NUCLEAR THEORY

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1. INTRODUCTION

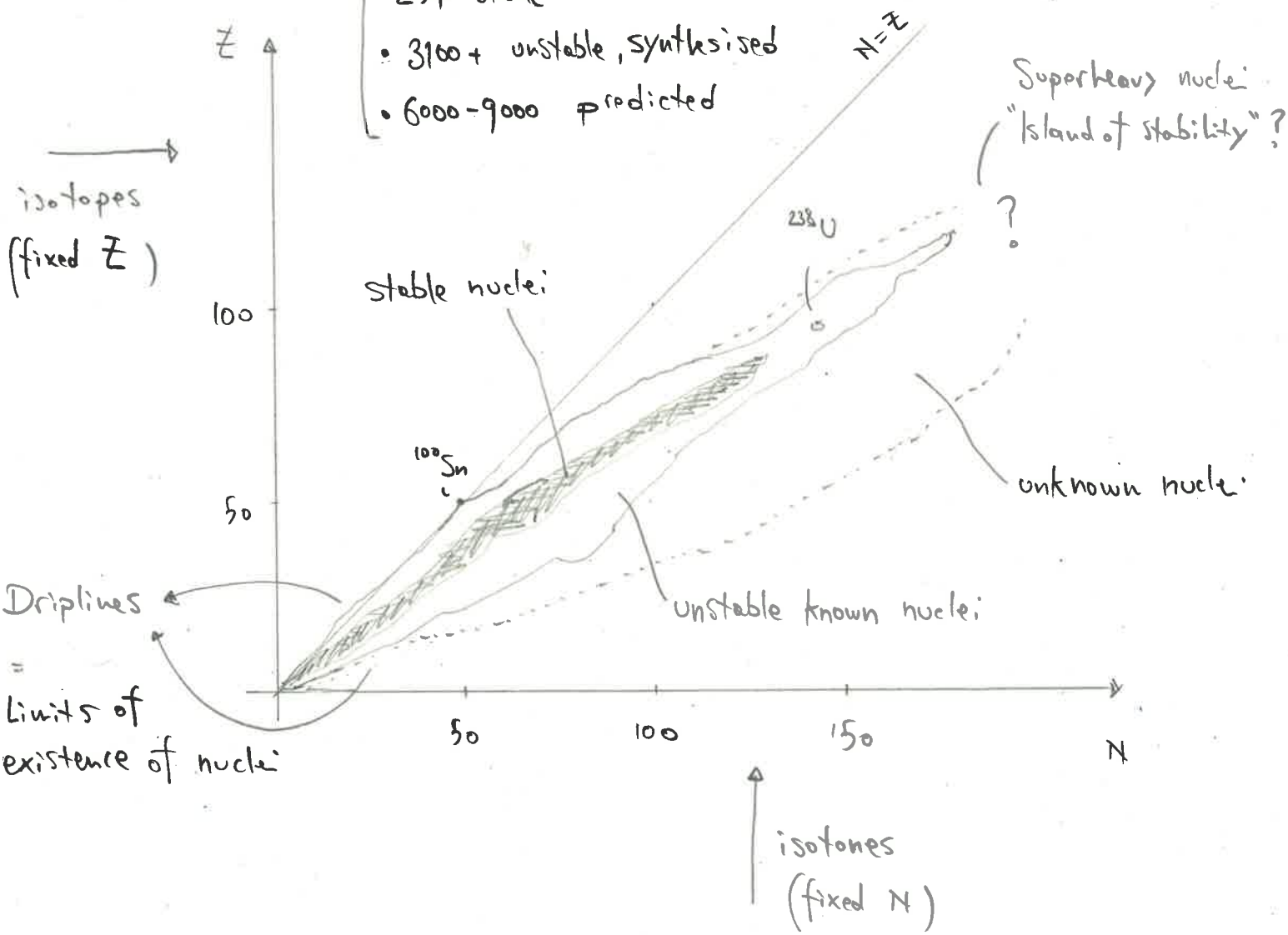
$A = Z + N$

A: mass number

Segrè chart

How many nuclei do exist?

