Development of shell models for nuclear astrophysics

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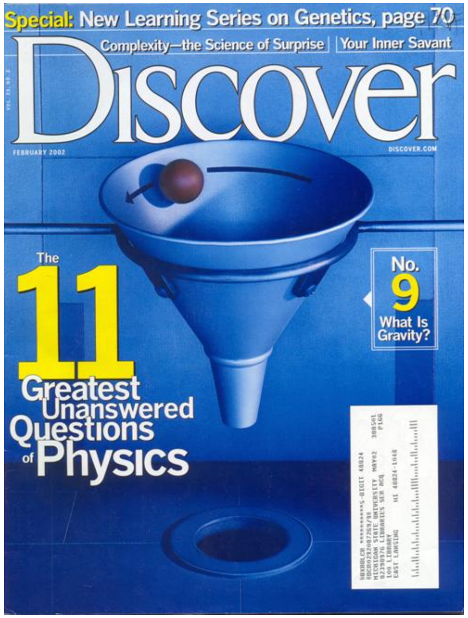
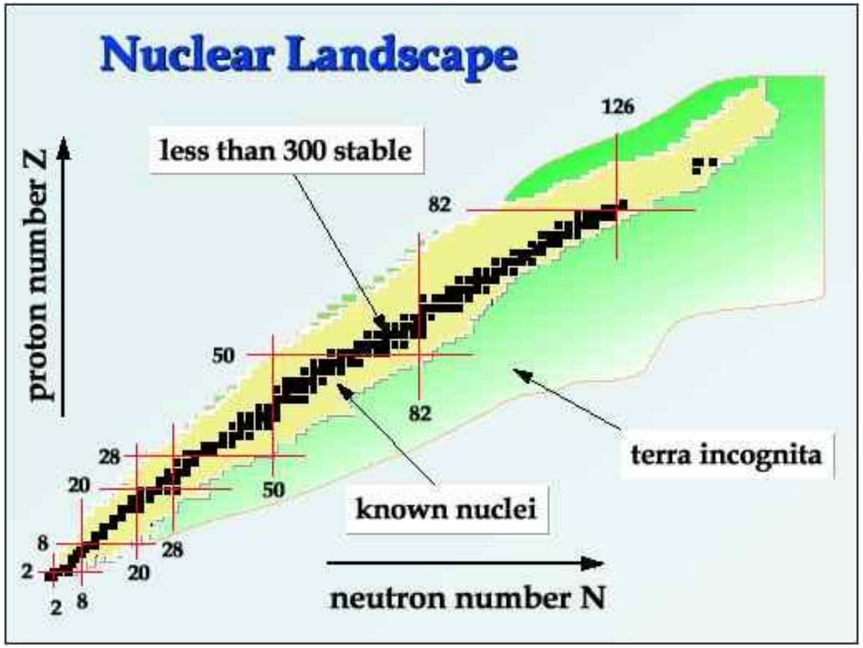
What is the Universe made of ?

- The origin of matter in the Universe is among the most fundamental questions in sciences
- What is the Universe made of ?
  - About 95% are of the dark matter and dark energy (don't know exactly what they are)
  - Nuclear astrophysics attempts to study the rest 5%
- One of the questions: How were the elements from iron to uranium made?



Nuclear landscape

- 118 elements are known
- < 300 stable isotopes with half-lives comparable to or longer than the age of the Earth
- Some unstable isotopes are known but not well-studied
- Several thousand isotopes are unexplored
- These are targets for FRIB, and at GSI, RIKEN, HIAF



Important role of nuclear structure in nucleosynthesis

- Nuclear structure controls the clock for the stellar processes
  - the total time along the reaction path entirely determines the speed of nucleosynthesis towards heavier nuclei and the produced isotopic abundances
- Need to know:
  - nuclear masses (ground state properties, energy gaps, single-particle levels, ...)
  - nuclear structure (nuclear deformation, collective excitations, quasiparticle excitations, isomeric states, …)
  - capture rates, β-decay rates
  - and under thermal conditions

