Chemical Engineering 412

Introductory Nuclear Engineering

Lecture 3

Atomic & Nuclear Models

Nuclear Energetics

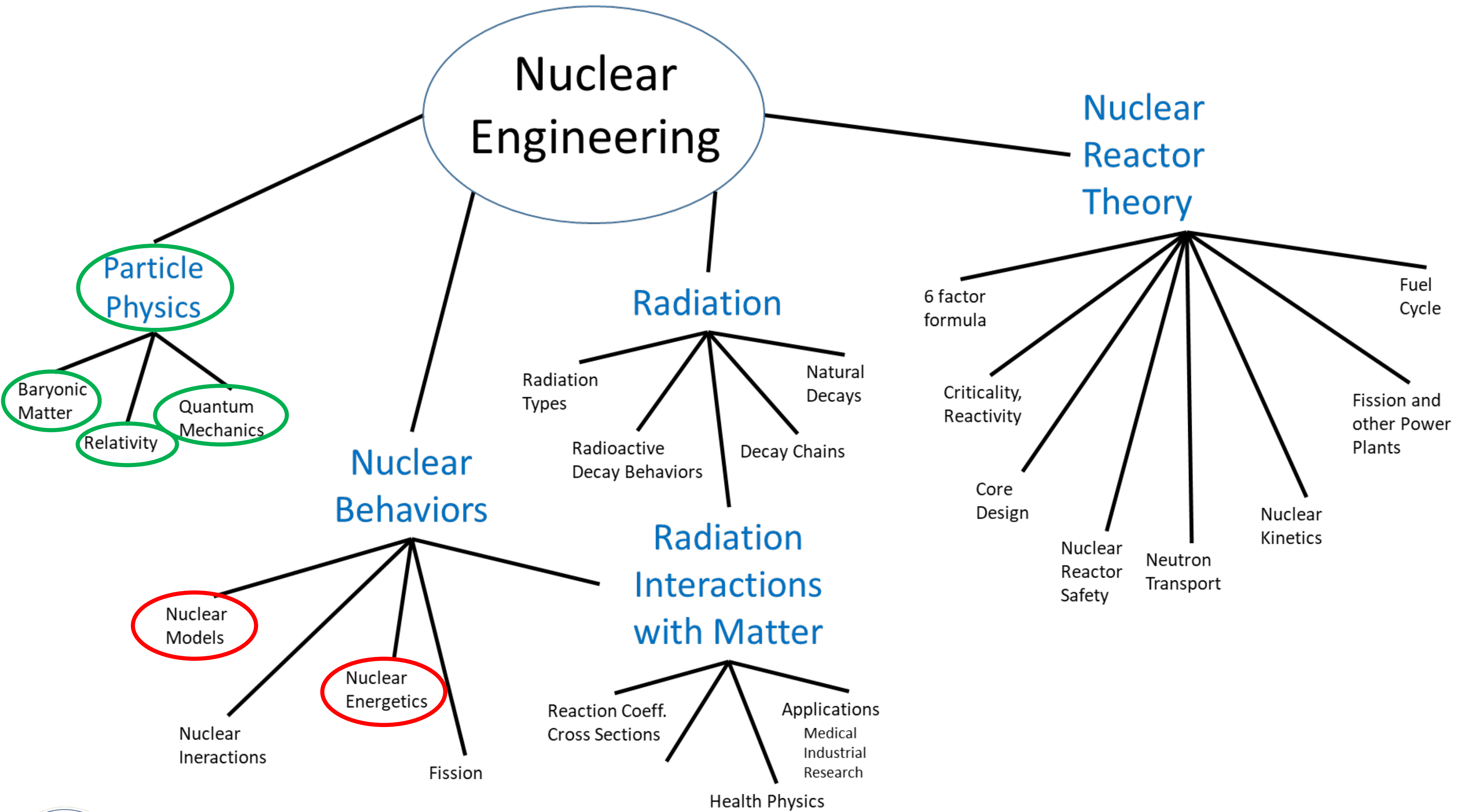
Spiritual Thought

D&C 122:7-8

7 …know thou, my son, that all these things shall give thee experience, and shall be for thy good.