- 254 Stable
- 3100+ unstable, synthesised
- 6000–9000 predicted



- Bound nuclei: stable with respect to the strong interaction
- Stable nuclei: stable with respect to all interactions

- Magic numbers: values of Z and/or N for which nuclear systems are particularly stable (a nucleus can be singly or doubly magic)
  ↳ 2, 8, 20, 28, 50, 82, ... for stable nuclei; they might change for unstable ones

Observables and energy scales

- Binding energy (ground-state energy)

$$E(N,Z) < 0$$

- Separation energies

neutron $$S_{xn}(N,Z) = |E(N,Z)| - |E(N-x),Z|$$

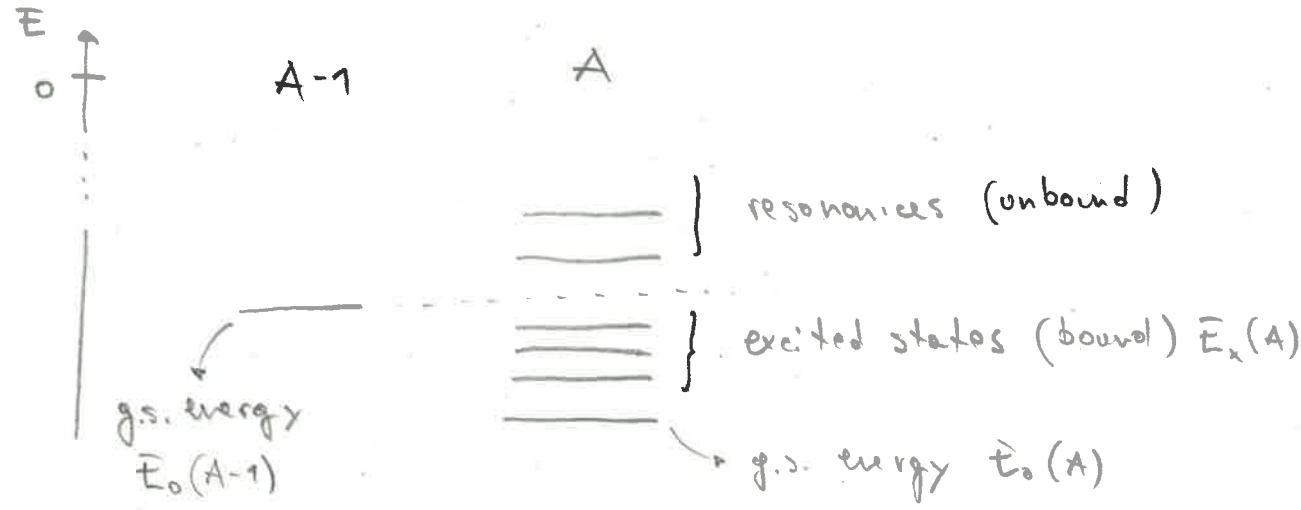
proton $$S_{xp}(N,Z) = |E(N,Z)| - |E(N,Z-x)|$$

→ if any of those is negative, then the system is unbound

→ usually S_1 and S_2 are considered

- Size and density
  - charge density distribution
  - charge radius
  - matter distribution and radius (model dependent)

- Excited states
  - excitation energies
  - corresponding EM transition rates



- Decays (types, rates, ...)
- Reaction processes (fusion, knockout, transfer, ...)

↓

ENERGY SCALES

- nucleon momenta 10^{8} eV
- E/A, S_1, S_2 10^{6-7} eV
- excitation energies $E_x - E_0$ 10^{4-6} eV

⇒ many different scales at play!

Complexity of atomic nuclei

- Mesoscopic systems

  - From two to few hundred constituents

    $2 \leq A < \sim 300$ ⇒ { Too many particles to solve the problem exactly
    Too few particles to apply statistical methods

  - Self-organisation, collective behaviours, emergent phenomena
  - Interplay between individual and collective excitations

- Self-bound quantum systems

  - In first approximation, nucleons occupy quantised orbits
    (In reality it's more complicated: single-nucleon states cannot be observed in a many-nucleon system)

- "Mean potential" generated by nucleon themselves
  ⇒ Filling of orbits may strongly depend on A
- Purely quantum effects (bubbles, halos, ...)