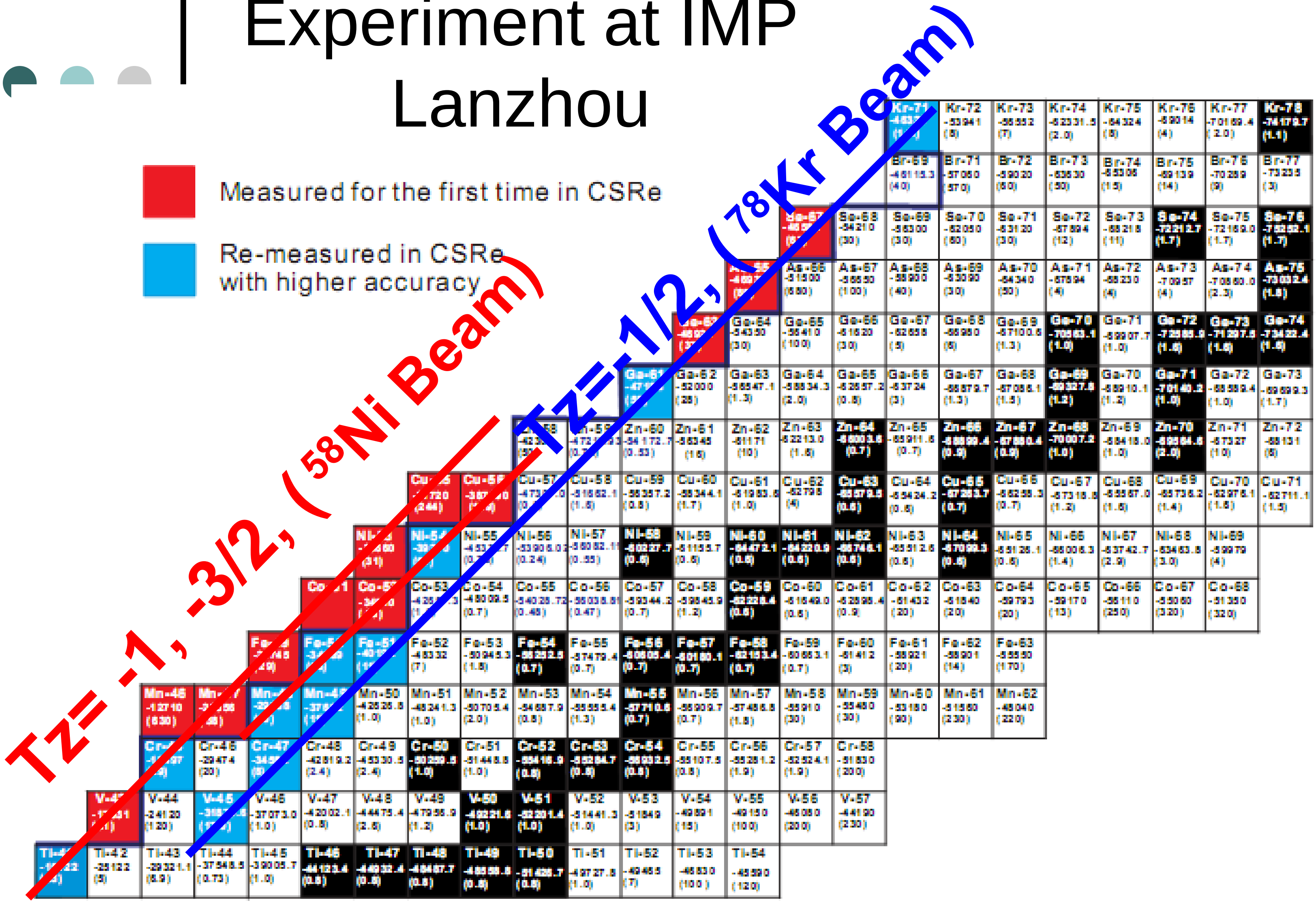
Tiny changes in nuclear structure and `big' effect in nucleosynthesis

- *Could a tiny change in nuclear structure cause big effects in nucleosynthesis?*

- Examples in rp-process of nucleosynthesis in nuclear astrophysics
  - Changes in mass near and at the waiting-points
  - Structures near waiting point nuclei

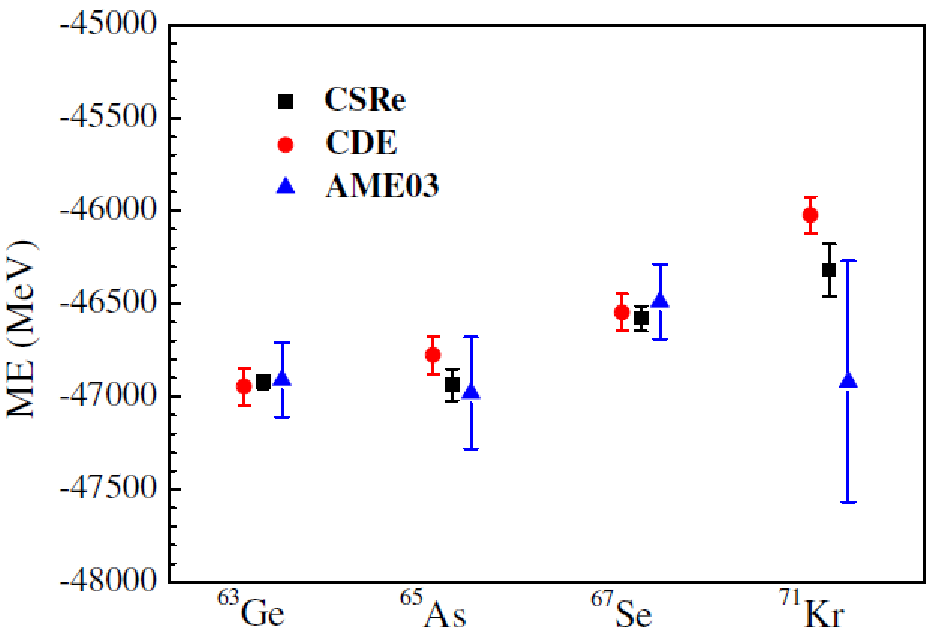
- These nuclei are very short-lived, close to the drip line, and therefore, very challenging experimentally,

