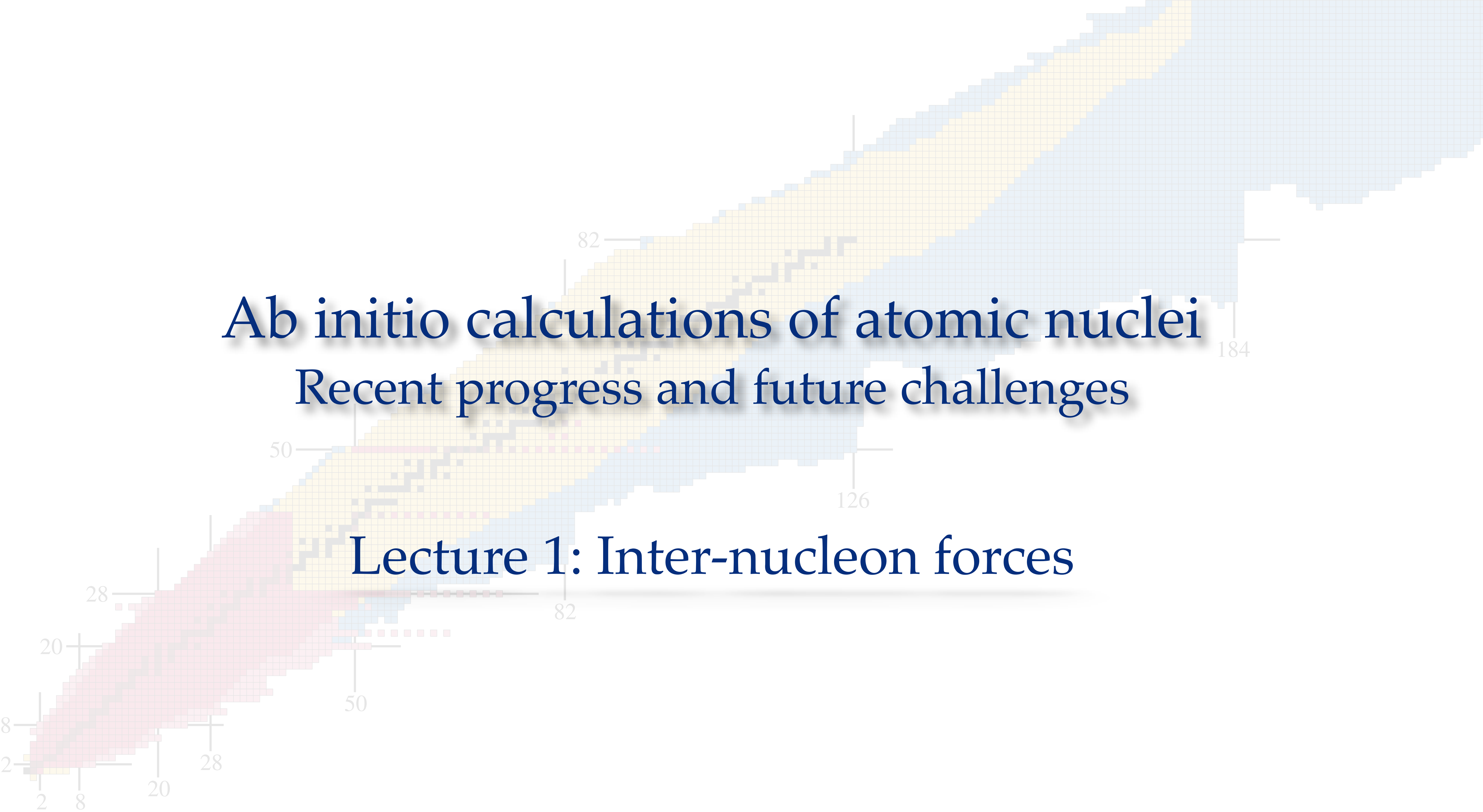


Ab initio calculations of atomic nuclei

Recent progress and future challenges

Lecture 1: Inter-nucleon forces

Università di Padova
7-10 June 2021

Vittorio Somà
CEA Saclay

Contents

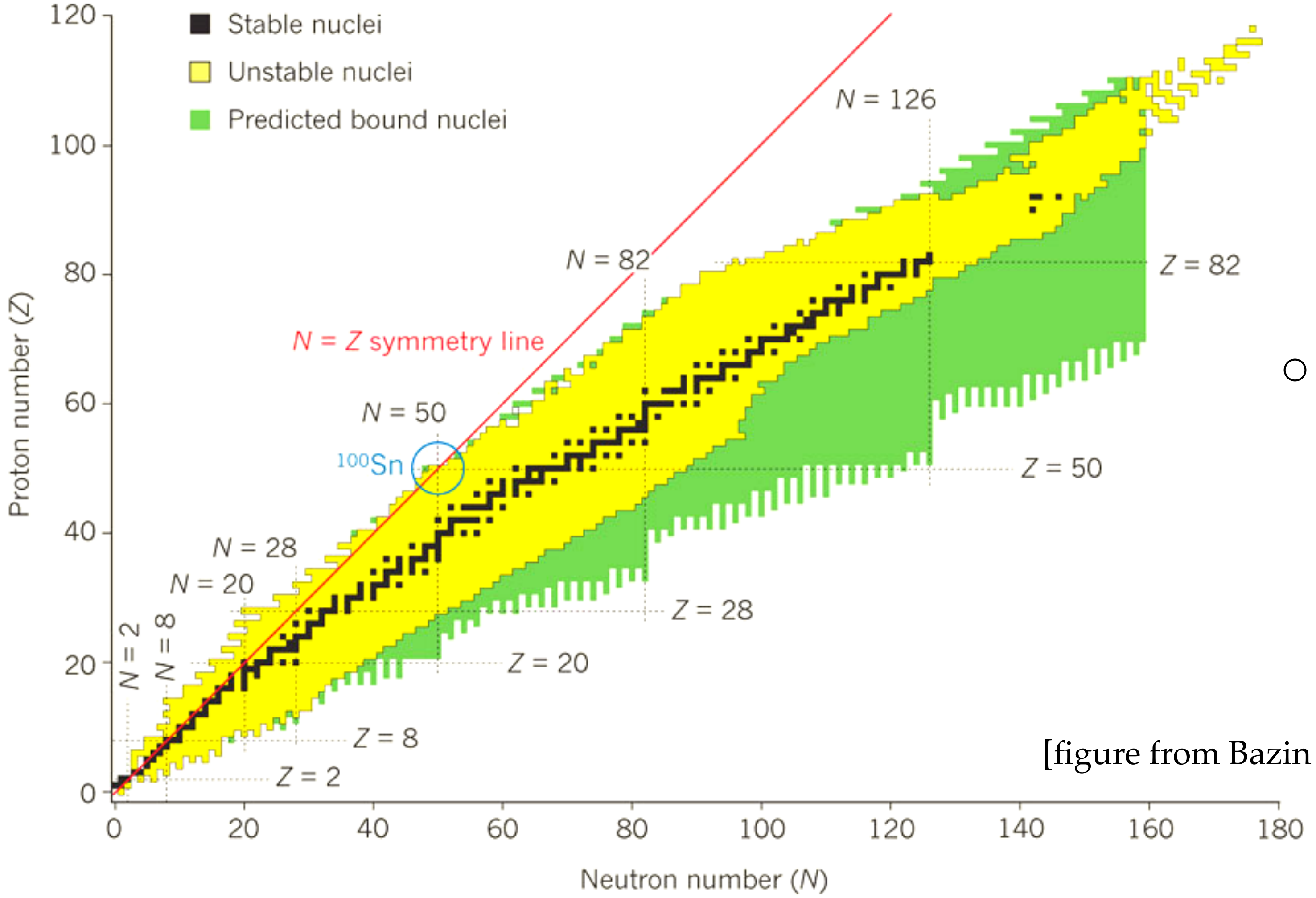
Acknowledgements

- **Thanks to (for slides and figures)**
  - B. Bally (Madrid Uni.)
  - T. Duguet (Saclay)
  - R. Roth and A. Tichai (TU Darmstadt)

Contents

Basic facts about nuclei

- 254 stable isotopes, ~3100 synthesised in the lab
- Heaviest synthesised element Z=118



[figure from Bazin 2012]

- Light/mid-mass elements produced in stellar fusion

- Neutron **drip-line** known up to Z=10 (24 neutrons)

- Over-stable magic nuclei (2, 8, 20, 28, 50, 82, …)