8 The Son of Man hath descended below them all. Art thou greater than he?

Roadmap

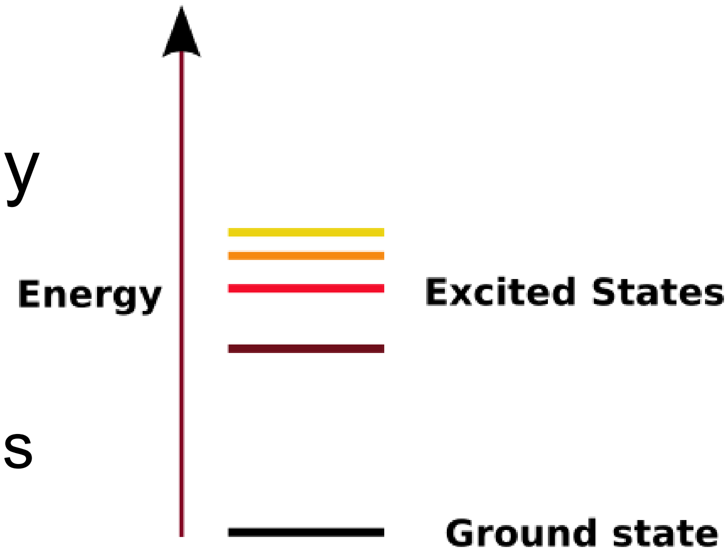

Nuclear Engineering
Particle Physics
Baryonic Matter
Relativity
Quantum Mechanics
Nuclear Behaviors
Nuclear Models
Nuclear Ineractions
Nuclear Energetics
Fission
Radiation
Radiation Types
Radioactive Decay Behaviors
Natural Decays
Decay Chains
Radiation Interactions with Matter
Reaction Coeff. Cross Sections
Health Physics
Applications
Medical
Industrial
Research
Nuclear Reactor Theory
6 factor formula
Criticality, Reactivity
Core Design
Nuclear Reactor Safety
Neutron Transport
Nuclear Kinetics
Fission and other Power Plants
Fuel Cycle

Objectives

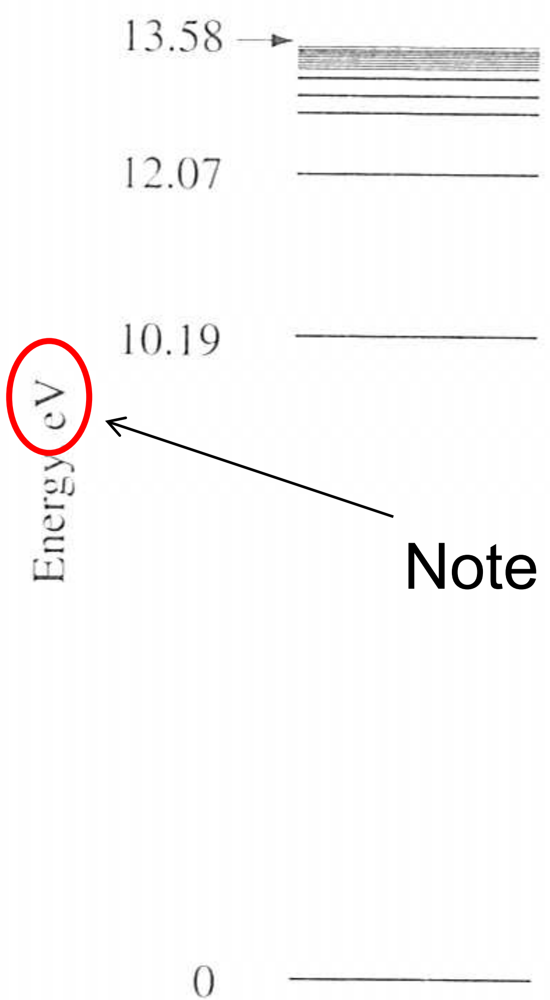
- Understand characteristics of nucleus energy states (quantized)
- Know how to approximate nuclear mass using atomic models
- Understand binding energy and mass defect and their implications
- Know how to identify, characterize, and create nuclear interaction equations
- Know how to assess energetics of nuclear interactions

