Nuclear Physics Tortoise Lecture Series 2026
@Yonsei Univ.

Nuclear Energy-Density Functional Method: From the Basics to the Physics of Exotic Nuclei

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大阪大学
THE UNIVERSITY OF OSAKA

Development of Physics in the 20th Century

1933

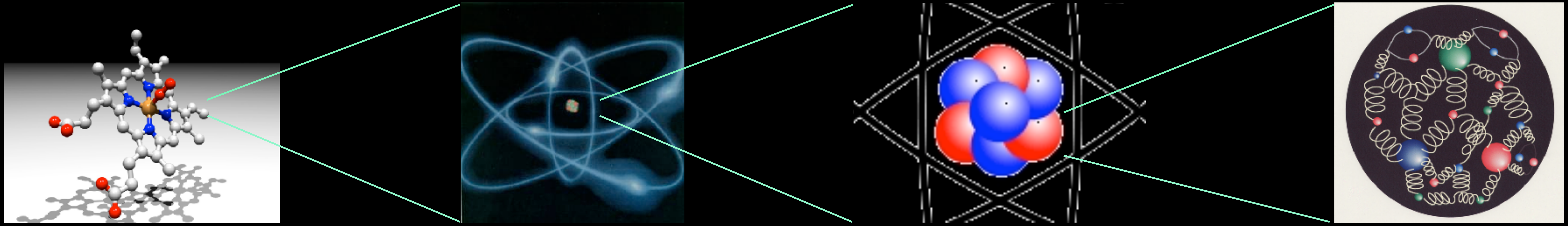
Schrödinger

Dirac

the birth of quantum mechanics

$$\Delta x \cdot \Delta p > \frac{\hbar}{2}$$

higher energy to explore the microscopic world



elementary particles and their interactions

What is the physics in the 21st century?

understanding of the diversity of matter/materials

designing of the quantum world

Quantum many-body problems in nature

Nuclear Physics		Condensed-matter Physics
MeV–GeV fm	scale	eV nm
nucleons, mesons, baryons quarks and gluons	ingredient	electrons
strong	interaction	electromagnetic

$$\hbar c = 200 \text{ MeV fm} = 200 \text{ eV nm}$$

universality and diversity in different hierarchies

From QCD to nuclear physics

The existence of atomic nuclei itself is an amazing emergent behavior!

Quantum Chromodynamics QCD

$$\mathcal{L}_{\mathrm{QCD}} = \bar{q}(i\gamma_\mu D^\mu - m)q - \frac{1}{2}\mathrm{tr}(G^a_{\mu\nu}G^{\mu\nu}_a)$$

2004

asymptotic freedom

Gross

Politzer

Wilczek

↓

pQCD for the internal structure of nucleons

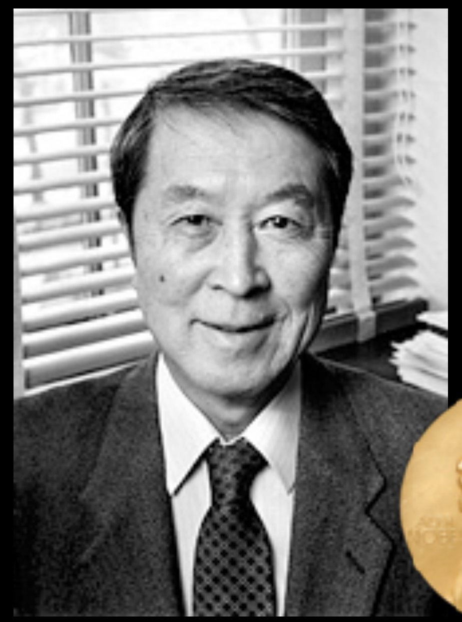
non-perturbative vacuum of QCD

↓ confinement ↓ hadron

↓ SSB of χ-symmetry ↓ pion ↓ nuclear force ↓ **nucleus**

1949

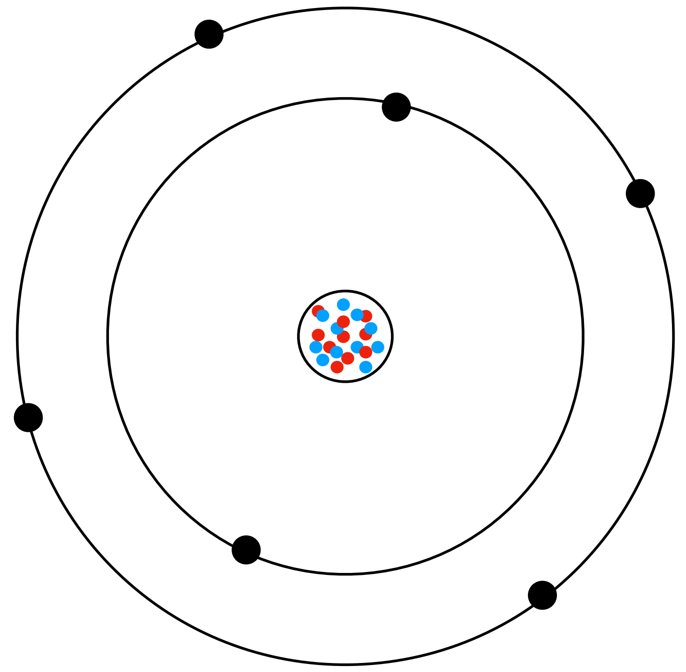
Yukawa



2008

Nambu

Nuclear mass: fundamental properties



- Atomic mass and nuclear mass

$$M(A,Z)c^2 = M_{\mathrm{nucl}}(A,Z)c^2 + Zm_ec^2 - B_{\mathrm{electron}}(Z)$$

atomic mass | nuclear mass | mass of *Z* electrons | electron binding energy

$m_ec^2 = 0.511\ (\mathrm{MeV})$ | a few eV–1 keV

mass excess: $\Delta = M(A,Z) - A \times u$

atomic mass unit: $u = \frac{1}{12}M(12,6) = 931.49\,\mathrm{MeV}/c^2$

- Nuclear biding energy

Nuclear mass $M_{\mathrm{nucl}}(A,Z)c^2 = Zm_pc^2 + Nm_nc^2 - B(A,Z)$

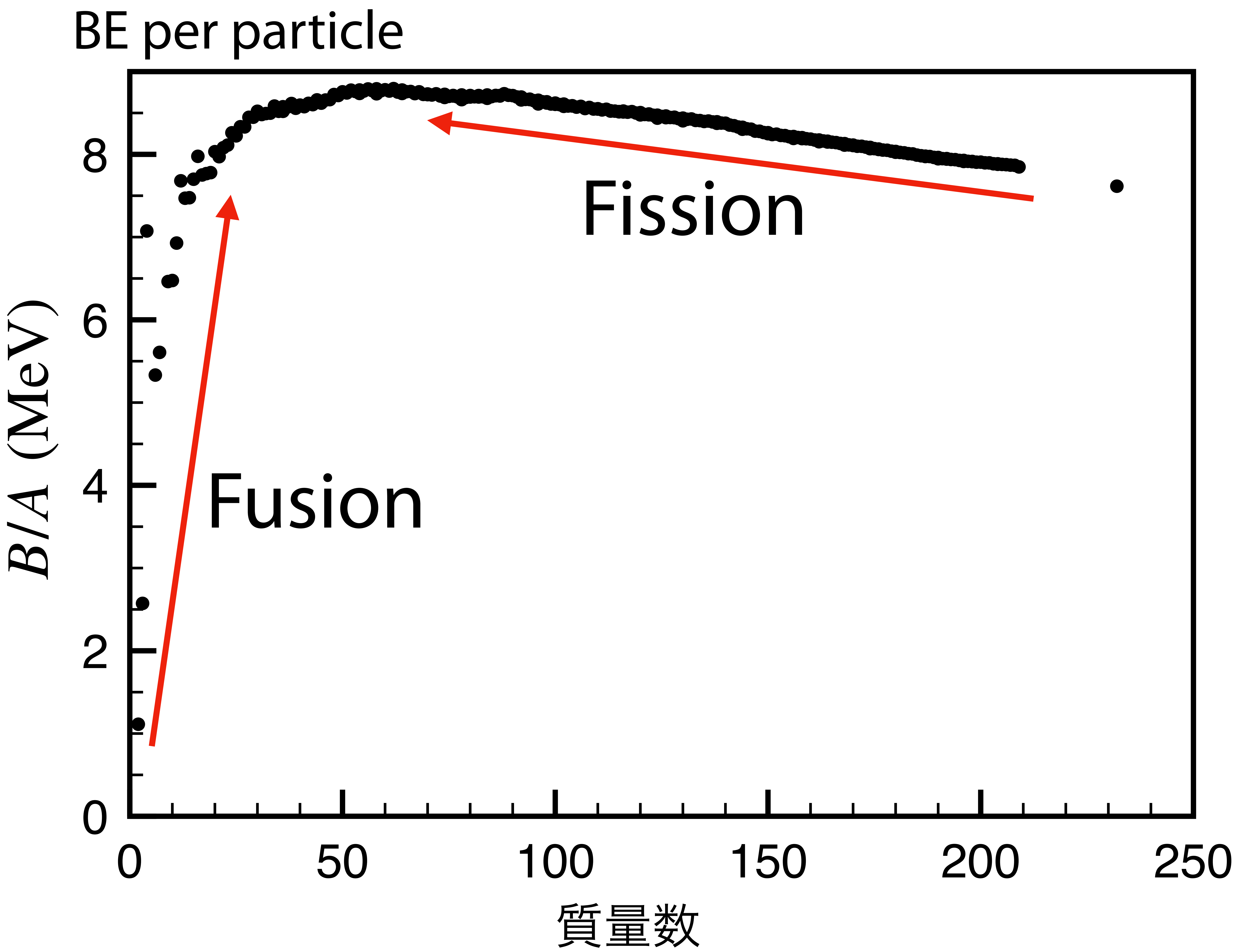
Nuclear biding energy

$$B(A,Z) = Zm_pc^2 + Nm_nc^2 - M_{\mathrm{nucl}}(A,Z)c^2$$

$$= Zm(^1\mathrm{H})c^2 + Nm_nc^2 - M(A,Z)c^2$$

mass of *Z* hydrogen atoms | atomic mass

Nuclear biding energy



Nuclear biding energy

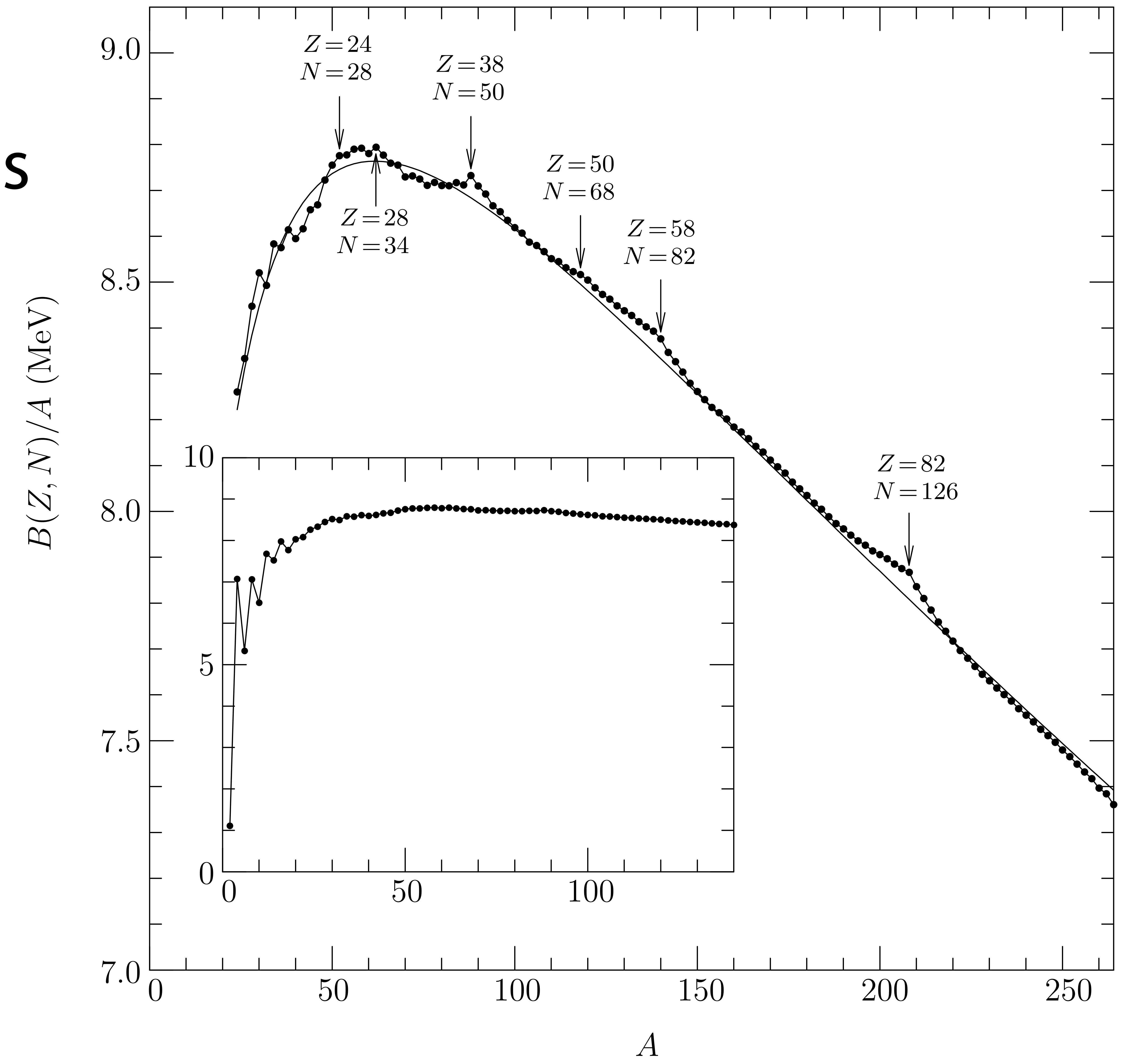
B/A is around 8 MeV

gradual change with some deviations

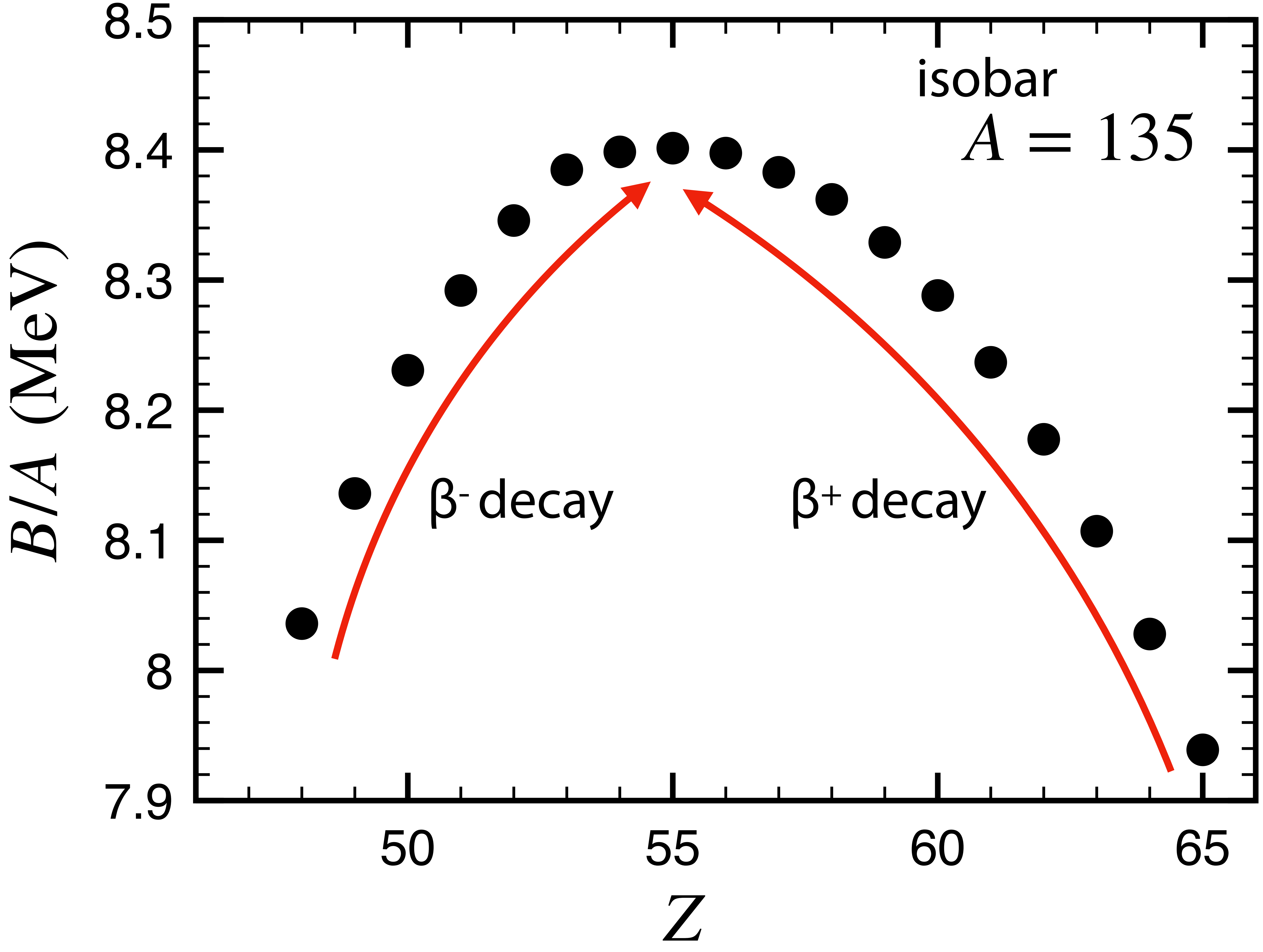
maximum (most stable) at

^{62}Ni: 8.794 MeV

^{58}Fe: 8.792 MeV



Heisenberg’s valley: stability against the beta decay



β- decay

$$n \to p + e^- + \bar{\nu}_e$$

$$(A, Z) \to (A, Z+1) + e^- + \bar{\nu}_e$$

β+ decay

$$p \to n + e^+ + \nu_e$$

$$(A, Z) \to (A, Z-1) + e^+ + \nu_e$$

*does not occur in vacuum

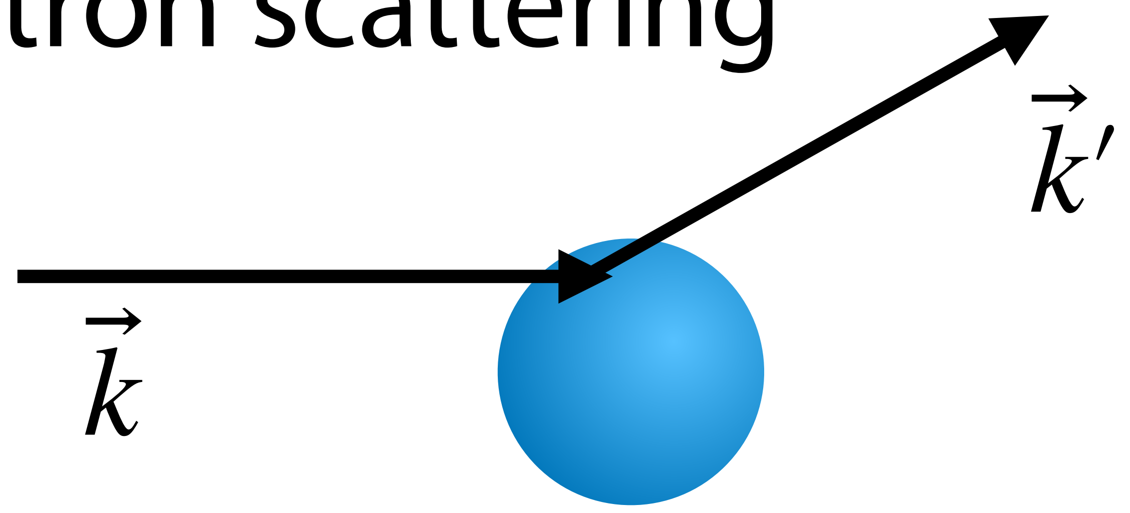
$$m_p < m_n$$

Nuclear density distribution

Rutherford: finding of nucleus with a radius $\sim 10^{-15}\,\mathrm{m}$

Density distribution

- electron scattering



$$\frac{d\sigma}{d\Omega} = \left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{point}} |F(\vec{q})|^2$$

momentum transfer

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

$$F(\vec{q}) \propto \int d\vec{r}\rho(\vec{r})e^{i\vec{q}\cdot\vec{r}}$$

Fourier transform of density

de Broglie wave $\lambda_e = \frac{h}{p} \approx \frac{2\pi\hbar c}{E_e} \sim 6\,\mathrm{fm}$ at $E_e = 200\,\mathrm{MeV}$

- X-rays from muonic atom

Bohr radius : $a_B = \frac{4\pi\varepsilon_0\hbar^2}{e^2 m} \sim 200\,\mathrm{fm}$

$$m_e c^2 = 0.511\,\mathrm{MeV}$$
$$m_\mu c^2 = 106\,\mathrm{MeV}$$

overlap with a nucleus

Coulomb potential: $V_{\mathrm{Coul}}(\vec{r}) = -Z\alpha\int d\vec{r}_N \frac{\rho(\vec{r}_N)}{|\vec{r}-\vec{r}_N|}$

Saturation of density distribution

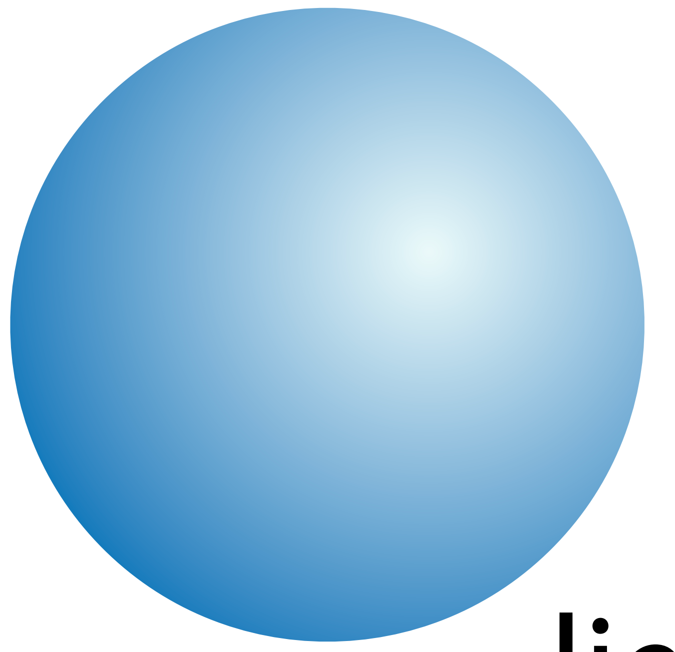
Nuclear radius

$$\boxed{\begin{aligned} R &= r_0 A^{1/3} \\ r_0 &\sim 1.1\ \mathrm{fm} \end{aligned}}$$

Nuclear density

$$\rho_0 = \frac{A}{V} = \frac{A}{\frac{4\pi R^3}{3}} = \frac{1}{\frac{4\pi r_0^3}{3}} \sim 0.17\ \mathrm{fm}^{-3}$$

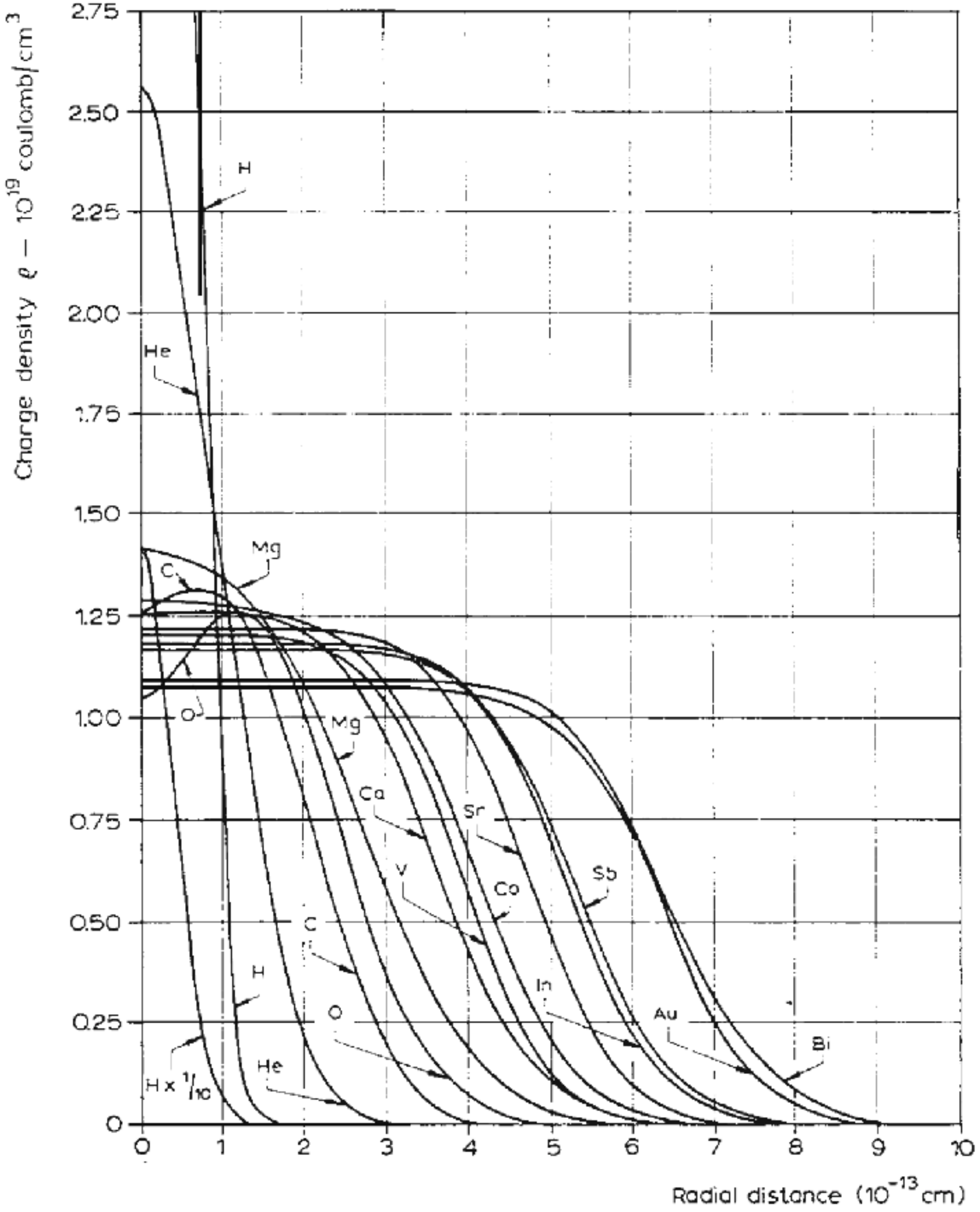
constant



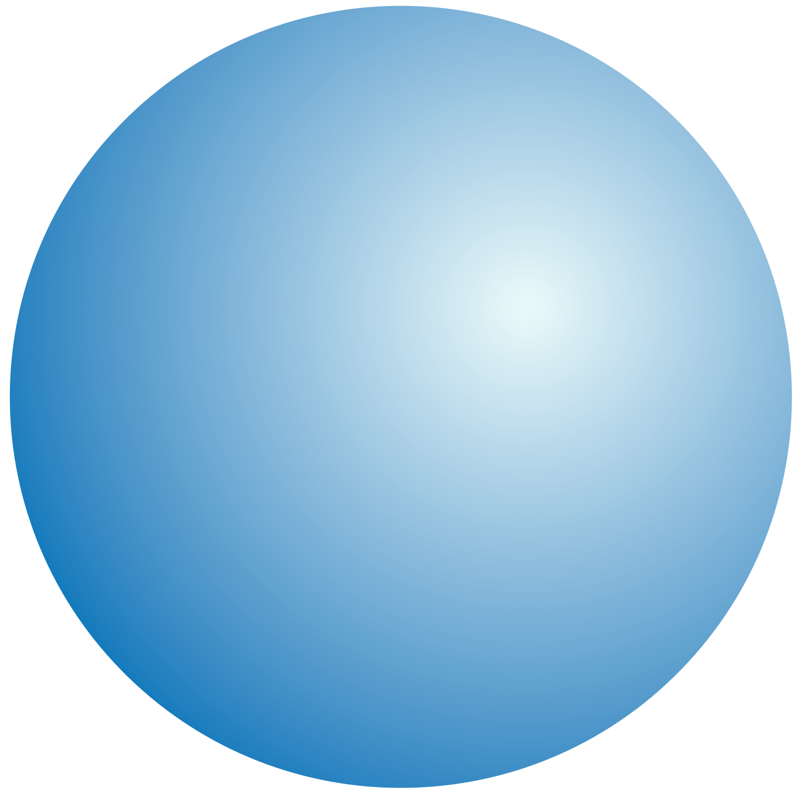
liquid-drop picture

Hofstadter

Nobel lecture (1961)