- All fundamental forces at play
  - Strong → binding (existence)
  - Weak → decays (stability)
  - EM → proton-neutron asymmetry, driplines, total mass

Many-body Schrödinger equation

- QCD non-perturbative at low energies
  ⇒ Lattice QCD might provide solution, but is costly and noisy for systems with many baryons
- Standard strategy: work directly with nucleon degrees of freedom
  ⇒ Three steps:
  1) Model the interaction between nucleons
  2) Solve many-body Schrödinger equation
  3) Compare to experimental data → feedback on points 1) and 2)

Do we know how? For all A?

How many? What form? Link to QCD?

- Time-independent Schrödinger equation

nuclear Hamiltonian — energy eigenvalues

$$\hat{H}\,|\Psi_k^A\rangle = E_k^A\,|\Psi_k^A\rangle$$

A-body wave function

↓

Any observable associated with a self-adjoint operator $\hat{O}$ is computed via

$$\sigma(A,k) = \langle \Psi_k^A | \hat{O} | \Psi_k^A \rangle$$

- Time-dependent Schrödinger equation

$$\hat{H}\,|\Psi^{A+B\to C+D}(t)\rangle = i\hbar \frac{\partial}{\partial t}\,|\Psi^{A+B\to C+D}(t)\rangle$$

↓

Solution typically yields the reaction cross section

$$\sigma(A_k + B_l \to C_m + D_n)$$

C_m: can be ground or excited state

(More complicated reactions possible)

Coordinate-space vs. configuration space approaches

- Coordinate-space approaches

→ Based on a direct phase-space sampling of the many-body wave function

- Typical example : Quantum Monte Carlo

1) Determine variational wave function $|\Psi_v\rangle$ by evaluating

$$E = \min\left[\frac{\langle\Psi_v|H|\Psi_v\rangle}{\langle\Psi_v|\Psi_v\rangle}\right]$$

Variational MC (VMC)

via Metropolis Monte Carlo integration

2) Improve on $|\Psi_v\rangle$ by projecting out excited state contaminations via Euclidean propagation

$$|\Psi(\tau)\rangle = \exp\left[-(H-E_0)\tau\right]|\Psi_v\rangle \xrightarrow[\tau\to\infty]{} |\Psi\rangle_{exact}$$

Green's function MC (GMC)

ADVANTAGES

- Virtually exact
- Flexible for what concerns spatial configurations

DRAWBACKS

- Wave function dimensionality scales exponentially with A
- Sign problem affects fermionic MC simulations (and worsens with A)

⇒ Computational cost strongly increases with A

- Configuration-space methods

Expand wave function on a basis of known many-body states

↳ Object of this course

ADVANTAGES

- Virtually exact, but controlled and systematically improveable approximation can be introduced

DRAWBACKS

- Exact calculations scale factorially with A
- Approximated calculations might not be accurate enough
- Spatial configurations constrained by those of the basis

Full configuration interaction

- One rewrites the Schrödinger equation as follows

1) Select a one-body basis $|\alpha\rangle$

2) Construct an A-body basis (Slater determinants) using all possible combinations of one-body states

$$|\Phi_i^A\rangle = |\underbrace{\alpha_1 \alpha_2 \cdots \alpha_A}_{i \text{ (collectively)}}\rangle$$

↓

These states form a complete basis of the A-body Hilbert space

* Any wave function can be written as

$$|\Psi^A\rangle = \sum_i c_i |\Phi_i^A\rangle$$

3) Apply to A-body Schrödinger equation

$$H|\Psi_k^A\rangle = E_k^A |\Psi_k^A\rangle$$

$$\Rightarrow H \sum_i c_i^{(k)} |\Phi_i^A\rangle = E_k^A \sum_i c_i^{(k)} |\Phi_i^A\rangle$$

left-multiply by $\langle \Phi_j^A |$

$$\Rightarrow \sum_i \underbrace{\langle \Phi_j^A | H | \Phi_i^A \rangle}_{\equiv H_{ji}} c_i^{(k)} = E_k^A \sum_i c_i^{(k)} \underbrace{\langle \Phi_j^A | \Phi_i^A \rangle}_{= \delta_{ij}}$$

$$\Rightarrow \sum_i H_{ji} c_i^{(k)} = E_k^A c_j^{(k)}$$

Eigenvalue equation for the coefficients of the linear combination

↓

Can be written in matrix form

$\Rightarrow$ Solution $\longleftrightarrow$ diagonalisation of H_N in the A-body basis

$$\begin{bmatrix} & \vdots & \\ \cdots & H_{ji} & \cdots \\ & \vdots & \end{bmatrix} \begin{bmatrix} \vdots \\ c_i^{(k)} \\ \vdots \end{bmatrix} = E_k^A \begin{bmatrix} \vdots \\ c_j^{(k)} \\ \vdots \end{bmatrix}$$

- What is the dimensionality of the problem ?