Excited energy states - Electrons

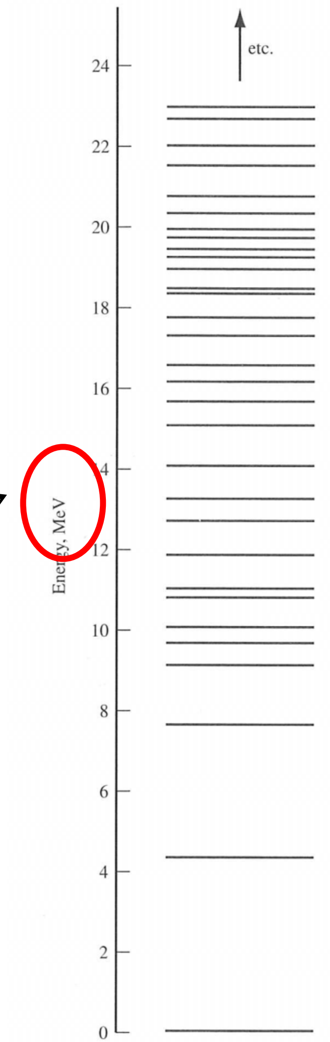
- Bound atomic electrons
  - specific energy levels
  - quantum numbers
- Transitions between energy levels requires:
  - absorption or emission
  - specific wavelengths/energies
  - light (or heat or other energy forms).



Nuclei Also Have Energy Levels



Note the scale change



Atomic Energy Levels (H)

Nuclear Energy Levels (^{12}C)

Nuclear Energy Levels

- Analogous to atomic energy levels
  - Discrete orbital configurations
  - Ground states
  - Excited states (except for smallest nuclei).
- Residual strong force
  - Far stronger
  - Much shorter range (a few nucleons)
  - Higher energy levels
  - Energy changes produce Gamma rays (γ-ray)

Nuclear Energy Levels (cont)

- Energy exchanged
  - innermost electrons (internal conversion)
  - ejection from the atom
  - collapse of an outer electron to the inner orbital with x-ray emission.
- Outer to an inner electronic state:
  - Highly energetic (hence the high-energy x-rays)
  - absorbed by a 2^{nd} electron
  - 2^{nd} electron is ejected – Auger Electron

Liquid Drop Model

- Nucleus is like a liquid drop.
  - Adding more mass (nucleons) does not change the density, just the size.
  - Surface tension and mass compete for droplet stability. In a nucleus, short-range nuclear attractive forces compete with longer range coulombic repulsive forces.
  - Total mass then is

$$M = \underbrace{NM_n}_{\text{neutron mass}} + \underbrace{ZM_p}_{\text{proton mass}} - \underbrace{\alpha A}_{\substack{\text{attractive}\\ \text{energy}}}$$

  - Surface nucleons are not as tightly bound (fewer neighbors)

$$M = \underbrace{NM_n}_{\text{neutron mass}} + \underbrace{ZM_p}_{\text{proton mass}} - \underbrace{\alpha A}_{\substack{\text{attractive}\\ \text{energy}}} + \underbrace{\beta A^{2/3}}_{\text{surface effect}}$$

Liquid Drop Model (contd)

- Coulombic repulsion decreases force, increases mass

$$M = \underbrace{NM_n}_{\text{neutron mass}} + \underbrace{ZM_p}_{\text{proton mass}} - \underbrace{\alpha A}_{\text{attractive energy}} + \underbrace{\beta A^{2/3}}_{\text{surface effect}} + \underbrace{\gamma Z^2 / A^{1/3}}_{\text{coulombic repulsion}}$$

- Different numbers of neutrons and protons increase mass

$$M = \underbrace{NM_n}_{\text{neutron mass}} + \underbrace{ZM_p}_{\text{proton mass}} - \underbrace{\alpha A}_{\text{attractive energy}} + \underbrace{\beta A^{2/3}}_{\text{surface effect}} + \underbrace{\gamma Z^2 / A^{1/3}}_{\text{coulombic repulsion}} + \underbrace{\frac{\zeta (A-2Z)^2}{A}}_{\text{asymmetry}}$$