Liquid drop model



Binding energy = [volume term] — liquid part (matter)

+[surface term] — finite-size effect

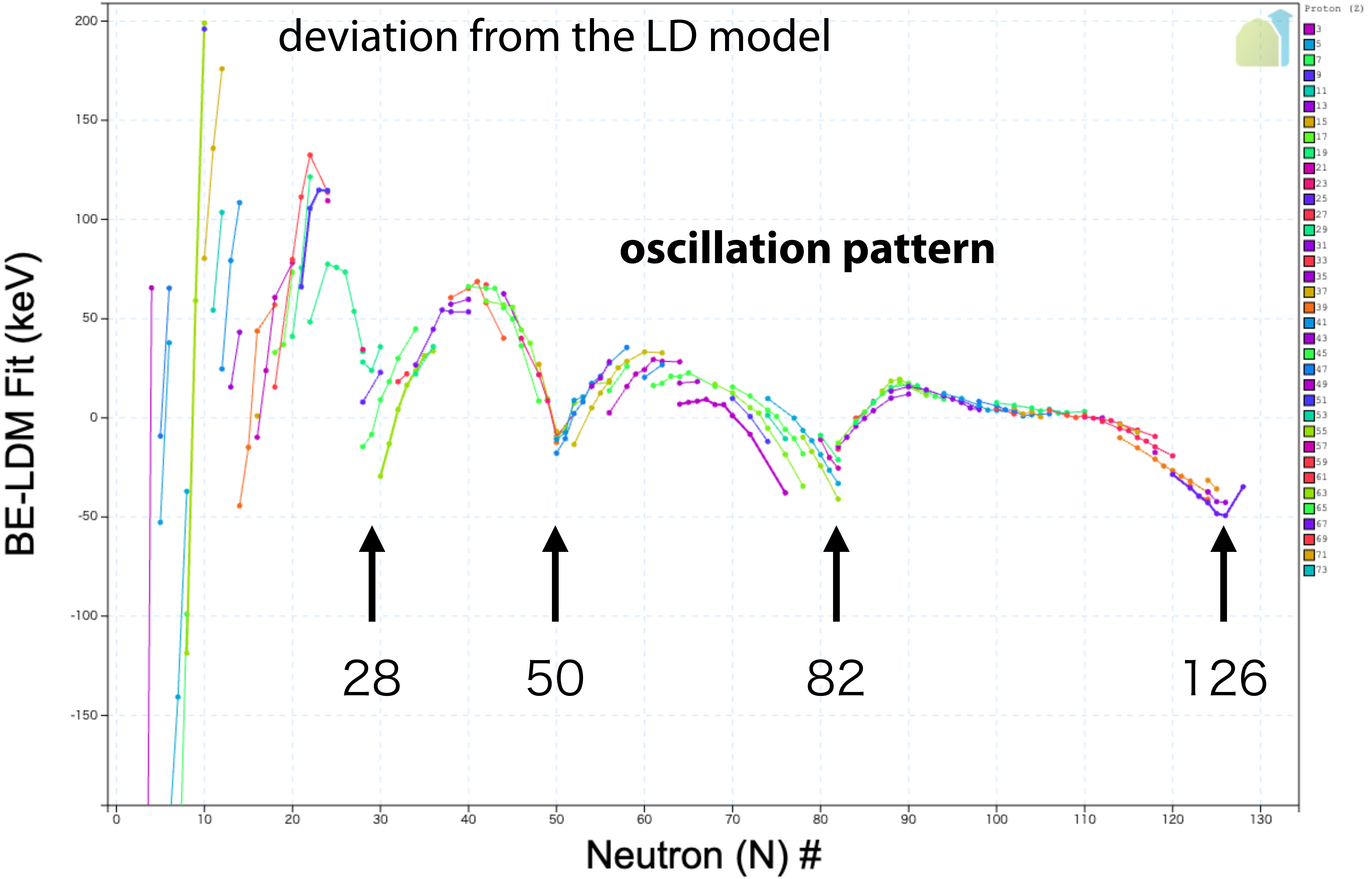
+[symmetry energy] — stable along N=Z

+[Coulomb energy] — charged system

$$\boxed{B(A,Z) = a_{\mathrm{vol}}A - a_{\mathrm{surf}}A^{2/3} - a_{\mathrm{sym}}\frac{(N-Z)^2}{A} - a_{\mathrm{Coul}}\frac{Z^2}{A^{1/3}} + \delta(A)}$$

Bethe–Weizsäcker

Quantum effect in BE



Magic number

For neutrons

$$N = 2,8,20,28,50,82,126$$

For protons

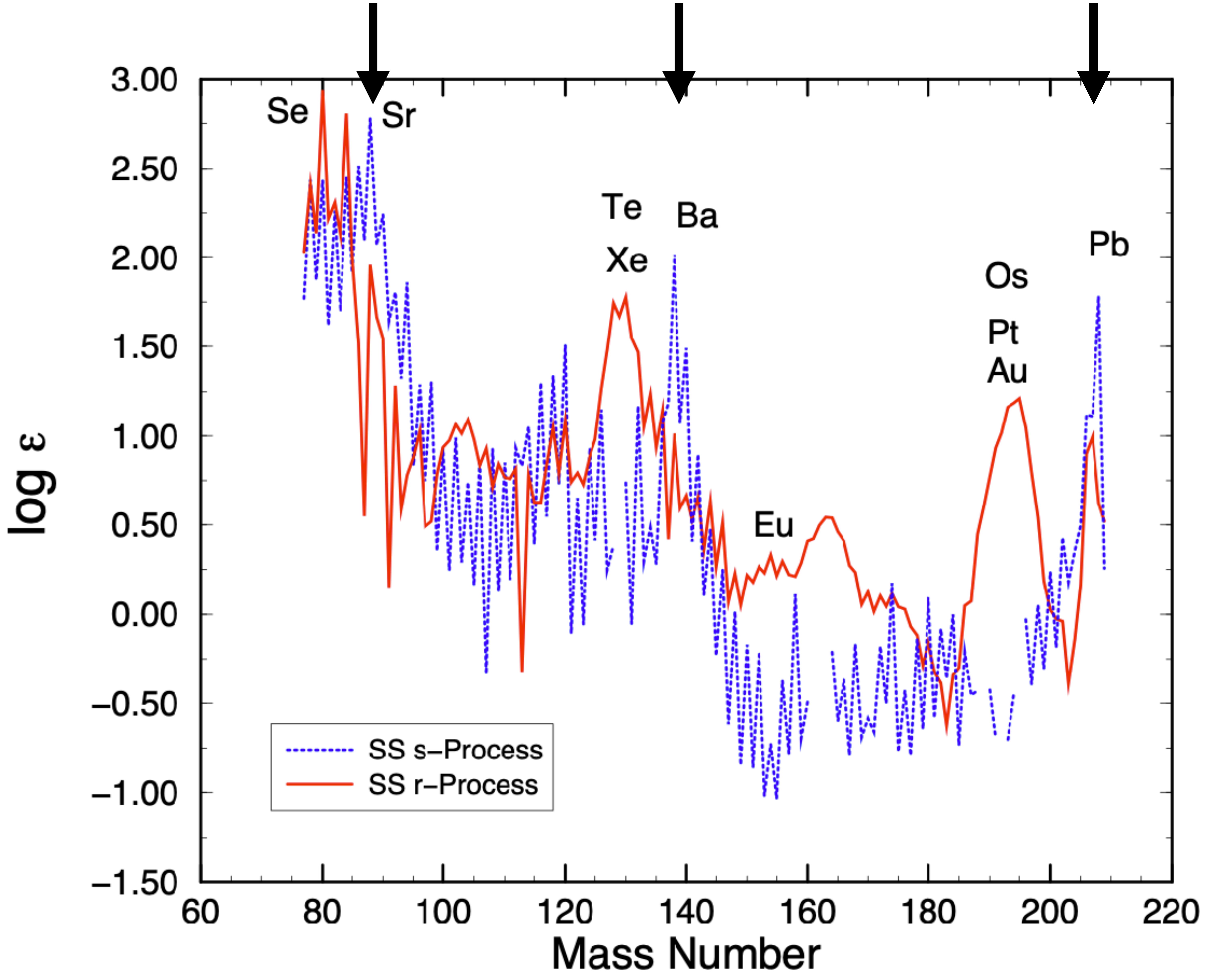
$$Z = 2,8,20,28,50,82$$

When the number of nucleons equals these magic numbers,

the nucleus exhibits special properties.

An example of the quantum effects

solar-system elemental abundances



high abundance with
$A \sim 90,140,210$

corresponding to
$N = 50,82,126$

Cowan and Sneden

Limit of existence: stability against particle emission

Neutron separation energy

$$S_n(N,Z) = M(N-1,Z)c^2 + m_n c^2 - M(N,Z)c^2 = B(N,Z) - B(N-1,Z)$$

Proton separation energy

$$S_p(N,Z) = M(N,Z-1)c^2 + m_p c^2 - M(N,Z)c^2 = B(N,Z) - B(N,Z-1)$$

$S_n \simeq S_p \sim 8\,\mathrm{MeV}$ due to $B(N,Z)/A \sim 8\,\mathrm{MeV}$

decreasing S_n as increasing the neutron number in isotopes

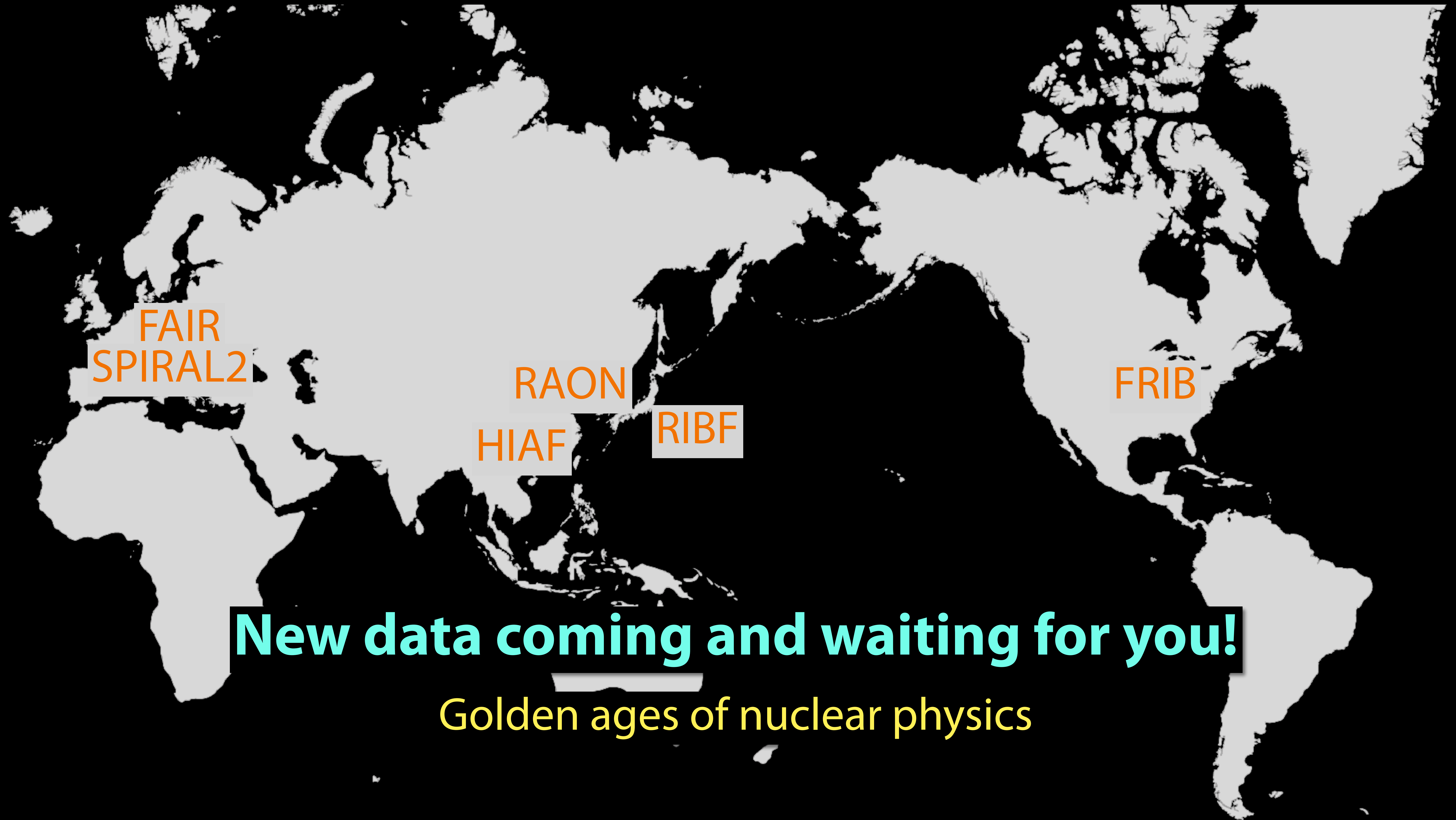
decreasing S_p as increasing the proton number in isotones

$S_n = 0$: limit against neutron emission

$S_p = 0$: limit against proton emission

drip line

Radioactive beam facilities under operation/construction



New data coming and waiting for you!

Golden ages of nuclear physics

RIKEN RI Beam Factory: RIBF since 2007

Rich phenomena revealed by RIBF

220 new isotopes discovered at RIKEN

32: pre-RIBF

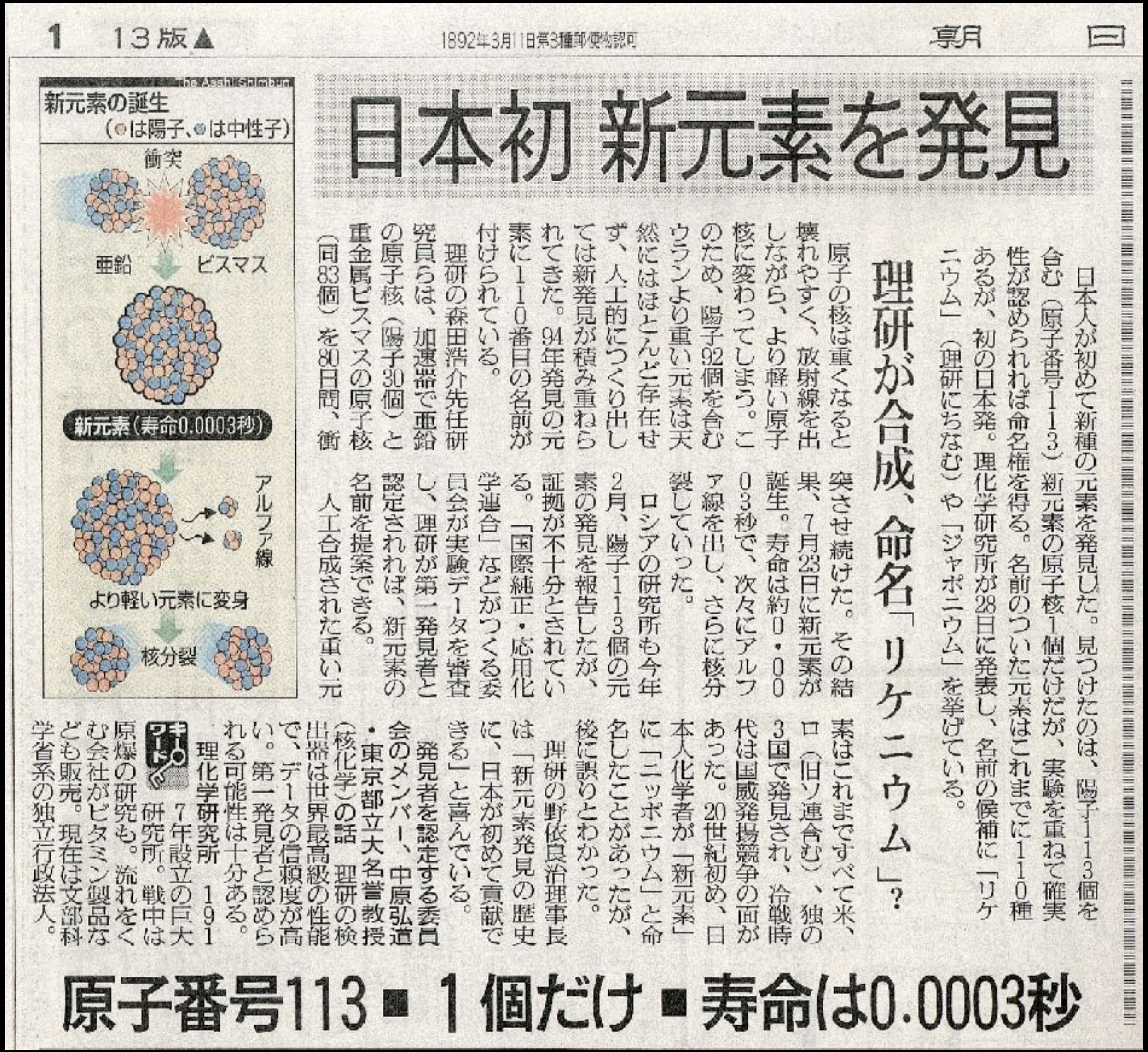
136: 2007–2017

52: 2018–

new insights into nuclei

A new element: the limit of heavy mass

The Asahi (Sep. 29, 2004)



1　13版▲　1892年3月11日第3種郵便物認可　朝日

日本初　新元素を発見

原子番号113■1個だけ■寿命は0.0003秒

日本人が初めて新種の元素を発見した。見つけたのは、陽子113個を含む（原子番号113）新元素の原子核1個だけだが、実験を重ねて確実性が認められれば命名権を得る。名前のついた元素はこれまでに110種あるが、初の日本発。理化学研究所が28日に発表し、名前の候補に「リケニウム」（理研にちなむ）や「ジャポニウム」を挙げている。

理研が合成、命名「リケニウム」？

原子の核は重くなると壊れやすく、放射線を出しながら、より軽い原子核に変わってしまう。このため、陽子92個を含むウランより重い元素は天然にはほとんど存在せず、人工的につくり出しては新発見が積み重ねられてきた。94年発見の元素に110番目の名前が付けられている。

理研の森田浩介先任研究員らは、加速器で亜鉛の原子核（陽子30個）と重金属ビスマスの原子核（同83個）を80日間、衝突させ続けた。その結果、7月23日に新元素が誕生。寿命は約0・0003秒で、次々にアルファ線を出し、さらに核分裂していった。

ロシアの研究所も今年2月、陽子113個の元素の発見を報告したが、証拠が不十分とされている。「国際純正・応用化学連合」などがつくる委員会が実験データを審査し、理研が第一発見者と認定されれば、新元素の名前を提案できる。

人工合成された重い元素はこれまですべて米、独、ロ（旧ソ連含む）の3国で発見され、冷戦時代は国威発揚競争の面があった。20世紀初め、日本人化学者が「新元素」に「ニッポニウム」と命名したことがあったが、後に誤りとわかった。

理研の野依良治理事長は「新元素発見の歴史に、日本が初めて貢献できる」と喜んでいる。

発見者を認定する委員会のメンバー、中原弘道・東京都立大名誉教授（核化学）の話　理研の検出器は世界最高級の性能で、データの信頼度が高い。第一発見者と認められる可能性は十分ある。

キーワード　理化学研究所　1917年設立の巨大研究所。戦中は原爆の研究も。流れをくむ会社がビタミン製品なども販売。現在は文部科学省系の独立行政法人。

新元素の誕生
（●は陽子、●は中性子）
衝突
亜鉛　ビスマス
新元素（寿命0.0003秒）
アルファ線
より軽い元素に変身
核分裂

Prof. Morita (RIKEN/Kyushu)

Sep. 27, 2012

the third event

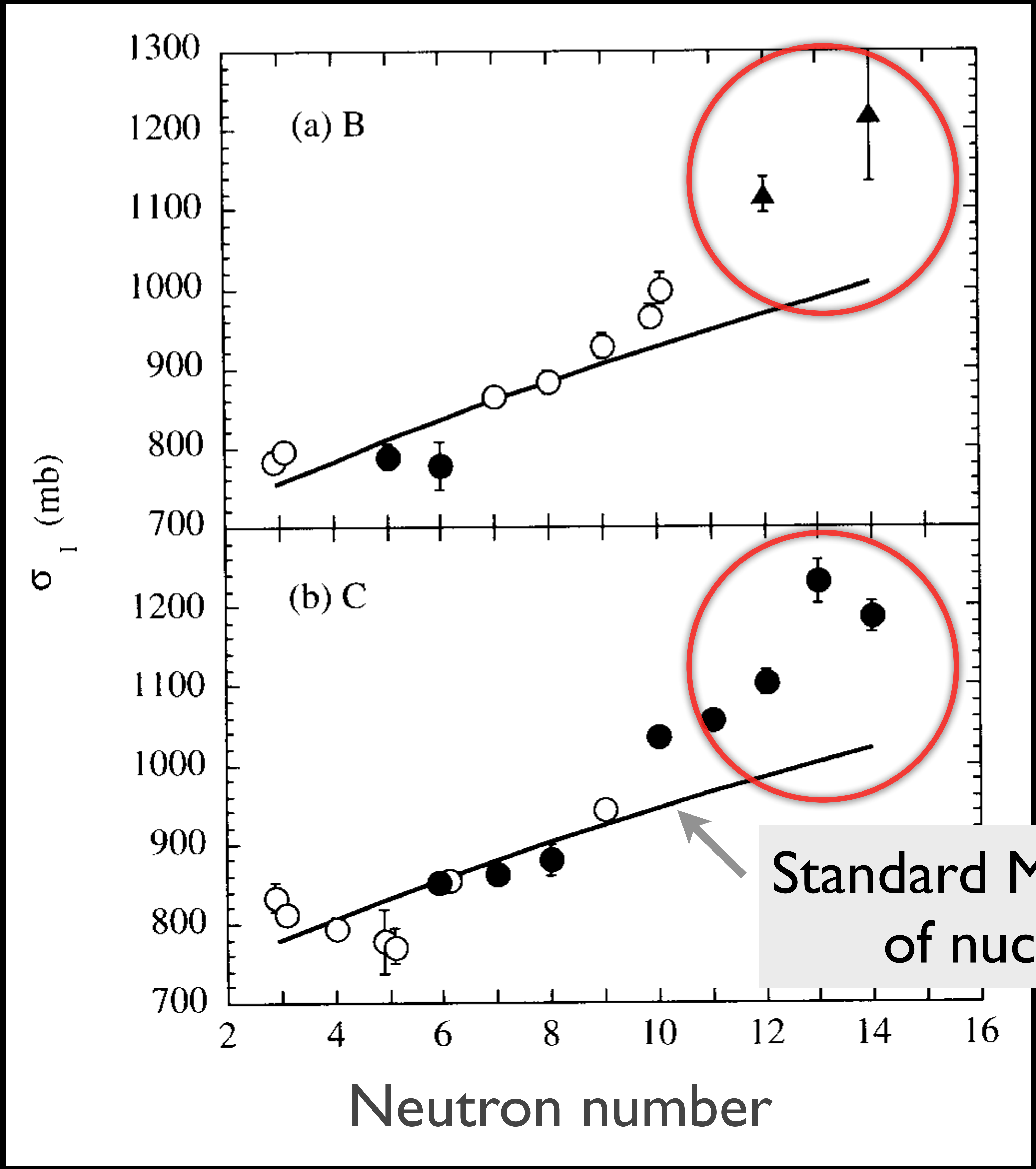
November, 2016

the element 113 named Nihonium

Neutron-rich nuclei out of the «common sense»

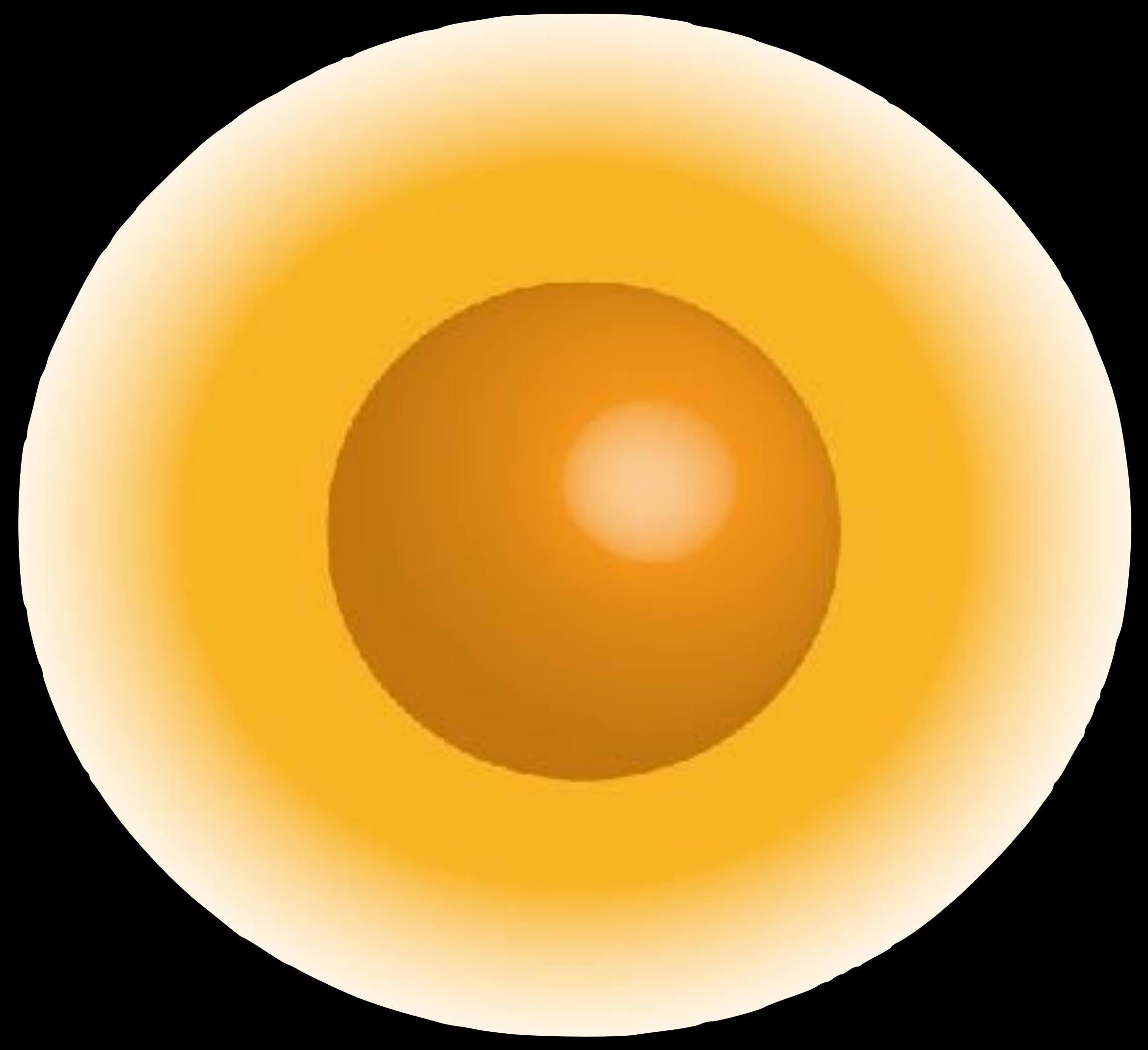
A. Ozawa *et al.*, Nucl. Phys. A691 (2001) 599

