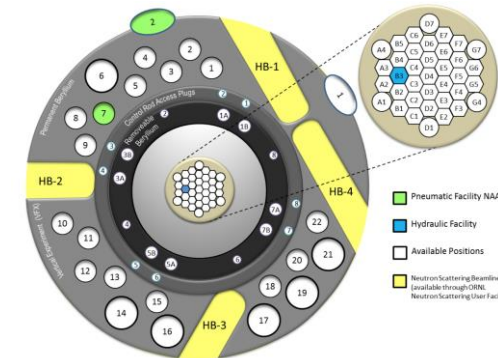
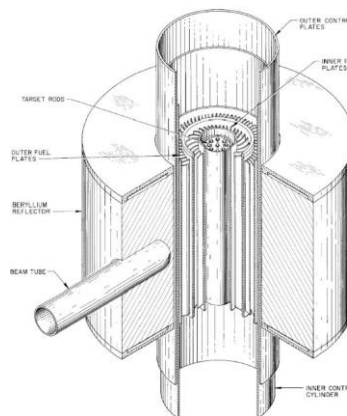
THE HIGH FLUX ISOTOPE REACTOR: Highest Steady-state Thermal Flux 2.6×10^5 neutrons/(cm² · s)



Reactor power, MW	85	
Active core height, cm	50.8	
Number of fuel elements	2	
Fuel type	U ₃ O ₈ —aluminum	
Total ²³⁵ U loading, kg	9.43	
Enrichment, %	93.1	
Fuel element parameters	<i>Inner fuel element</i>	<i>Outer fuel element</i>
Number of fuel plates	171	369
²³⁵ U loading, kg	2.60	6.83
Average fuel uranium density, gU/cm ³	0.776	1.151
²³⁵ U per plate, g	15.18	18.44
Burnable poison in element (¹⁰ B), g	2.8	None
Fuel plate thickness, cm	0.127	0.127
Coolant channel between plates, cm	0.127	0.127
Minimum aluminum clad thickness, mm	0.25	0.25
Fuel plate width, cm	8.1	7.3
Fuel cycle length, d	~24	
Cycle 400 length, d	24.6	
Coolant inlet temperature, °F	120	
Coolant outlet temperature, °F	169	
Fuel plate centerline temperature, °F	323	