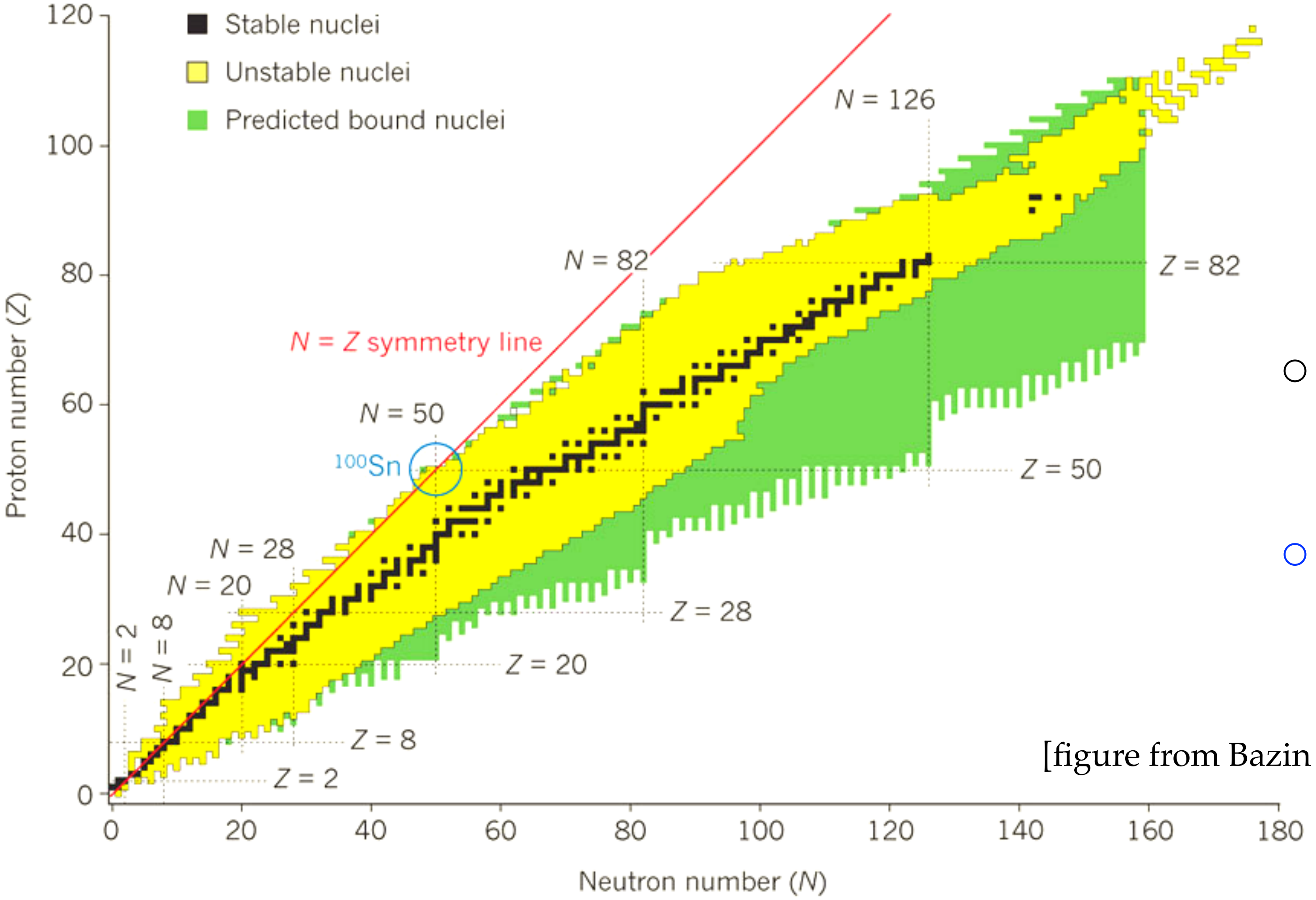
Basic questions about nuclei

○ 254 stable isotopes, ~3100 synthesised in the lab

○ **How many** bound nuclei exist? (~6000-8000?)

○ Heaviest synthesised element *Z*=118

○ **Heaviest possible** element?
Enhanced stability near *Z*=120?



[figure from Bazin 2012]

○ Light/mid-mass elements produced in stellar fusion

○ How have heavy elements been produced?

○ Neutron **drip-line** known up to *Z*=10 (24 neutrons)

○ Where is the neutron drip-line beyond *Z*=10?

○ Over-stable magic nuclei (2, 8, 20, 28, 50, 82, …)

○ Are **magic numbers** the same for unstable nuclei?

Diversity of nuclear phenomena

Nucleus: bound (or resonant) state of Z protons and N neutrons

Several scales at play:

p & n momenta ~ **10^8** eV

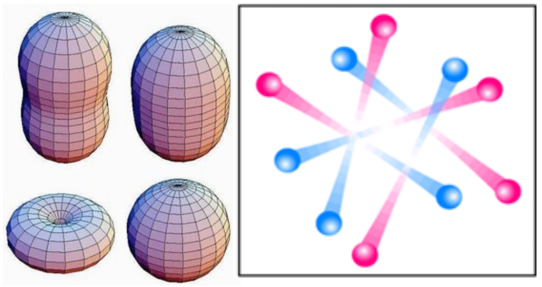
Separation energies ~ **10^7** eV

Vibrational excitations~ **10^6** eV

Rotational excitations ~ **10^4** eV

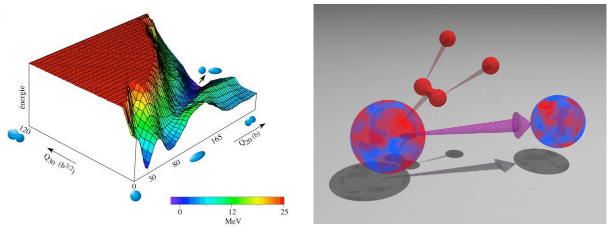
Ground state

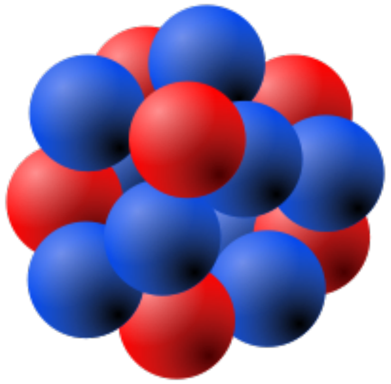
Mass, size, superfluidity, …



Radioactive decays

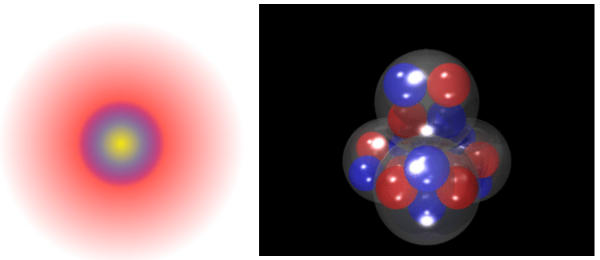
β, 2β, α, p, 2p, fission, …





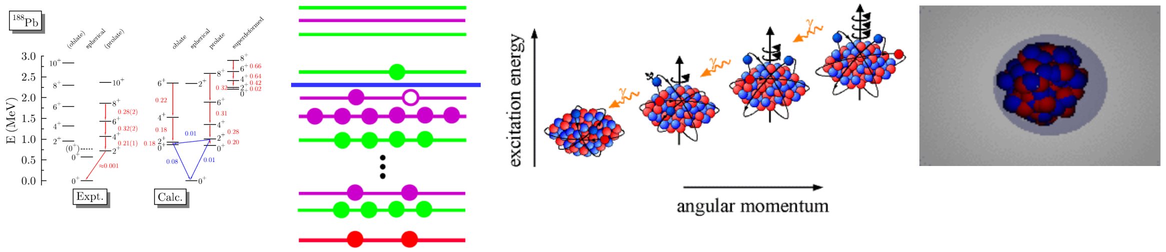
Exotic structures

Clusters, halos, …



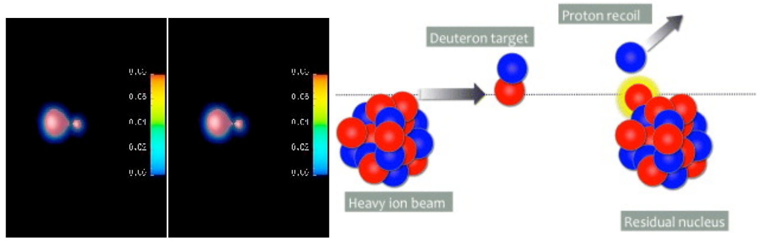
Spectroscopy

Excitation modes



Reaction processes

Fusion, transfer, knockout, …



What makes atomic nuclei so complex?