Size



Standard Model prediction
of nuclear physics

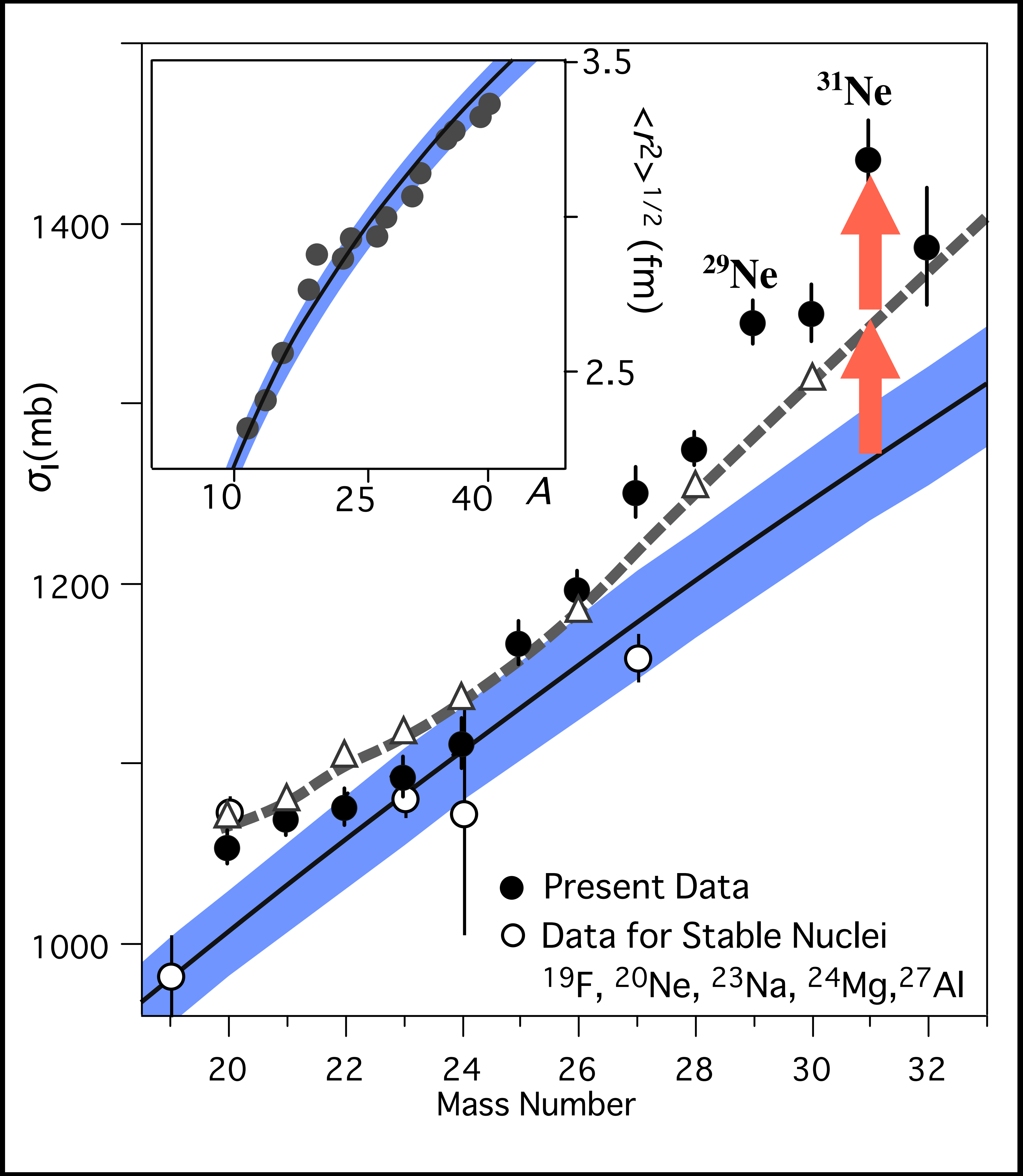
neutron halo



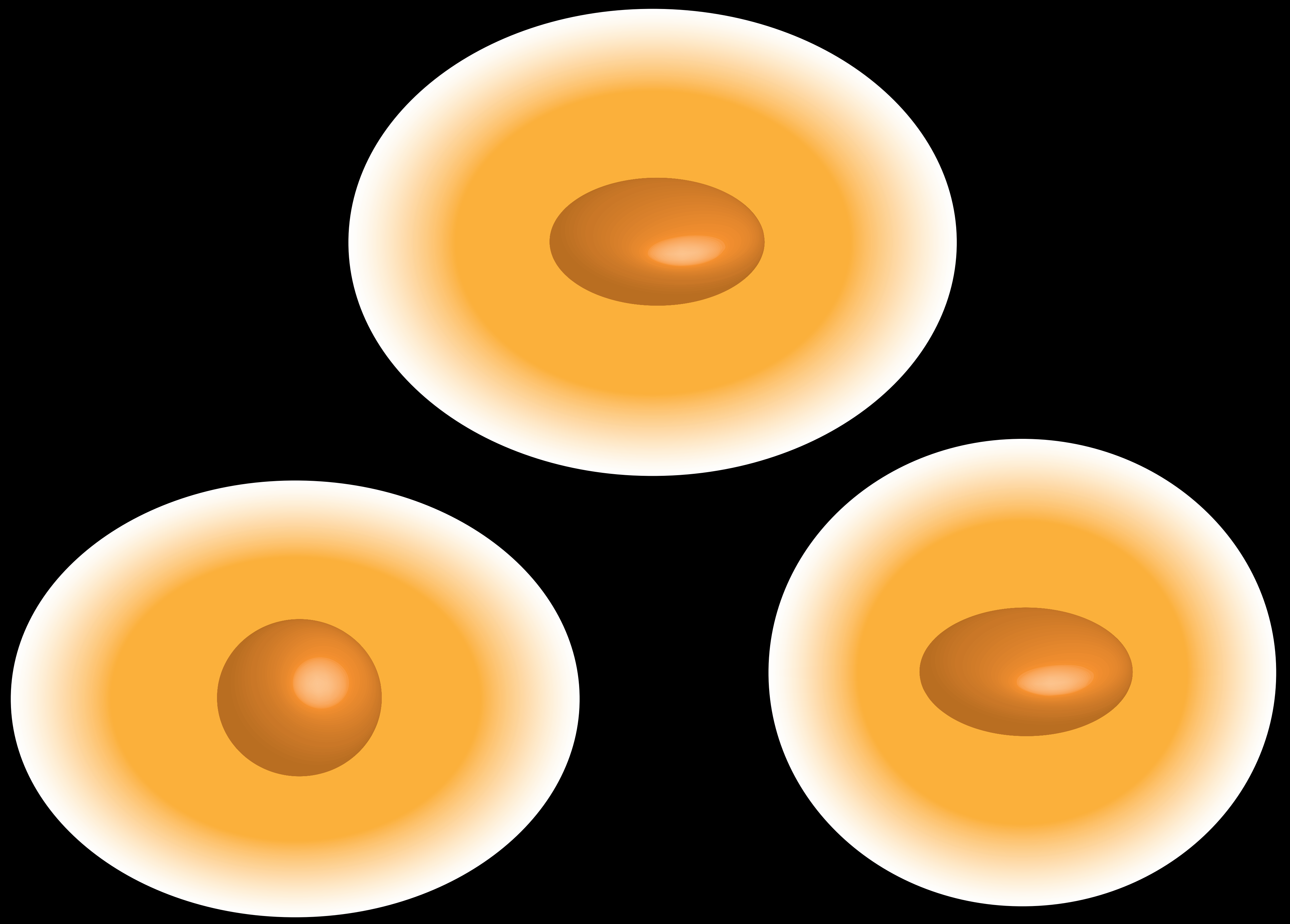
low-density neutrons
a new degree of freedom

Discovery of "deformed halo"

M. Takechi *et al*., Phys. Lett. B707 (2012) 357



systematics considering the deformation



still a mystery

Quest for the origin of heavy elements beyond Fe and Ni

Neutrons play a key role: Protons feel the repulsive Coulomb force

$$
\begin{aligned}
{}^{A}_{Z}\mathrm{X}_{N} + n &\rightarrow {}^{A+1}_{Z}\mathrm{X}_{N+1} + \gamma && (1) \\
{}^{A+1}_{Z}\mathrm{X}_{N+1} &\rightarrow {}^{A+1}_{Z+1}\mathrm{Y}_{N} + e^{-} + \bar{\nu}_e && (2)
\end{aligned}
$$

Neutron-rich nuclei are created by the neutron capture (1)

The beta-decay increases the atomic number (2)

neutron-rich environment: Supernova explosion, neutron-star mergers

gravitational-wave observation

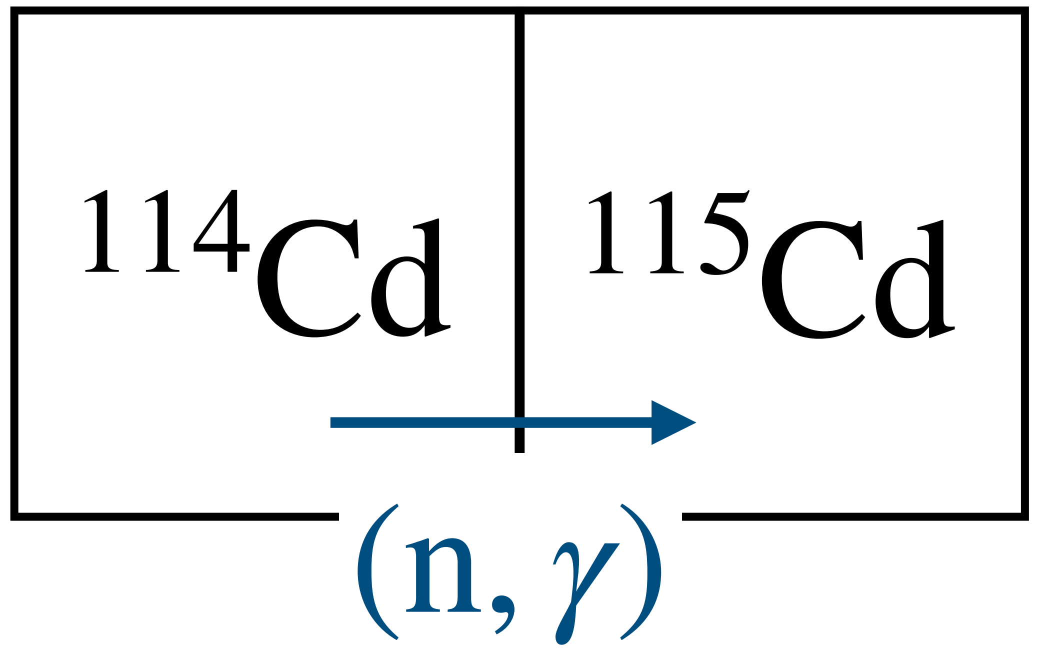
Nucleosynthesis induced by neutron capture

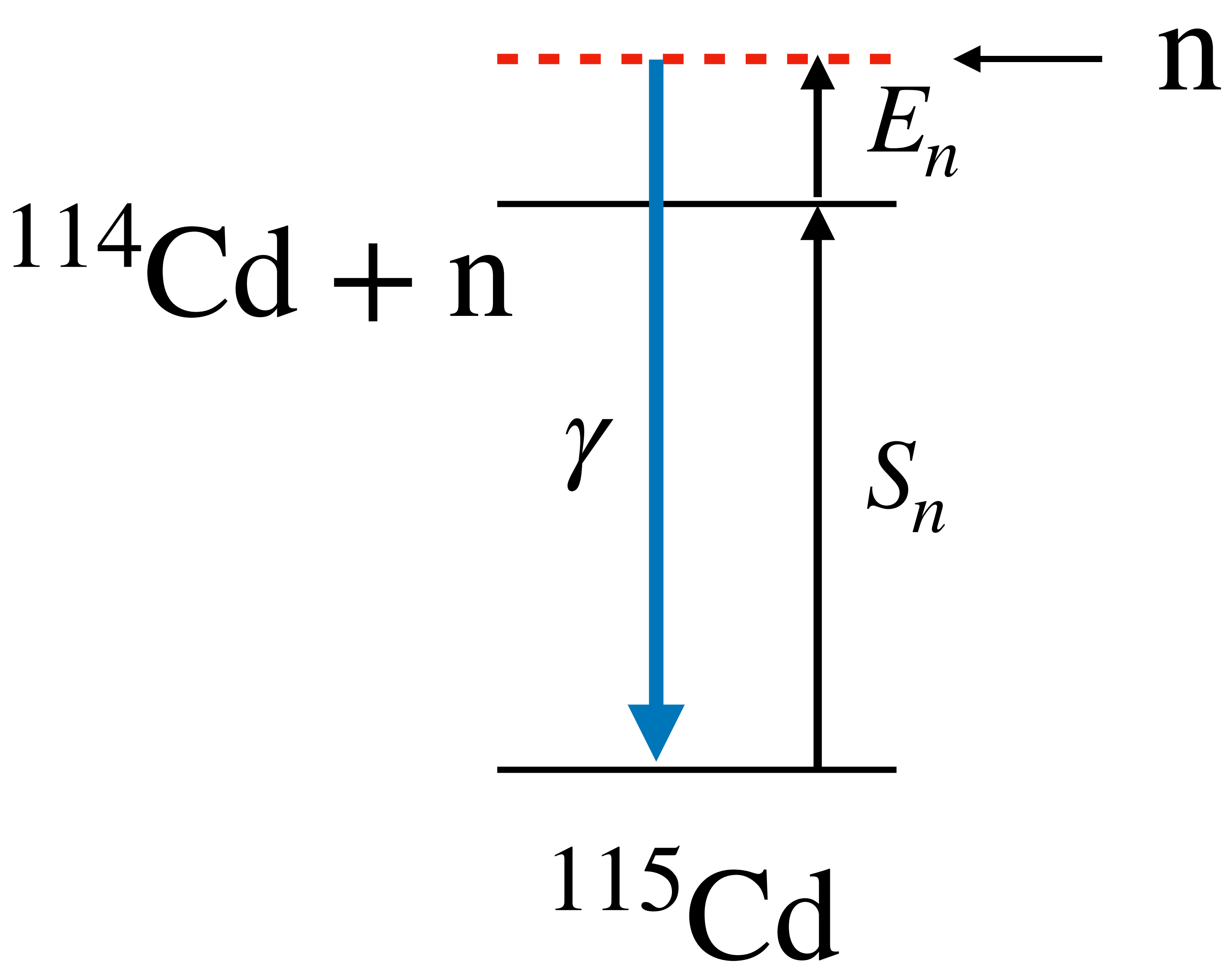
Ex.

$$^{114}_{48}\mathrm{Cd}_{66} + \mathrm{n} \rightarrow {}^{115}_{48}\mathrm{Cd}^{*}_{67} \rightarrow {}^{115}_{48}\mathrm{Cd}_{67}(\mathrm{gs}) + \gamma$$

(n, γ) reaction

on the nuclear chart

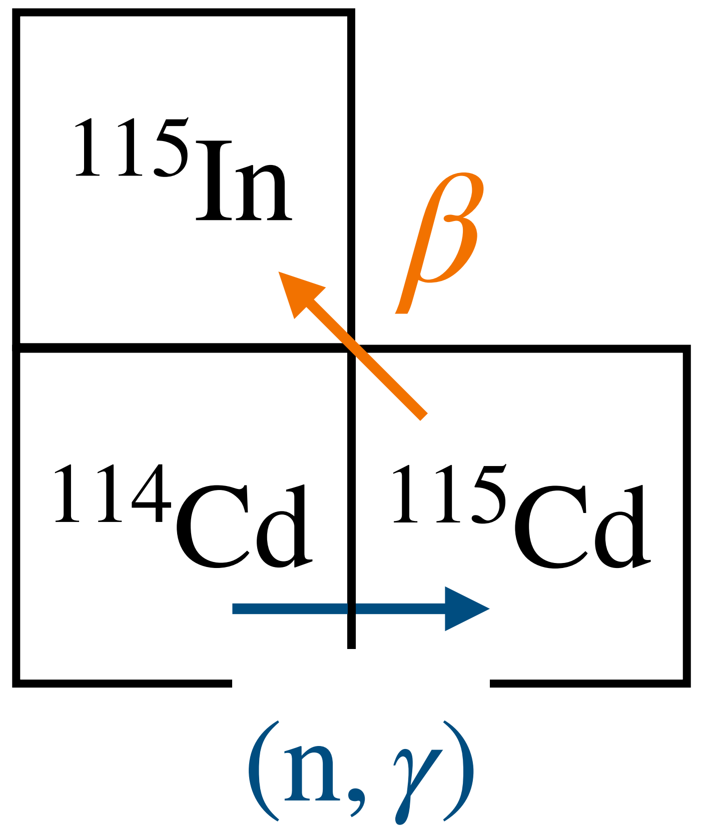




After capturing a neutron

- n-capture is ***slower*** than beta decay

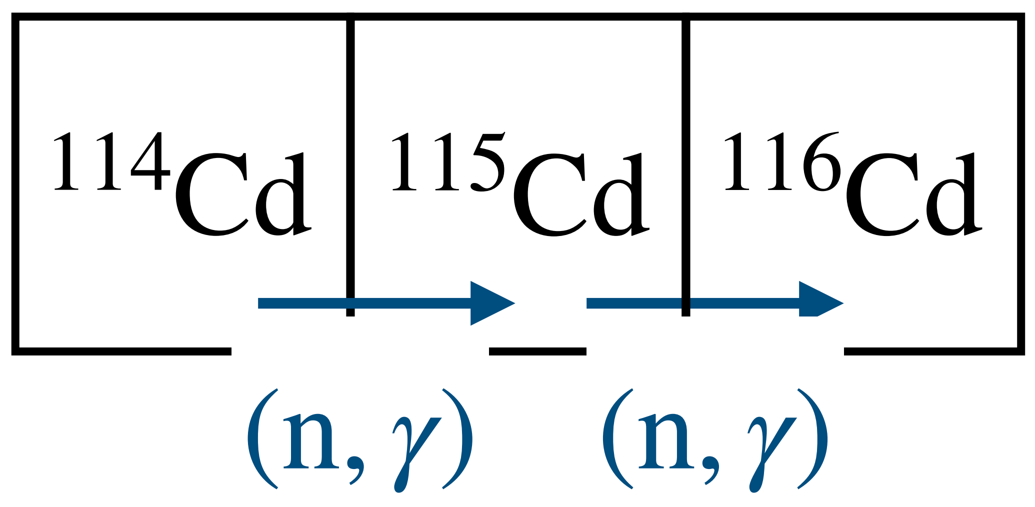
$$^{114}\mathrm{Cd} \rightarrow {}^{115}\mathrm{Cd} \rightarrow {}^{115}\mathrm{In}$$



s(low)-process

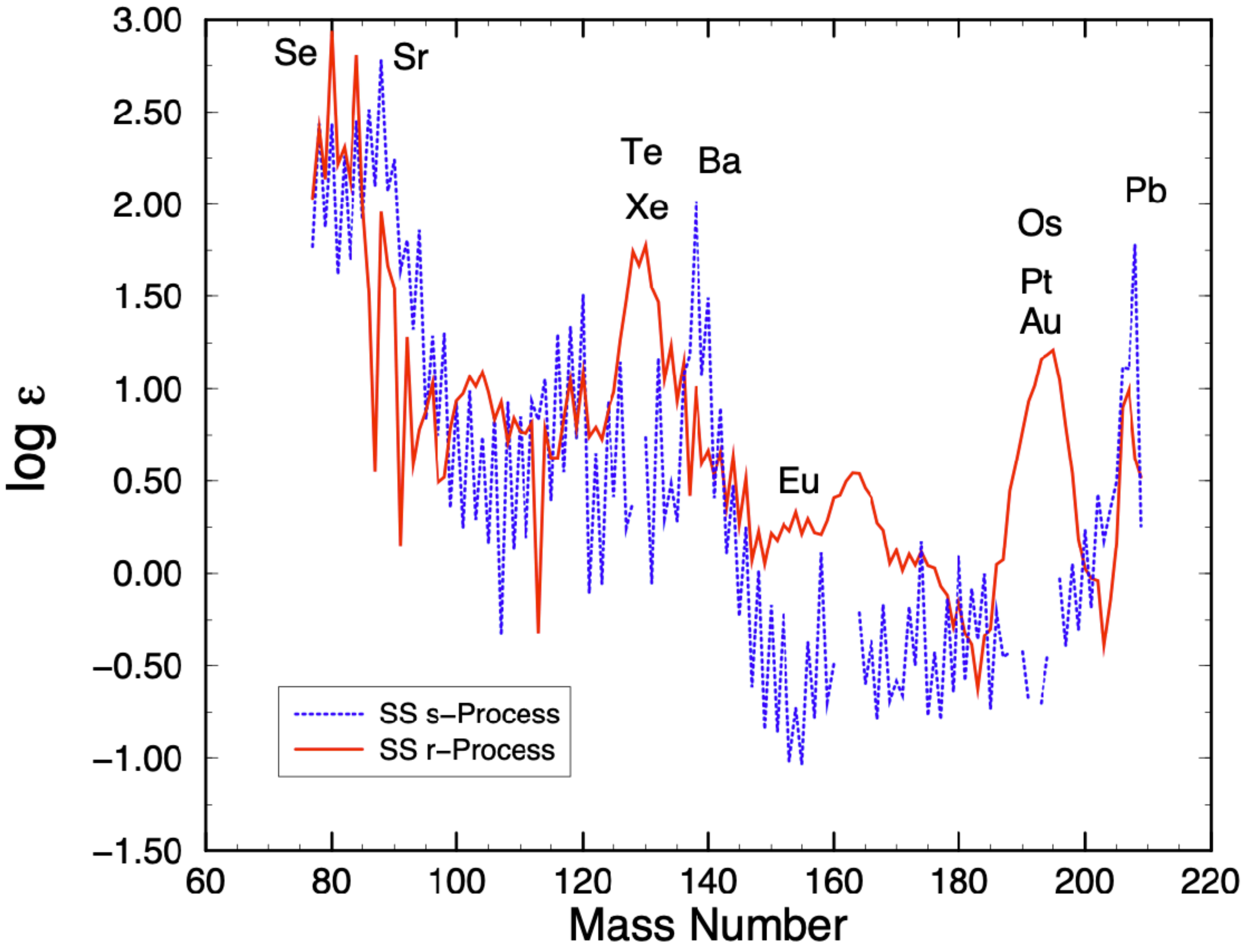
- n-capture is ***faster*** than beta decay

$$^{114}\mathrm{Cd} \rightarrow {}^{115}\mathrm{Cd} \rightarrow {}^{116}\mathrm{Cd}$$