Experiment at IMP Lanzhou



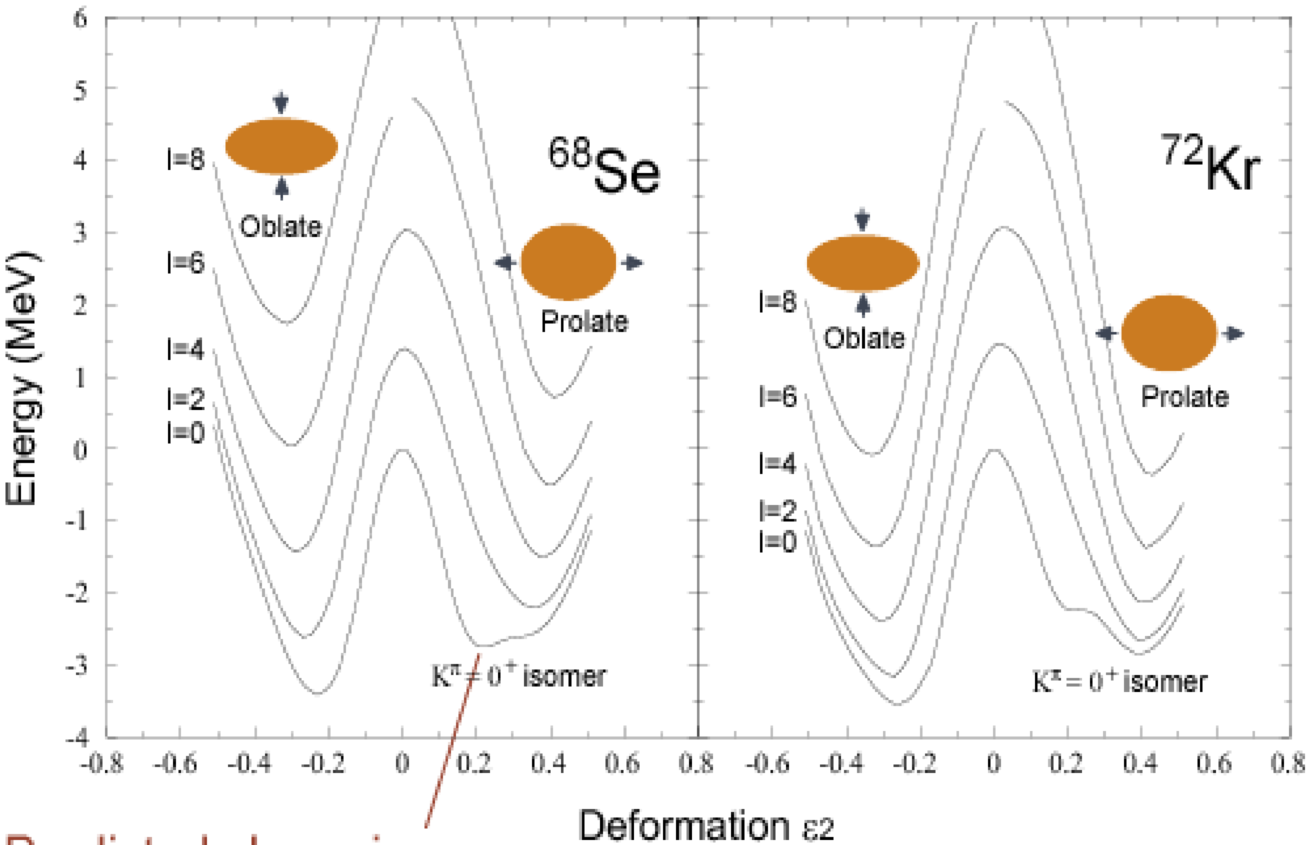
Recent mass measurement at IMP

- Masses of these nuclei are measured for the first time
- Test of reliability of model predictions
- Reduce error bars in previous measurements
- For example: new data show some differences for ^{65}As and ^{71}Kr.

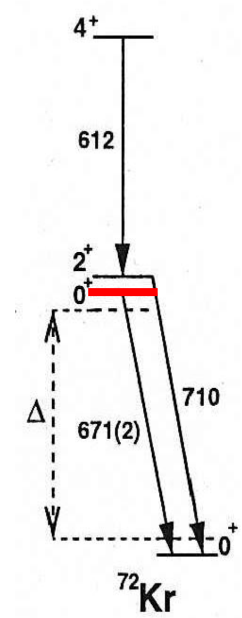


X. Tu et al., Phys. Rev. Lett. 106 (2011) 112501

Shape coexistence in waiting-point nuclei ^{68}Se and ^{72}Kr



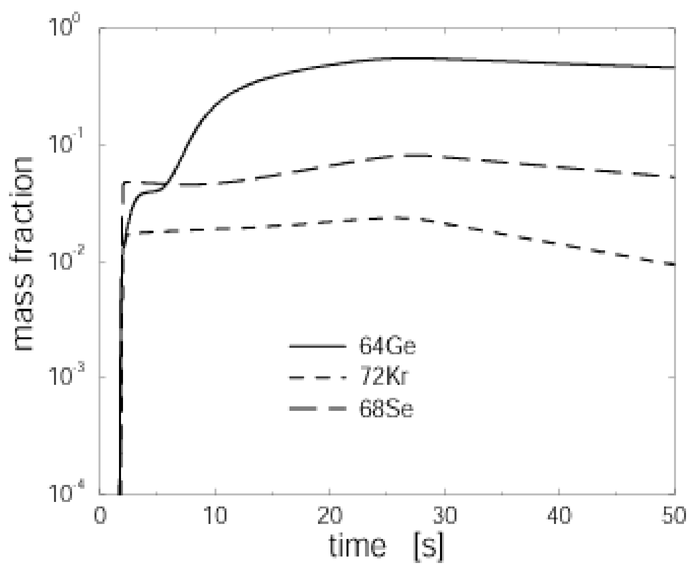
Predicted shape isomer



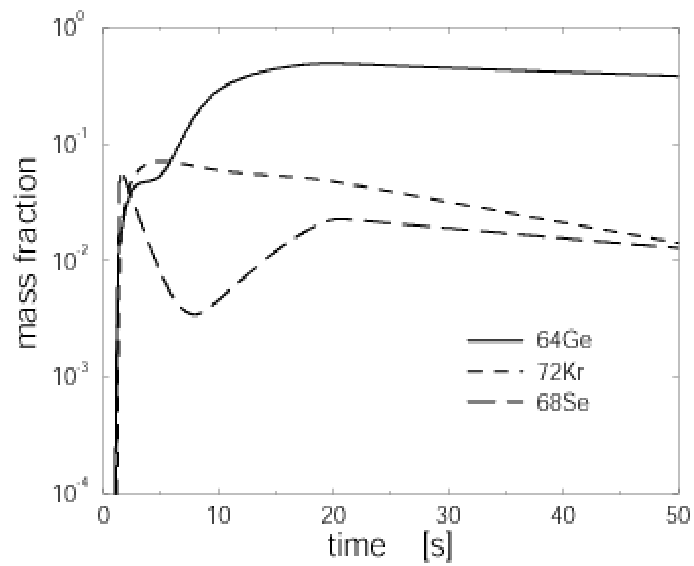
Bouchez *et al*, *PRL* (2003)

Abundances in X-ray burst environment

- It is possible that a flow towards higher mass through the isomer branch can occur (calculations using multi-mass-zone x-ray burst model)
  - Sun, Wiescher, Aprahamian, Fisker, *Nucl. Phys.* A758 (2005) 765