- **Mesoscopic** systems
  - From 2 to few hundreds nucleons → Statistical approaches can not be applied
  - Enough particles to prompt collective behaviours → Interplay with individual excitations
  - Self-organisation and emergent phenomena

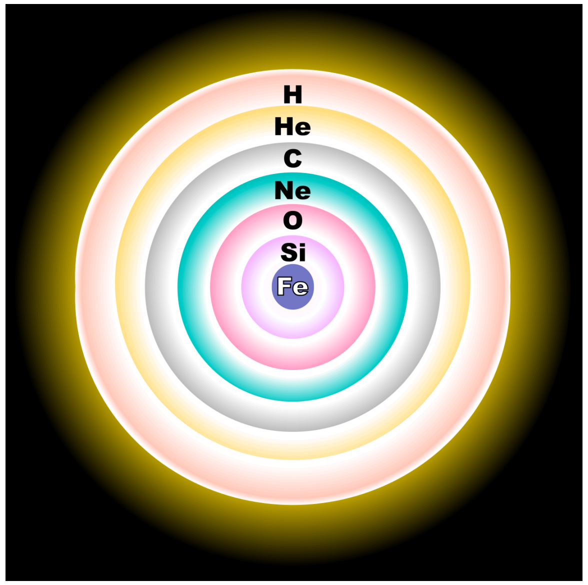
- **Self-bound quantum** systems
  - In a first approximation, nucleons occupy quantised orbits
  - Filling and energies strongly depend on A → each nucleus displays a specific structure
  - Purely quantum effects (e.g. halos, bubble-nuclei)

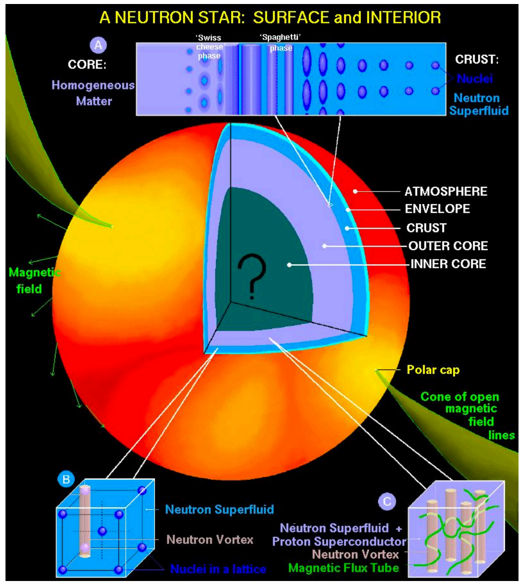
- Interacting via **strong**, **weak** and **EM** forces
  - Strong interaction responsible for binding and saturation
  - Weak interaction triggers decays of unstable nuclei towards the ‘valley of stability’
  - EM interaction determines proton-neutron asymmetry and limits the mass

Interdisciplinary aspects

Astrophysics

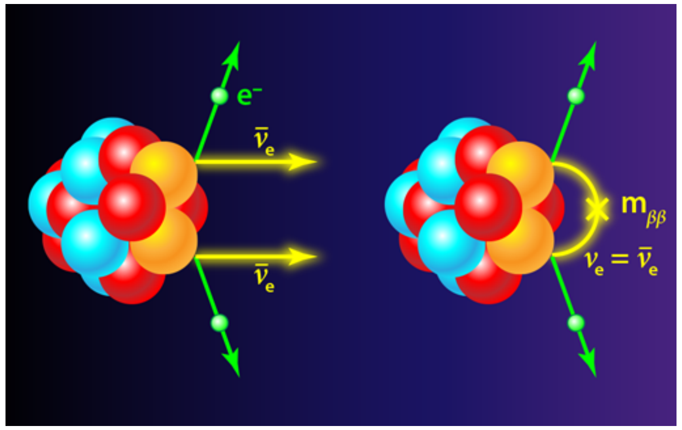
- ○ Nucleosynthesis (BB, stellar, r-process, …)
- ○ Neutron stars (birth, life & death)





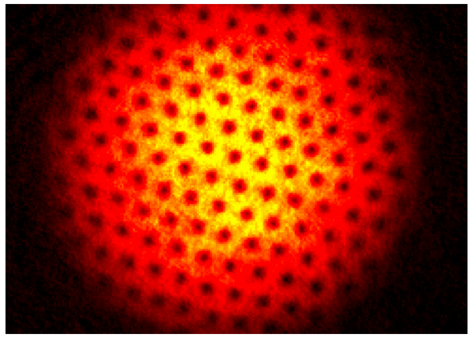
Particle physics

- ○ Neutrinoless 2β decay
- ○ Neutrino-nucleus scattering
- ○ Tests of standard model
- ○ Dark matter (nucleus-WIMP scattering)



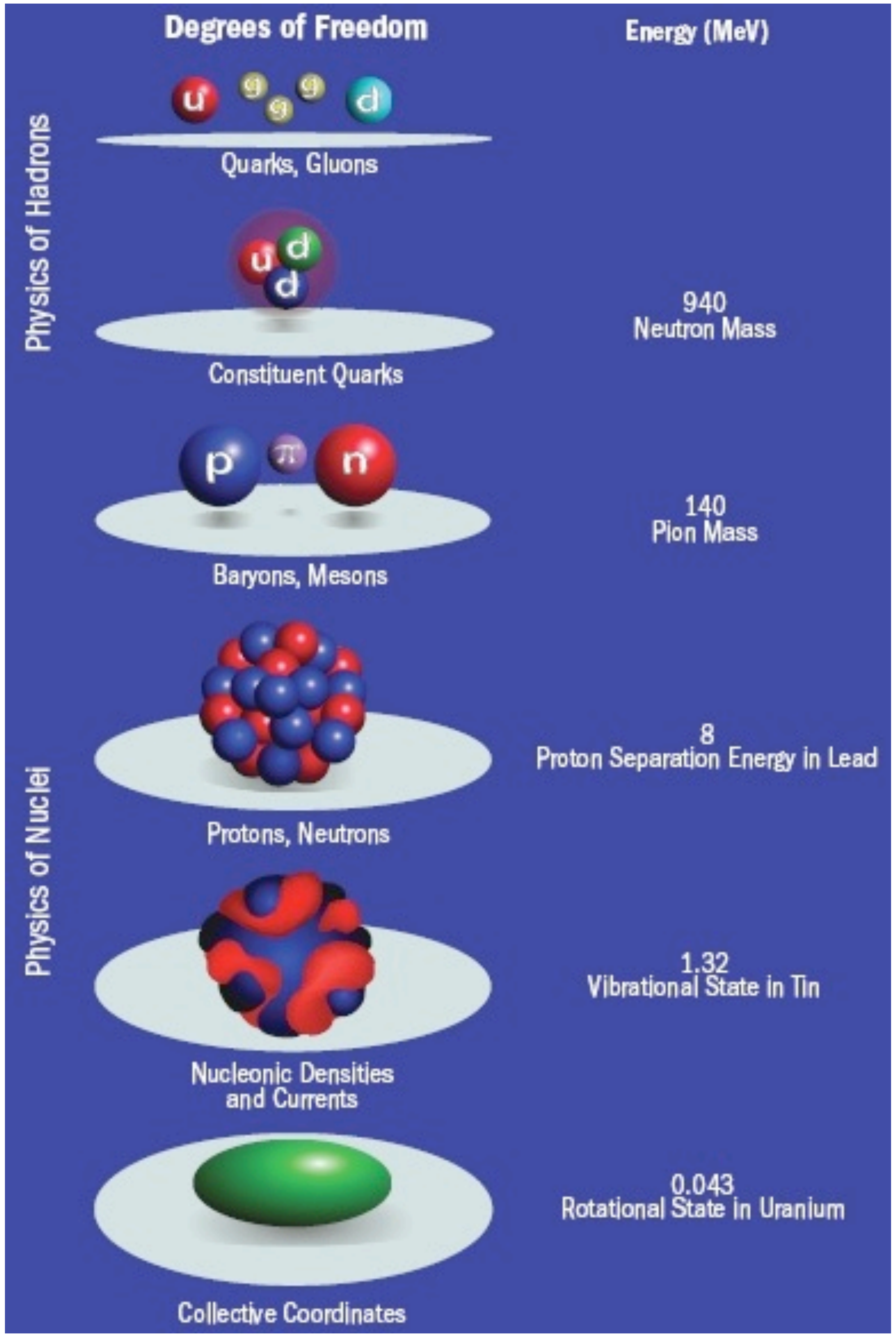
Other mesoscopic systems

- ○ Ultracold fermionic gases → universality classes, superfluidity, ….
- ○ Atoms & molecules → cross-fertilisation of many-body techniques



Which is the most appropriate theoretical description?