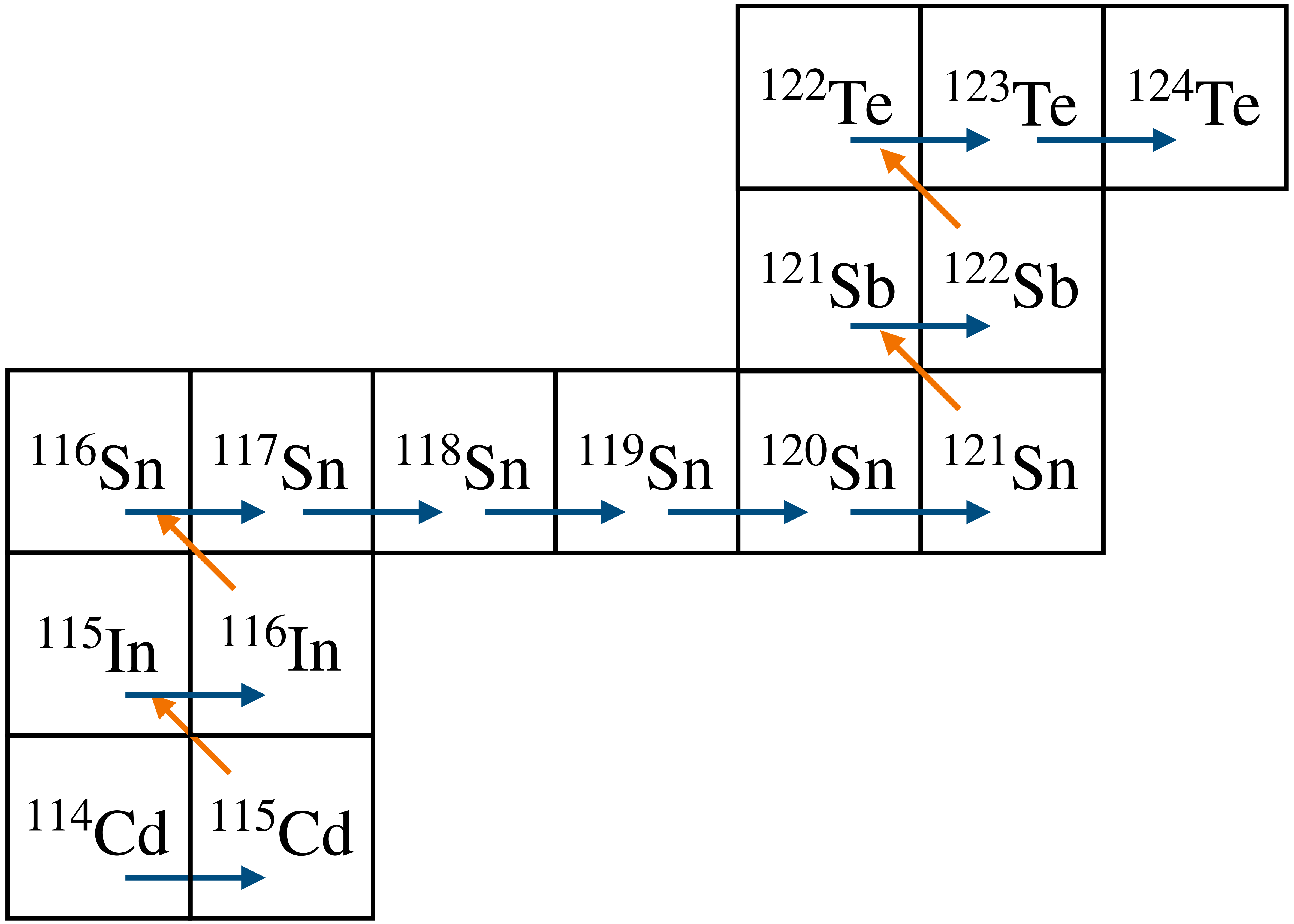
r(apid)-process

Two-peak structure in the solar-system elemental abundances



Cowan and Sneden

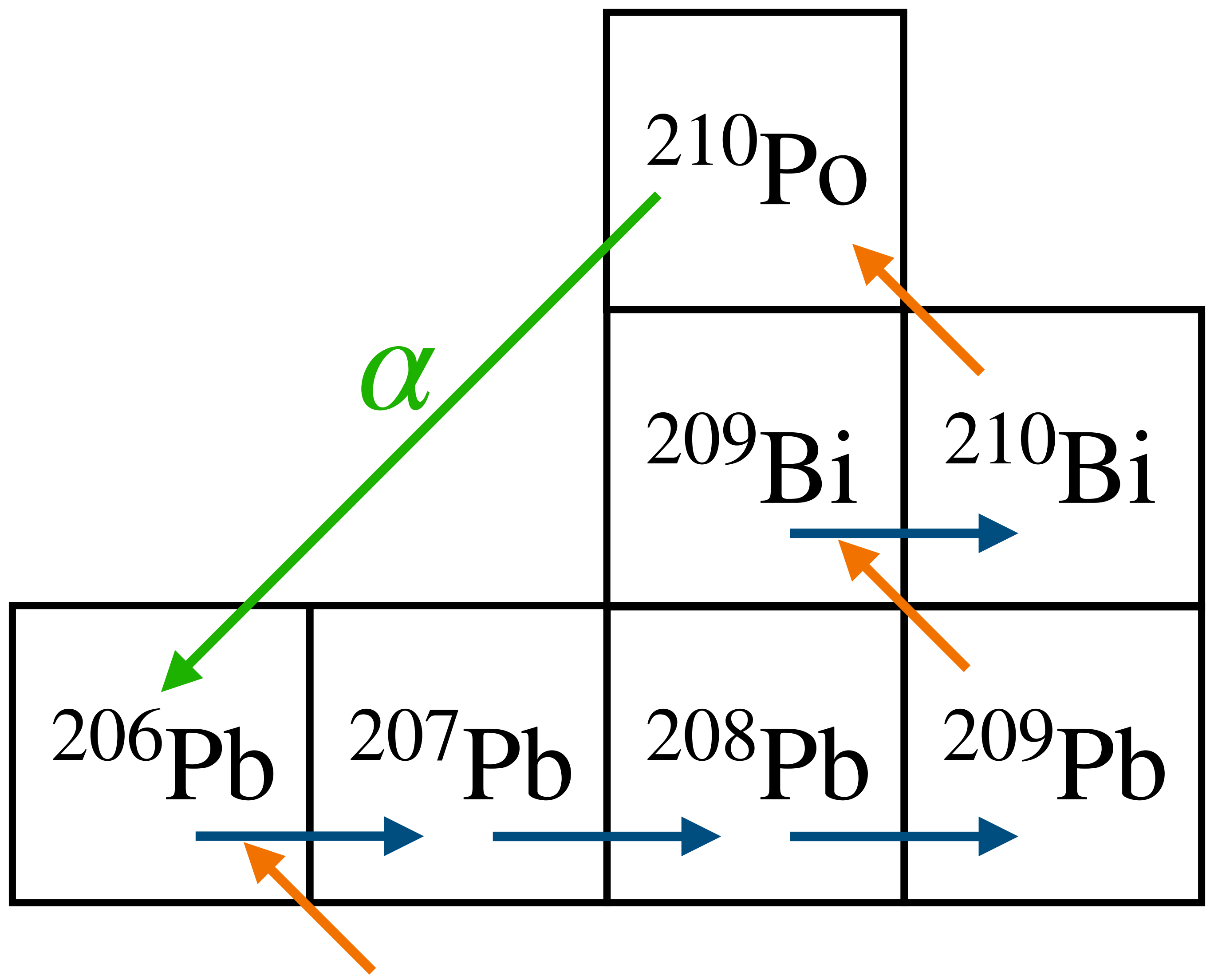
s-process nucleosynthesis



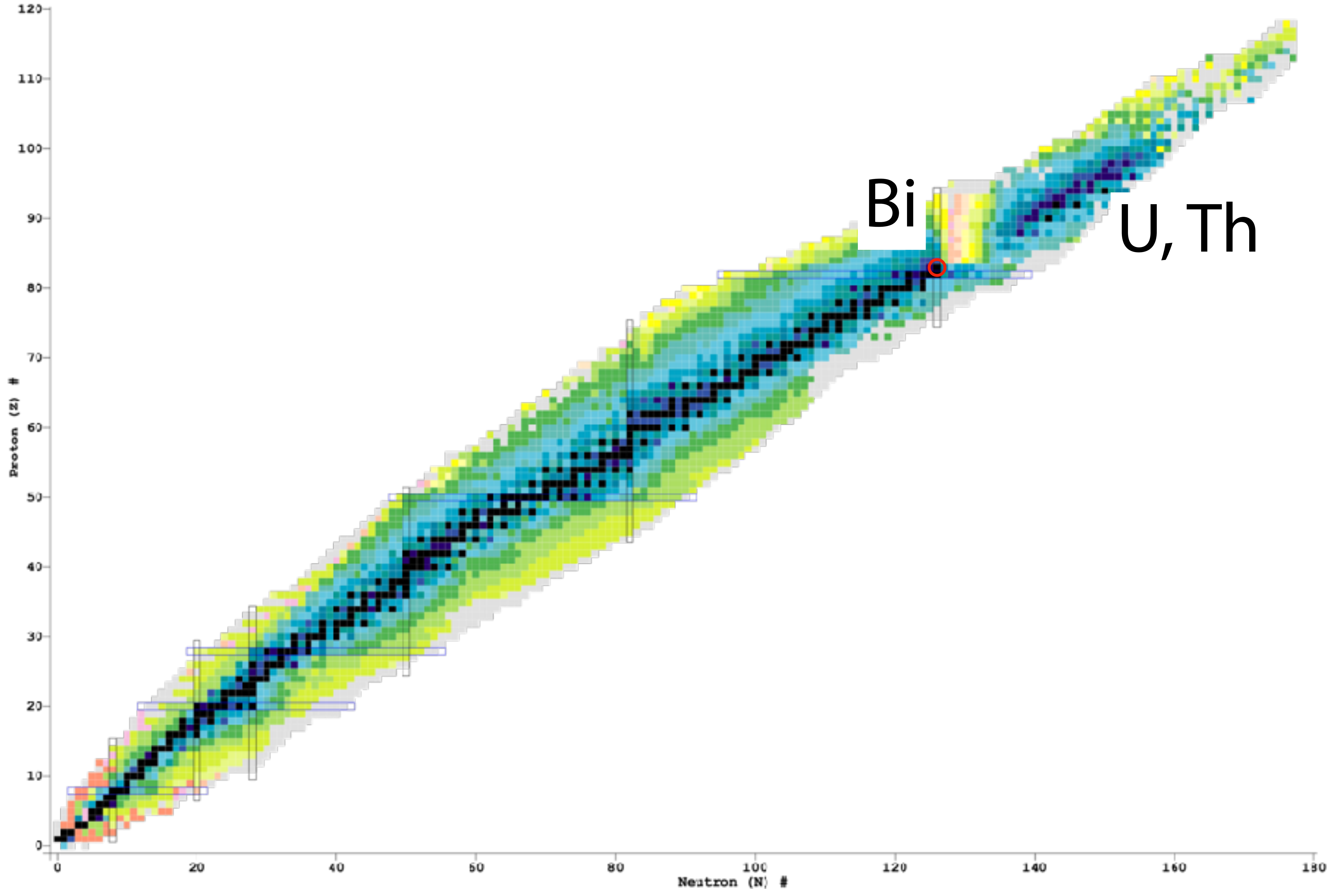
Element synthesis proceeds along the valley of stability.

s-process nucleosynthesis

termination of the s-process



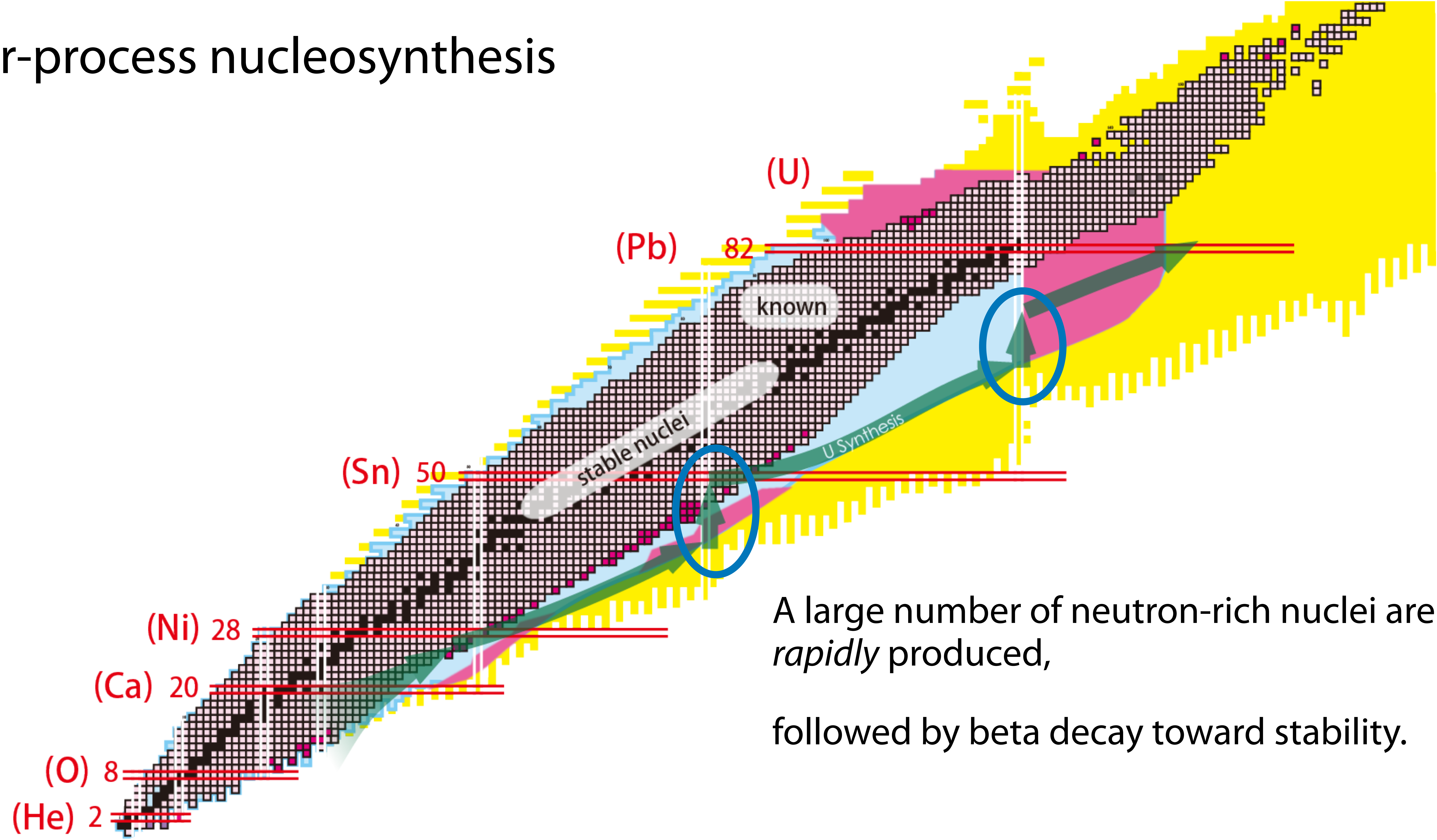
up to ^{209}Bi



does not reach U and Th

r-process

r-process nucleosynthesis

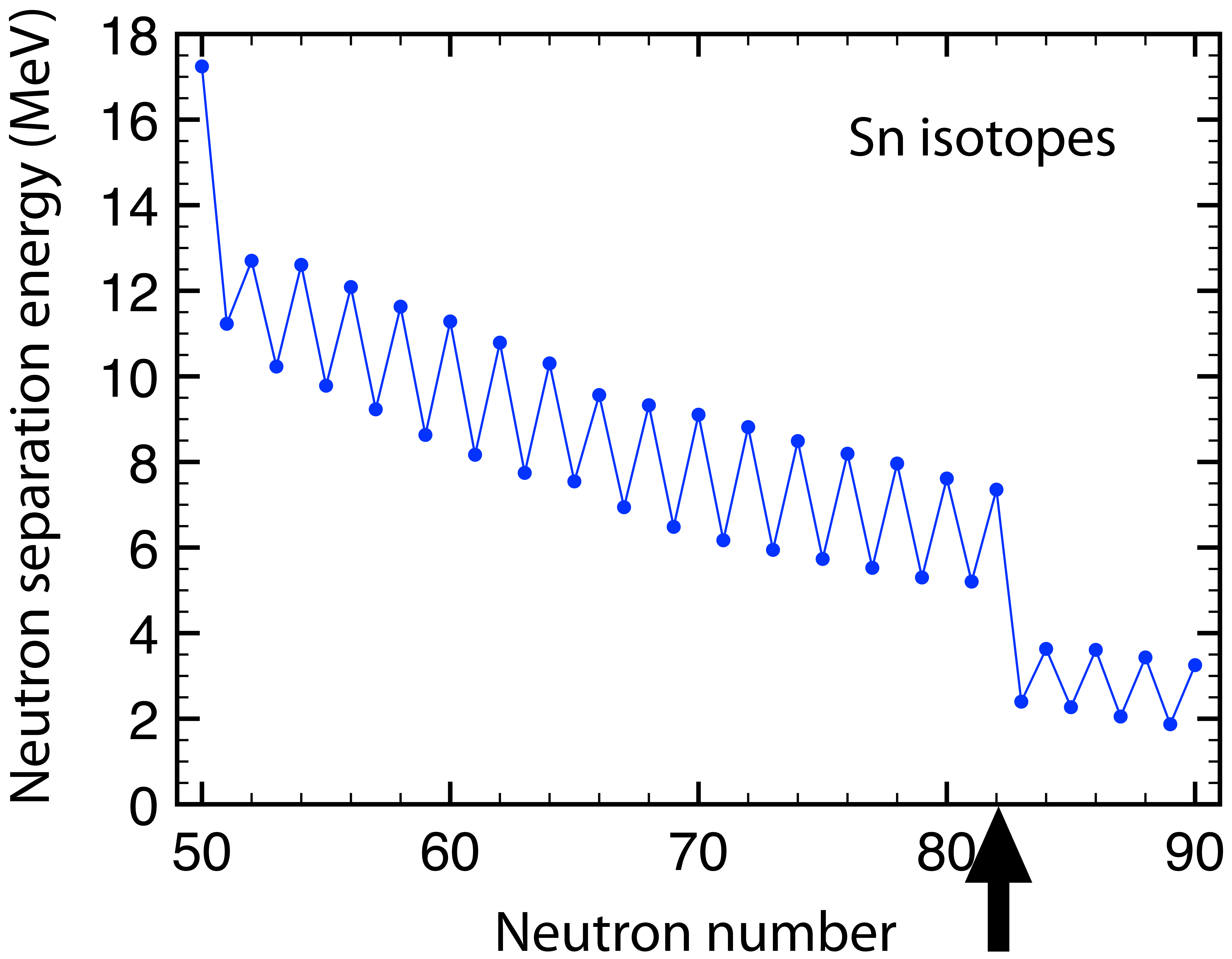


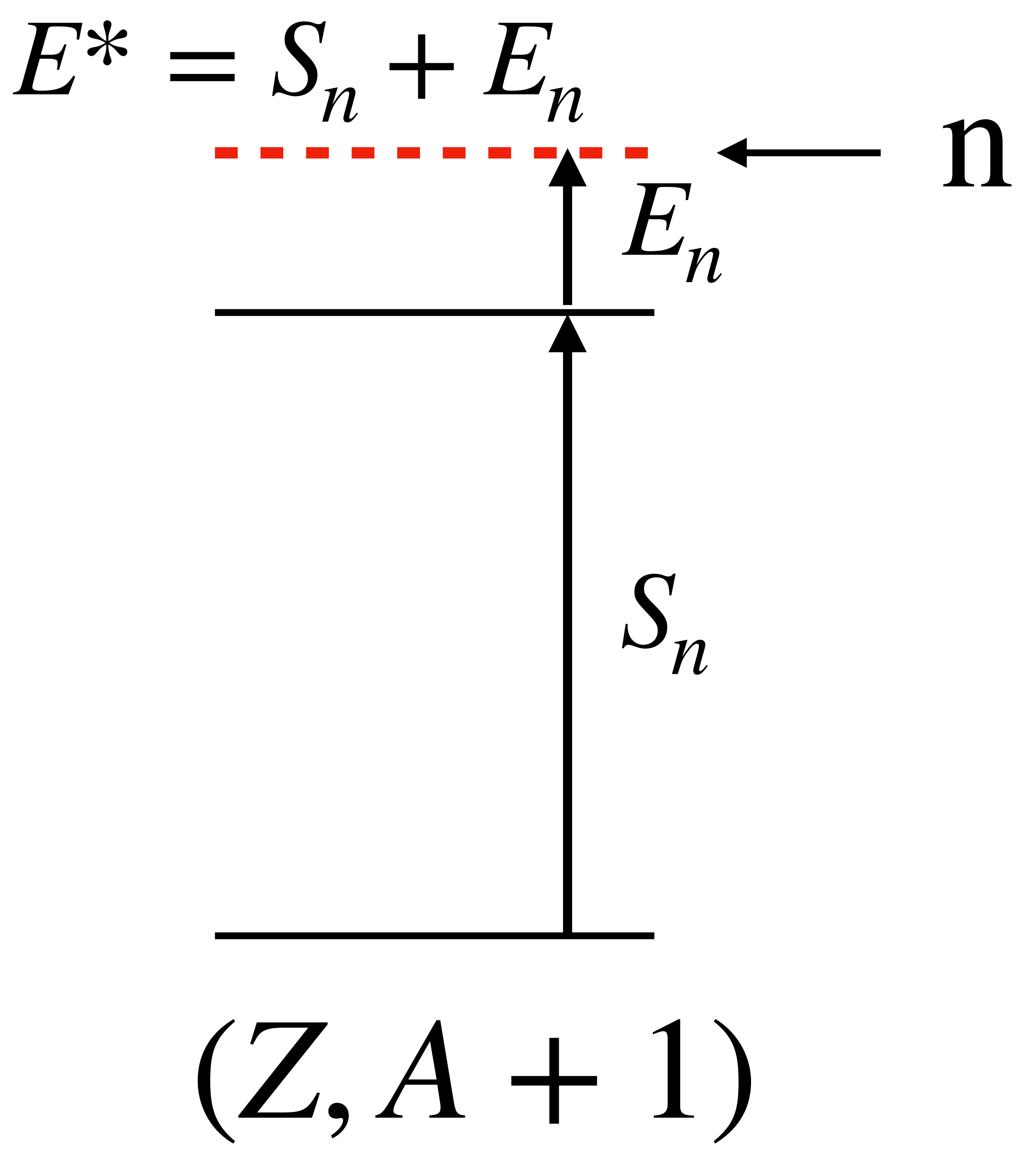
A large number of neutron-rich nuclei are *rapidly* produced,

followed by beta decay toward stability.

waiting point nuclei

low capture rate

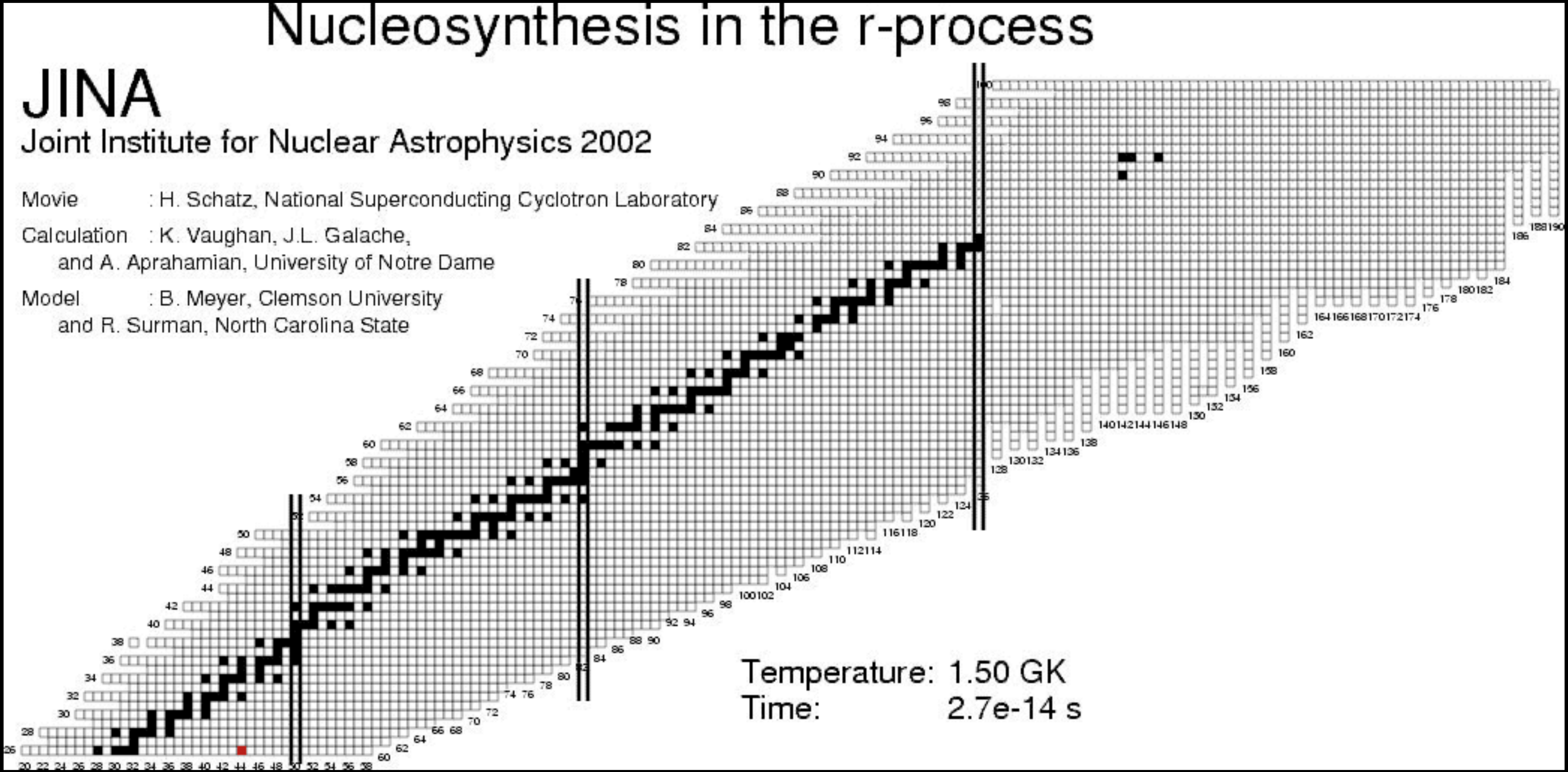




sudden decrease in S_n

low level density $\rho(E^*)$

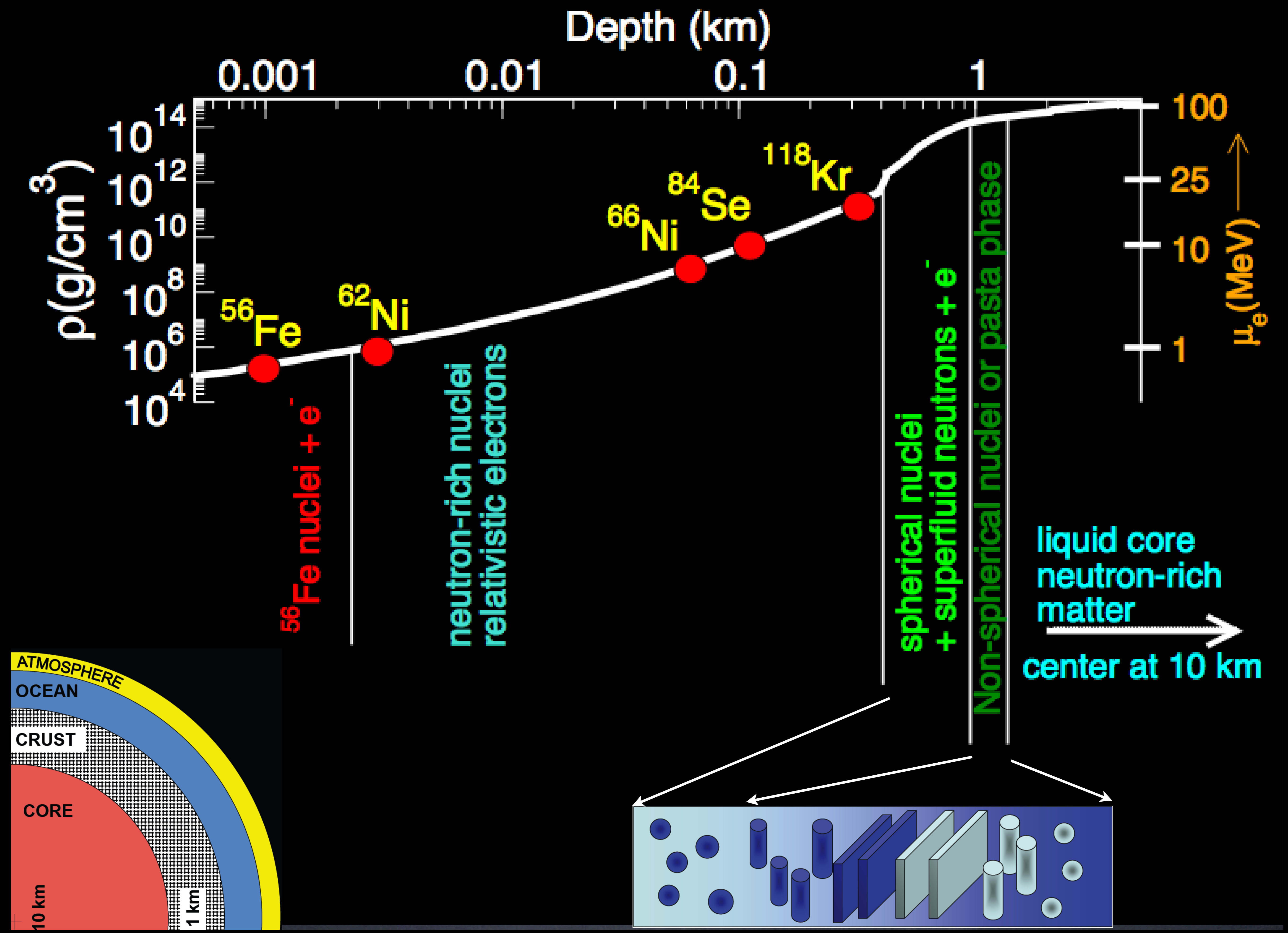
$$\Gamma_{i\to f} = \frac{2\pi}{\hbar} |\langle f | H_{\text{int}} | i \rangle|^2 \rho(E_f)$$



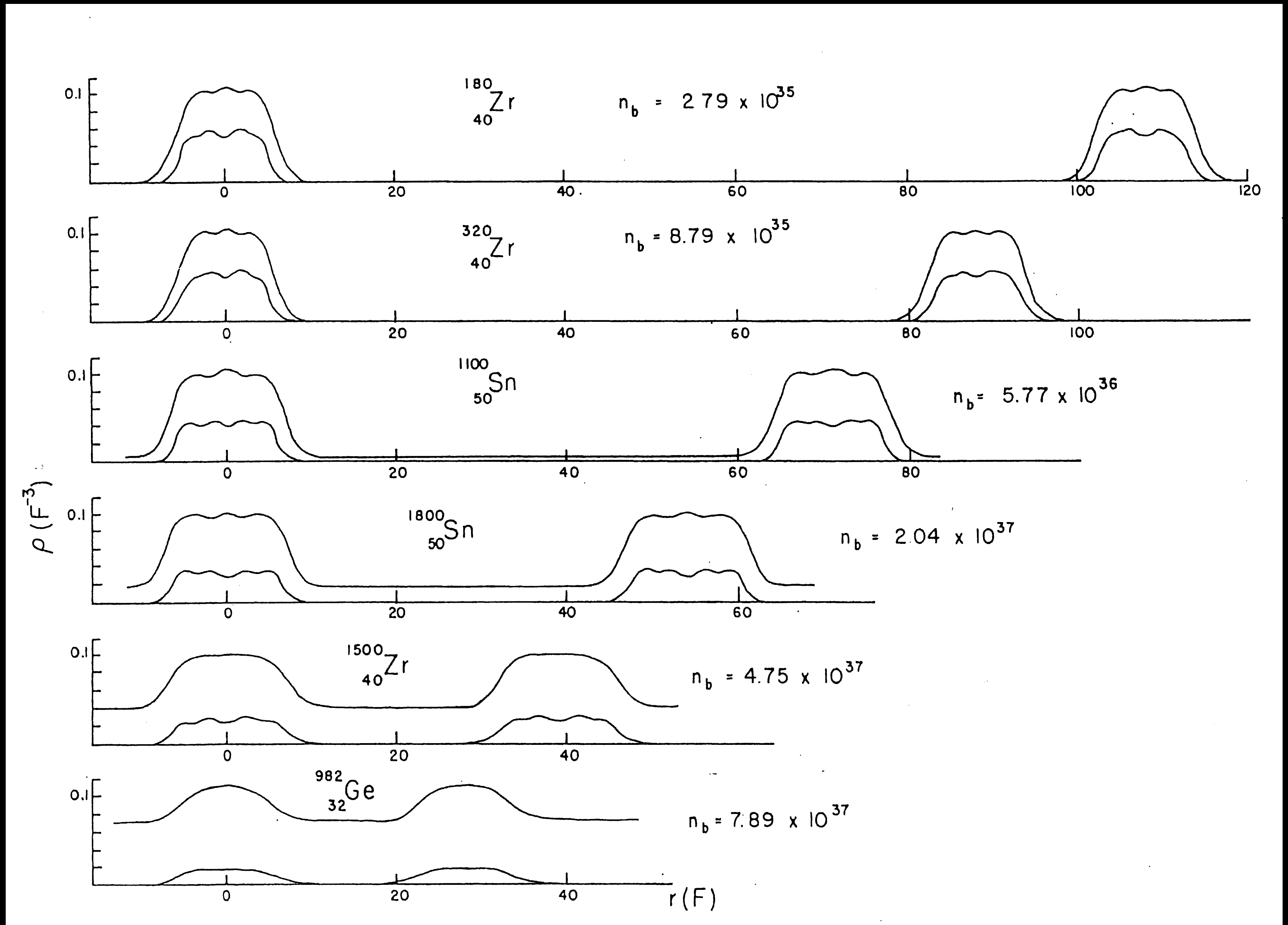
We need data of neutron-rich nuclei: beta-decay rates, neutron-capture rates,…

Nuclear physics in the inner part of neutron star

Page and Reddy, 2012



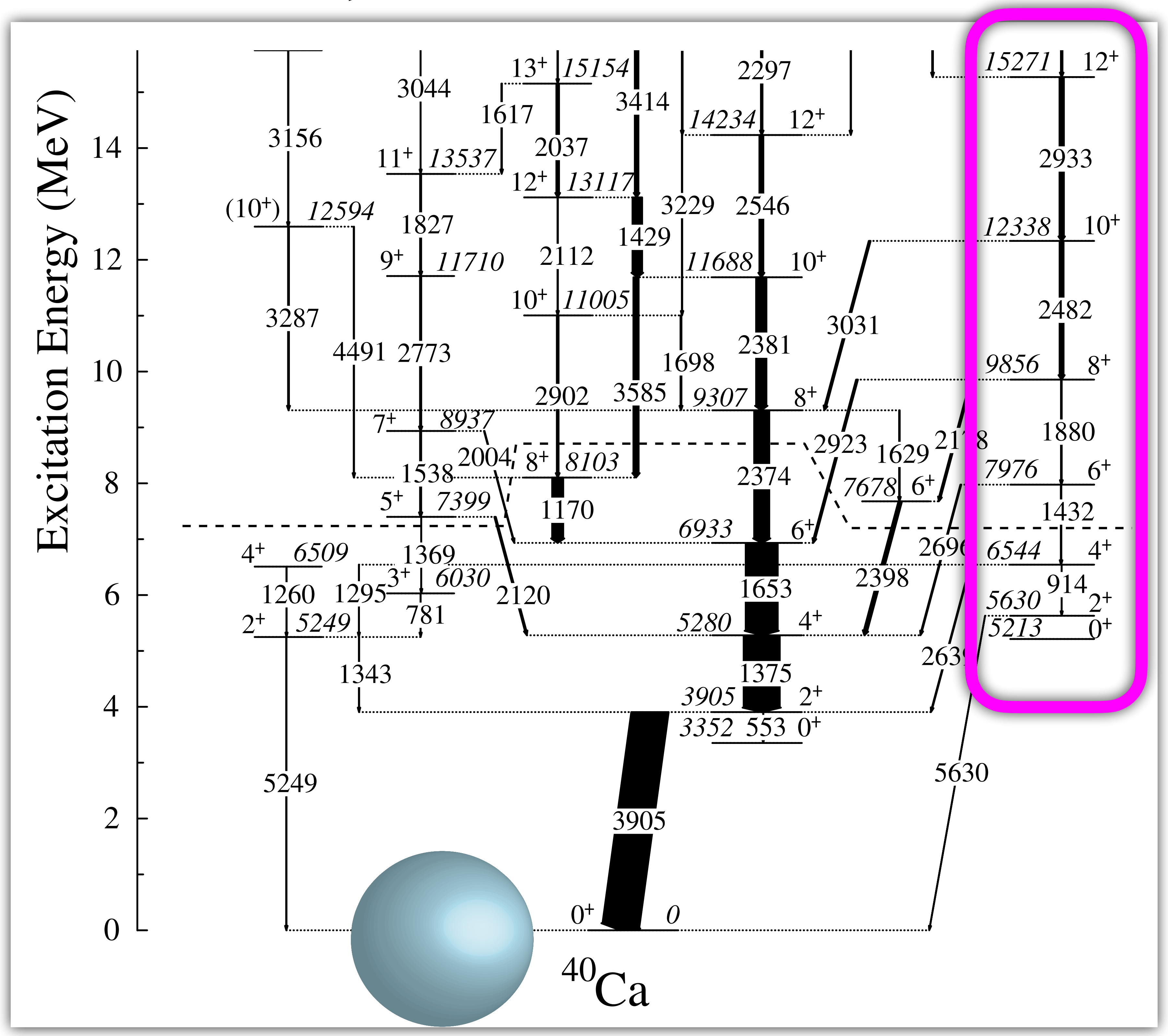
J. W. Negele and D. Vautherin, Nucl. Phys. A207 (1973) 298



We need to describe the structure of extremely-neutron-rich nuclei.