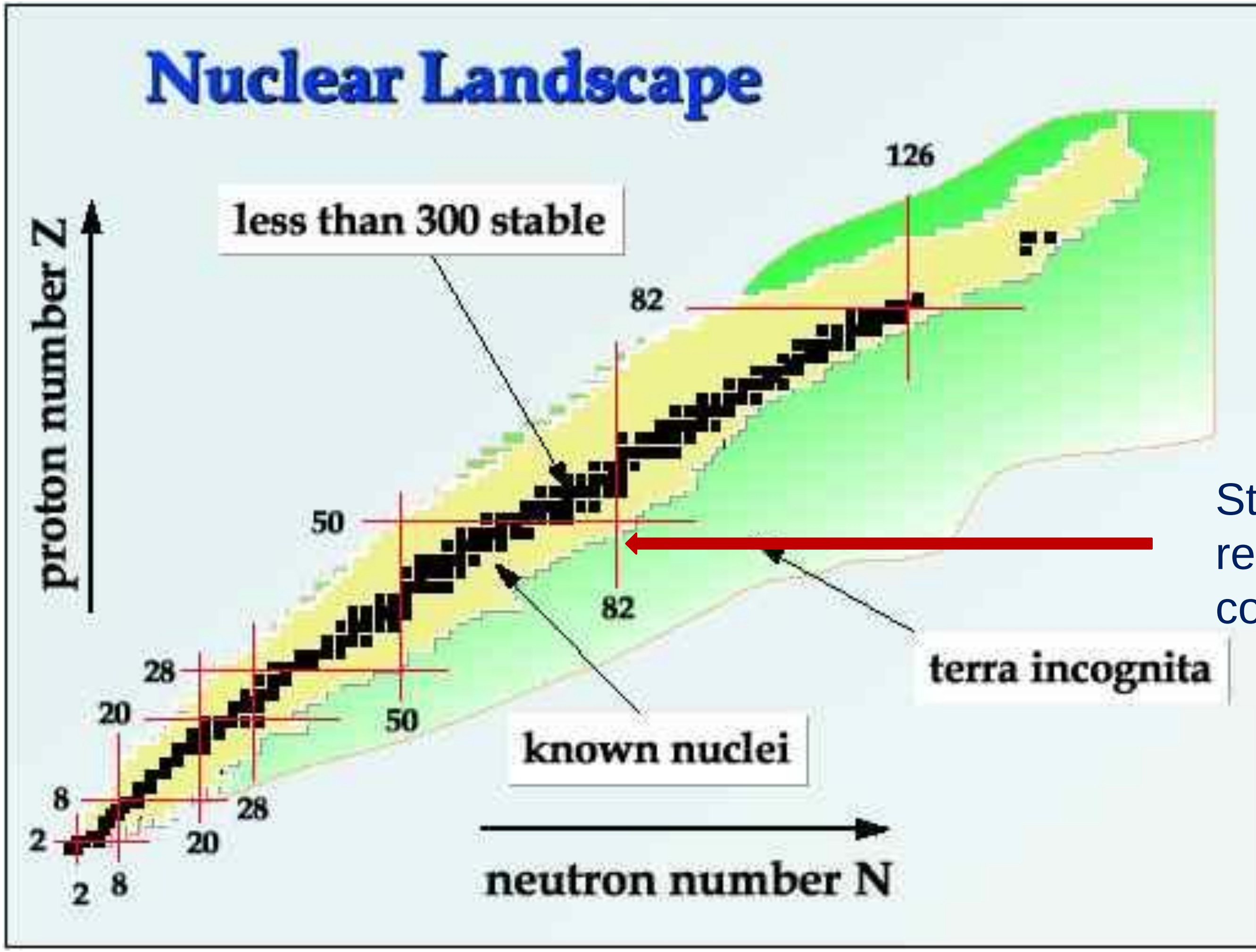
Without any possible isomer contribution



Full flow through isomers rather than g-states

Many structures unexplored

K. L. Kratz et al., Z. Phys. A 325, 489 (1986).



Identification of the classical N = 82 r-process wait-point isotope ^{130}Cd

30 years later

Structure of south-east region of ^{132}Sn is still completely unknown

A. Jungclaus et al., Phys. Rev. C 93, 041301(R) (2016).

Theoretical description of heavy, deformed nuclei

- Physical observables is a combination of operators and wave functions
- This lecture discuss mainly how to build many-body wave functions
- Once you know this, simply pick up a workable Hamiltonian, calculate the matrix elements, do the diagonalization, numerically.