More reductionist / elementary / "fundamental" description



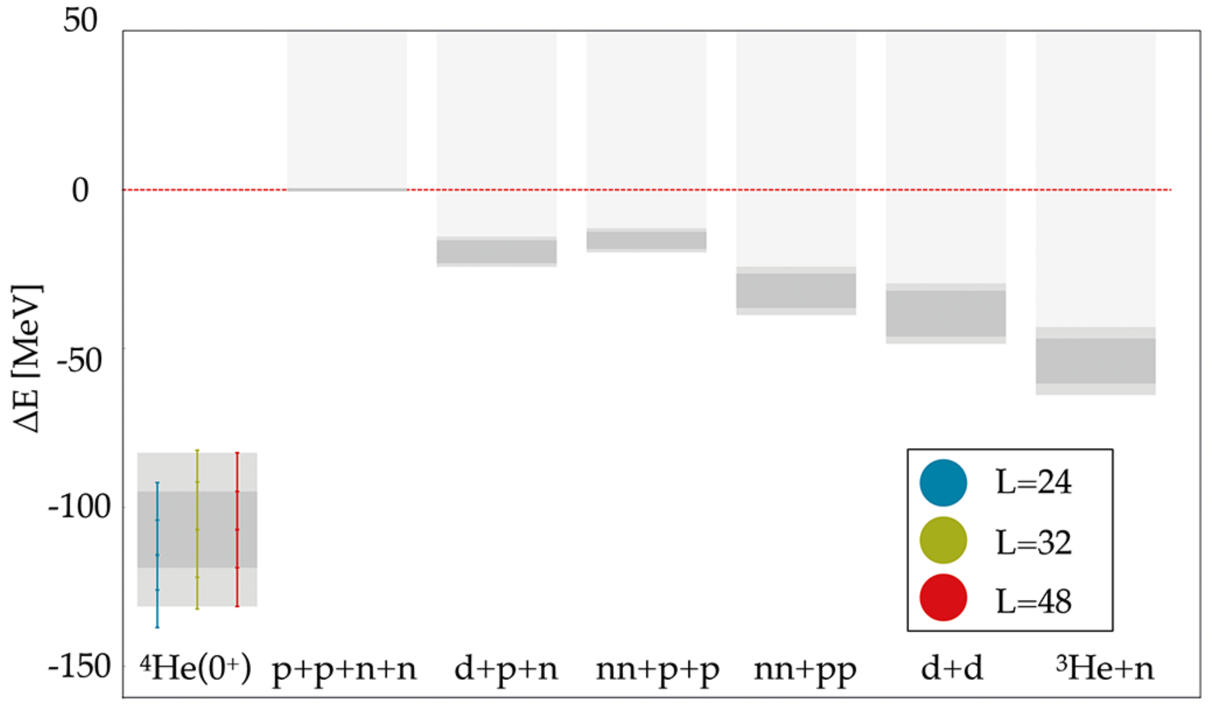
Emergent phenomena amenable to effective descriptions

- **Nuclei from QCD d.o.f.?**
  - Nonperturbative at low energy

    → Lattice QCD

- Noise-to-signal ratio of *A*-nucleon correlation functions scales as $e^{A\left(M_N-\frac{3}{2}m_\pi\right)t}$

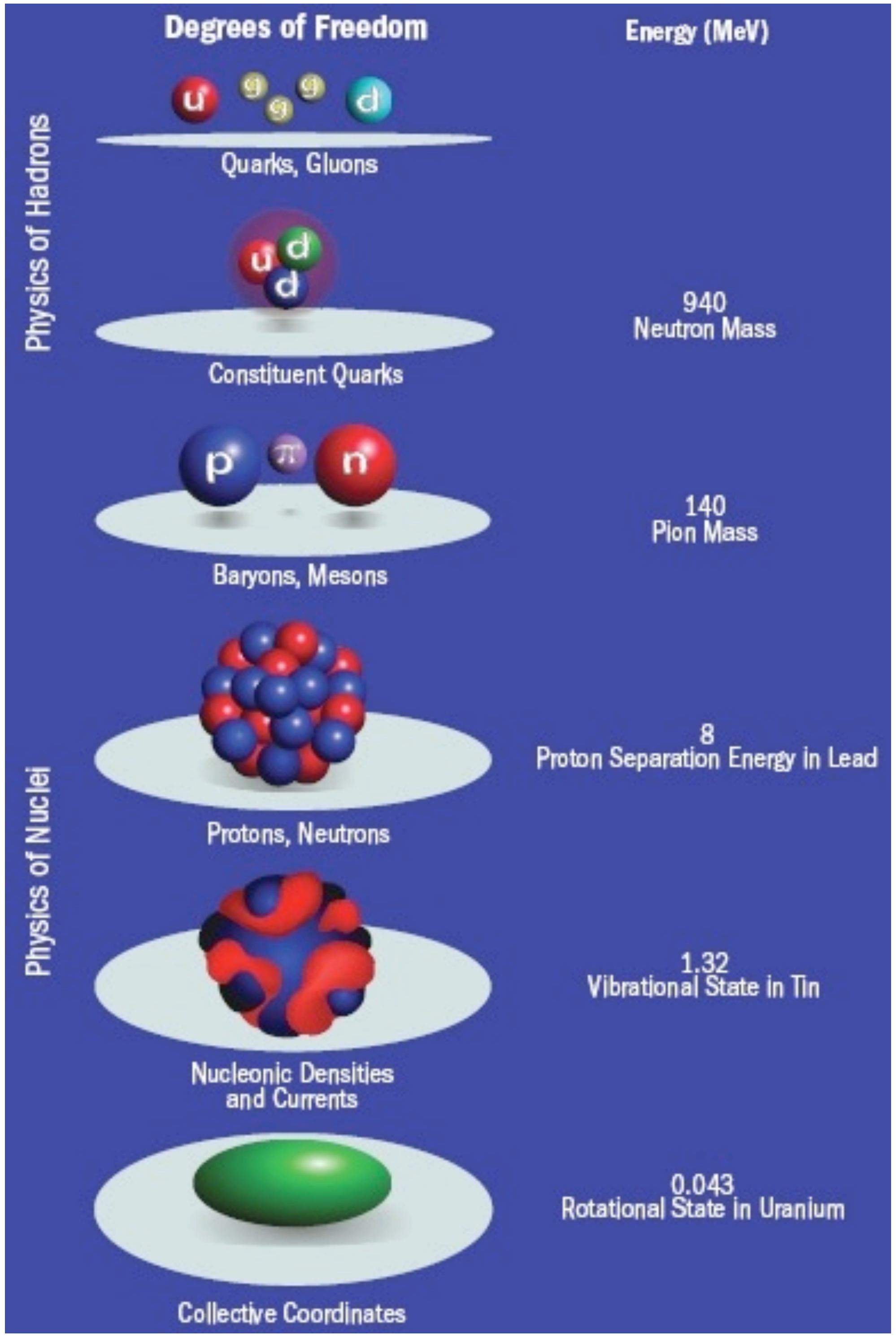
→ Calculations possible for small *A*



[Beane *et al.* 2013]

Which is the most appropriate theoretical description?

More reductionist/elementary/“fundamental” description



Emergent phenomena amenable to effective descriptions

⊙ **Nuclei from QCD d.o.f.?**

○ Nonperturbative at low energy

→ Lattice QCD

⊙ **Nuclei from nucleonic d.o.f.?**

○ Do we know inter-nucleon interactions?

○ Can we solve A-body Schrödinger eq.?

⊙ **Nuclei from collective d.o.f.?**

○ Can we do it systematically?

○ Which observables can we describe?

➪ Current trend: from a plurality of nuclear models to an articulated **“tower” of EFTs**

Ab initio nuclear many-body problem

- This course focuses on the **ab initio nuclear many-body problem**

- Ab initio = "from scratch"
  - Describe the nucleus as a system of A interacting **structure-less nucleons**
  - Model the Hamiltonian to describe **inter-nucleon interactions** in free space
  - Solve **many-body Schrödinger equation** for all A nucleons (non-relativistic)
  - **Systematically improvable** solution + **error** estimates

$$\frac{\vec{p}}{m} \approx \frac{200 \text{ MeV}}{1000 \text{ MeV}} \quad \rightarrow \quad \left(\frac{v}{c}\right)^2 < 0.1$$

- ***A*-body Schrödinger equation**

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

  - **Strategy**:

1. Derive / build / model basic interactions between nucleons
2. Solve many-body Schrödinger equation
3. Compare to data and give feedback on points 1 and 2.