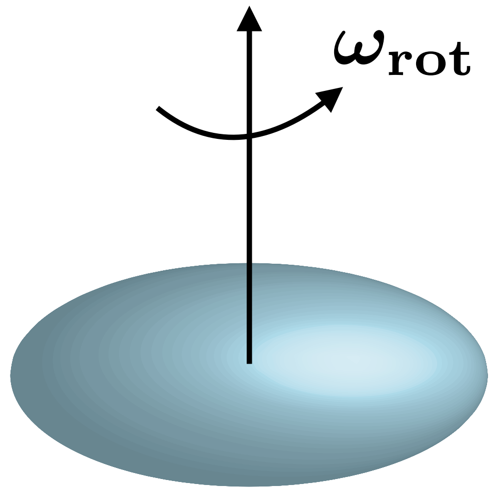
Appearance of new types of state

Excitation energy, Spins, …



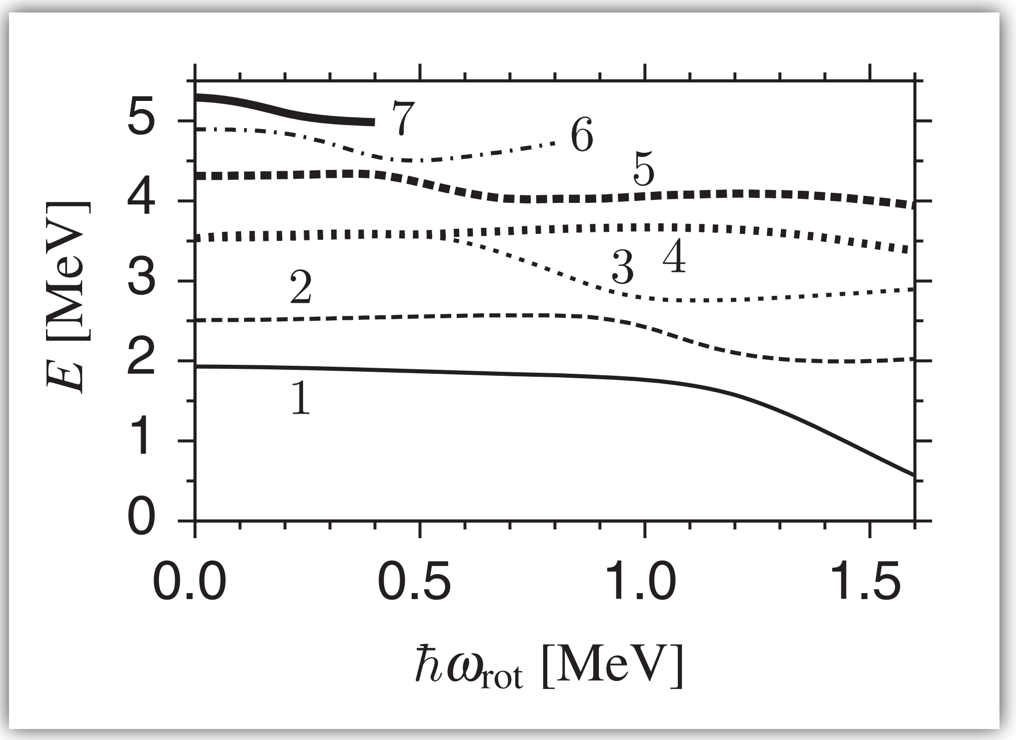
E. Ideguchi, *et al.*, PRL87(2001)22501

doubly magic！

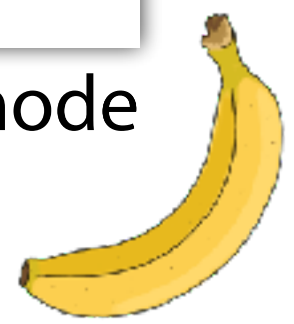


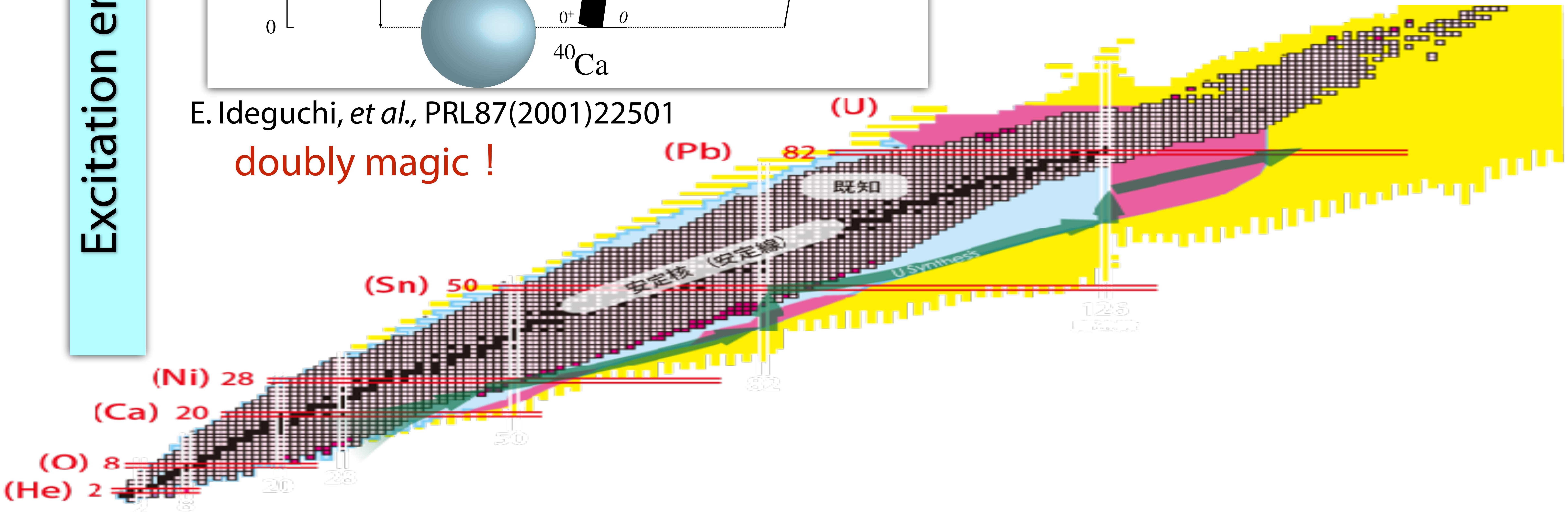
highly-deformed state

H. Ogasawara, KY, *et al.*, PTP121(2009)357



softening of octupole mode





RIBF upgrade

RIBF高度化：原子核物理学の多次元展開

Nuclear physics in a multi-dimensional view

KEK

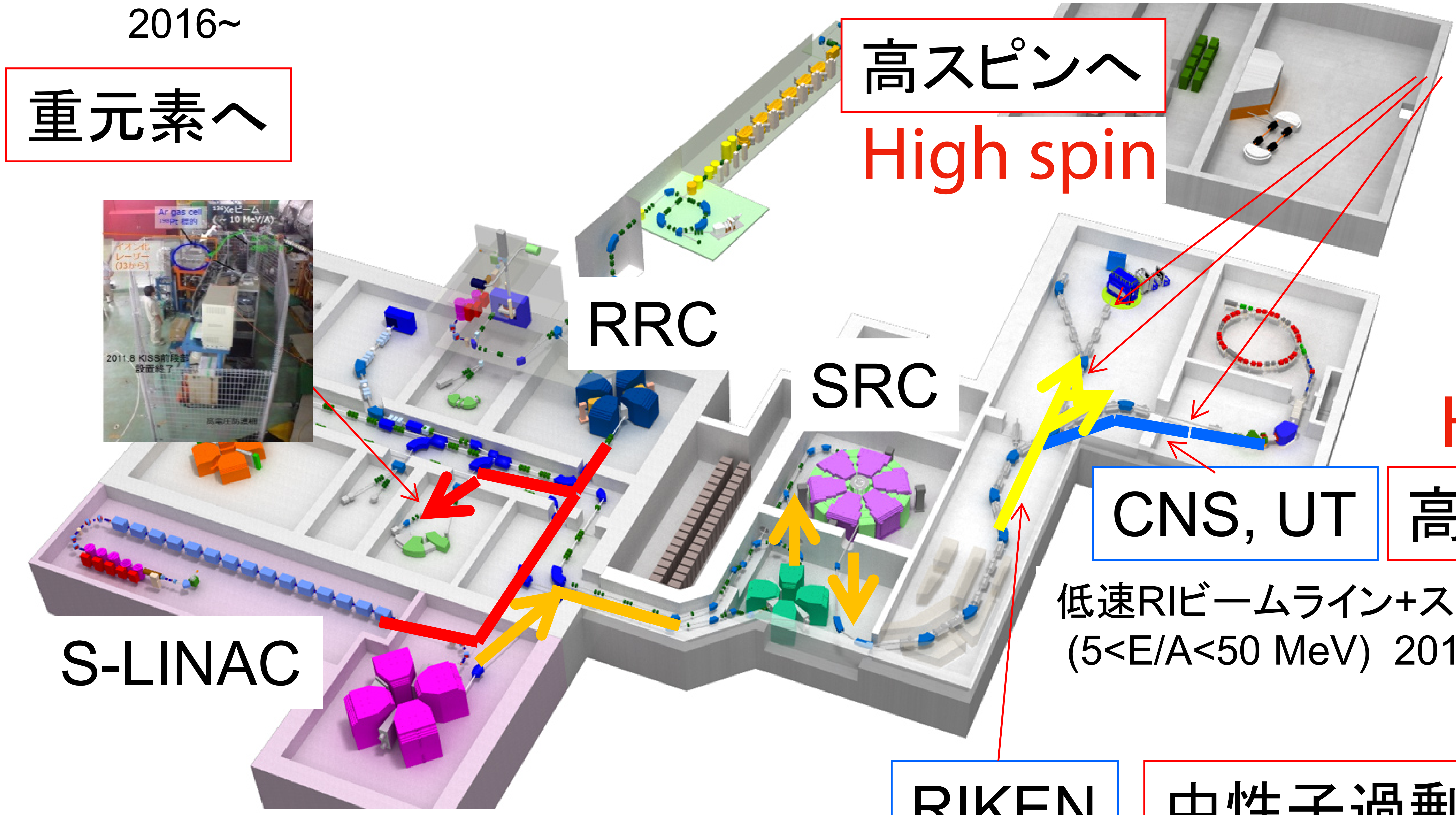
多核子移行反応などによる
超低速(E<30 keV)
RIビーム
2016~

Heavy 重元素へ

RCNP, Osaka

次世代ガンマ線検出器　2016～

高スピンへ
High spin



High energy

CNS, UT　高励起へ

低速RIビームライン+スペクトロメータ
(5<E/A<50 MeV)　2017～

RIKEN　中性子過剰へ　High isospin

高速2次RIビーム(50<E/A<300 MeV)
既存基幹実験装置にビーム配給

courtesy of H. Sakurai

Current issues in (low-energy) nuclear physics

How and where were heavy elements made?

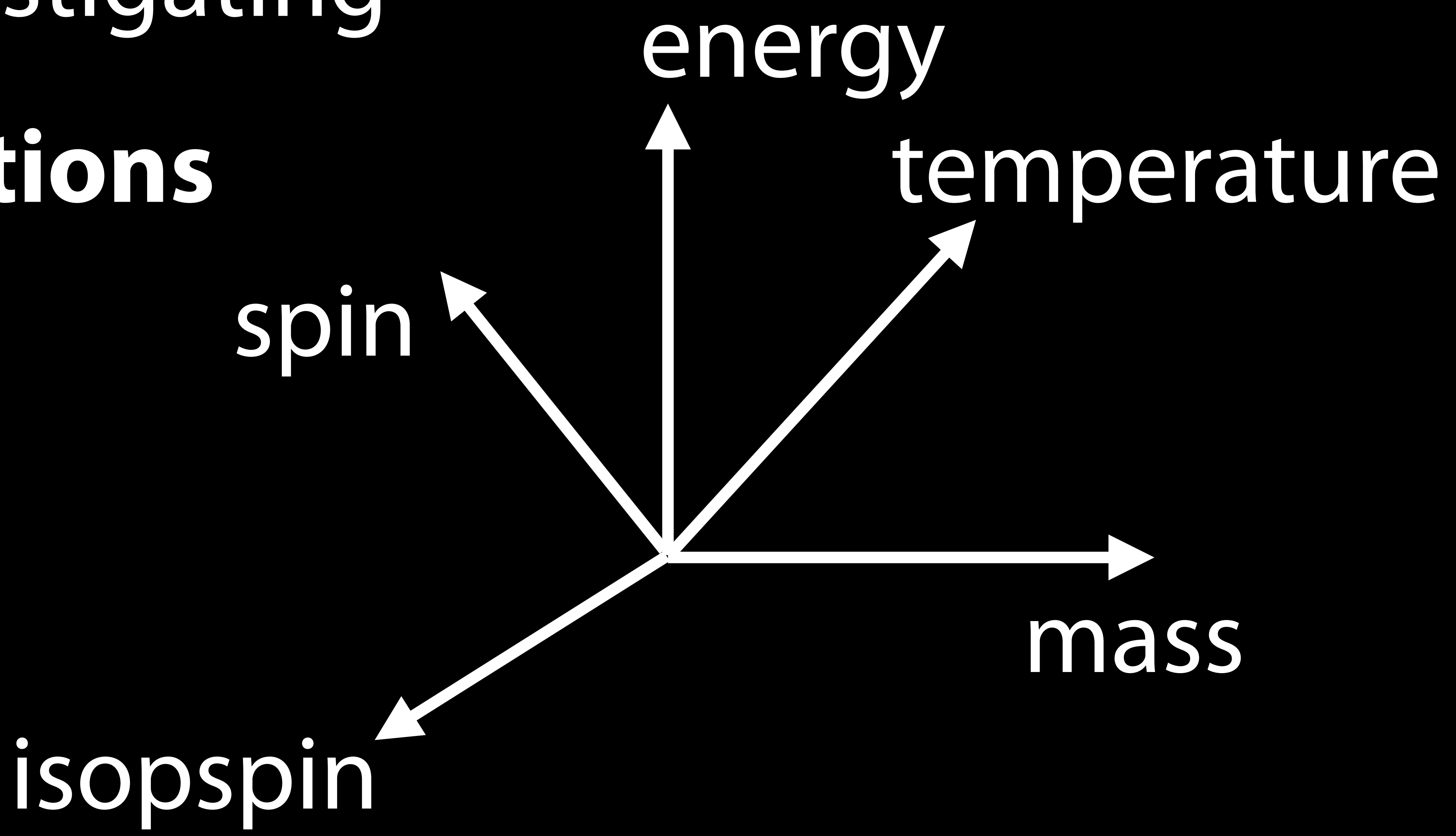
How many elements can exist?

We are studying **what material is**.

To answer these questions, we have been investigating

properties of **nuclei under extreme conditions**

exotic nuclei



Quantum many-body theory for nuclear problems

$$H = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i \neq j} v(i,j)$$

one can solve the equation for up to A~12

w/modern supercomputers

↓

We need a theory applicable to medium-heavy nuclei and infinite systems

our strategy:

to give up obtaining the many-body wave functions with 6A dim.

to construct a theory in which **densities** are a basic ingredient

radius, shape,…

Aim of this lecture

to understand the mean-field (MF) theory as an approximation to the quantum theory of many-body system

to understand the similarity and difference between MF theory and Density-Functional theory

to obtain physical picture characterizing the system from experimental data with the help of mean field

to understand physics behind the recent experiments

Nuclear collective phenomena and scopes of this lecture

Superfluidity **Deformation** **Collective excitation**

microscopic approach:

nucleonic degrees of freedom

Monday: Nuclear mean-field theory for pairing

Tuesday: Nuclear deformation and collective excitations (rotation)

Wednesday: Collective vibration and the physics of exotic nuclei

Prof. Tajima will also give a lecture on the pairing and superfluidity on Thursday.

Nuclear mean-field theory

Second quantization

A nucleus as a **many fermion system**

Two fermions cannot occupy the same quantum state.

The sign of the many-body wave function changes under the exchange of two particles.

a two-particle system

$$\Psi(x_1, x_2) = -\Psi(x_2, x_1) \qquad x = (\vec{r}st)$$

product

$$\Psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1)]$$

$$= \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_1(x_1) & \psi_1(x_2) \\ \psi_2(x_1) & \psi_2(x_2) \end{vmatrix}$$

U : ex. harmonic-oscillator potential

$$h = -\frac{\hbar^2}{2m}\Delta + U$$

$$h\psi_i = \epsilon_i \psi_i$$

Second quantization

Slater determinant for the *A*-body w.f.

$$\Psi(\vec{r}_1 s_1 t_1, \cdots, \vec{r}_A s_A t_A) = \frac{1}{\sqrt{A!}} \sum_{\pi} (-1)^{\pi} \prod_{k=1}^{A} \psi_k(x_{k_\pi})$$

permutation π :1,2,…*A*

+1 for even permutation,
-1 for odd permutation

$$= \frac{1}{\sqrt{A!}} \begin{vmatrix} \psi_1(x_1) & \psi_1(x_2) & \cdots & \psi_1(x_A) \\ \psi_2(x_1) & \psi_2(x_2) & \cdots & \psi_2(x_A) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_A(x_1) & \psi_A(x_2) & \cdots & \psi_A(x_A) \end{vmatrix}$$

Second quantization

An easy way to write down the Slater det. w.f.

a particle is occupied or not $\Longleftrightarrow$ creation and annihilation $c_i^\dagger, c_i$

anti-commutation relation

$$\{c_i, c_j^\dagger\} := c_i c_j^\dagger + c_j^\dagger c_i = \delta_{ij}$$

$$\{c_i, c_j\} = 0,\ \{c_i^\dagger, c_j^\dagger\} = 0$$

single-particle state : $|k\rangle := c_k^\dagger |0\rangle$

vacuum: $c_i |0\rangle = 0$

Slater determinant is given as $|\Psi\rangle = \prod_i^A c_i^\dagger |0\rangle$

$$c_i^\dagger c_j^\dagger + c_j^\dagger c_i^\dagger = 0$$

zero if two particles occupy the same s.p. state $c_i^\dagger c_i^\dagger = 0$

The sign changes under the exchange of two particles.

$$c_i^\dagger c_j^\dagger = -c_j^\dagger c_i^\dagger$$

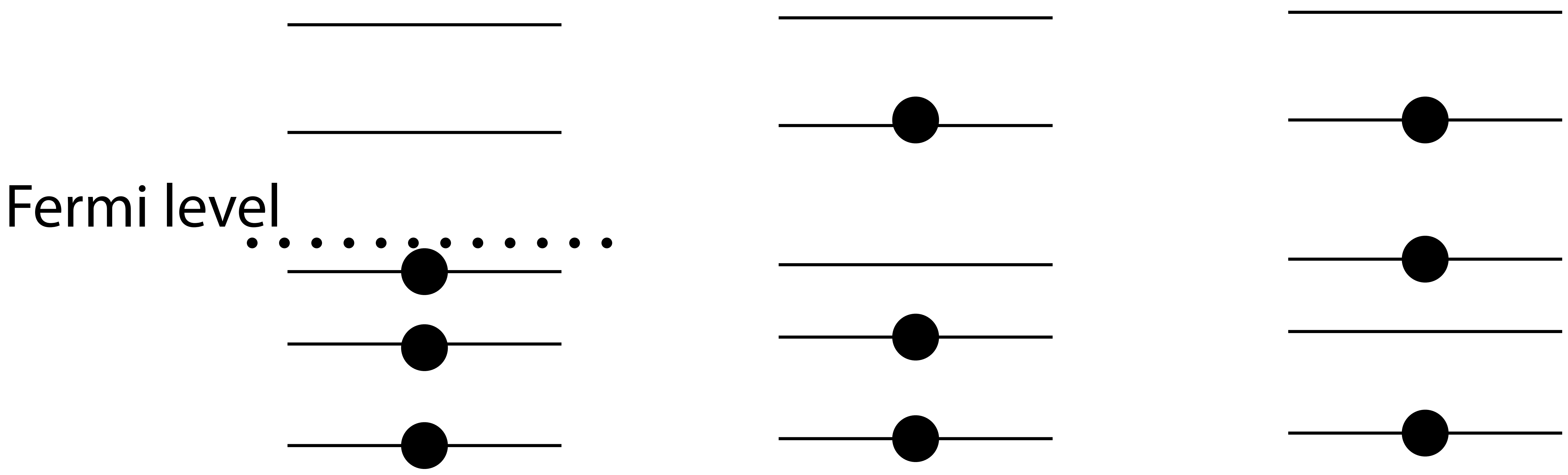
Simplest case: free particles

many-body Hamiltonian
$$H = \sum_i \epsilon_i c_i^\dagger c_i$$
$$= \sum_i h_i$$

single-particle Hamiltonian
$$h_i = \epsilon_i c_i^\dagger c_i$$

$$H|\Psi_\lambda\rangle = E_\lambda|\Psi_\lambda\rangle$$
$$H|k\rangle = h_k|k\rangle = \epsilon_k|k\rangle$$

$$E_\lambda = \sum_i^A \epsilon_i$$



ground state: $|\Psi_0\rangle$ $\quad|\Psi_1\rangle\quad|\Psi_2\rangle$

one-particle–one-hole

Simplest case: free particles

$|k\rangle$: known, e.g., HO basis $\qquad H = \sum_{ij} h_{ij} c_i^\dagger c_j$

$D_{k\alpha}$: unitary matrix

unknown single-particle states $|\alpha\rangle$ $\qquad a_\alpha^\dagger = \sum_k D_{k\alpha} c_k^\dagger$

$$D^\dagger D = DD^\dagger = 1$$

D is determined such that h_{ij} is diagonal $\qquad H = \sum_{ij} h_{ij} c_i^\dagger c_j = \sum_\alpha e_\alpha a_\alpha^\dagger a_\alpha$

new fermion creation/annihilation operators satisfy the anti-commutation relations

$$\{a_\alpha, a_\beta^\dagger\} = \delta_{\alpha\beta}, \quad \{a_\alpha, a_\beta\} = 0, \ \{a_\alpha^\dagger, a_\beta^\dagger\} = 0$$

Slater det. wf: $\qquad |\mathrm{SD}\rangle = \prod_\alpha^A a_\alpha^\dagger |0\rangle \quad \Rightarrow \quad H|\mathrm{SD}\rangle = \sum_\alpha^A e_\alpha |\mathrm{SD}\rangle$

SD is an eigenstate of the Hamiltonian for non-interacting systems

Hartree–Fock approximation for interacting many-fermion systems

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} c_i^\dagger c_j^\dagger c_l c_k$$

$$\bar{v}_{ijkl} = v_{ijkl} - v_{ijlk}$$

$$\bar{v}_{ijkl} = \bar{v}_{klij}$$

Model assumption $\quad |\Phi_{\mathrm{HF}}\rangle = \prod_{\alpha=1}^{A} a_\alpha^\dagger |0\rangle \qquad$ SD w.f.

then find the optimal s.p. states $\quad a_\alpha^\dagger = \sum_l D_{l\alpha} c_l^\dagger$

$$\langle \Phi_{\mathrm{HF}} | H | \Phi_{\mathrm{HF}} \rangle = \sum_{ij} t_{ij} \langle \Phi_{\mathrm{HF}} | c_i^\dagger c_j | \Phi_{\mathrm{HF}} \rangle + \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} \langle \Phi_{\mathrm{HF}} | c_i^\dagger c_j^\dagger c_l c_k | \Phi_{\mathrm{HF}} \rangle$$

$$= \sum_{ij} t_{ij} \rho_{ji} + \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} (\rho_{ki}\rho_{lj} - \rho_{kj}\rho_{li}) = \sum_{ij} t_{ij}\rho_{ji} + \frac{1}{2} \sum_{ijkl} \rho_{ki} \bar{v}_{ijkl} \rho_{lj}$$

one-body density matrix: $\quad \rho_{ij} := \langle \Phi_{\mathrm{HF}} | c_j^\dagger c_i | \Phi_{\mathrm{HF}} \rangle = \sum_{\alpha=1}^{A} D_{i\alpha} D_{j\alpha}^*$