Nuclear structure models

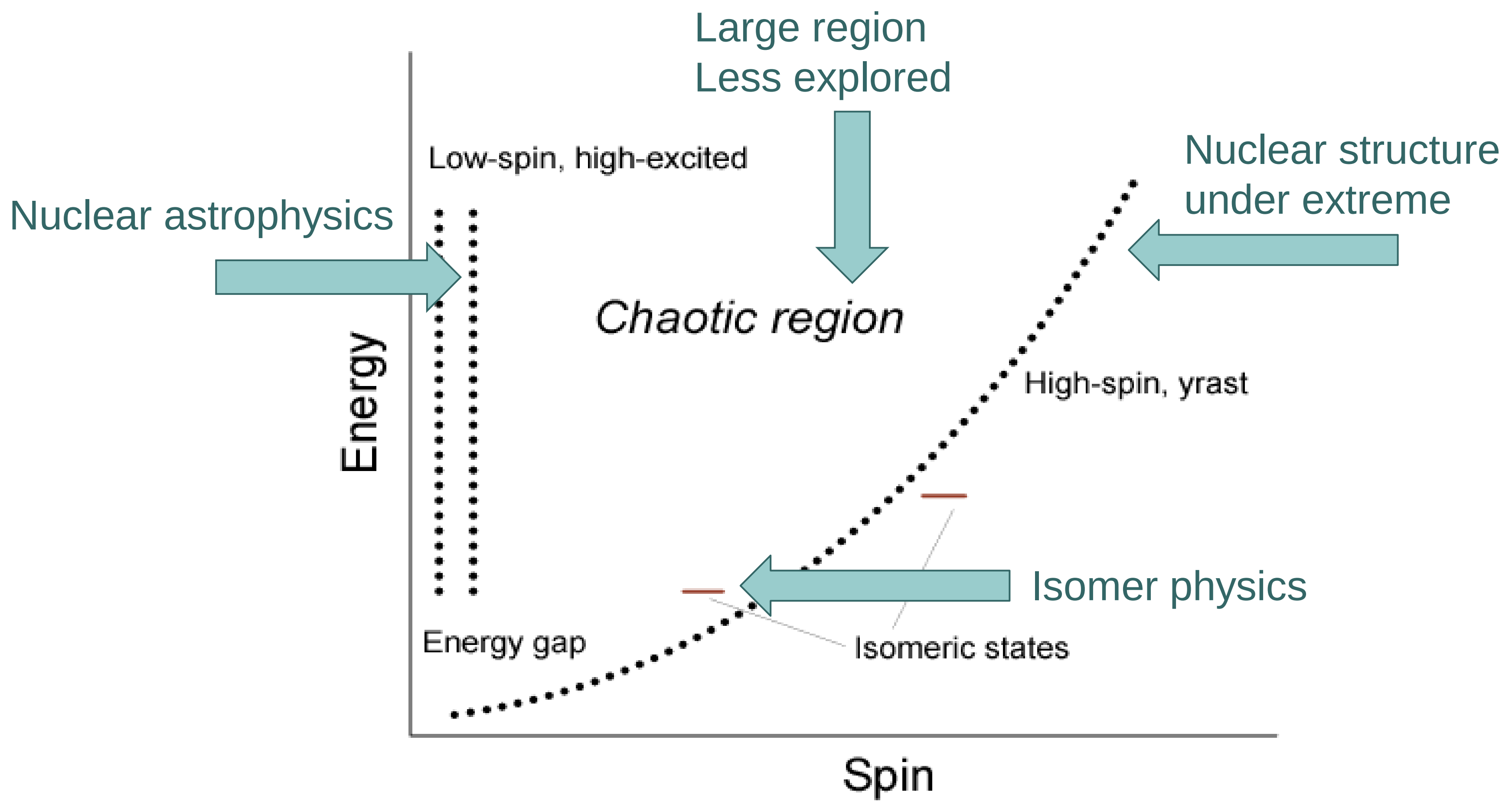
- Description of the strongly correlated many-body systems – two popular methods:
- Shell-model diagonalization method
  - Based on quantum mechanical principles
  - Growing computer power helps extending applications
  - A single configuration contains no physics
  - Huge basis dimension required, severe limit in applications
- Density functional theory
  - Applicable to any size of systems
  - Fruitful physics around minima of energy surfaces
  - No configuration mixing, results depending on quality of mean-field
  - States with broken symmetry, usually cannot study transitions

Shell models are needed

- Network calculations involve many nuclear data
  - currently, only very few data can be measured
  - some may be measured, but technically difficult
  - some others cannot be measured in ordinary labs with traditional methods

- Must rely on theoretical calculations
  - most traditional mean-filed type models are excluded
  - ab initio no core type models are not applicable
  - traditional shell models have limited use
  - new many-body techniques must be developed

Excited nuclear states



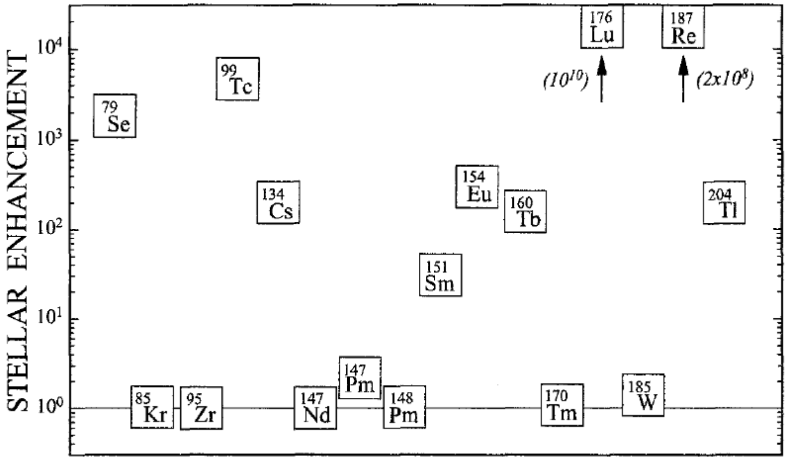
Stellar enhancement of decay rate

- A stellar enhancement can result from the thermal population of excited states

$$\lambda_\beta = \sum_i \left(p_i \times \sum_j \lambda_{\beta ij} \right)$$

$$p_i = \frac{(2I_i + 1) \times \exp(-E_i / kT)}{\sum_m (2I_m + 1) \times \exp(-E_m / kT)}$$