- Protons and neutrons separately prefer pairs

$$M = \underbrace{NM_n}_{\text{neutron mass}} + \underbrace{ZM_p}_{\text{proton mass}} - \underbrace{\alpha A}_{\text{attractive energy}} + \underbrace{\beta A^{2/3}}_{\text{surface effect}} + \underbrace{\gamma Z^2 / A^{1/3}}_{\text{coulombic repulsion}} + \underbrace{\frac{\zeta (A-2Z)^2}{A}}_{\text{pairing}} + \underbrace{\delta / \sqrt{A}}_{p/n \text{ pairing}}$$

Nuclear Mass Equation

$$m = Zm_p + (A - Z)m_n - \frac{E_B}{c^2}$$

$$E_B = a_v A - a_s A^{\frac{2}{3}} - a_c \frac{Z^2}{A^{\frac{1}{3}}} - a_a \frac{(A - 2Z)^2}{A} + \frac{a_p[(-1)^Z + (-1)^N]}{2\sqrt{A}}$$

(All units MeV)	Lamarsh	Least-squares	Wapstra	Rohlf	Text (Shultis)	Bertsch et al.
M_n	939.565	939.565	939.565	939.565	939.565	939.565
M_p	938.272	938.272	938.272	938.272	938.272	938.272
a_v	15.56	15.8	14.1	15.75	15.835	15.74063
a_s	17.23	18.3	13	17.8	18.33	17.61628
a_c	0.697	0.714	0.595	0.711	0.714	0.71544
a_a	23.285	23.2	19	23.7	23.20	23.42742
a_p	12	12	33.5	11.18	11.2	12.59898

These semi-empirical models work best for large A.

Example

Estimate the atomic mass of ^{40}Ca based on the liquid drop model.

Term	Magnitude (MeV)
volume	633.4
surface	214.389
Coulombic	83.51
n-p asymetry	0
pairing	-1.77088