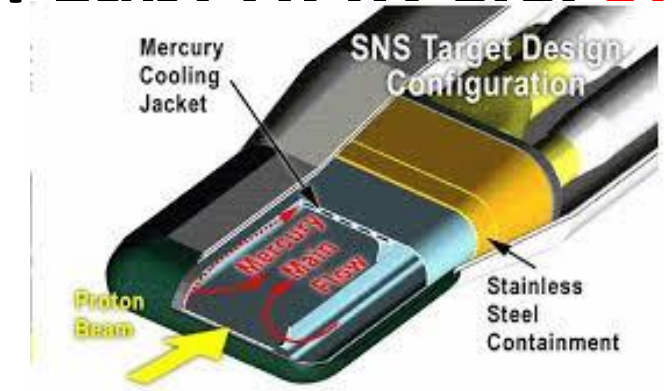


9.4 kg ²³⁵U + 2.8 g ¹⁰B

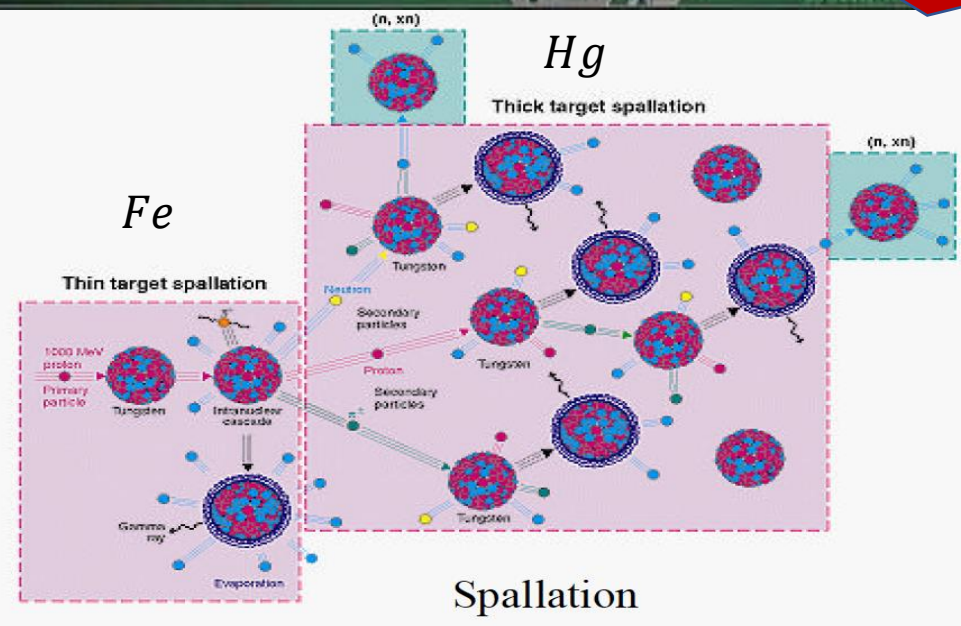


Two Neutron Sources in Oak Ridge National Lab: HFIR & SNS

Spallation Neutron Source



World's most intense pulsed, accelerator-based neutron source
NEUTRONS.ORNL.GOV



- Backscattering Spectrometer (BASIS) - BL-2**: Dynamics of macromolecules, constrained molecular systems, polymers, biology, chemistry, materials science.
- Nanoscale-Ordered Materials Diffractometer (NOMAD) - BL-18**: Liquids, solutions, glasses, polymers, nanocrystalline and partially ordered complex materials.
- Wide Angular-Range Chopper Spectrometer (ARCS) - BL-16**: Atomic-level dynamics in materials science, chemistry, condensed matter, materials science.
- Fine-Resolution Fermi Chopper Spectrometer (SEQUOIA) - BL-17**: Dynamics of complex fluids, quantum fluids, magnetism, condensed matter, materials science.
- Ultra-Small-Angle Neutron Scattering Instrument (USANS) - BL-1A**: Life sciences, polymers, materials science, earth and environmental sciences.
- Vibrational Spectrometer (VISION) - BL-16B**: Vibrational dynamics in molecular systems, chemistry.
- Spallation Neutrons and Pressure Diffractometer (SNAP) - BL-3**: Materials science, geology, earth and environmental sciences.
- Neutron Spin Echo Spectrometer (NSE) - BL-15**: High-resolution dynamics of slow processes, polymers, biological macromolecules.
- Hybrid Spectrometer (HYSPEC) - BL-14B**: Atomic-level dynamics in single crystals, magnetism, condensed matter sciences.
- Magnetism Reflectometer - BL-4A**: Chemistry, magnetism of layered systems and interfaces.
- Liquids Reflectometer - BL-4B**: Interfaces in complex fluids, polymers, chemistry.
- Cold Neutron Chopper Spectrometer (CNCS) - BL-5**: Condensed matter physics, materials science, chemistry, biology, environmental science.
- Fundamental Neutron Physics Beam Line - BL-13**: Fundamental properties of neutrons.
- Extended Q-Range Small-Angle Neutron Scattering Diffractometer (EQ-SANS) - BL-6**: Life science, polymer and colloidal systems, materials science, earth and environmental sciences.
- BL-8A** and **BL-8B**: (No specific callout text provided).
- Elastic Diffuse Scattering Spectrometer (CORELLI) - BL-9**: Detailed studies of disorder in crystalline materials.
- Versatile Neutron Imaging Instrument at SNS (VENUS) - BL-10**: Energy selective imaging in materials science, engineering, materials processing, environmental sciences and biology.
- Macromolecular Neutron Diffractometer (MaNDI) - BL-11B**: Atomic-level structures of membrane proteins, drug complexes, DNA.
- Single-Crystal Diffractometer (TOPAZ) - BL-12**: Atomic-level structures in chemistry, biology, earth science, materials science, condensed matter physics.
- Engineering Materials Diffractometer (VULCAN) - BL-7**: Mechanical behaviors, materials science, materials processing.
- Powder Diffractometer (POWGEN) - BL-11A**: Atomic-level structures in chemistry, materials science, and condensed matter physics including magnetic spin structures.