Note for the derivation

$$|\Phi_{\mathrm{HF}}\rangle = \prod_{\alpha=1}^{A} a_\alpha^\dagger |0\rangle$$

$$a_\alpha^\dagger = \sum_l D_{l\alpha} c_l^\dagger$$

$$c_l^\dagger = \sum_\alpha D_{l\alpha}^* a_\alpha^\dagger$$

$$\rho_{ij} := \langle \Phi_{\mathrm{HF}} | c_j^\dagger c_i | \Phi_{\mathrm{HF}} \rangle = \sum_{\alpha=1}^{A} D_{i\alpha} D_{j\alpha}^*$$

$$\sum_{ij} t_{ij} \langle \Phi_{\mathrm{HF}} | c_i^\dagger c_j | \Phi_{\mathrm{HF}} \rangle = \sum_{ij} t_{ij} \sum_{\alpha,\beta=1}^{A} D_{i\alpha}^* D_{j\beta} \underbrace{\langle \Phi_{\mathrm{HF}} | a_\alpha^\dagger a_\beta | \Phi_{\mathrm{HF}} \rangle}_{= \delta_{\alpha,\beta}}$$

$$= \sum_{ij} \sum_{\alpha=1}^{A} t_{ij} D_{i\alpha}^* D_{j\alpha} = \sum_{ij} t_{ij} \rho_{ji}$$

$$\frac{1}{4} \sum_{ijkl} v_{ijkl} \langle \Phi_{\mathrm{HF}} | c_i^\dagger c_j^\dagger c_l c_k | \Phi_{\mathrm{HF}} \rangle = \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} \sum_{\alpha,\beta,\gamma,\delta=1}^{A} D_{i\alpha}^* D_{j\beta}^* D_{l\delta} D_{k\gamma} \underbrace{\langle \Phi_{\mathrm{HF}} | a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma | \Phi_{\mathrm{HF}} \rangle}_{= \delta_{\alpha,\gamma}\delta_{\beta,\delta} - \delta_{\alpha,\delta}\delta_{\beta,\gamma}}$$

$$= \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} \sum_{\alpha,\beta=1}^{A} D_{i\alpha}^* D_{j\beta}^* (D_{l\beta} D_{k\alpha} - D_{l\alpha} D_{k\beta})$$

$$= \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} (\rho_{ki}\rho_{lj} - \rho_{kj}\rho_{li}) = \frac{1}{2} \sum_{ijkl} \bar{v}_{ijkl} \rho_{ki} \rho_{lj}$$

*Note for the derivation by using the **Wick's theorem***

to reduce arbitrary products of creation and annihilation operators to sums of products of pairs of these operators

$$c_i^\dagger c_j^\dagger c_l c_k =: c_i^\dagger c_j^\dagger c_l c_k : + : \wick{\c1 c_i^\dagger \c1 c_j^\dagger c_l c_k} : + : \wick{c_i^\dagger \c1 c_j^\dagger \c1 c_l c_k} : + : \wick{c_i^\dagger c_j^\dagger \c1 c_l \c1 c_k} : + : \wick{\c1 c_i^\dagger c_j^\dagger \c1 c_l c_k} : + : \wick{\c1 c_i^\dagger c_j^\dagger c_l \c1 c_k} : + : \wick{c_i^\dagger \c1 c_j^\dagger c_l \c1 c_k} :$$

$$+ : \wick{\c1 c_i^\dagger \c1 c_j^\dagger \c2 c_l \c2 c_k} : + : \wick{\c1 c_i^\dagger \c2 c_j^\dagger \c2 c_l \c1 c_k} : + : \wick{\c1 c_i^\dagger \c2 c_j^\dagger \c1 c_l \c2 c_k} :$$

$$\wick{\c1 A \c1 B} := \langle \Phi | AB | \Phi \rangle$$

contraction

$$\langle \Phi | : X : | \Phi \rangle = 0$$

$$\langle \Phi | c_i^\dagger c_j^\dagger c_l c_k | \Phi \rangle = \langle \Phi | c_i^\dagger c_j^\dagger | \Phi \rangle \langle \Phi | c_l c_k | \Phi \rangle + \langle \Phi | c_i^\dagger c_k | \Phi \rangle \langle \Phi | c_j^\dagger c_l | \Phi \rangle - \langle \Phi | c_i^\dagger c_l | \Phi \rangle \langle \Phi | c_j^\dagger c_k | \Phi \rangle$$

$$= \rho_{ki}\rho_{lj} - \rho_{li}\rho_{kj}$$

Hartree–Fock approximation

$$\rho_{ij} := \langle \Phi_{\mathrm{HF}} | c_j^\dagger c_i | \Phi_{\mathrm{HF}} \rangle = \sum_{\alpha=1}^{A} D_{i\alpha} D_{j\alpha}^*$$

Idempotency $\quad \rho^2 = \rho$

$$\sum_l \rho_{il}\rho_{lj} = \sum_l \sum_{\alpha,\beta=1}^{A} D_{i\alpha} D_{l\alpha}^* D_{l\beta} D_{j\beta}^* = \sum_\alpha D_{i\alpha} D_{j\alpha}^* = \rho_{ij}$$

using $\; D^\dagger D = 1$

the eigenvalues are zero or one

"unoccupied" "occupied"

$|\Phi\rangle$ is SD$\Longleftrightarrow \rho^2 = \rho$

when $\mathrm{Tr}\rho = A$

$$D^\dagger \rho D = \begin{array}{cc} & A \\ A & \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \end{array}$$

Hartree–Fock approximation

$$E_{\mathrm{HF}}[\rho] = \langle \Phi_{\mathrm{HF}} | H | \Phi_{\mathrm{HF}} \rangle = \sum_{ij} t_{ij}\rho_{ji} + \frac{1}{2}\sum_{ik} \Gamma_{ik}\rho_{ki}$$

Hartree–Fock potential: $\Gamma_{ik}[\rho] = \sum_{jl} \bar{v}_{ijkl}\rho_{lj}$

$$h_{ij} := \frac{\partial E_{\mathrm{HF}}[\rho]}{\partial \rho_{ji}} = t_{ij} + \Gamma_{ij}[\rho]$$

one-body potential: mean field

$$H_{\mathrm{HF}} = \sum_{ij} h_{ij} c_i^\dagger c_j$$

The energy, mean field, and the Hamiltonian are a functional of density matrix.

Hartree–Fock approximation **nonlinear problem**

input of the cal.: (effective) interaction, basis set, and initial values of the SD (density matrix)

density matrix $$\rho_{ij} = \sum_{k=1}^{A} D_{ik} D_{jk}^{*}$$

mean field $$\Gamma_{ik}[\rho] = \sum_{jl} \bar{v}_{ijkl} \rho_{lj}$$

diagonalization $$h_{ij} = t_{ij} + \Gamma_{ij}[\rho]$$

$$\sum_{j} h_{ij} D_{jk} = \epsilon_k D_{ik}$$

self-consistency

find the s.p. orbital giving the lowest total energy

Hartree–Fock equation

(HF eq.)*

$$\sum_j h_{ij} D_{jk} = \epsilon_k D_{ik} \qquad \rho_{ij} = \sum_{k=1}^{A} D_{ik} D_{jk}^* \qquad \sum_j D_{jk}^* h_{ij}^* = \epsilon_k D_{ik}^*$$

$$\Rightarrow \quad \sum_j h_{ij}\rho_{jm} = \sum_j \sum_{k=1}^{A} h_{ij} D_{jk} D_{mk}^* = \sum_{k=1}^{A} \epsilon_k D_{ik} D_{mk}^* = \sum_j \sum_{k=1}^{A} D_{ik} D_{jk}^* h_{mj}^*$$

$$= \sum_j \rho_{ij} h_{mj}^*$$

$$= \sum_j \rho_{ij} h_{jm}$$

$$\Rightarrow \quad [h[\rho], \rho] = 0$$

one can diagonalize the HF Hamiltonian and the density matrix simultaneously

Hartree–Fock equation in the coordinate-space rep.

$$\sum_j h_{ij} D_{jk} = \epsilon_k D_{ik}, \quad h_{ij} = t_{ij} + \sum_{ln} \sum_{m=1}^{A} \bar{v}_{injl} D_{lm} D_{nm}^*$$

i, j, n, l :arbitrary basis

grid basis: $\psi^\dagger(\vec{r})|0\rangle = c_{\vec{r}}^\dagger |0\rangle = |\vec{r}\rangle$

$$\{c_{\vec{r}}, c_{\vec{r}'}^\dagger\} = \delta(\vec{r} - \vec{r}')$$

$$\{c_{\vec{r}}, c_{\vec{r}'}\} = 0, \ \{c_{\vec{r}}^\dagger, c_{\vec{r}'}^\dagger\} = 0$$

$$a_k^\dagger = \int d\vec{r} \underbrace{\varphi_k(\vec{r})}_{= D_{\vec{r}k}} c_{\vec{r}}^\dagger$$

$\bar{v}(\vec{r}_1, \vec{r}_1')$ local potential

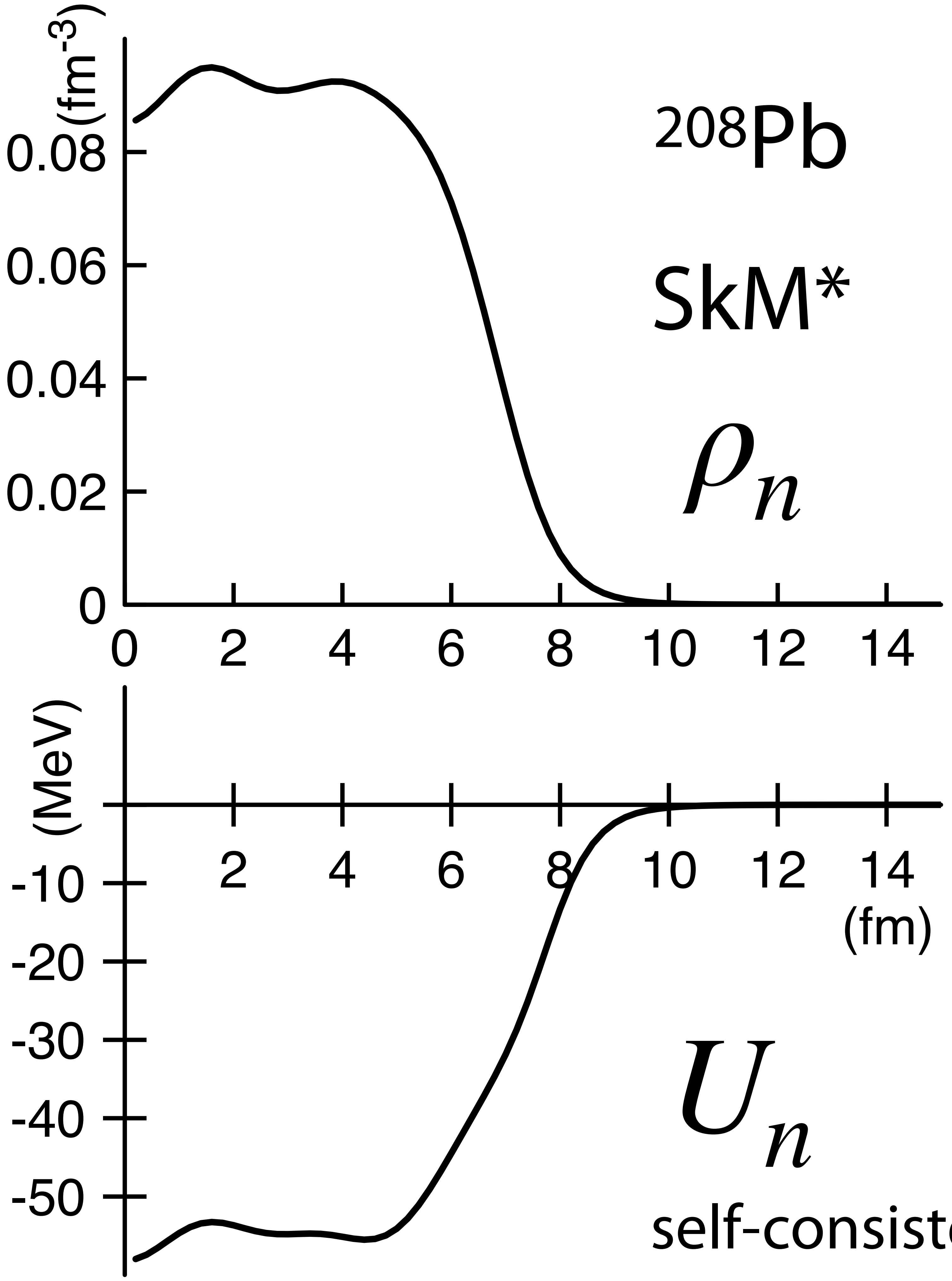
$$-\frac{\hbar^2}{2m}\Delta\varphi_k(\vec{r}) + \sum_{m=1}^{A} \int d\vec{r}' \bar{v}(\vec{r}, \vec{r}')\varphi_m^*(\vec{r}')[\varphi_m(\vec{r}')\varphi_k(\vec{r}) - \varphi_m(\vec{r})\varphi_k(\vec{r}')] = \varepsilon_k \varphi_k(\vec{r})$$

Hartree potential: $\Gamma_{\mathrm{H}}(\vec{r}) = \int d\vec{r}' \bar{v}(\vec{r}, \vec{r}') \sum_{m=1}^{A} |\varphi_m(\vec{r}')|^2 = \int d\vec{r}' v(\vec{r}, \vec{r}')\rho(\vec{r}')$

Fock potential: $\Gamma_{\mathrm{F}}(\vec{r}, \vec{r}') = -\bar{v}(\vec{r}, \vec{r}') \sum_{m=1}^{A} \varphi_m^*(\vec{r}')\varphi_m(\vec{r}) = -v(\vec{r}, \vec{r}')\rho(\vec{r}, \vec{r}')$

Mean field potential

$$\Gamma_{\mathrm{H}}(\vec{r}) = \int d\vec{r}' v(\vec{r}, \vec{r}')\rho(\vec{r}') \quad \propto \rho(\vec{r})$$ when the interaction is short-ranged



self-consistent mean field

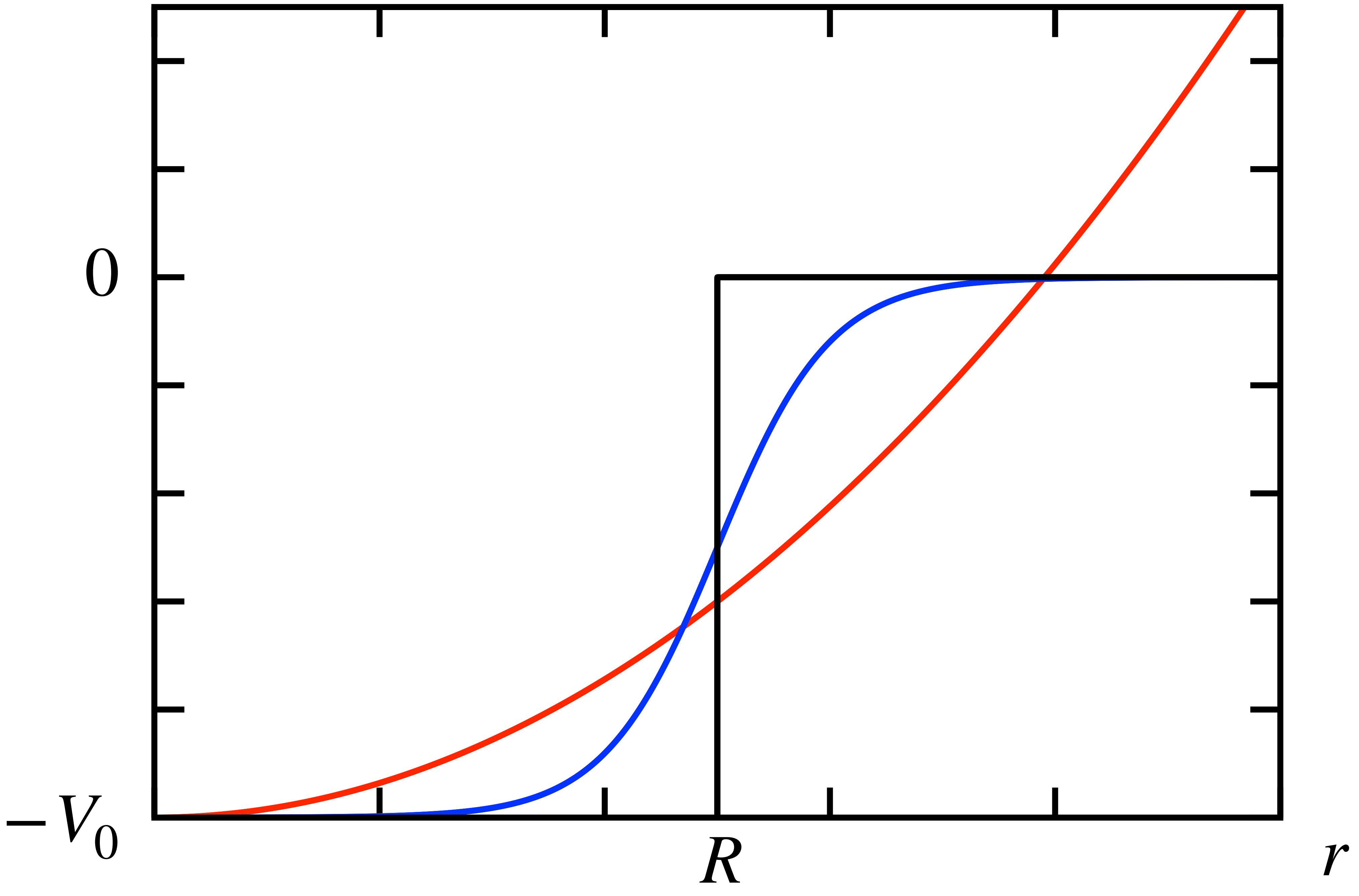
phenomenological mean-field potentials

Woods–Saxon (WS)

$$V(\vec{r}) = -V_0 \frac{1}{1+\exp[(r-R)/a]}$$

Harmonic oscillator (HO)

Square well



Density matrix and local densities

$$T = -i\sigma_y K$$

$$T\varphi_i(\vec{r}\sigma) = -2\sigma\varphi_i^*(\vec{r}-\sigma)$$

Density matrix: $\rho(\vec{r}\sigma, \vec{r}'\sigma') = \langle \Phi | \psi^\dagger(\vec{r}'\sigma')\psi(\vec{r}\sigma) | \Phi \rangle$

time-reversal operation

$$\boxed{\rho^T(\vec{r}\sigma, \vec{r}'\sigma') = 4\sigma\sigma'\rho^*(\vec{r}-\sigma, \vec{r}'-\sigma')}$$

Density matrix in terms of the scalar and vector parts

$2 \times 2 = 4 \qquad = 1 + 3$

$$\rho(\vec{r}, \vec{r}') = \sum_\sigma \rho(\vec{r}\sigma, \vec{r}'\sigma) \qquad \boldsymbol{s}(\vec{r}, \vec{r}') = \sum_{\sigma\sigma'} \rho(\vec{r}\sigma, \vec{r}'\sigma)\langle \sigma' | \boldsymbol{\sigma} | \sigma \rangle$$

hermitian

$$\rho(\vec{r}\sigma, \vec{r}'\sigma') = \frac{1}{2}[\rho(\vec{r}, \vec{r}')\delta_{\sigma,\sigma'} + \sum_\nu \langle \sigma | \sigma_\nu | \sigma' \rangle s_\nu(\vec{r}, \vec{r}')]$$

$$\boxed{\begin{aligned} \rho^T(\vec{r}, \vec{r}') &= \rho^*(\vec{r}, \vec{r}') = \rho(\vec{r}', \vec{r}) \\ \boldsymbol{s}^T(\vec{r}, \vec{r}') &= -\boldsymbol{s}^*(\vec{r}, \vec{r}') = -\boldsymbol{s}(\vec{r}', \vec{r}) \end{aligned}}$$

Local densities: ingredients of energy density functional

particle density: $\rho(\boldsymbol{r}) = \rho(\boldsymbol{r}, \boldsymbol{r})$

spin density: $\boldsymbol{s}(\boldsymbol{r}) = \boldsymbol{s}(\boldsymbol{r}, \boldsymbol{r})$

kinetic density: $\tau(\boldsymbol{r}) = (\nabla \cdot \nabla')\rho(\boldsymbol{r}, \boldsymbol{r}')\Big|_{\boldsymbol{r}=\boldsymbol{r}'}$

current density: $\boldsymbol{j}(\boldsymbol{r}) = \dfrac{1}{2i}(\nabla - \nabla')\rho(\boldsymbol{r}, \boldsymbol{r}')\Big|_{\boldsymbol{r}=\boldsymbol{r}'}$

time reversal

$$\boxed{\begin{aligned} \rho^T(\vec{r}, \vec{r}') &= \rho^*(\vec{r}, \vec{r}') = \rho(\vec{r}', \vec{r}) \\ \boldsymbol{s}^T(\vec{r}, \vec{r}') &= -\boldsymbol{s}^*(\vec{r}, \vec{r}') = -\boldsymbol{s}(\vec{r}', \vec{r}) \end{aligned}}$$

$\rho^T(\boldsymbol{r}) = \rho(\boldsymbol{r}), \qquad \tau^T(\boldsymbol{r}) = \tau(\boldsymbol{r}),$

"time-even" densities

$\boldsymbol{s}^T(\boldsymbol{r}) = -\boldsymbol{s}(\boldsymbol{r}), \qquad \boldsymbol{j}^T(\boldsymbol{r}) = -\boldsymbol{j}(\boldsymbol{r})$

"time-odd" densities

If the situation is invariant under time-reversal,
the time-odd densities vanish.

Skyrme Hartree–Fock model: A nuclear energy-density functional method

$$E_{\mathrm{Sky}} = \sum_{t=0,1} \int d\vec{r} \chi_t$$

$$\chi_t^{\mathrm{even}} = C_t^{\rho}[\rho_0]\rho_t^2 + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\tau}\rho_t\tau_t + C_t^{\nabla J}\rho_t\nabla\cdot\boldsymbol{J}_t + C_t^{J}\overleftrightarrow{J}_t^2$$

$$\chi_t^{\mathrm{odd}} = C_t^{s}[\rho_0]\boldsymbol{s}_t^2 + C_t^{\Delta s}\boldsymbol{s}_t\cdot\Delta\boldsymbol{s}_t + C_t^{j}\boldsymbol{j}_t^2 + C_t^{\nabla j}\boldsymbol{s}_t\cdot(\nabla\times\boldsymbol{j}_t) + C_t^{T}\boldsymbol{s}_t\cdot\boldsymbol{T}_t + C_t^{\nabla s}(\nabla\cdot\boldsymbol{s}_t)^2$$

Total energy of a system as density functional:

$$E = \int d\vec{r}\,\mathscr{E}[\rho(\vec{r})]$$

$$= E_{\mathrm{kin}} + E_{\mathrm{Sky}} + E_{\mathrm{Coul}} + \underline{E_{\mathrm{pair}}}$$

introduced in the next session

$$h := \frac{\delta\mathscr{E}[\rho]}{\delta\rho} = t + v_{\mathrm{KS}}[\rho] + v_{\mathrm{Coul}}[\rho]$$

Kohn–Sham eq.

$$h\phi_i = \varepsilon_i\phi_i$$

very similar to the HF eq.

Mean-field theory for open-shell nuclei

—pairing—

Odd–even effect in the nuclear mass

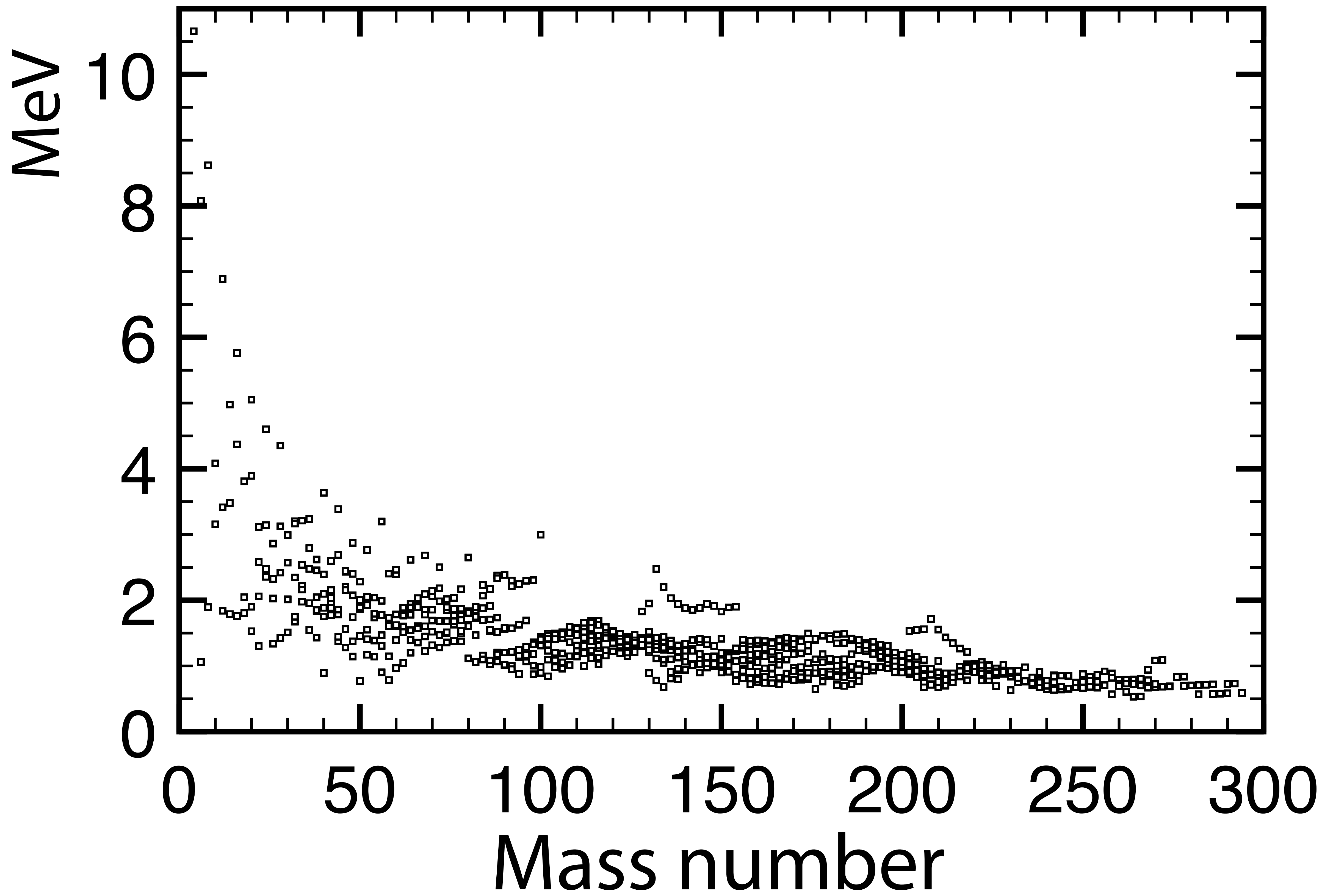
Bethe–Weizsäcker mass formula

$$B(A,Z) = a_{\mathrm{vol}}A - a_{\mathrm{surf}}A^{2/3} - a_{\mathrm{sym}}\frac{(N-Z)^2}{A} - a_{\mathrm{Coul}}\frac{Z^2}{A^{1/3}} + \delta(A)$$