Binding energy =
633.4-214.389-83.51-0-(-1.77088)=337.27

BE/A =
337.27/40=8.431

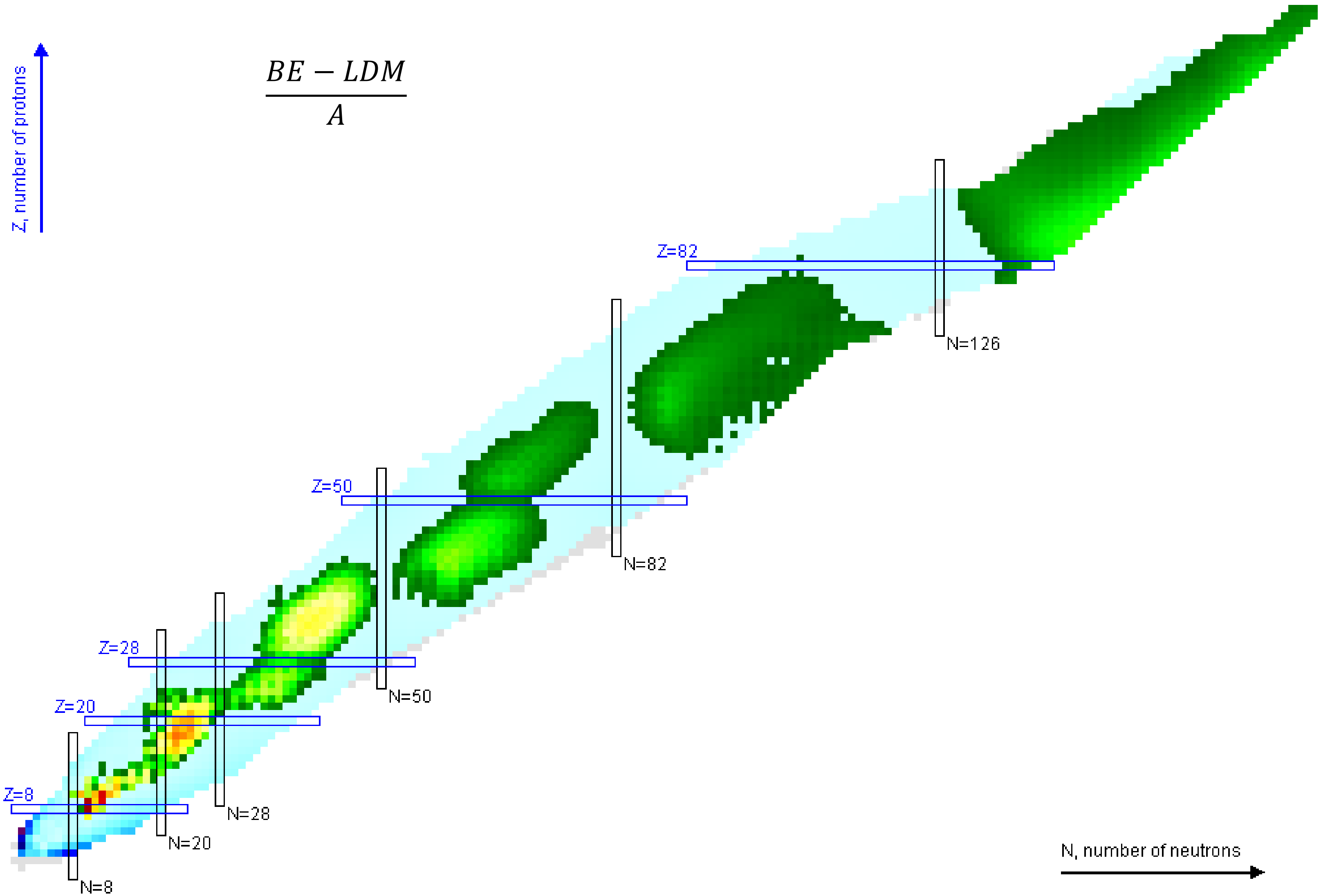
Observed BE/A =
337.27/40=8.551

Estimated Atomic Mass =
(20*939.565+20*938.272+20*0.510999-337.27)/931.5 MeV/u = 39.956 u
(20*939.565+20*938.789-337.27)/ 931.5 MeV/u = 39.96759 u

Observed Atomic Mass = 39.9674 u

Atomic Mass based on sum of parts = 40.329 u

Accuracy of Liquid Drop Model



Source: Brookhaven Nat. Labs http://www.nndc.bnl.gov/chart/reColor.jsp?newColor=be-ldm

Shell Model (Quantum Model)

- Assume each nucleon acts independently of all others
- All nucleons move in a potential well that is flat inside the nucleus but increases sharply at the edge.
- Much math leads to theoretical prediction of "magic" numbers of nucleons consistent with observations. These are: 2, 8, 20, 28, 50, 82, 126
- Some lists include 14 and sometimes 6 as magic.
- These are analogous to the closed shells of electron orbitals that give rise to noble gases and apply to the neutrons and protons separately. That is, nuclei with a magic number protons or a magic number of neutrons are especially stable, and those with magic numbers of both are doubly magic and exceptionally stable.