LEGEND

- Operating instrument in user program
- In design or construction
- Under consideration

*Scheduled commissioning date

Neutron Scattering by Crystals

Strong interaction. && Electromagnetic Interaction

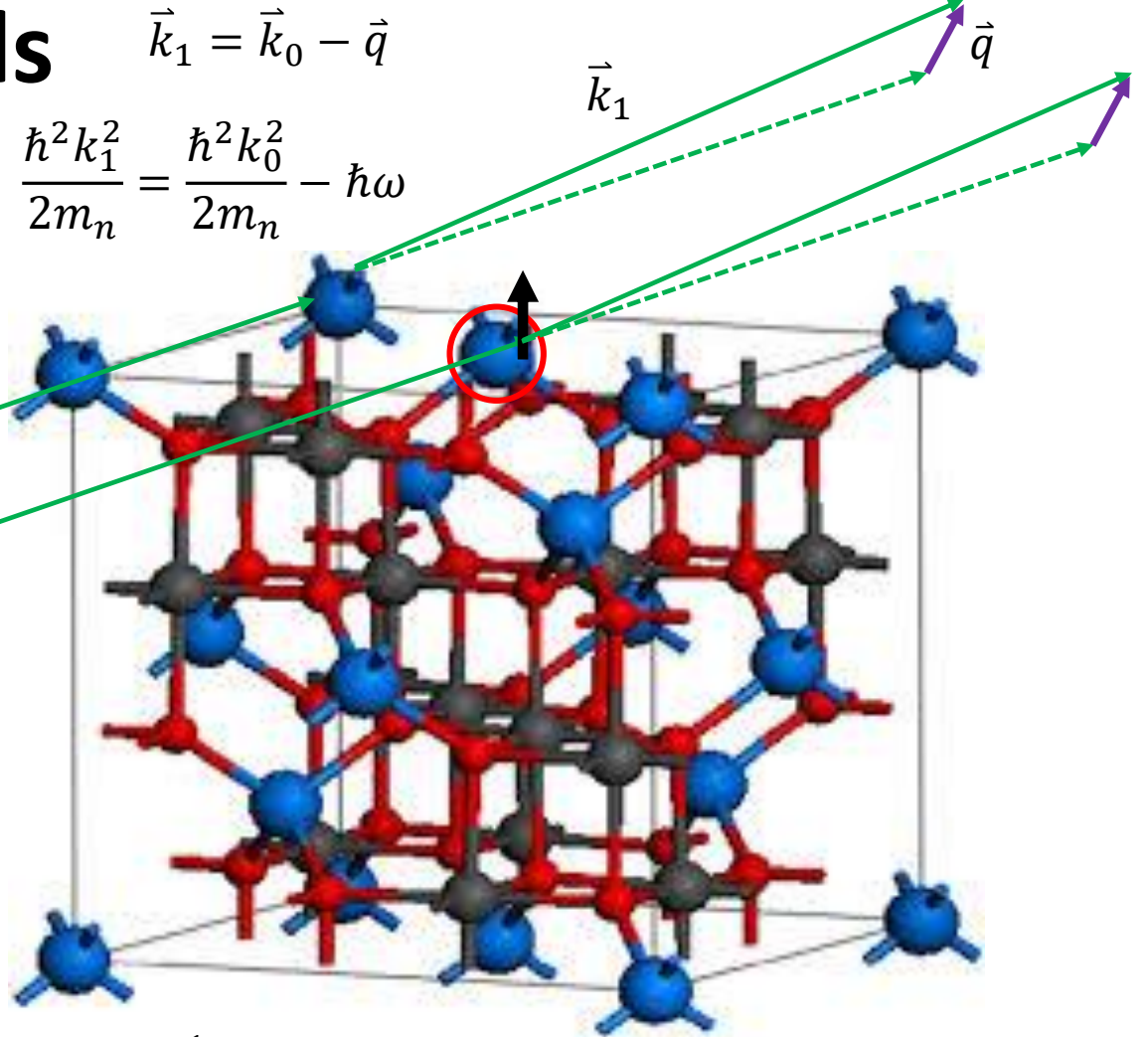
1) Neutron-Nucleus Interaction: Fermi pseudopotential

$$V(\vec{r}) = \frac{4\pi\hbar^2}{m} b_c \delta(\vec{r})$$

$$\left(\frac{d\sigma}{d\Omega d\omega}\right)_N = \left(\frac{d\sigma}{d\Omega d\omega}\right)_{N;c} + \left(\frac{d\sigma}{d\Omega d\omega}\right)_{N;inc}$$

$$\left(\frac{d\sigma}{d\Omega d\omega}\right)_{N;\alpha} \equiv b_\alpha^2 \frac{k_1}{k_0} N S_\alpha(\vec{q}, \omega), \alpha = c, inc$$