In principle, one-body basis infinite $\Rightarrow$ A-body basis infinite.

$$|\Psi_k^A\rangle = \sum_{i=1}^{\infty} c_i^{(k)} |\Phi_i^A\rangle$$

In practice

$$|\Psi_k^A\rangle = \sum_{i=1}^{D} c_i^{(k)} |\Phi_i^A\rangle$$

↘ i) Ritz variational principle

$$E_0(D) \geq E_{exact} = E_0(\infty)$$

ii) Hylleraas-Undheim theorem

$$E_k(D) \geq E_k(D+1)$$

One must check convergence with D (model-space convergence)

- How many Slater determinants can be built from a given number of single-particle (i.e., one-body) states?

Take X particles and a one-body basis with n states.

⇒ Total number of Slater determinants is $\binom{n}{x} = \frac{n!}{(n-x)!\,x!}$

EXAMPLE

^{16}O $A=16$ $Z=8$ $N=8$

Let us take $n=20$

proton Slater = $\frac{20!}{(20-8)!\,8!} = 1.2 \cdot 10^5 = D_p$

neutron Slater = (same as above) $= 1.2 \cdot 10^5 = D_n$

⇒ total $D = D_p \times D_n = 1.6 \cdot 10^{10}$ determinants (i.e. A-body states)

One must now compute H in this basis, i.e. H_{ij}

⇒ corresponding matrix has dimensions $D^2 = 2.5 \cdot 10^{20}$.

⇒ exploiting sparsity takes from D^2 to $D^{1.2} = 1.7 \cdot 10^{12}$ / total number of non-zero entries (which must be stored in memory)

⇒ total size of $H_{ij} \sim 1.4 \cdot 10^{13}$ B : 14 TB / not far from limit of current supercomputers

↓

Correlation-expansion methods

- Controlled and improvable approximations
- From factorial (FCI) to polynomial scaling with basis dimension

Ab initio vs. effective approach

AB INITIO APPROACH

- H describes basic interactions between nucleons (in vacuum)
- Solution of the Schrödinger eq. is systematically improvable (ideally, exact)

$$H|\Psi_k\rangle = E_k|\Psi_k\rangle$$

ADVANTAGES

- Associated theoretical uncertainties can / should be evaluated
- High predictive power

DRAWBACKS

- High computational cost
  ⇒ limited to light and medium-mass nuclei
- Precision depends on quality of H

EFFECTIVE APPROACH

- H^{eff} effectively models interactions within the nuclear medium (phenomenologically adjusted)
- Solution of the Schrödinger eq. is approximated by construction

$$H^{eff}|\Psi_k^{eff}\rangle = E_k|\Psi_k^{eff}\rangle$$

ADVANTAGES

- Low computational cost
  ⇒ can access all nuclei
- Very precise where data exist

DRAWBACKS

- Low predictive power
- Hard / impossible to evaluate associated theoretical error

Two main classes of effective approaches exist

(INTERACTING) SHELL MODEL

Reduce one-body Hilbert space

→ FCI in a "valence" space

↓

$|\Psi^{eff}\rangle$ complicated but computed only for $A' \ll A$ nucleons

ADVANTAGE

- Locally, excellent description of experimental data

DRAWBACK

- Valence space becomes too large when $A > 100$ ⇒ limited applicability

ENERGY DENSITY FUNCTIONALS

Reduce many-body Hilbert space

→ Basic formulation $|\Psi^A\rangle = |\phi^A\rangle$

just one Slater determinant

↓

$|\Psi^{eff}\rangle$ computed for all A nucleons but kept "simple"

ADVANTAGE

- Low computational cost
  ⇒ can access all nuclei

DRAWBACK

- Difficult to optimise / improve