- Examples in the s-process



F. Kaeppeler,
Prog. Part. Nucl. Phys. 43 (1999) 419

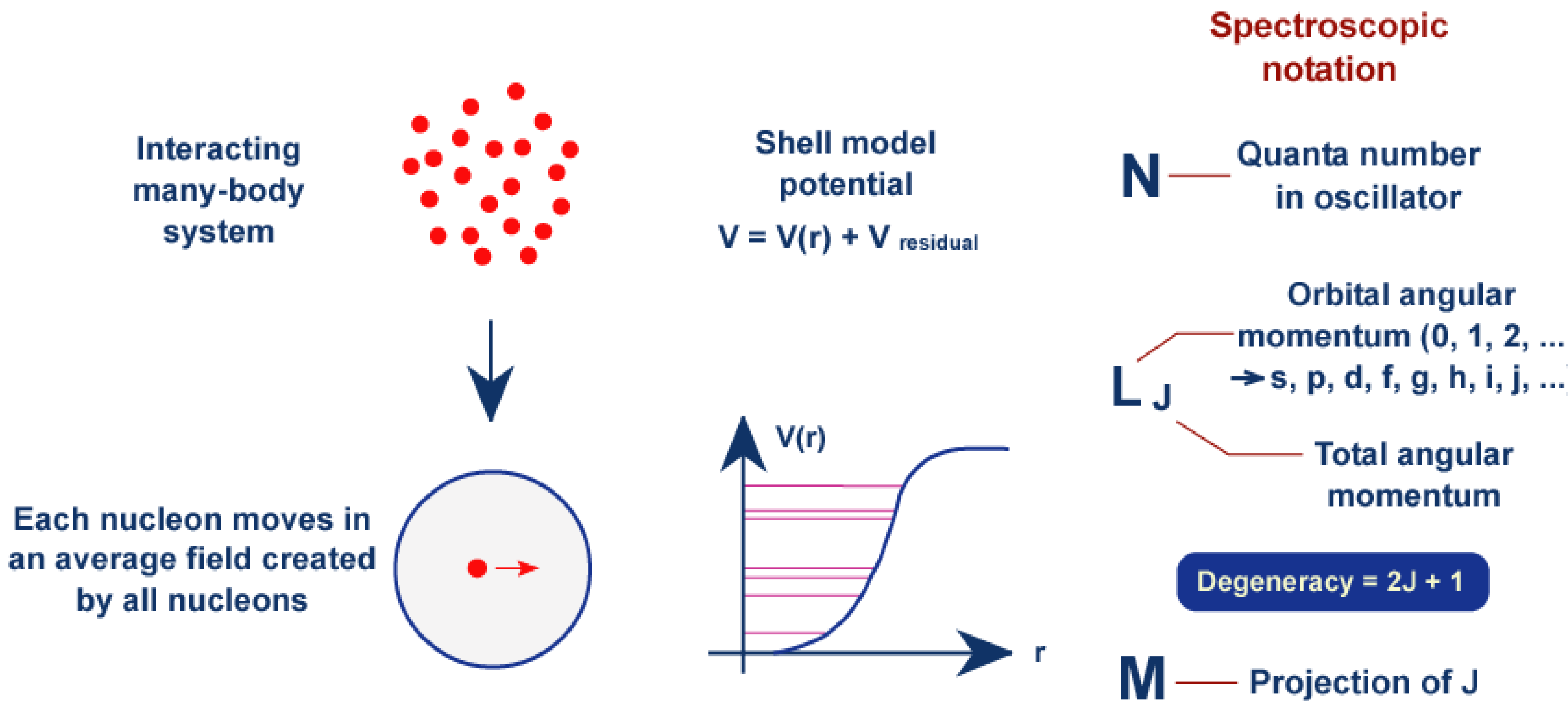
Properties of nuclei

- Nuclei are strongly correlated quantum many-body systems with particle number of the order $10^1 – 10^2$
  - The number is too big for obtaining an exact solution
  - The number is too small for applying statistical method
- Nucleon-nucleon interaction is via nuclear force
  - Property of nuclear force is still not clear
  - Effective interactions often used
- Nuclear deformation
  - Most nuclei are deformed
- Nuclear shell effect
  - Existence of magic numbers
    - Neutrons: 2, 8, 20, 28, 50, 82, 126, next ?
    - Protons: 2, 8, 20, 28, 50, 82, next ?

Assumption of average potential

- Unlike an atomic system, there is no real central force in nuclei
- To simplify the complicated many-body problem, assume that there is an average potential
- Individual particles move in bound orbitals in response to the remainder of the system
- Each orbital has a well designated energy, angular momentum, and parity associated with it
- Pauli Principle restricts the number of particles in each orbital and prohibits collisions between particles in nuclei

The average potential



Nuclear shells

orbital ang. mom. l .. s=0, p=1, d=2, f=3, g=4 ...(parity $\pi=(-1)^l$

spectroscopic notation: $0\,f_{7/2}$

"nodal" quantum number

total ang. mom. $j = l \pm 1/2$

For a given species of nucleon (protons *or* neutrons) we can put $2j+1$ particles into a j-orbit.

Shell gaps or **magic numbers** can be computed by adding up the occupancies below a certain level

intruder orbit

$0g_{9/2}$	10	[50]
$1p_{1/2}$	2	
$0f_{5/2}$	6	
$1p_{3/2}$	4	
$0f_{7/2}$	8	
$0d_{3/2}$	4	[20]
$1s_{1/2}$	2	
$0d_{5/2}$	6	
$0p_{1/2}$	2	[8]
$0p_{3/2}$	4	
$0s_{1/2}$	2	[2]

Nuclear many-body problem

- Introducing a mean-field potential *U*, a many-body Hamiltonian *H* = *T* + *V* can be written as

$$H = (T + U) + (V - U) = V_{average} + V_{residual}$$

- Success of nuclear structure calculations depends on how you treat the mean-field and the residual interaction
- Solution of Schrödinger equation is equivalent to diagonalizing the Hamiltonian *H* in a complete basis

$$|\Psi\rangle = \sum_i f_i |\phi_i\rangle$$

  - Problem of finding a solution is often related to basis truncation

Nuclear many-body problem

- To find mean field out of the microscopic two-body interactions, one applies variational principle
  - The solution corresponds to minimization in energy
  - The average pontential is called Hartree-Fock potential
  - Resulting average potential with a set of single particle states (energies and wave functions)
- Two widely used simple but powerful potentials
  - Woods-Saxon potential

$$V_{W.S.}(r) = -V_0\left[1+\exp\left(\frac{r-R_0}{a}\right)\right]^{-1}$$

  - Harmonic oscillator potential

$$V_{H.O.}(r) = -V_0\left[1-\left(\frac{r}{R_0}\right)^2\right]$$

Slater determinant

- Using an average potential, the general many-body Schroedinger equation can be reduced to a much simpler form

$$H\Psi = \left\{ \sum_{i=1}^{A} \left[-\frac{\hbar^2}{2m} \Delta_i^2 + V(x_i) \right] \right\} \Psi = \left\{ \sum_{i=1}^{A} h_i \right\} \Psi = E\Psi$$