\vec{k}_0
 n



$$\vec{k}_1 = \vec{k}_0 - \vec{q}$$

$$\frac{\hbar^2 k_1^2}{2m_n} = \frac{\hbar^2 k_0^2}{2m_n} - \hbar\omega$$

	Coherent	Incoherent
Elastic	Bragg diffraction: $\vec{q} = \vec{G}$	Local structure
Inelastic	Single-Phonon excitation	NMR

$$S_\alpha(\vec{q}, \omega) \equiv \frac{1}{2\pi\hbar} \int d\vec{r} dt G(\vec{r}, t) e^{i(\vec{q}\cdot\vec{r} - \omega t)}$$

$$G(\vec{r}, t) \equiv \frac{1}{N} \int d\vec{r}' \langle \rho(\vec{r}', 0) \rho(\vec{r}' - \vec{r}, t) \rangle \quad \rho(\vec{r}', t) \equiv \sum_j \delta(\vec{r}' - \vec{R}_j(t))$$

$$G_s(\vec{r}, t) \equiv \frac{1}{N} \sum_i \int d\vec{r}' \langle \delta(\vec{r}' - \vec{R}_i(0)) \delta(\vec{r}' - \vec{r} - \vec{R}_i(t)) \rangle$$

Neutron Scattering by Crystals

Strong interaction. && Electromagnetic Interaction

2) Neutron-Electron Interaction: dipole-dipole interaction

If $L = 0$, some iron group 3d ions

$$\left(\frac{d\sigma}{d\Omega d\omega}\right)_M = \left(\frac{d\sigma}{d\Omega d\omega}\right)_{Bragg} + \left(\frac{d\sigma}{d\Omega d\omega}\right)_{diff}$$

$$\left(\frac{d\sigma}{d\Omega d\omega}\right)_{Brag} \equiv (1.91 \frac{e}{\hbar c})^2 \frac{k_1}{k_0} \int \frac{dt}{2\pi} e^{-i\omega t} \langle \mathbf{M}_\perp(\vec{q}) \rangle \langle \mathbf{M}_\perp(-\vec{q}) \rangle$$

$$\equiv \left(1.91 \frac{e}{\hbar c}\right)^2 \frac{k_1}{k_0} \delta(\omega) \langle \mathbf{M}_\perp(\vec{q}) \rangle \langle \mathbf{M}_\perp(-\vec{q}) \rangle \quad \mathbf{M}(\vec{q}) \equiv \sum_j \mu_j e^{-i\vec{q} \cdot \vec{R}_j} \quad \mathbf{M}_\perp(\vec{q}) \equiv \mathbf{M}(\vec{q}) \cdot \vec{q}$$

$$\left(\frac{d\sigma}{d\Omega d\omega}\right)_{diff} \equiv (1.91 \frac{e}{\hbar c})^2 \frac{k_1}{k_0} \int \frac{dt}{2\pi} e^{-i\omega t} [\langle \mathbf{M}_\perp(\vec{q}, 0) \mathbf{M}_\perp(-\vec{q}, t) \rangle - \langle \mathbf{M}_\perp(\vec{q}) \rangle \langle \mathbf{M}_\perp(-\vec{q}) \rangle]$$

If \vec{q} is small

$$\mu_j = \mu_{Lj} + \mu_{Sj}$$

$$= \mu_B(\mathbf{L} + 2\mathbf{S})$$

If $L \neq 0$, but orbital ground state singlet or nonmagnetic doublet (some 3d ions)

$$\mathbf{L} + 2\mathbf{S} \rightarrow g\mathbf{S}$$

If small ion radius (rare earth ions)

$$\mathbf{L} + 2\mathbf{S} \rightarrow g\mathbf{J}$$

$$\mathbf{J} = \mathbf{L} + \mathbf{S}$$

g : Lander factor

	Coherent	Incoherent
Elastic	Bragg diffraction: $\vec{q} = \vec{G}$	Critical Scattering
Inelastic	Magnon Excitation	Crystal Field splitting Spin-Orbital Coupling