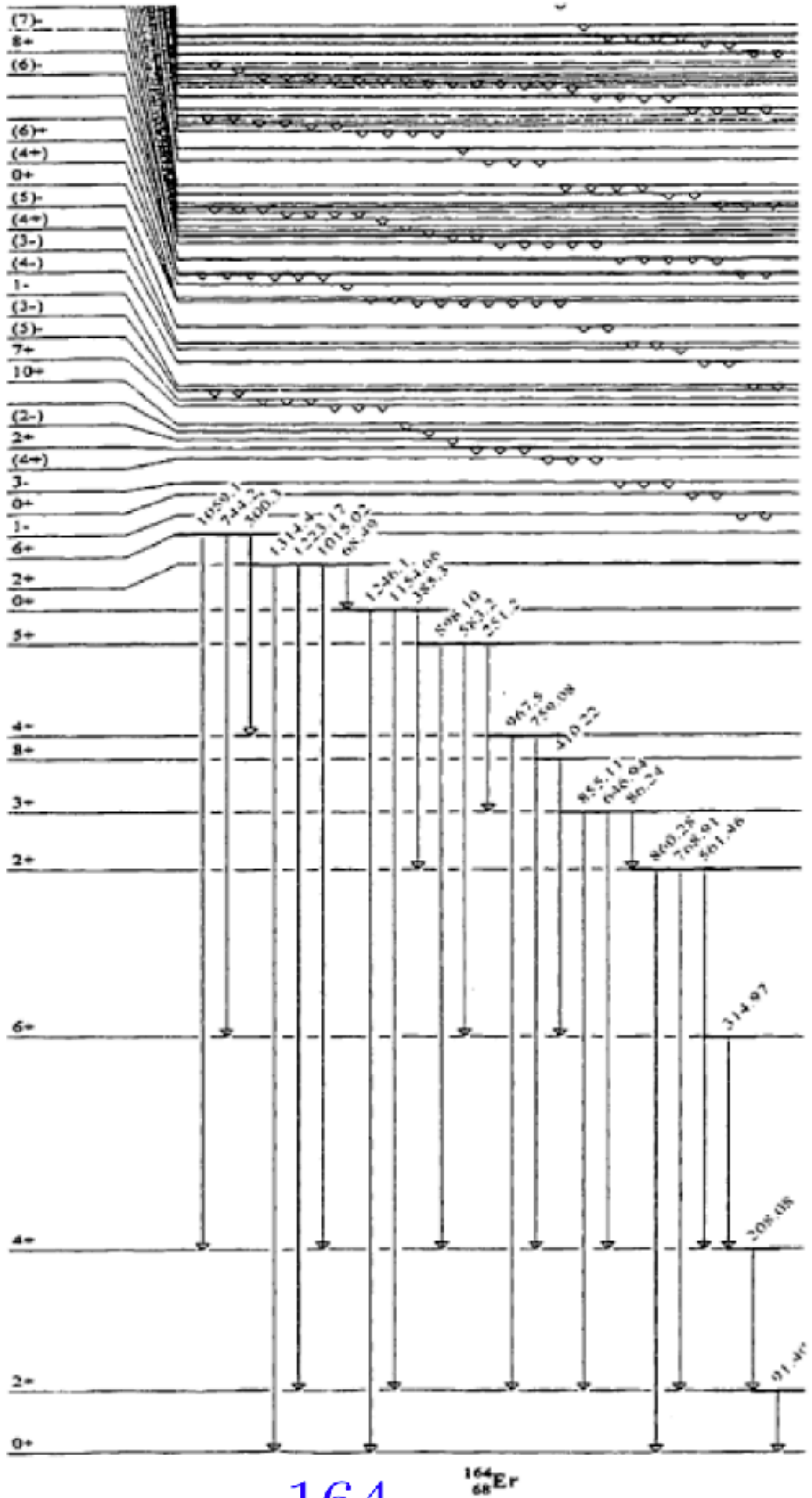
strong binding for even-even nuclei

$$\Delta_n^{(3)}(N,Z) = \frac{1}{2}[M(N+1,Z) - 2M(N,Z) + M(N-1,Z)]$$

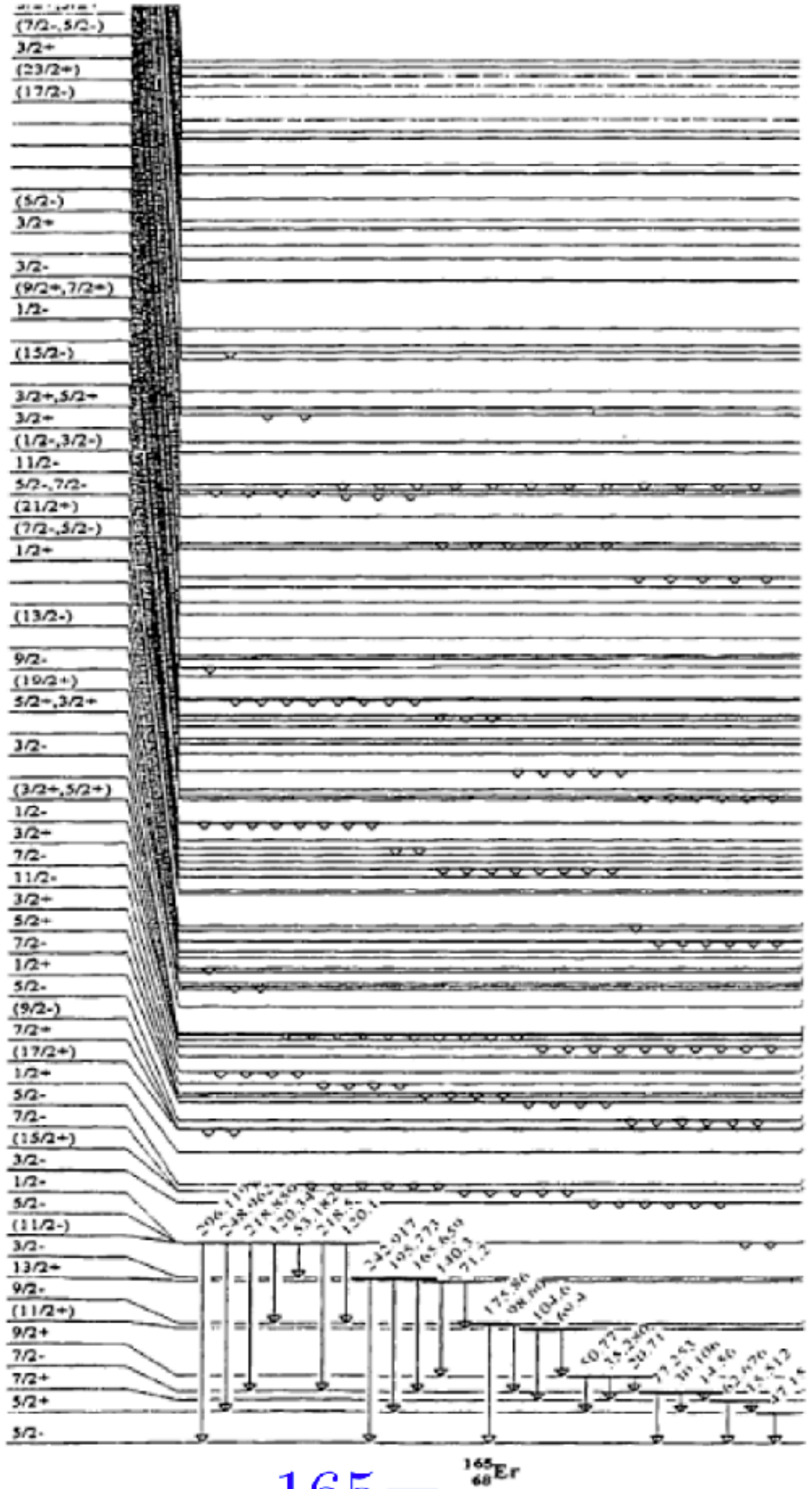
$$\Delta_p^{(3)}(N,Z) = \frac{1}{2}[M(N,Z+1) - 2M(N,Z) + M(N,Z-1)]$$



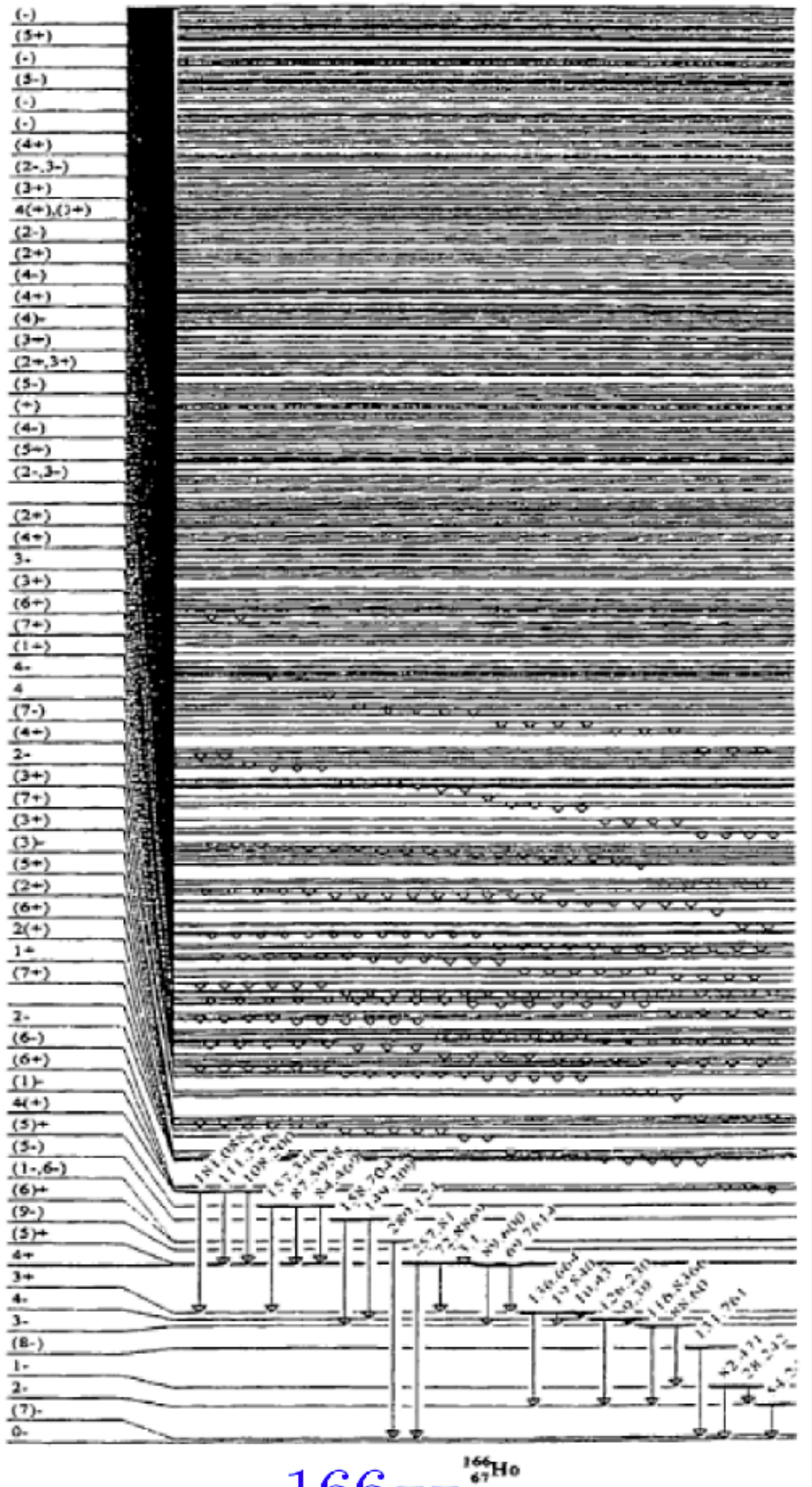
Odd–even effect in the low-lying spectra



$^{164}_{68}\mathrm{Er}_{96}$



$^{165}_{68}\mathrm{Er}_{97}$



$^{166}_{67}\mathrm{Ho}_{99}$

Bardeen–Cooper–Schrieffer (BCS) theory

HF basis

$J = 0$ pair (in spherical nuclei)

$$h|i\rangle = \varepsilon_i |i\rangle \qquad i = (nljm), \quad \tilde{i} = (nlj\ -m)$$

$$A_i^\dagger := c_i^\dagger c_{\tilde{i}}^\dagger$$

$|\tilde{i}\rangle$ is a time-reversed state of $|i\rangle$

large overlap

Cooper pair $A^\dagger := \sum_i \varphi_i A_i^\dagger$ like a boson $\langle 0|[A, A^\dagger]|0\rangle = 1$

n Cooper-pairs condensed state: $|\Phi\rangle \propto (A^\dagger)^n |0\rangle, \quad n = N/2$

BCS state:

$$\begin{aligned} |\mathrm{BCS}\rangle &= \prod_{i>0} (u_i + v_i A_i^\dagger)|0\rangle \\ &= \prod_{i>0} u_i (1 + \varphi_i A_i^\dagger)|0\rangle \\ &= \prod_{i>0} u_i e^{\varphi_i A_i^\dagger}|0\rangle \\ &\propto \frac{1}{n!} e^{A^\dagger}|0\rangle \end{aligned}$$

$u_i = \cos\theta_i (\neq 0), v_i = \sin\theta_i, \varphi_i = \tan\theta_i$

$$\frac{v_i}{u_i} = \tan\theta_i = \varphi_i$$

$$(A_i^\dagger)^2|0\rangle = 0$$

superposition of the condensed states with **different numbers of particle**

BCS theory

$J = 0$ pair

$$|\mathrm{BCS}\rangle = \prod_{i>0} (u_i + v_i A_i^\dagger)\,|0\rangle \qquad A_i^\dagger := c_i^\dagger c_{\tilde{i}}^\dagger$$

normalization $1 = \langle \mathrm{BCS}\,|\,\mathrm{BCS}\rangle$ $\qquad u_i^2 + v_i^2 = 1$

particle # $\quad N = \langle \mathrm{BCS}\,|\,\hat{N}\,|\,\mathrm{BCS}\rangle = 2\sum_{i>0} v_i^2$ $\qquad v_i^2$: **occupation prob.**

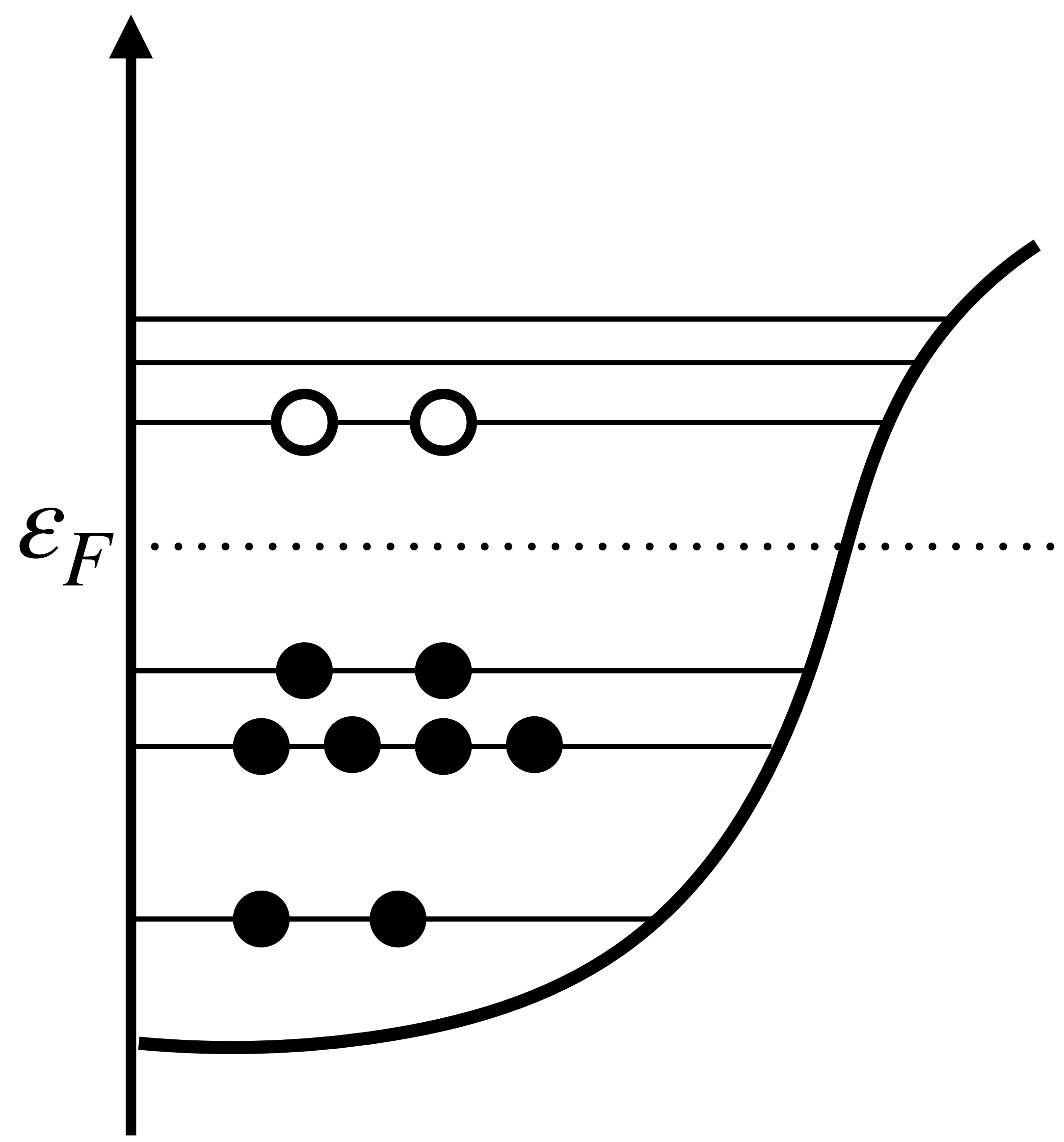
The Hartree–Fock and the BCS states

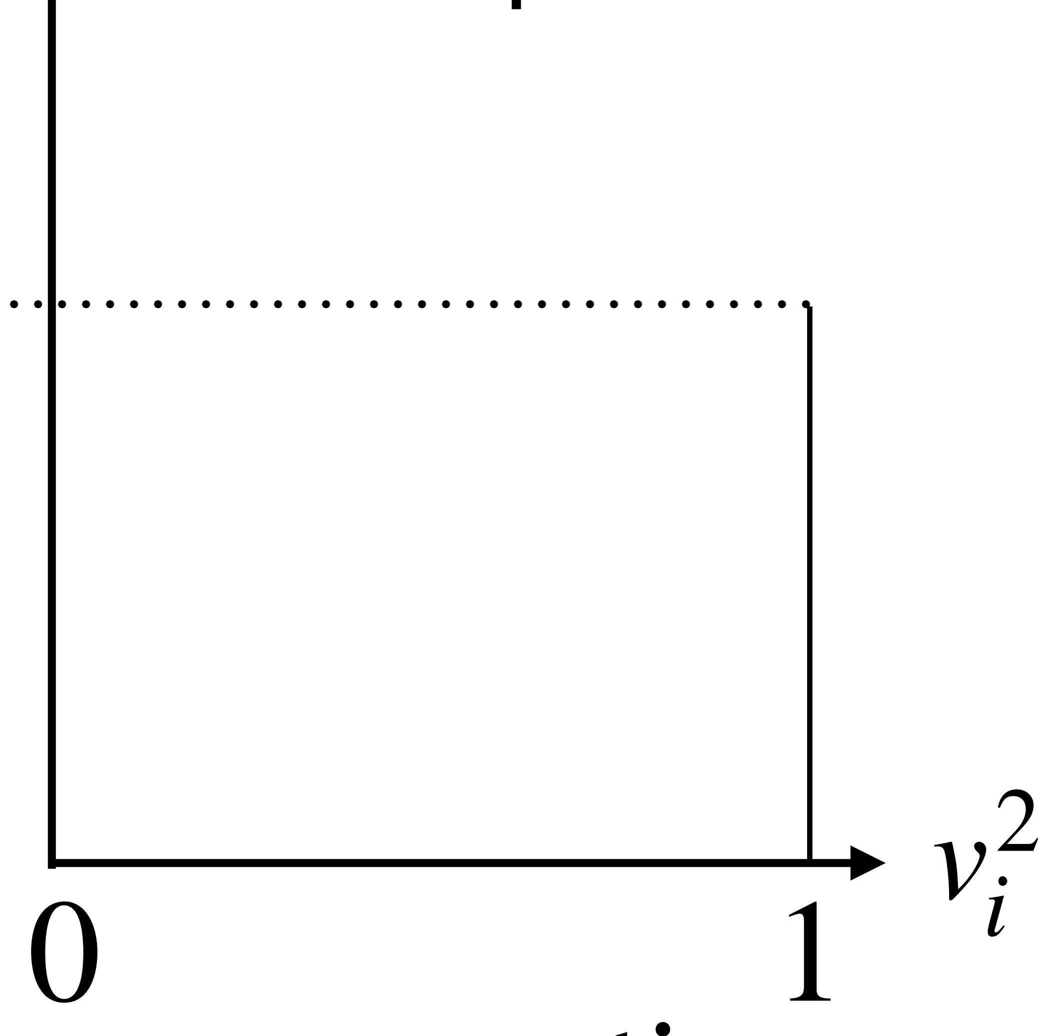
$$|\Phi_{\mathrm{HF}}\rangle = \prod_{i=1}^{A} a_i^\dagger |0\rangle = \prod_i b_i |0\rangle$$

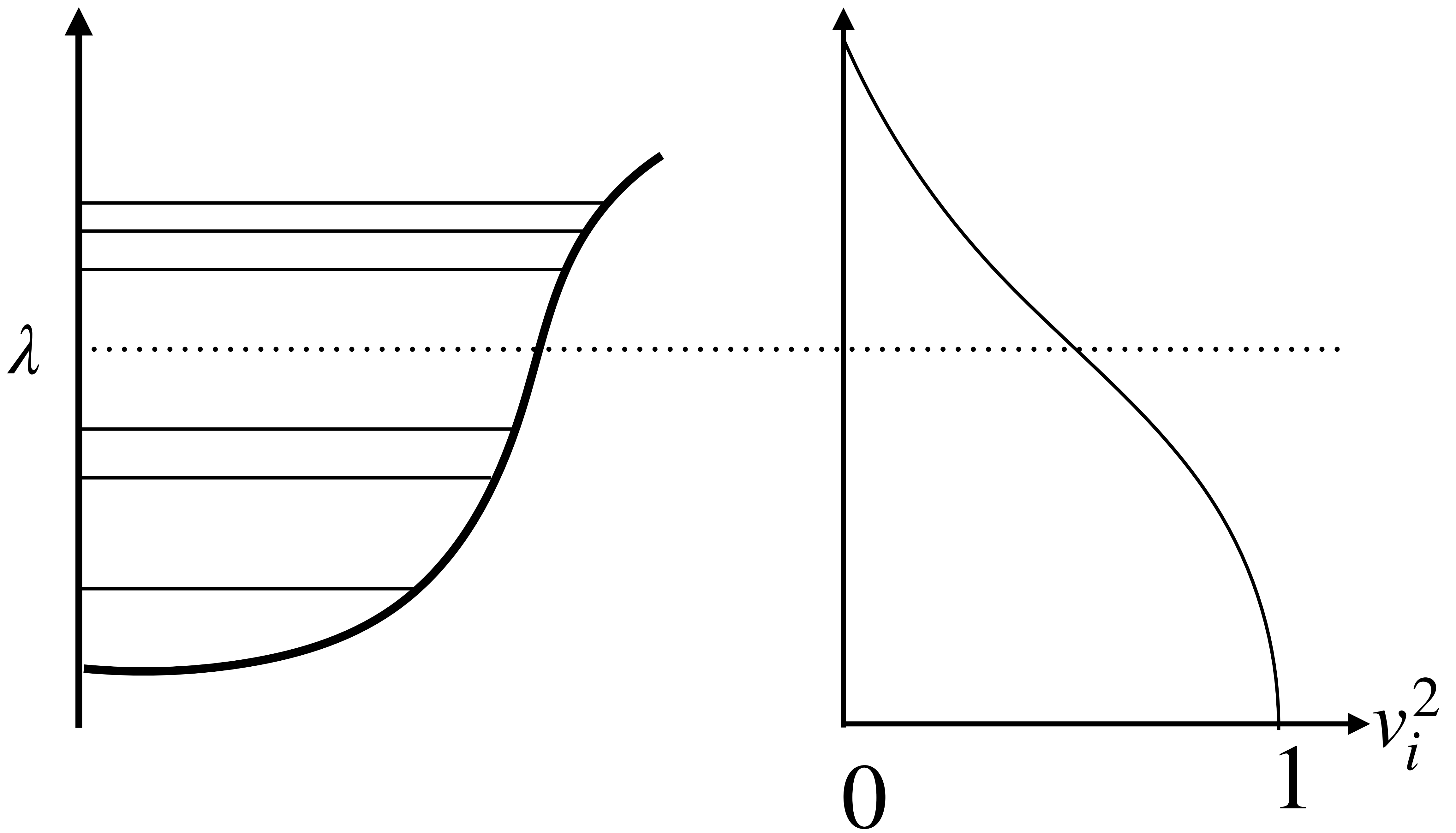
$$|\Phi_{\mathrm{BCS}}\rangle = \prod_{i>0} (u_i + v_i a_i^\dagger a_{\tilde{i}}^\dagger) |0\rangle$$

$$a_i^\dagger = \theta_i a_i^\dagger + (1-\theta_i) a_i^\dagger$$
$$=: b_i + d_i^\dagger$$

hole particle







s.p. states are occupied up to the Fermi energy

s.p. orbitals are partially occupied

BCS theory

The particle # is broken

$$H' = H - \lambda N \qquad \lambda: \text{ Lagrange multiplier}$$

$$= \sum_{i>0} (\varepsilon_i - \lambda)(c_i^\dagger c_i + c_{\tilde{i}}^\dagger c_{\tilde{i}}) - \sum_{i,j>0} G_{ij} A_i^\dagger A_j$$

variation $\delta\langle \mathrm{BCS} | \hat{H}' | \mathrm{BCS} \rangle = 0$

$$0 = \frac{\partial}{\partial v_i}\left[2\sum_{j>0}(\varepsilon_j - \lambda)v_j^2 - \sum_{j,k>0} G_{jk}\sqrt{1-v_j^2}\,v_j\sqrt{1-v_k^2}\,v_k\right] \qquad u_i^2 + v_i^2 = 1$$

$$= u_i^{-1}\left[4(\varepsilon_i - \lambda)u_i v_i - 2(u_i^2 - v_i^2)\sum_{j>0} G_{ij} u_j v_j\right]$$

pair potential

$$\Delta_i := \sum_{j>0} G_{ij} u_j v_j$$

variational eq.

$$2(\varepsilon_i - \lambda)u_i v_i = \Delta_i (u_i^2 - v_i^2)$$

BCS theory

gap eq. $$\Delta_i = \frac{1}{2}\sum_{j>0} G_{ij}\frac{\Delta_j}{\sqrt{(\varepsilon_i - \lambda)^2 + \Delta_i^2}}$$

particle # $$N = \frac{1}{2}\sum_{i>0}\left(1 - \frac{\varepsilon_i - \lambda}{\sqrt{(\varepsilon_i - \lambda)^2 + \Delta_i^2}}\right)$$

trivial solution:

$\Delta_i = 0$ normal(fluid)

$v_i = 1,\ u_i = 0$ or $v_i = 0,\ u_i = 1$

hole particle

in the case $G_{ij} = G$, $\frac{G}{2}\sum_{j>0}\frac{1}{|\varepsilon_j - \lambda|} < 1$ stays as normal

⟷ Cooper instability in infinite systems

shell structure around the Fermi level is important in finite systems

HF+BCS scheme

solve the HF eq. $h|i\rangle = \varepsilon_i|i\rangle$

---

initial values for Δ_i

particle # condition

the chemical potential λ is determined with $N = \langle \mathrm{BCS}|\hat{N}|\mathrm{BCS}\rangle = 2\sum_{i>0} v_i^2$