- Slater determinant is used to represent basis states, with antisymmetry property for Fermionic wave functions

$$\Psi = \begin{vmatrix} \varphi_1(x_1) & \varphi_1(x_2) & \cdots & \varphi_1(x_A) \\ \varphi_2(x_1) & \varphi_2(x_2) & \cdots & \varphi_2(x_A) \\ \vdots & & & \vdots \\ \varphi_A(x_1) & \varphi_A(x_2) & \cdots & \varphi_A(x_A) \end{vmatrix}$$

$$\Psi(\cdots, x_a, \cdots, x_b, \cdots) = -\Psi(\cdots, x_b, \cdots, x_a, \cdots)$$

$\Psi = 0$ if $x_1 = x_2$

Second quantization

- The basis states are Slater determinants, but it is most convenient to use an equivalent formalism, the second quantization, by introducing creation and annihilation operators

$$a_i^+|0\rangle = |i\rangle, \quad a_i^+|i\rangle = 0$$

$$a_i|i\rangle = |0\rangle, \quad a_i|0\rangle = 0$$

$$\{a_i^+, a_j^+\} = \{a_i, a_j\} = 0$$

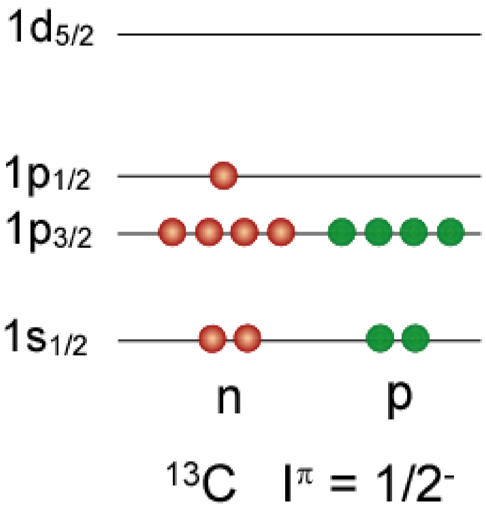
$$\{a_i, a_j^+\} = \{a_j^+, a_i\} = a_i a_j^+ + a_j^+ a_i = \delta_{ij}$$

- A Slater determinant can then be written as

$$|\Psi\rangle = a_1^+ a_2^+ a_3^+ \cdots a_A^+|0\rangle$$

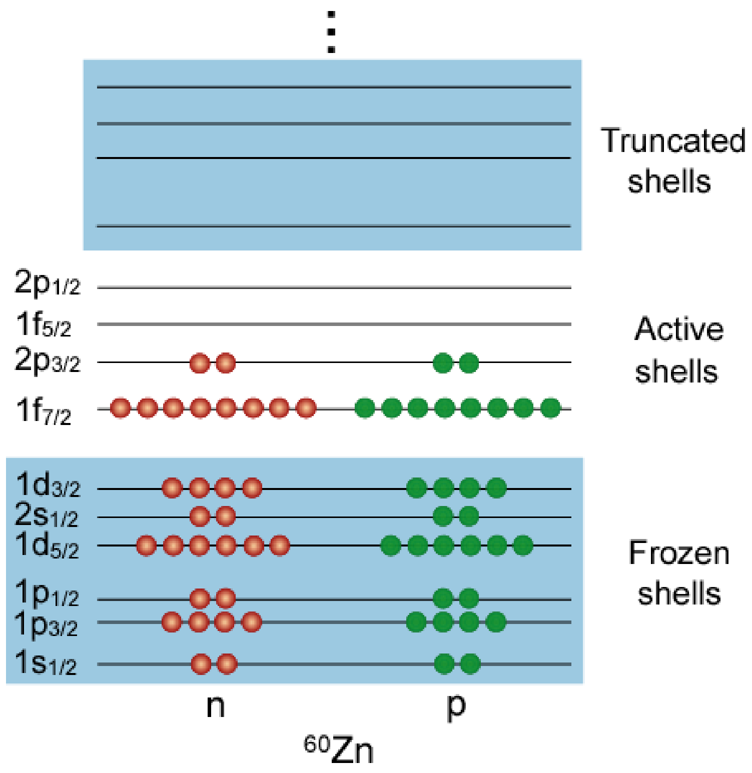
Occupation representation of basis states

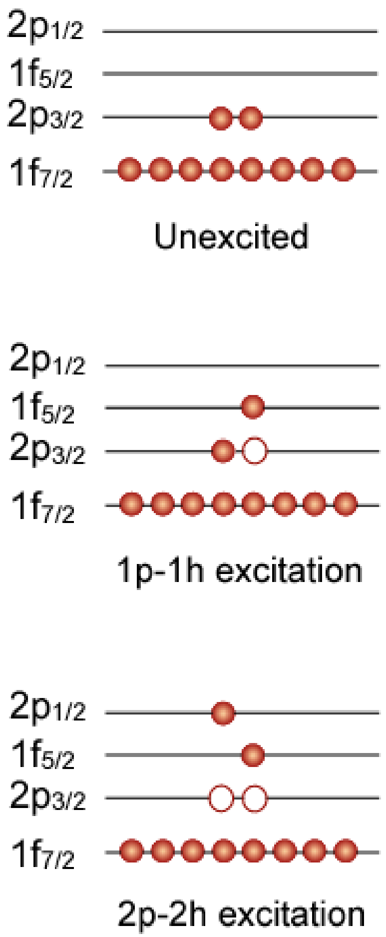
- Construct independent-particle wave function for the ground state by filling up, in order of energy, the single particle orbits
- What is the ground state angular momentum I and parity π of a nucleus?
  - even-*N*, even-*Z* nucleus has $I^{\pi} = 0^{+}$
  - odd-*A* nucleus has I^{π} of the last nucleon
- To add more nucleons and build states with good angular momentum, one can perform angular-momentum-coupling