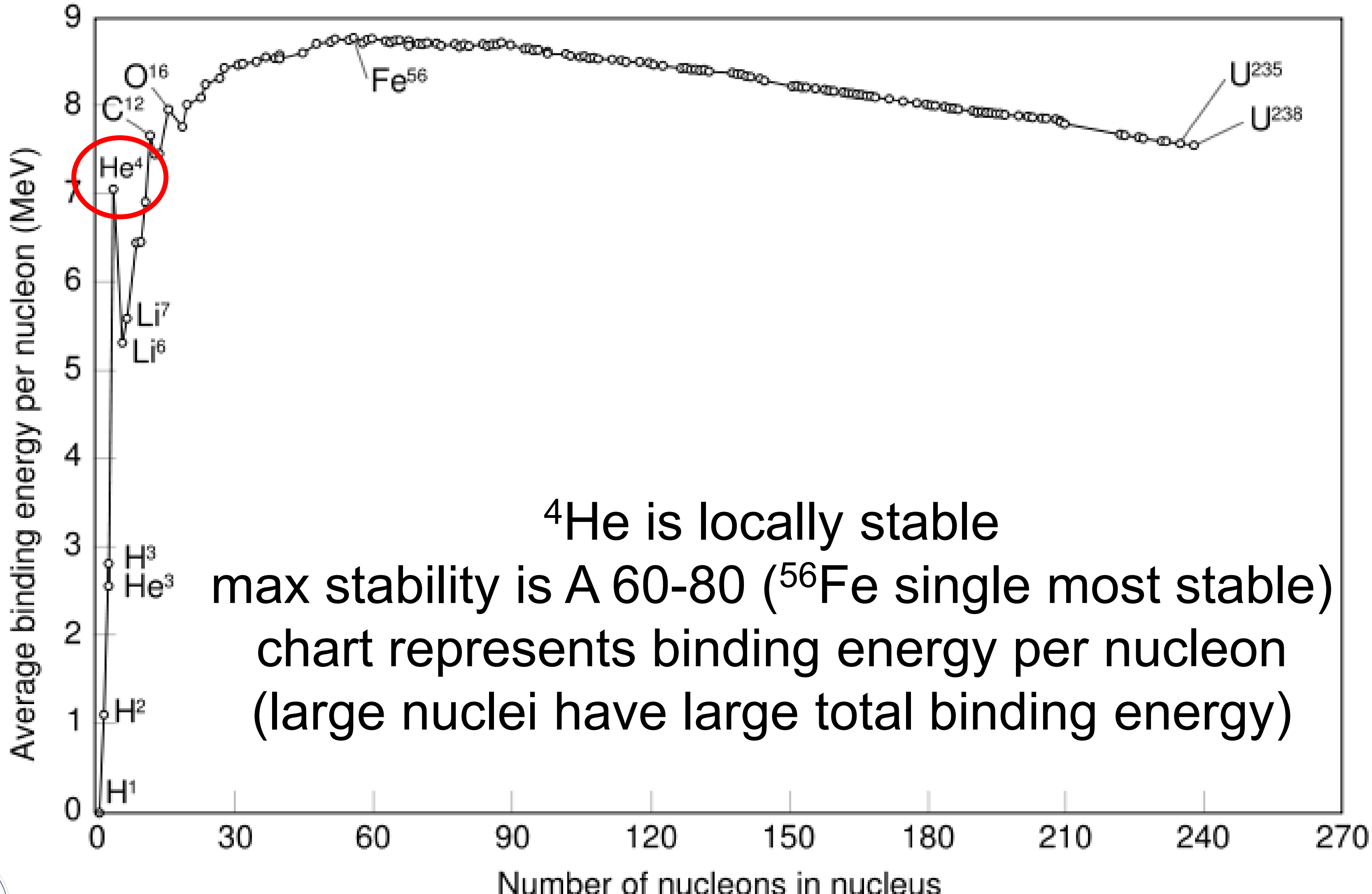
Nuclear Stability

- Proton excess leads to decay (coulombic repulsion)
- Neutron excess leads to decay (too large – nuclear force is short-range)
- Odd numbers of either neutrons or protons leads to decay (nucleons like to be paired, especially with like nucleons)
- Certain numbers of nucleons are exceptionally stable
- Neutrons easier to accommodate than protons (coulombic repulsion)