BCS amplitudes u_i, v_i

$$u_i^2 = \frac{1}{2}\left[1 + \frac{\varepsilon_i - \lambda}{\sqrt{(\varepsilon_i - \lambda)^2 + \Delta_i^2}}\right], \quad v_i^2 = \frac{1}{2}\left[1 - \frac{\varepsilon_i - \lambda}{\sqrt{(\varepsilon_i - \lambda)^2 + \Delta_i^2}}\right]$$

the pair field Δ_i is updated $\Delta_i = \sum_{j>0} G_{ij} u_j v_j$

Excited states in the BCS model

$$H'_{\rm MF} = \sum_{i>0} E_i(a_i^\dagger a_i + a_{\tilde{i}}^\dagger a_{\tilde{i}}) + \text{const}$$

$$E_i = \sqrt{(\varepsilon_i - \lambda)^2 + \Delta_i^2}$$

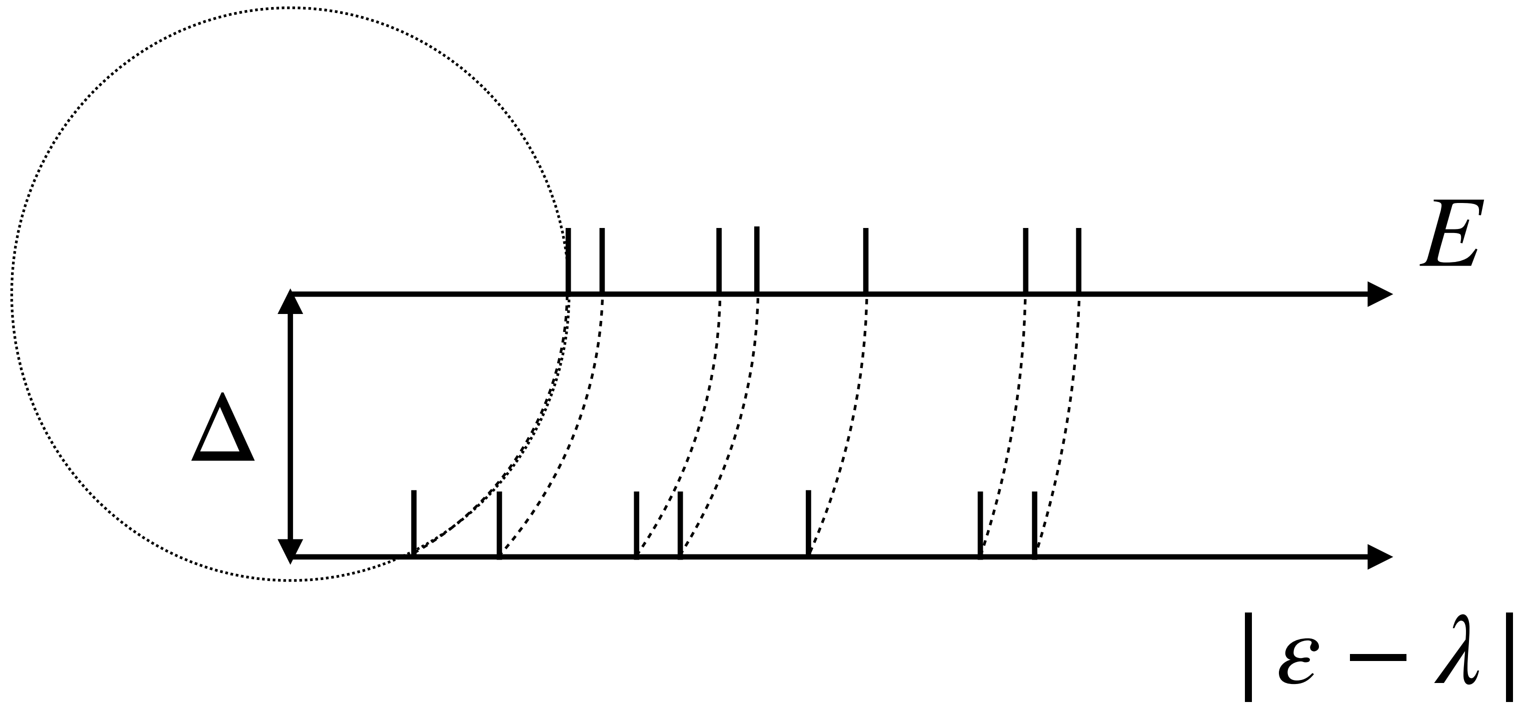
vacuum for q.p.: $|\Phi_{\rm BCS}\rangle = \prod_{i>0}(u_i + v_i \underbrace{c_i^\dagger c_{\tilde{i}}^\dagger}_{J=0 \text{ pair}})|0\rangle$

||

g.s. of an even–even nucleus

excited states = 2qp excitations: $a_i^\dagger a_j^\dagger |\Phi_{\rm BCS}\rangle$

Excitation energy $E_i + E_j \geq 2\Delta$



g.s. of a neighboring odd nucleus =
lowest 1qp excitation: $a_0^\dagger |\Phi_{\rm BCS}\rangle$

excited states of a neighboring odd nucleus =
1qp excitations: $a_i^\dagger |\Phi_{\rm BCS}\rangle$

Excitation energy $E_i - E_0 \sim E_i - \Delta$

different level densities in low energy in e-e and odd nuclei

Generalized mean-field theory: Hartree–Fock–Bogoliubov

HF+BCS: the s.p. orbitals are unchanged

➡ simultaneous optimization of the HF field and the pair field

$$\rho_{ji} = \langle \Phi | c_i^\dagger c_j | \Phi \rangle, \quad \kappa_{ji} = \langle \Phi | c_i c_j | \Phi \rangle, \quad \kappa_{ij}^* = \langle \Phi | c_i^\dagger c_j^\dagger | \Phi \rangle$$

Wick's theorem

$$c_i^\dagger c_j = \rho_{ji} + : c_i^\dagger c_j :$$

$$\begin{aligned} c_i^\dagger c_j^\dagger c_l c_k = {} & \rho_{ki}\rho_{lj} - \rho_{li}\rho_{kj} + \kappa_{ij}^* \kappa_{kl} \\ & + \rho_{ki} : c_j^\dagger c_l : + \rho_{lj} : c_i^\dagger c_k : - \rho_{li} : c_j^\dagger c_k : - \rho_{kj} : c_i^\dagger c_l : \\ & \underline{+ \kappa_{ij}^* : c_l c_k : + \kappa_{kl} : c_i^\dagger c_j^\dagger :} \quad \text{not considered in the HF approx.} \\ & + : c_i^\dagger c_j^\dagger c_l c_k : \end{aligned}$$

Generalized mean-field theory: Hartree–Fock–Bogoliubov

mean-field approx.

$$H - \lambda N = \sum_{ij} (t_{ij} - \lambda\delta_{ij}) c_i^\dagger c_j + \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} c_i^\dagger c_j^\dagger c_l c_k \qquad \cancel{+\frac{1}{4}\sum_{ijkl} \bar{v}_{ijkl} : c_i^\dagger c_j^\dagger c_l c_k :}$$

$$= \text{const} + \sum_{ij} (t_{ij} - \lambda\delta_{ij}) : c_i^\dagger c_j : + \sum_{ijkl} \bar{v}_{ijkl} \rho_{ki} : c_j^\dagger c_l : + \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} (\kappa_{ij}^* : c_l c_k : + \kappa_{kl} : c_i^\dagger c_j^\dagger :)$$

$$H'_{\mathrm{MF}} = \text{const} + \sum_{ij} (t_{ij} + \Gamma_{ij} - \lambda\delta_{ij}) : c_i^\dagger c_j : + \frac{1}{2} \sum_{ij} (\Delta_{ij} : c_i^\dagger c_j^\dagger : + \Delta_{ij}^* : c_j c_i :)$$

$$= \text{const} + \frac{1}{2} \sum_{ij} : \psi_i^\dagger \begin{bmatrix} h - \lambda & \Delta \\ -\Delta^* & -(h^* - \lambda) \end{bmatrix}_{ij} \psi_j :$$

$$\parallel$$

$$\mathscr{H}$$

we want to diagonalize it

$$= \text{const} + \sum_\alpha E_\alpha a_\alpha^\dagger a_\alpha$$

$$\psi_j = \begin{pmatrix} c_j \\ c_j^\dagger \end{pmatrix}$$

Nambu–Gorkov

$$\Gamma_{ij} = \sum_{kl} \bar{v}_{ikjl} \rho_{lk}$$

$$\Delta_{ij} = \frac{1}{2} \sum_{kl} \bar{v}_{ikjl} \kappa_{kl}$$

Generalized mean-field theory: Hartree–Fock–Bogoliubov

$$\sum_j \begin{bmatrix} h-\lambda & \Delta \\ -\Delta^* & -(h^*-\lambda) \end{bmatrix}_{ij} \phi_{\alpha j} = E_\alpha \phi_{\alpha i}, \quad \phi_{\alpha i} = \begin{pmatrix} U_{\alpha i} \\ V_{\alpha i} \end{pmatrix}$$

when $E_\alpha, (U_{\alpha i}, V_{\alpha i})^T$ is the solution, then $-E_\alpha, (V^*_{\alpha i}, U^*_{\alpha i})^T$ is also the solution

any vectors (fields) are given by the linear combination $\quad \psi_i = \sum_\alpha \left[a_\alpha \begin{pmatrix} U_{\alpha i} \\ V_{\alpha i} \end{pmatrix} + b_\alpha \begin{pmatrix} V^*_{\alpha i} \\ U^*_{\alpha i} \end{pmatrix} \right]$

promote the fields to the operators $\quad \hat{\psi}_i = \sum_\alpha \left[\hat{a}_\alpha \begin{pmatrix} U_{\alpha i} \\ V_{\alpha i} \end{pmatrix} + \hat{b}_\alpha \begin{pmatrix} V^*_{\alpha i} \\ U^*_{\alpha i} \end{pmatrix} \right] = \begin{pmatrix} \hat{c}_i \\ \hat{c}^\dagger_i \end{pmatrix}$

Generalized mean-field theory: Hartree–Fock–Bogoliubov

hermicity $\hat{c}_i = (\hat{c}_i^\dagger)^\dagger$

$$\hat{c}_i = \sum_\alpha (\hat{a}_\alpha U_{\alpha i} + \hat{b}_\alpha V^*_{\alpha i})$$

$$(\hat{c}_i^\dagger)^\dagger = \sum_\alpha (\hat{a}_\alpha V_{\alpha i} + \hat{b}_\alpha U^*_{\alpha i})^\dagger$$

$$= \sum_\alpha (\hat{a}_\alpha^\dagger V^*_{\alpha i} + \hat{b}_\alpha^\dagger U_{\alpha i})$$

$\Rightarrow$ $\hat{b}_\alpha = \hat{a}_\alpha^\dagger$ annihilation of the hole=creation of the particle

quasiparticles: $\hat{a}_\alpha^\dagger = \sum_i U_{i\alpha}\hat{c}_i^\dagger + V_{i\alpha}\hat{c}_i$

U, V :matrices

BCS:

$a_{\tilde{i}}^\dagger = u_i c_{\tilde{i}}^\dagger + v_i c_i$

u, v :amplitudes

Generalized mean-field theory: Hartree–Fock–Bogoliubov

generalized Bogoliubov trans.: $\alpha^\dagger_\alpha = \sum_i U_{i\alpha} c_i^\dagger + V_{i\alpha} c_i$

$$\begin{pmatrix} \alpha_\alpha \\ \alpha^\dagger_\alpha \end{pmatrix} = \sum_i \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix}_{\alpha i} \begin{pmatrix} c_i \\ c_i^\dagger \end{pmatrix} = \mathscr{W}^\dagger \begin{pmatrix} c_i \\ c_i^\dagger \end{pmatrix}$$

unitary matrix $\mathscr{W} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}, \quad \mathscr{W}\mathscr{W}^\dagger = \mathscr{W}^\dagger\mathscr{W} = 1$

$$U^\dagger U + V^\dagger V = 1, \qquad UU^\dagger + V^* V^T = 1$$

$$U^T V + V^T U = 0, \qquad UV^\dagger + V^* U^T = 0$$

BCS:

$$u_i^2 + v_i^2 = 1$$

Hartree–Fock–Bogoliubov (HFB) equation

$$\rho_{ij} = \langle \Phi | c_j^\dagger c_i | \Phi \rangle, \quad \kappa_{ij} = \langle \Phi | c_j c_i | \Phi \rangle$$
$$= (V^* V^T)_{ij} \qquad\qquad = (V^* U^T)_{ij} = -(UV^\dagger)_{ij}$$

properties of U, V matrices $\quad \rho^2 - \rho = -\kappa\kappa^\dagger, \quad \rho\kappa = \kappa\rho^*$

generalized density matrix

$$\mathscr{R} := \begin{pmatrix} \langle \Phi | c_j^\dagger c_i | \Phi \rangle & \langle \Phi | c_j c_i | \Phi \rangle \\ \langle \Phi | c_j^\dagger c_i^\dagger | \Phi \rangle & \langle \Phi | c_j c_i^\dagger | \Phi \rangle \end{pmatrix} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1 - \rho^* \end{pmatrix}, \qquad \mathscr{R}^2 = \mathscr{R}$$

$$\mathscr{H} = \begin{pmatrix} h - \lambda & \Delta \\ -\Delta^* & -h^* + \lambda \end{pmatrix} \qquad [\mathscr{H}, \mathscr{R}] = 0 \qquad \text{HFB eq}$$

Hartree–Fock:

$$[h, \rho] = 0, \quad \rho^2 = \rho$$

HFB scheme

initial values for ρ_{ij} and κ_{ij}

ph-channel: HF potential   pp-channel: pair potential

mean fields $$\Gamma_{ij} = \sum_{kl} \bar{v}_{ikjl}\rho_{lk}, \qquad \Delta_{ij} = \frac{1}{2}\sum_{kl} \bar{v}_{ikjl}\kappa_{kl}$$

the chemical potential λ is determined with $N = \langle \Phi | \hat{N} | \Phi \rangle = 2 \sum_{i,\alpha>0} V^*_{i\alpha} V_{i\alpha}$

eigenvalue prob. $$\sum_j \begin{bmatrix} h-\lambda & \Delta \\ -\Delta^* & -(h^*-\lambda) \end{bmatrix}_{ij} \begin{pmatrix} U_{\alpha j} \\ V_{\alpha j} \end{pmatrix} = E_\alpha \begin{pmatrix} U_{\alpha i} \\ V_{\alpha i} \end{pmatrix}$$

α: quasiparticle basis

the densities are updated

$$\rho_{ij} = \langle \Phi | c_j^\dagger c_i | \Phi \rangle = \sum_\alpha V^*_{i\alpha} V_{j\alpha}, \quad \kappa_{ij} = \langle \Phi | c_j c_i | \Phi \rangle = \sum_\alpha V^*_{i\alpha} U_{j\alpha}$$

Exercise 1

Basics of the mean-field calculation

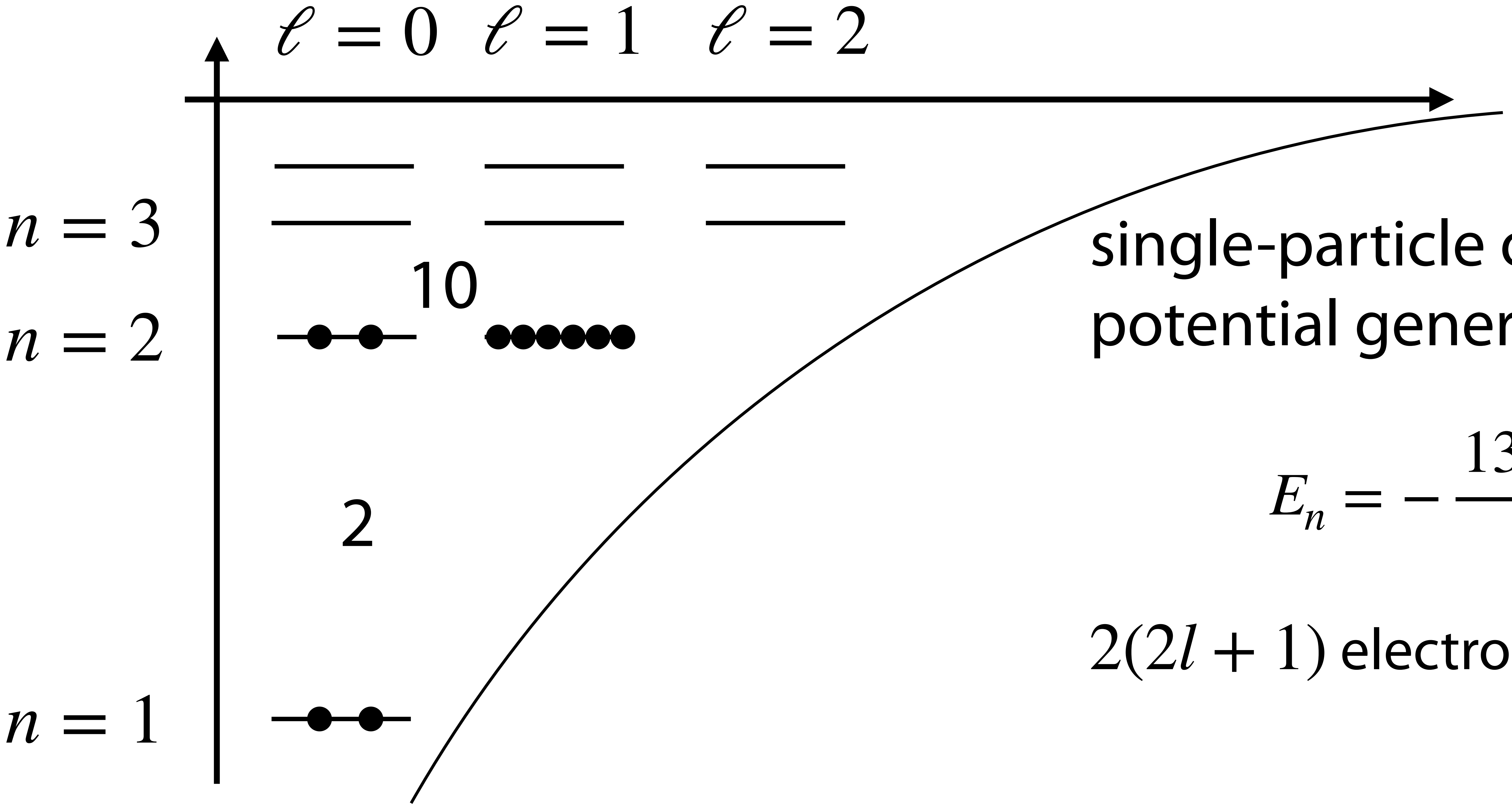
Eigen-value problem

Independent-particle model: mean field approach

understanding the shell effect–magic number

cf. atomic periodicity

stability of novel gas: He, Ne, Ar, Kr, Xe,... (2, 10, 18, 36, 54,…)



single-particle orbital in the Coulomb potential generated by a nucleus with Ze

$$E_n = -\frac{13.6Z^2}{n^2}\ \mathrm{eV}, \qquad n = n_r + \ell + 1$$

$2(2l+1)$ electrons in each orbital

Hartree potential: $\Gamma_{\mathrm{H}}(\vec{r}) = \int d\vec{r}' v(\vec{r}, \vec{r}') \sum_{j=1}^{A} |\varphi_j(\vec{r}')|^2 = \int d\vec{r}' v(\vec{r}, \vec{r}') \rho(\vec{r}')$

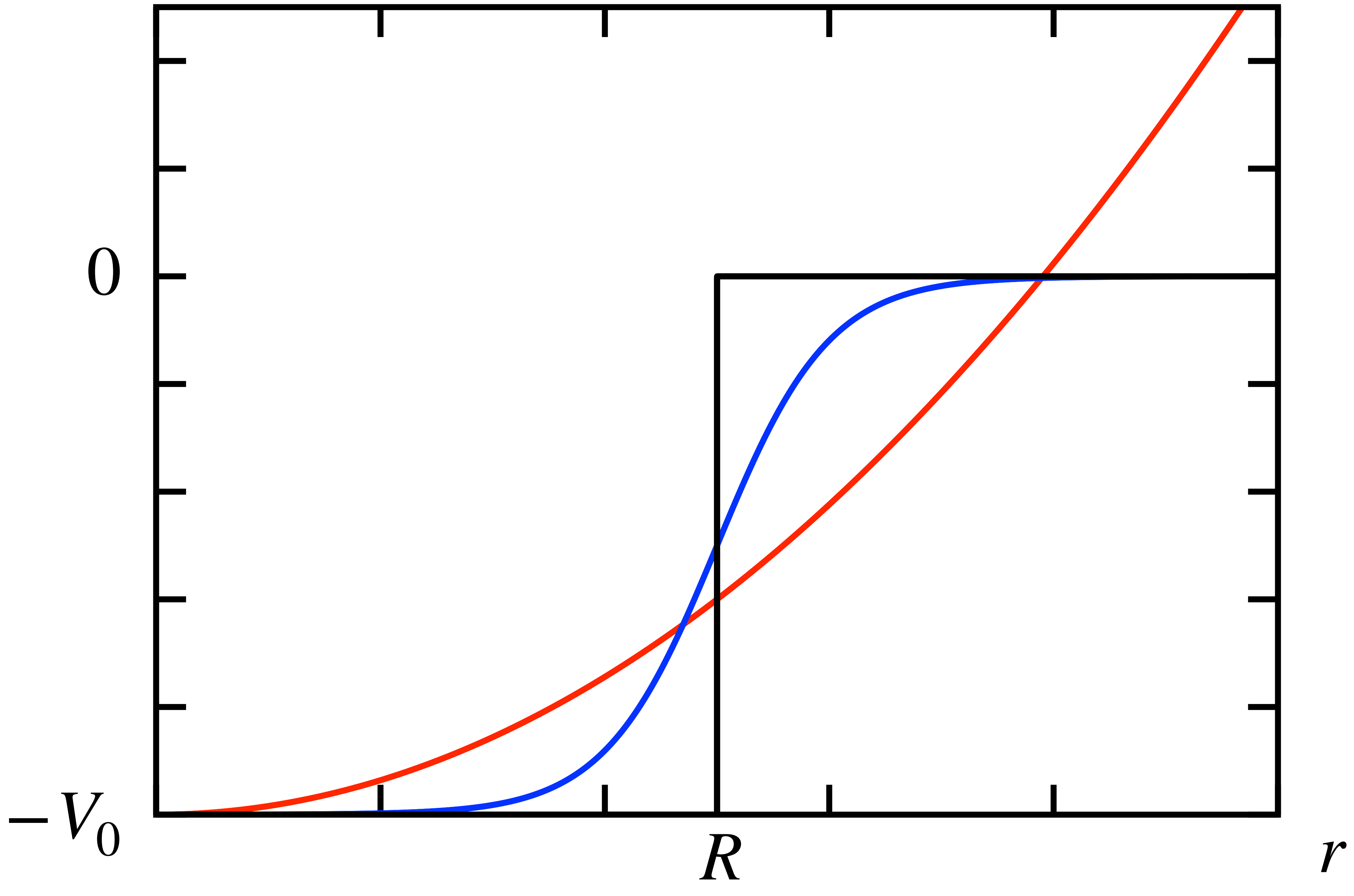
proportional to the density distribution

phenomenological shell model potential

Woods–Saxon potential $V(\vec{r}) = -V_0 \dfrac{1}{1 + \exp[(r-R)/a]}$

Harmonic Oscillator potential $V(\vec{r}) = -V_0 + \dfrac{1}{2} k r^2$

Square well potential



Single-particle orbital

$$-\frac{\hbar^2}{2m}\Delta\varphi_k(\vec{r}) + V(\vec{r})\varphi_k(\vec{r}) = \varepsilon_k\varphi_k(\vec{r})$$

neglecting the spin d.o.f

polar coordinate:

$$\varphi_{n\ell m}(\vec{r}) = \frac{u_{n\ell}(r)}{r}Y_{\ell m}(\theta\phi)$$

ℓ is a good quantum number for the central potential

m: magnetic quantum number

Schrödinger eq.

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u_{n\ell}(r) + \left(V(r) + \frac{\hbar^2\ell(\ell+1)}{2mr^2}\right)u_{n\ell}(r) = \varepsilon_{n\ell}u_{n\ell}(r)$$

Woods–Saxon (WS) potential — solved numerically

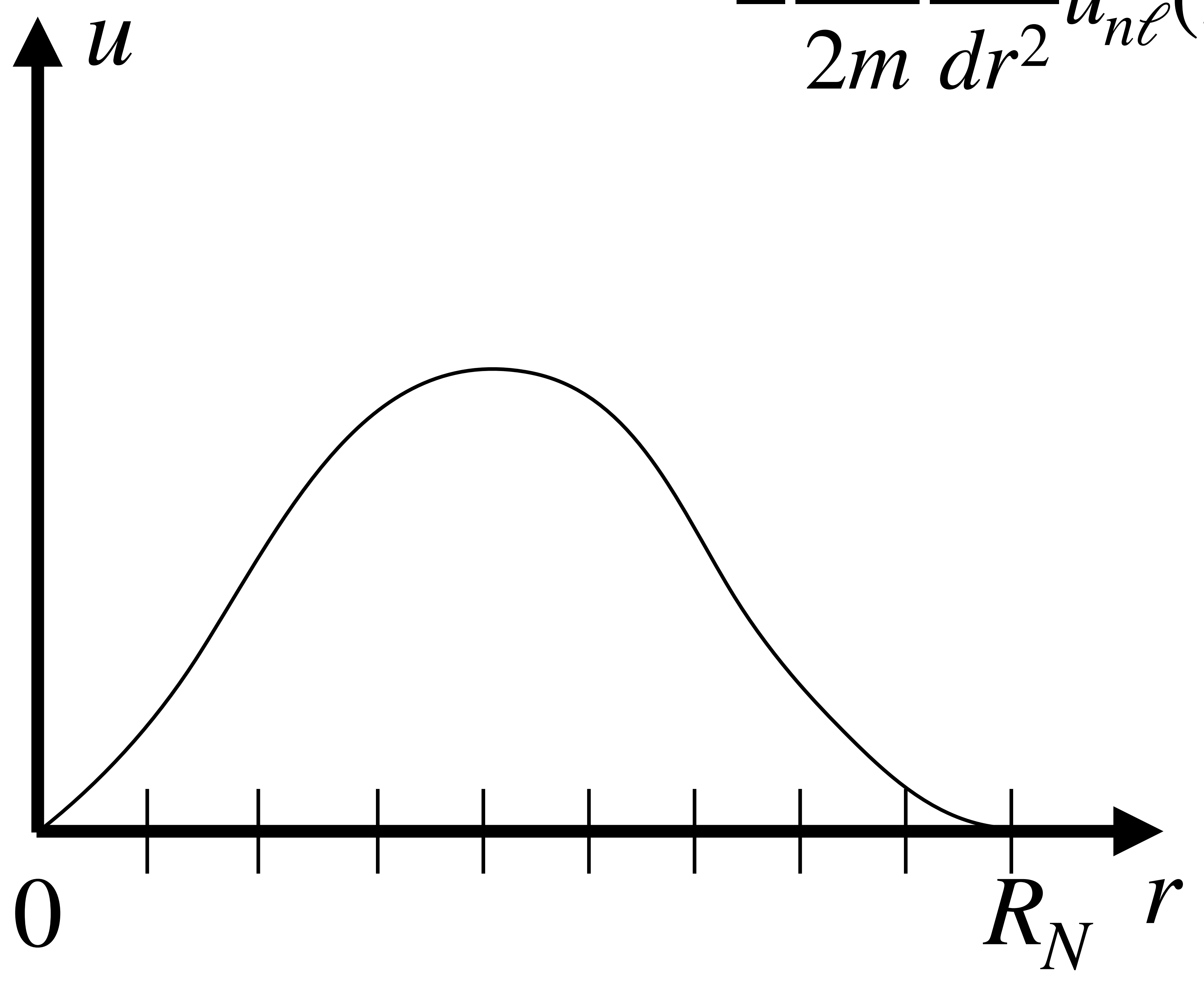
Harmonic Oscillator (HO) potential — solved analytically — $\varepsilon_{nl} = \hbar\omega(N + \frac{3}{2}),\ N = 2n + \ell$

Square well potential — solved analytically for infinite well — $\varepsilon_{n\ell} = -V_0 + \frac{\hbar^2 k_{n\ell}^2}{2m}$

$j_\ell(k_{n\ell}R) = 0$

Let's try to solve the Sc. eq. numerically

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u_{n\ell}(r) + \left(V(r) + \frac{\hbar^2\ell(\ell+1)}{2mr^2}\right)u_{n\ell}(r) = \varepsilon_{n\ell}u_{n\ell}(r)$$



discretization of the radial coordinate

$$r(i) = r_i = i \times \Delta, \qquad i = 0,1,\cdots N_r$$

Δ: radial mesh size — should be small

N_r: number of mesh points — should be large

representation of differential operator

$$\frac{d^2u_i}{dr^2} \simeq \frac{1}{\Delta^2}(u_{i+1} - 2u_i + u_{i-1})$$

three-point formula of the finite-difference method

Boundary conditions important!

$$r(i) = r_i = i \times \Delta$$

$$u(0) = u_1 = 0$$

$$u(R_N) = u_N = 0$$ box boundary condition (bound-state approximation)

= infinite square well potential

The kinetic energy is represented as

$$\frac{\hbar^2}{2m} = B = \frac{197^2}{2 \times 939} = 20.7\,\mathrm{MeV\,fm^2}$$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} = -B \begin{pmatrix} -2 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \cdots & 0 \\ 0 & 1 & -2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 1 \\ 0 & \cdots & 0 & 1 & -2 \end{pmatrix} \begin{pmatrix} u_2 \\ u_3 \\ u_4 \\ \vdots \\ u_{N-1} \end{pmatrix}$$

For $\ell = 0$, $$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u_n(r) + V(r)u_n(r) = \varepsilon_n u_n(r)$$

Solve the Sc. equation with the HO potential by diagonalizing the matrix numerically

$$V(r) = \frac{m\omega^2}{2}r^2, \qquad \hbar\omega = 41 \times A^{-1/3}\,\mathrm{MeV}$$

mass number

then find the optimal values of Δ and N_r by comparing with the analytical solution.

$$\varepsilon_1 = 3/2\hbar\omega$$

$$\varepsilon_2 = 7/2\hbar\omega$$

$$\varepsilon_n = [2(n-1) + 3/2]\hbar\omega$$

Find the solutions for every ℓ.