Nuclear shell model

- This is an example for ^{60}Zn





Building many-body basis

- In principle, one allows all possible configurations within the valence space

  number of configuration:

$$\begin{pmatrix} N_{s.p.\ orbitals} \\ N_{particles} \end{pmatrix}$$

avaliable states = 6, particles = 2

110000, 101000, 100100, 100010, 100001
011000, 010100, 010010, 010001,
001100, 001010, 001001,
000110, 000101,
000011

# of configurations = 15

- For an average potential with spherical symmetry, s.p. states have good j and m
- A many-body configuration has good M = sum of all s.p. m
- For total angular momentum I, one must apply the rule of angular momentum coupling (much more complicated)

Limitation of spherical shell model

- A serious problem: configuration space becomes too big for heavy nuclei
- Size of a configuration space (n particles in N single-particle states)

$$Dimension \sim \binom{N_n}{n_n}\binom{N_p}{n_p}$$

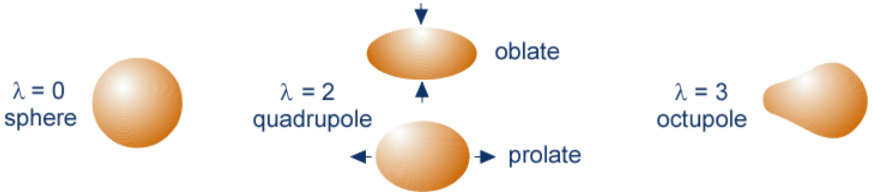
Example: ^{60}Zn

$$\binom{20}{10}\binom{20}{10} = \left(\frac{20!}{10!10!}\right)^2 = 3.4\times 10^{10}$$

- Conclusion: this method can not be used for heavy nuclei

Nuclear deformation

- A. Bohr and B. Mottelson, Nobel Prize 1975
- Most nuclei in nuclear chart are deformed
  - Quadrupole
    - Axially symmetric (prolate or oblate)
    - Axially asymmetric (γ-deformed)
  - Octupole, …
- Collective motion
  - Rotation – rotational spectrum, …
  - Vibration – β, γ, scissors, …



Experimental evidence for nuclear deformation

- Existence of rotational bands
  - Nuclear excitation spectra show band energies E(I) ~ I(I+1), collective rotation in deformed nuclei
- Large quadrupole moments
  - Possible only for deformed nuclei
  - Using Bohr model, one can derive deformation parameters β and γ for nuclear shapes that deviate from spherical symmetry
- Deformed single particle structure
  - A very sensitive experimental test comes from observed single particle energies – they are very different from those with zero deformation

Novel method connecting mean-field and shell models

- Angular-momentum projection method based on deformed mean-field solutions
  - Start from intrinsic bases (e.g. solutions of deformed mean-field) and select most relevant configurations
  - Use angular momentum projection technique to transform them to laboratory basis (many-body technique)
  - Diagonalize Hamiltonian in the projected basis (configuration mixing, a shell-model concept)
- It is an efficient way, and probably the only way to treat heavy, deformed nuclei with a shell model concept

The Projected Shell Model (PSM):

- K. Hara, Y. Sun, *Int. J. Mod. Phys.* E 4 (1995) 637
- Y. Sun, *Phys. Scr.* 91 (2016) 043005

Features of GT calculation by PSM

- As a shell model, PSM can be applied to any heavy, deformed nuclei without a size limitation.
- Its wavefunctions contain correlations beyond mean-field and are written in laboratory frame having definite good quantum numbers (angular-momentum and parity).
- A state-by-state evaluation of GT transition rates is computationally feasible, which enables calculations of GT transitions of excited states in a parent nucleus connecting to many states in a daughter.

Features of GT calculation by PSM

- Calculations of forbidden transitions require multishell model spaces, not possible for most of conventional shell models working in one-major shell bases. PSM is a multishell shell model, and can treat situations when forbidden transitions are dominated.
- Isomeric states belong to a special group of nuclear states because of their long half-lives, which could alter significantly the elemental abundances produced in nucleosynthesis. PSM is capable of describing the detailed structure of isomeric states.
  - A. Aprahamian and Y. Sun, Nature Phys. 1, 81 (2005).

Development of two kinds of shell model

- Large-scale shell model based on spherical basis
  - adopt useful effective interactions
  - develop simpler quadrupole+pairing interactions
  - include monopole force or monopole corrections in the Hamiltonian
  - include isospin symmetry-breaking forces (Coulomb, INC)
  - develop new computation algorithms
- Projected shell model based on deformed basis
  - use Generate coordinate method to describe effect of shapes
  - introduce Pfaffian method to allow computation for high excitations
  - develop codes for beta-decay matrix elements for heavy, deformed nuclei
  - work closely with structure experiments to test the models

Nuclear astrophysics center (CNA) at Shanghai Jiao Tong University

- Associated institution of JINA-CEE
- Promote nuclear astrophysics development in China
- Promote international collaborations and academic exchanges in this field
- Carry out conversations from different fields in China
  - Nuclear experimental facilities in IMP (Lanzhou), CIAE (Beijing)
  - Jinping underground lab (Sichuan)
  - Da-Ya Bay neutrino lab (Guangdong)
  - Shanghai synchrotron light (upgrade to provide gamma rays)
  - Strong laser facilities, ELI-like (Shanghai)
  - Large telescope LAMOST (Beijing)
  - Supercomputer Tian-He (Tianjin)

CGS16
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