Ab initio vs effective approach

***Ab initio* (= “from scratch”) approach**

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

A-body Hamiltonian

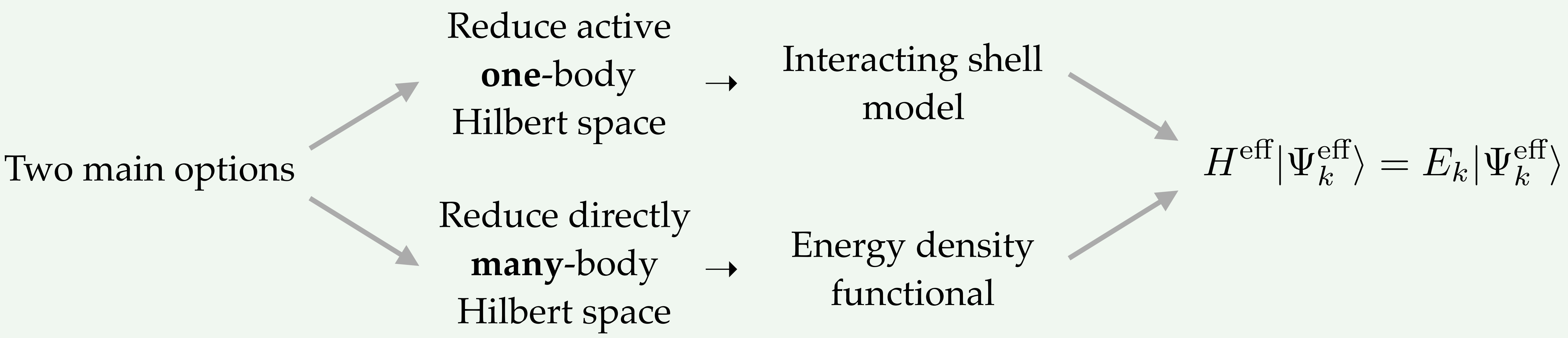
$$H = T + V^{2\mathrm{N}} + V^{3\mathrm{N}} + ... + V^{A\mathrm{N}}$$

A-body wave-function

5 variables x A *nucleons*

Unfavourable scaling for large A

Effective approach



Two main options

Reduce active **one**-body Hilbert space → Interacting shell model

Reduce directly **many**-body Hilbert space → Energy density functional

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

- ⊙ Complementary approaches
- ⊙ Choice depends on the goals (accuracy, predictive power, reach across the mass table, …)

Contents

1. Inter-nucleon forces

- Brief introduction to the nuclear many-body problem
- **Properties and modelling of nuclear forces**
- The modern view: chiral effective field theory

2. Ab initio techniques for the nuclear many-body problem

- Configuration-interaction approaches
- Techniques to mitigate the “curse of dimensionality” (SRG, NO2B, IT)
- Mean field and correlations
- Expansion methods for closed-shell nuclei
- Symmetry breaking
- Expansion methods for open-shell nuclei
- State of the art and open problems

3. Equation of state of nuclear matter & connections to astrophysics

- Neutron stars & Tolman-Oppenheimer-Volkoff equations
- Equation of state of neutron-star matter
- Astrophysical constraints on the nuclear EoS

Nuclear Hamiltonian

⊙ **Hamiltonian containing strong + Coulomb forces**

First quantisation

$$H \equiv \sum_{i=1}^{A} \frac{p_i^2}{2m} + \frac{1}{2}\sum_{i\neq j}^{A} V^{\rm 2N}(i,j) + \frac{1}{6}\sum_{i\neq j\neq k}^{A} V^{\rm 3N}(i,j,k) + \cdots$$

Second quantisation

$$= \sum_{\alpha\beta} t_{\alpha\beta}\, a^\dagger_\alpha a_\beta + \left(\frac{1}{2!}\right)^2 \sum_{\alpha\beta\gamma\delta} \bar{v}^{\rm 2N}_{\alpha\beta\gamma\delta}\, a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma + \left(\frac{1}{3!}\right)^2 \sum_{\alpha\beta\gamma\delta\zeta\epsilon} \bar{v}^{\rm 3N}_{\alpha\beta\gamma\delta\zeta\epsilon}\, a^\dagger_\alpha a^\dagger_\beta a^\dagger_\gamma a_\epsilon a_\zeta a_\delta + \cdots$$

○ **Are there forces beyond pairwise interactions? Why?**

→ Yes, because nucleons are themselves composite particles

○ **How many of them do we need to include?**

→ In principle all of them, in practice up to 3N

○ **Which form do the various terms take? What constraints/information do we have?**

→ They are operators in space/spin/isospin, constrained by symmetries & experiments

○ **Can we derive these interactions directly from QCD?**

→ In principle yes, in practice…

Basic properties of inter-nucleon interactions

- Interactions between effective point-like four-component fermions

nucleons = $p\,/\,n$ with spin up / down

- Most general form $V_{NN} = V(1,2) = V(\vec{r}_1, \vec{p}_1, \vec{\sigma}_1, \vec{\tau}_1; \vec{r}_2, \vec{p}_2, \vec{\sigma}_2, \vec{\tau}_2)$

position momentum spin isospin

- Constraints

1. Symmetry requirements (continuous and discrete symmetries, isospin)
2. Experimental information (**NN scattering, deuteron properties**) to fix parameters

- Complicated operator
  - Several operatorial structures contribute
  - Both **infrared** and **ultraviolet** sources of non-perturbativeness
    - Infrared related to large scattering length (⟷ *nn* virtual state, *np* bound state)
    - Ultraviolet related to short-range repulsion

Symmetries & operator structure

- Nuclear interactions are **invariant** under exchange of the two nucleons, translation, rotation, Galilean boost, parity, time evolution, time reversal, ~isospin

  ➪ Constraints on the mathematical form of the operator

$$\boxed{V(1,2) = V^0 + V^\sigma(\vec{\sigma}_1 \cdot \vec{\sigma}_2) + V^\tau(\vec{\tau}_1 \cdot \vec{\tau}_2) + V^{\sigma\tau}(\vec{\sigma}_1 \cdot \vec{\sigma}_2)(\vec{\tau}_1 \cdot \vec{\tau}_2)}$$

with

$$V^i = \sum_{k=1}^{5} c_k^i \, f_k^i(\vec{r}^{\,2}, \vec{p}^{\,2}, \vec{L}^{\,2}) \, O_k$$

where $\vec{x} \equiv \vec{x}_1 - \vec{x}_2$

and

$$O_k = \begin{cases} \mathbb{1} & \\ \vec{L} \cdot \vec{S} & \text{spin-orbit} \\ S_{12}^r \equiv 3(\vec{\sigma}_1 \cdot \bar{r})(\vec{\sigma}_2 \cdot \bar{r}) - (\vec{\sigma}_1 \cdot \vec{\sigma}_2) & \text{tensor } (r) \\ S_{12}^p \equiv 3(\vec{\sigma}_1 \cdot \bar{p})(\vec{\sigma}_2 \cdot \bar{p}) - (\vec{\sigma}_1 \cdot \vec{\sigma}_2) & \text{tensor } (p) \\ Q_{12} \equiv \frac{1}{2}\left[(\vec{\sigma}_1 \cdot \vec{L})(\vec{\sigma}_2 \cdot \vec{L}) + (\vec{\sigma}_2 \cdot \vec{L})(\vec{\sigma}_1 \cdot \vec{L})\right] & \text{quadratic spin-orbit} \end{cases}$$

where $\bar{x} \equiv \dfrac{\vec{x}}{|\vec{x}|}$

Experimental constraints: NN scattering

- **Extensive dataset of nucleon-nucleon scattering observables exists**
  - Few thousand cross-section data points over several decades are available
  - Partial-wave analysis of data with **$T_{lab} \leq 350$ MeV** usually employed to **fit V_{NN}**

→ see e.g. **https://nn-online.org/**

- **Reaction types**
  - **np** scattering: the **easiest**
  - **pp** scattering: technically easy to perform experiments, but **EM interaction needs to be subtracted** (might be non-trivial when aiming for high precision)
  - **nn** scattering: technically difficult (no n targets), **indirect information**
    - nd scattering (then subtract np component)
    - reactions with nn in final state, e.g. n+d → n+n+p
    - comparison between different reactions

^{3}He+^{3}He → ^{4}He+p+p

^{3}He+^{3}H → ^{4}He+p+n

^{3}H+^{3}H → ^{4}He+n+n

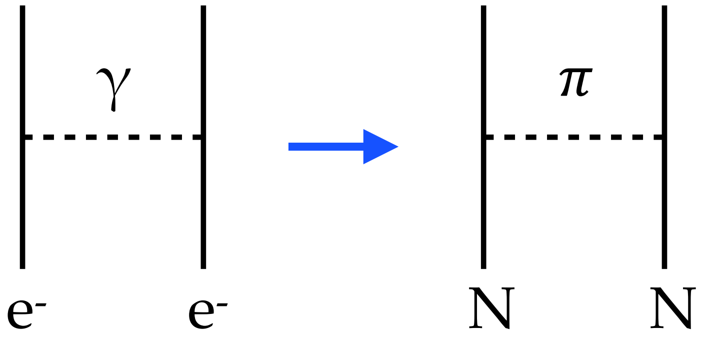
Yukawa potential

What was known:
- ○ Coulomb interaction between charged particles (infinite range)
- ○ Nuclear interaction is short range ~ 2 fm

➪ **Idea: nuclear force mediated by massive spin-0 boson** (the "mesotron" → later, pion)

[Yukawa, Proca]

1935



Yukawa potential

$$V(r) \propto \frac{e^{-mr}}{r}$$

m ~ 100 MeV ← r ~ 2 fm

Range ~ Compton wavelength of exchanged boson ~ 1/m

⊙ **One-pion exchange describes** long-range attraction **between nucleons**

- ○ Generate tensor and τ · τ structures
- ○ Works so well that, as of today, it is part of most sophisticated potential models!