266 (255) total stable nuclides

		Protons	
		Even	Odd
Neutrons	Even	159	50
	Odd	53	4

Binding Energy



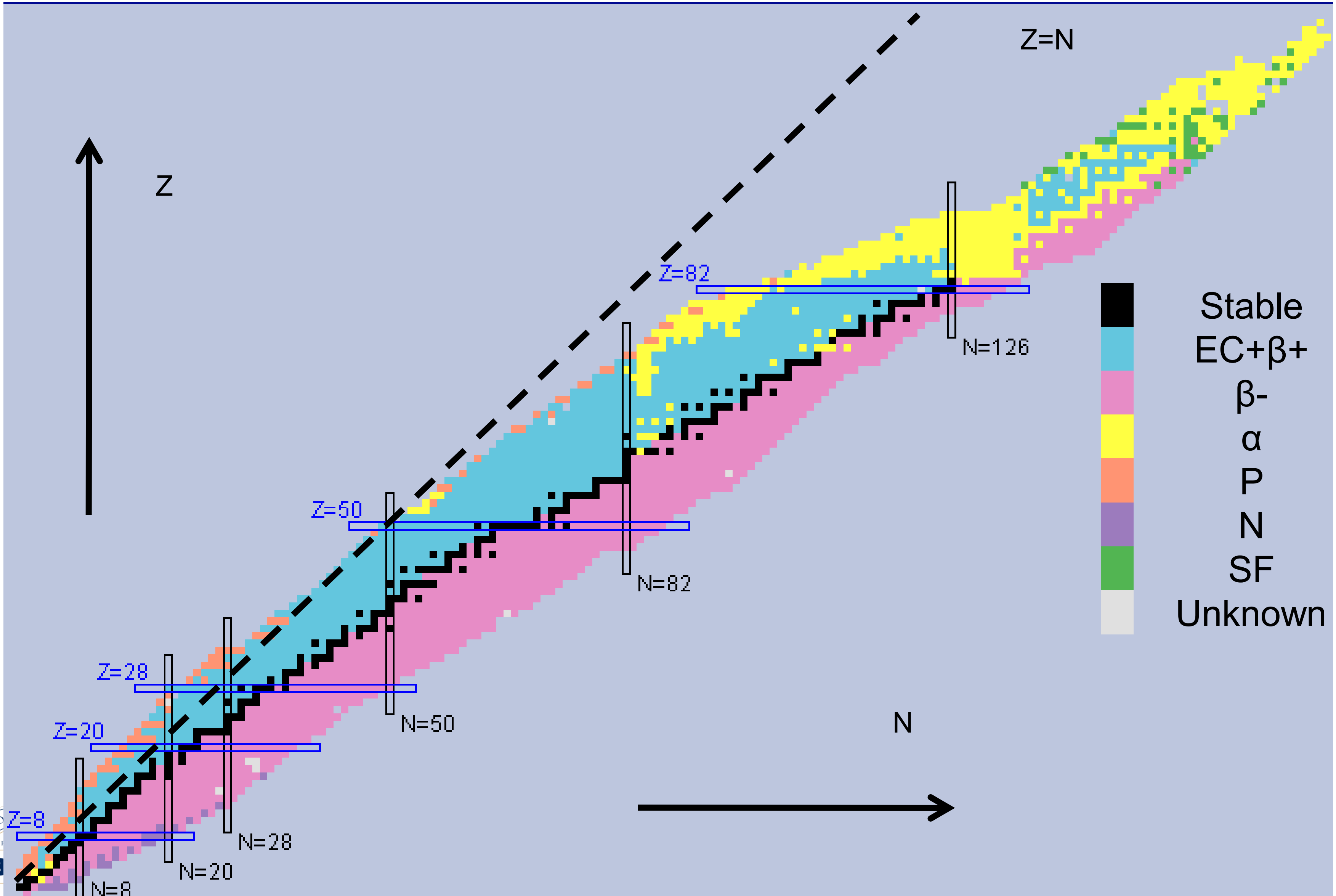
^{4}He is locally stable

max stability is A 60-80 (^{56}Fe single most stable)

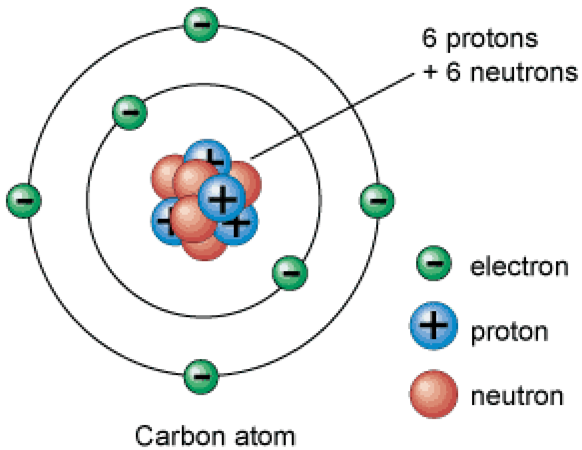
chart represents binding energy per nucleon

(large nuclei have large total binding energy)

Chart of the Nuclides



Modern Nucleus Concepts



- Much smaller relative to electron shells than typically depicted (picture at left misleading).
- Includes protons and neutrons, but not as discrete particles. Pairs of protons and neutrons typically share the same physical location (as waves) but have different quantum numbers (spin number differs).
- Slight density variation with increasing distance from center.
- Not necessarily spherical.
- Measurable charge separation in many cases.