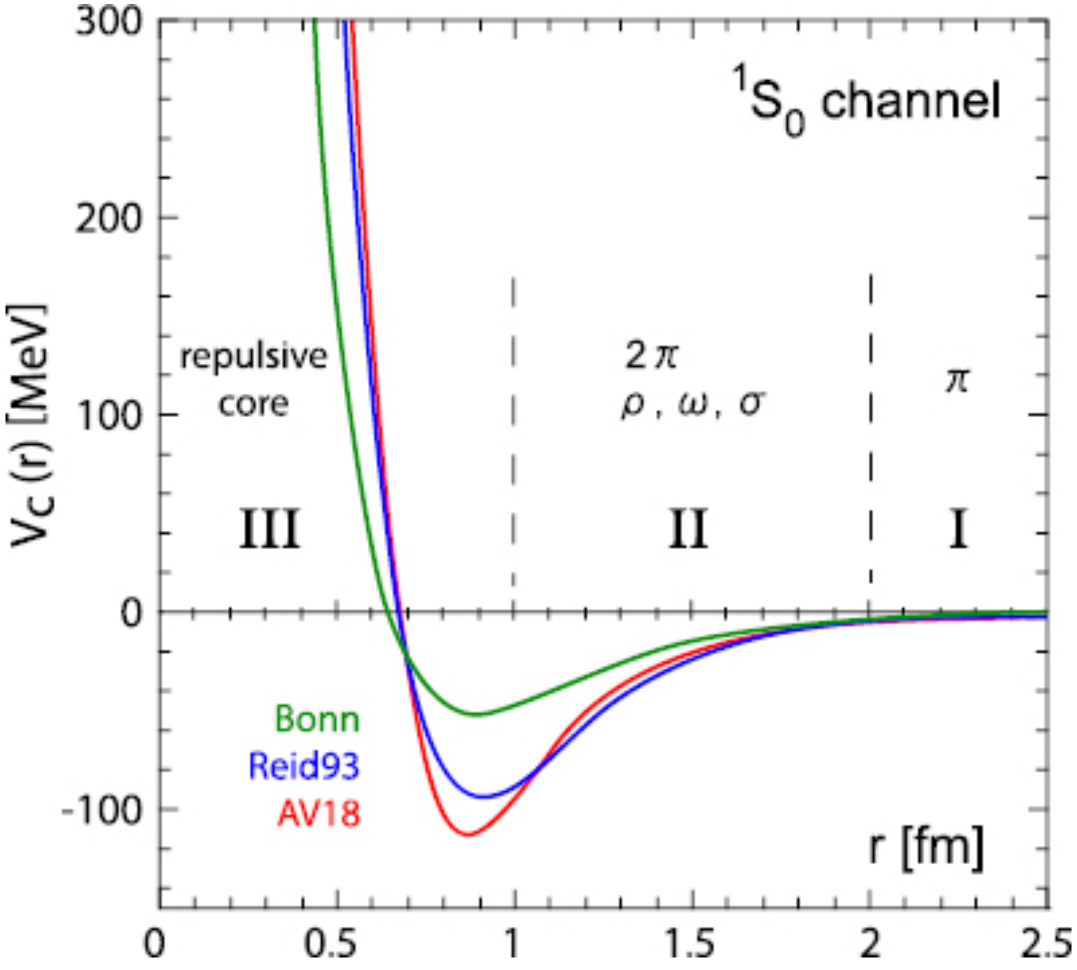
⊙ **However, not the full story.** Short-range **part?**

- ○ 1950's: Multi-pion exchange: disaster
- ○ 1960's: More mesons discovered → multi-pion resonances ≈ exchange of heavier mesons

One-boson-exchange potentials

1970's

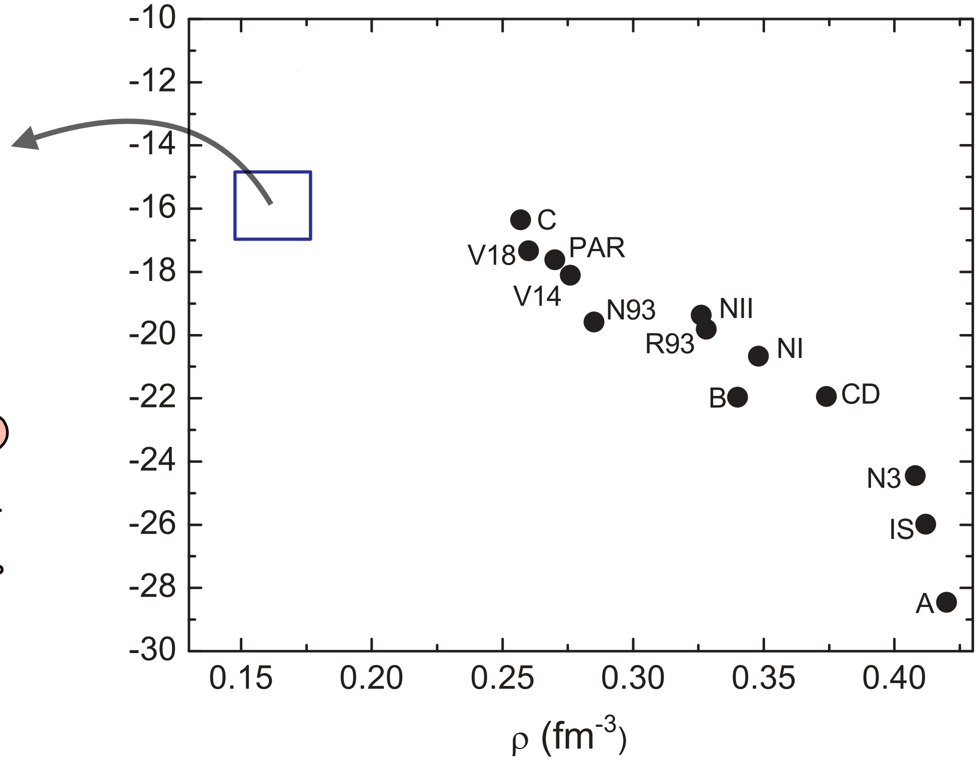
- Meson with **larger masses** (ρ , ω, σ) can model **ranges smaller than 1/m$_\pi$**
  - Different spin/isospin structures generated
  - Parts sometimes phenomenological (usually the short-range repulsion)



- **Experimental** side: more and more precise *NN* data
- **Theoretical** side: more sophisticated potentials → $\chi^2 \approx 2$ in the 1980's, $\chi^2 \approx 1$ in the 1990's

Three-nucleon forces

- ⦿ Calculations with accurate ($\chi^2 = 1$) OBE potentials show **deficiencies in systems with *A*>2**
  - ○ Lightest nuclei do not match experiment
  - ○ Saturation point of nuclear matter is not reproduced



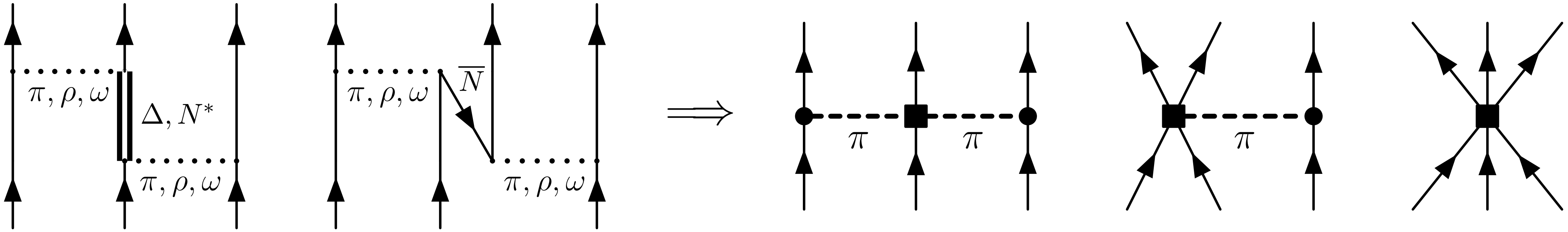
[Li *et al.* 2006]

Three-nucleon forces must be considered

1980's

➪ **Fundamental reason**: nucleons are composite particles, but we treat them as structureless

- ○ Certain processes, e.g. involving nucleon excitations, can not be described as 2-body



[Fujita, Miyazawa, …]

- ○ Three-nucleon forces are added mostly phenomenologically to OBE potentials

Contents

1. Inter-nucleon forces

- ○ Brief introduction to the nuclear many-body problem
- ○ Properties and modelling of nuclear forces
- ○ **The modern view: chiral effective field theory**

2. Ab initio techniques for the nuclear many-body problem

- ○ Configuration-interaction approaches
- ○ Techniques to mitigate the "curse of dimensionality" (SRG, NO2B, IT)
- ○ Mean field and correlations
- ○ Expansion methods for closed-shell nuclei
- ○ Symmetry breaking
- ○ Expansion methods for open-shell nuclei
- ○ State of the art and open problems

3. Equation of state of nuclear matter & connections to astrophysics

- ○ Neutron stars & Tolman-Oppenheimer-Volkoff equations
- ○ Equation of state of neutron-star matter
- ○ Astrophysical constraints on the nuclear EoS

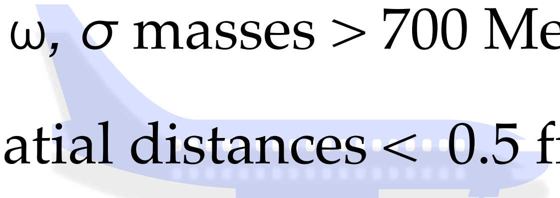
Resolution scale of nucleon-nucleon interactions

⊙ **Two main problems** with OBE potentials

1. Substantial part remains **phenomenological**
2. Strong repulsive short-range component ("**hard core**")

Hard core ↔ Strong coupling between low and high momenta ↔ High resolution

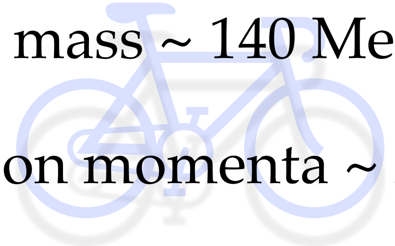
Do we really need such high resolution to compute properties of nuclei?



ρ, ω, σ masses > 700 MeV

spatial distances $<$ 0.5 fm
cf. nucleon radius ~ 0.8 fm

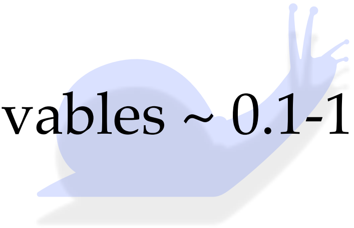
↔



pion mass ~ 140 MeV

av. nucleon momenta ~ 200 MeV

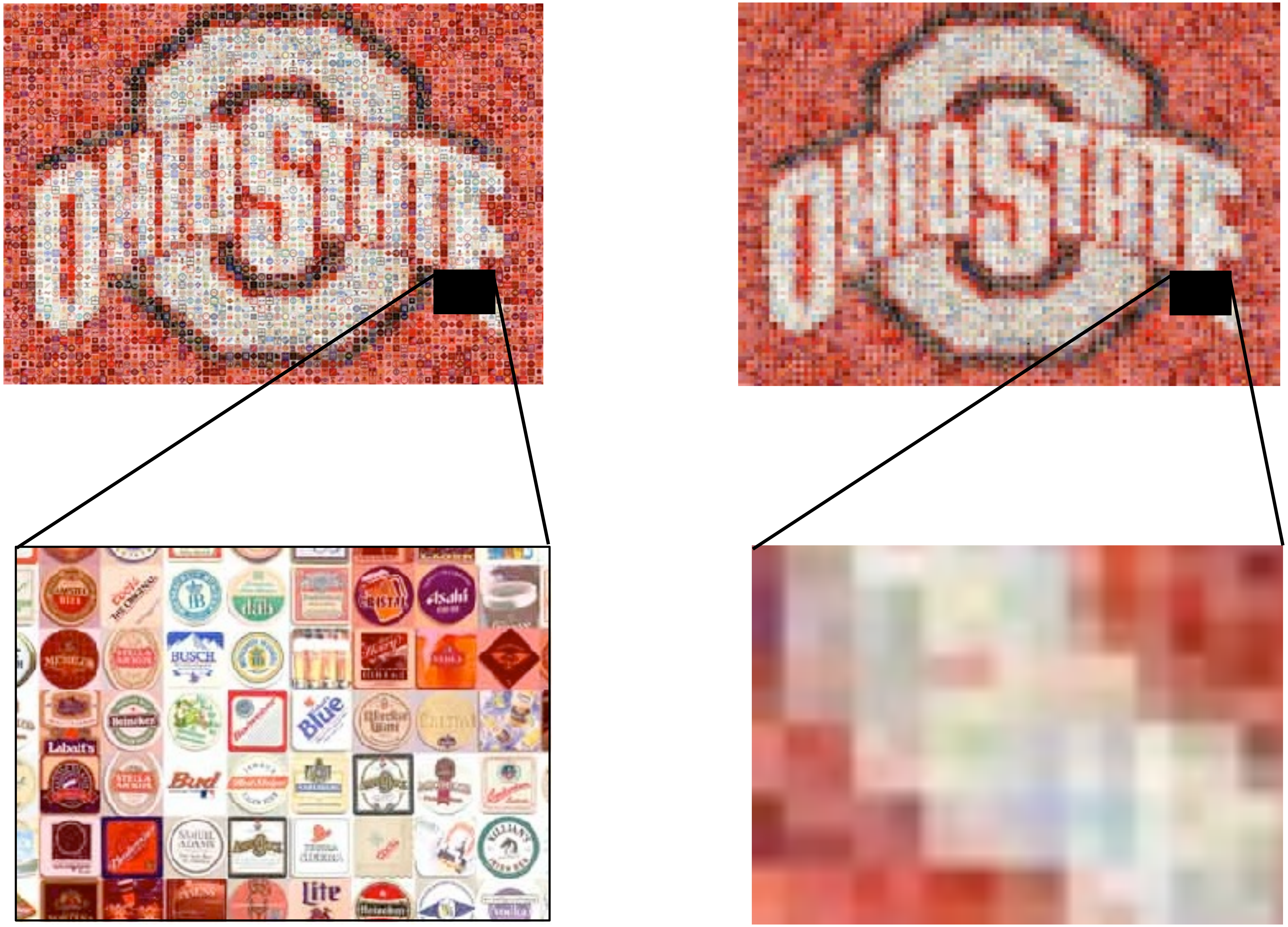
↔



observables ~ 0.1-10 MeV

➪ For many of the observables we are interested in, the answer is **no**

Resolution scale of nucleon-nucleon interactions



[figures from K. Hebeler]

Effective field theory

⦿ The principles

[Weinberg, van Kolck, ..]

1990's

1. Use separation of scales to define d.o.f. & expansion parameter

   Typical momentum at play ← $\frac{Q}{M}$ → High energy scale (not included explicitly)

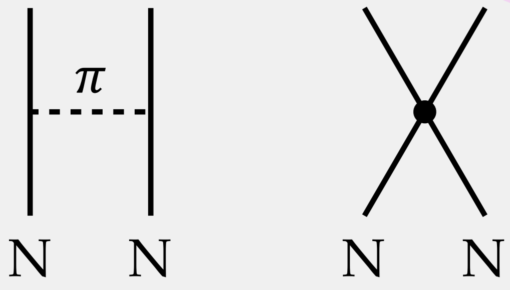
2. Write all possible terms allowed by symmetries of underlying theory (QCD)
3. Order by size all possible terms → **systematic** expansion (= "power counting")
4. Truncate at a given order and adjust coupling constants (use underlying theory or data)

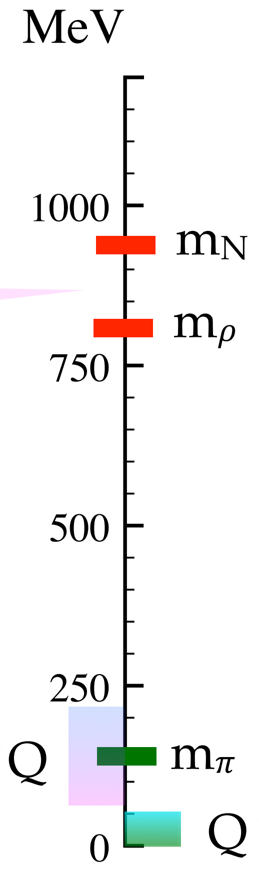
Chiral EFT

➪ Expand around Q ~ m_π

High-energy via contact interactions

Keep pion dynamic explicit

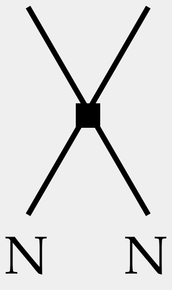




Pionless EFT

➪ Expand around Q ~ 0

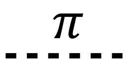
Integrate out pions too
→ only contact terms



Chiral effective field theory (à la Weinberg)

⊙ **Building blocks**

1. Nucleon propagator = 

2. Pion propagator = 

3. Pion-nucleon vertex = •, ●, …
4. k-nucleon contact = ■, □, …

→

Goal of the power counting:
Estimate the power ν of the law $(Q/M)^\nu$ with which each contribution (=diagram) scales

⊙ **Naive dimensional analysis**

1. Nucleon propagator ~ Q^{-1}
2. Pion propagator ~ Q^{-2}
3. Derivative operator ~ Q
4. Loop integration ~ Q^4

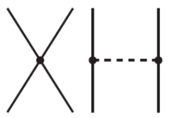
➡

Equation for *k*-nucleon connected diagrams

$$\nu = 2k - 4 + \underbrace{2L}_{\text{loops}} + \underbrace{\sum_i}_{\text{vertices}} \Delta_i \quad \text{with} \quad \Delta_i \equiv \underbrace{d_i}_{\text{derivatives}} + \underbrace{\frac{n_i}{2}}_{\text{nucleon fields}} - 2$$