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Nuclear Energetics

- Study of mass/energy changes in nucleus
  - Reactions
    - Binary (2) or ternary (rare) reactions
    - Decays (1 nucleus)
  - Stability
  - Mass Defect
  - Binding Energy/Separation Energy
- Foundational to understanding radioactive decay

Reaction Terminology

- Chemistry
  - Exothermic reactions
    - Generate heat
    - Negative heat of reaction
  - Endothermic reactions
    - Consume heat
    - Positive heat of reaction
- Nuclear chemistry
  - Exothermic = Exoergic
    - Positive Q-values
  - Endothermic = Endoergic
    - negative Q-values

Not "thermal", because it's not traditional heat transfer; atomic scale with wave emission and kinetic energy

Mass Defect/Binding Energy

- $E=mc^2$ -----> $\Delta E = \Delta mc^2$
  - Even for Macroscopic effects, but tiny
    - 10^{-8} % for formation of CO_2 molecule
- Δm = mass defect
    - m = nuclear, M = atomic → How to define M?
    - $M({}^{A}_{Z}X) = m({}^{A}_{Z}X) + Zm_e - \frac{BE_{Ze}}{c^2}$ → How to define m?
  - $\Delta m = \frac{BE}{c^2} = Zm_p + (A-Z)m_n - m({}^{A}_{Z}X)$
- Binding Energy
  - $BE({}^{A}_{Z}X) = [ZM({}^{1}_{1}H) + (A-Z)m_n - M({}^{A}_{Z}X)]c^2$
- Separation Energy
  - $Sn({}^{A}_{Z}X) = BE({}^{A}_{Z}X) - BE({}^{A-1}_{Z}X)$

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Fundamental Particles

- Neutron = 1 up + 2 down quarks
  - 1.67492729(28) × 10−27 kg
  - 1.008664915(6) u
  - 939.56536 MeV/c2
- Proton = 2 up + 1 down quark
  - 1.67262171(29) × 10−27 kg
  - 1.007276466(13) u
  - 938.27203 MeV/c2
- Neutron mass > Proton + electron
- Electron – lepton
  - 9.109 382 15(45) × 10^{-31} kg
  - 5.485 799 09(27) × 10^{-4} u
  - 0.51099892 MeV/c^2

931.5MeV/u

Reactions

- Nuclear reactions
  - 1, 2, or 3 (rare) particles
  - Sometimes written like Chemical reactions:

$$ {}^{4}_{2}He + {}^{14}_{7}N \rightarrow {}^{17}_{8}O + {}^{1}_{1}H $$

- For single reactions this is common
- For binary nuclear reactions a more compact nomenclature is typical,

$$ {}^{14}_{7}N(\alpha, p)\,{}^{17}_{8}O $$

Lightest nuclides in parentheses

Note: this is the first nuclear reaction detected, by Rutherford

Nuclear Conservation

- Chemical reactions
  - conserve enthalpy, elements, and total mass.
- Nuclear reactions
  - Don't conserve any of those
  - Do conserve
    - Total energy (mass + kinetic/radiative energy)
    - Nucleons (protons + neutrons)
    - Electrical charge.
  - Note ***sum*** of protons and neutrons (nucleons) is conserved.
  - Electrons <u>**NOT**</u> conserved; charge is.

Parallel reactions

- Chemistry – multiple possible reactions
  - Large quantities of reactants
  - Branching ratios, equilibrium, etc.
- Nuclear – single nuclei at a time
  - Statistical probabilities for various outcomes
- Example, neutron interacting with sulfur
  - ${}^{32}_{16}S(n,n){}^{32}_{16}S$ α%
  - ${}^{32}_{16}S(n,n'){}^{32}_{16}S^{*}$ β% where β=0% if E_n<XX
  - ${}^{32}_{16}S(n,p){}^{32}_{15}P$ δ% where δ =0% if E_n<YY
  - ${}^{32}_{16}S(n,\gamma){}^{33}_{16}S$ (1-α-β-δ)%