Weinberg power counting

Chiral effective field theory (à la Weinberg)

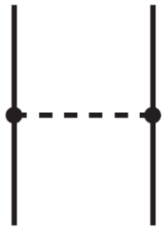
	2N Force	**3N Force**	**4N Force**
LO $(Q/\Lambda_\chi)^0$			

Pure contact term

$$V_{\rm ct}^{(0)}(\boldsymbol{p}',\boldsymbol{p}) = C_S + C_T\,\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2$$

Central operator (no **q** dependence)

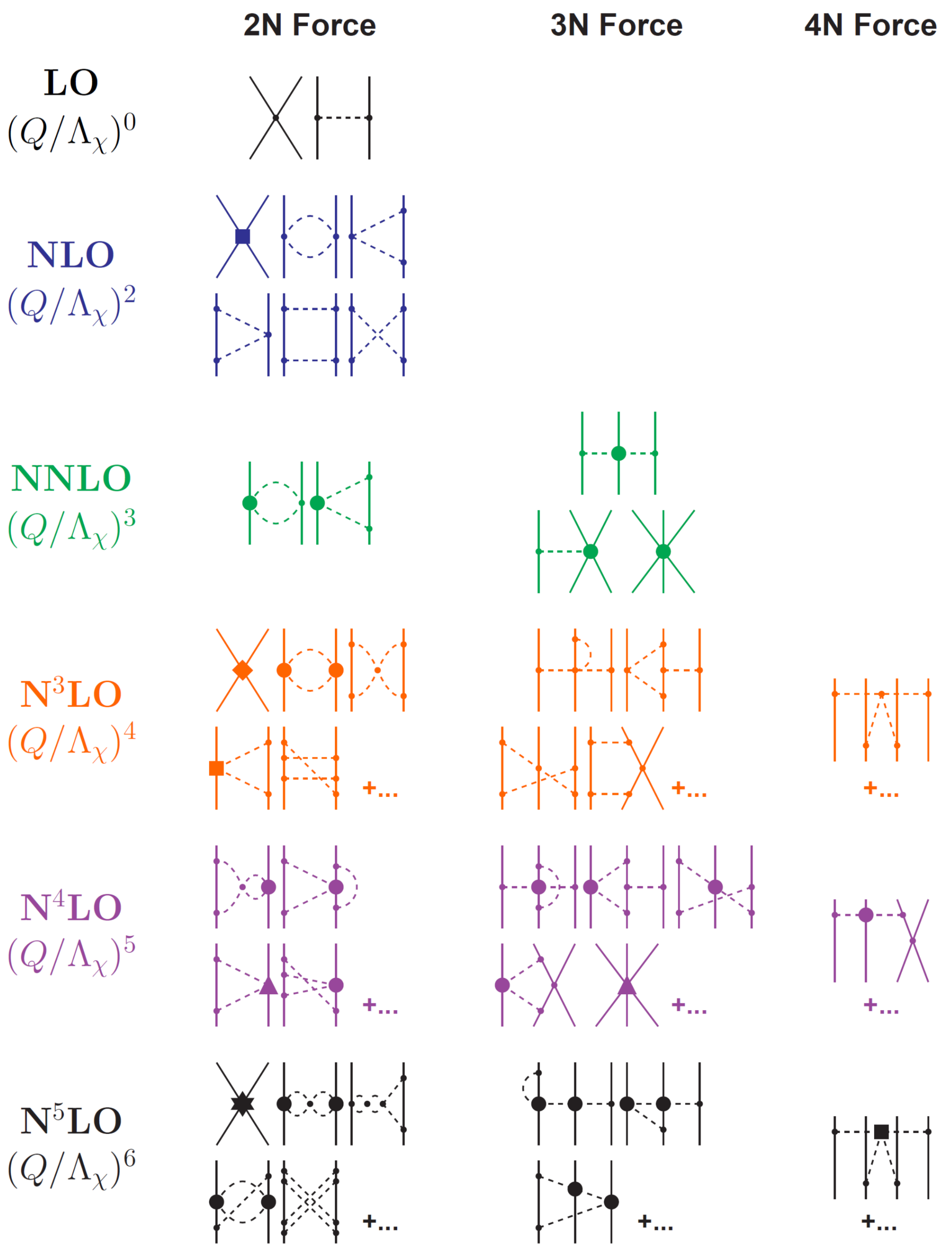
One-pion exchange



$$V_{1\pi}^{(0)}(\boldsymbol{p}',\boldsymbol{p}) = -\frac{g_A^2}{4f_\pi^2}\,\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2\,\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{q}\;\boldsymbol{\sigma}_2\cdot\boldsymbol{q}}{q^2+m_\pi^2}$$

Tensor operator

Chiral effective field theory (à la Weinberg)



○ Finite number of diagram at a given order

○ No $\nu=1$ due to symmetries

○ 3N force cancels at $\nu=2$

○ 3N enter at N^{2}LO, 4N at N^{3}LO

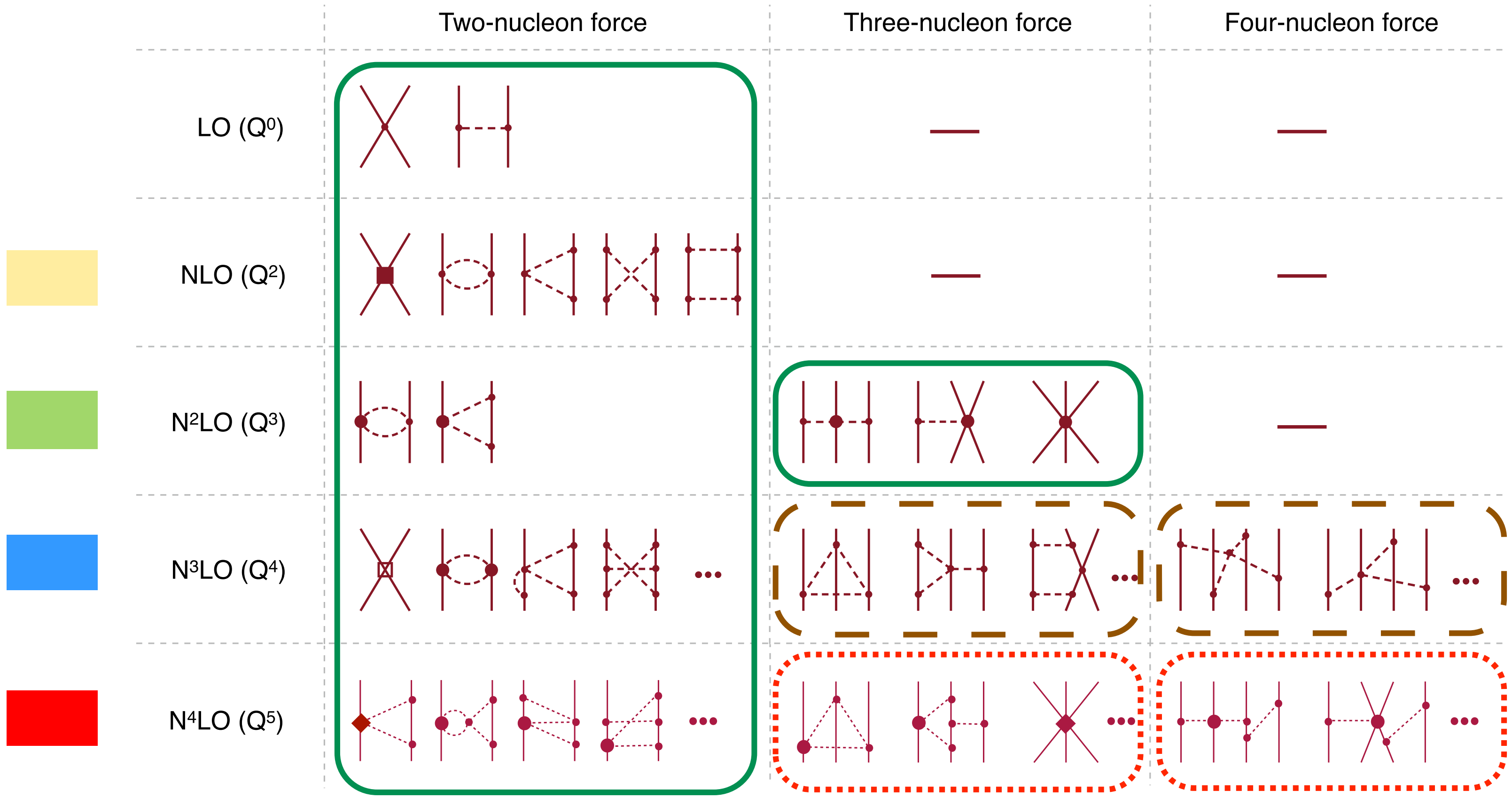
○ Consistency between *k*-body sectors

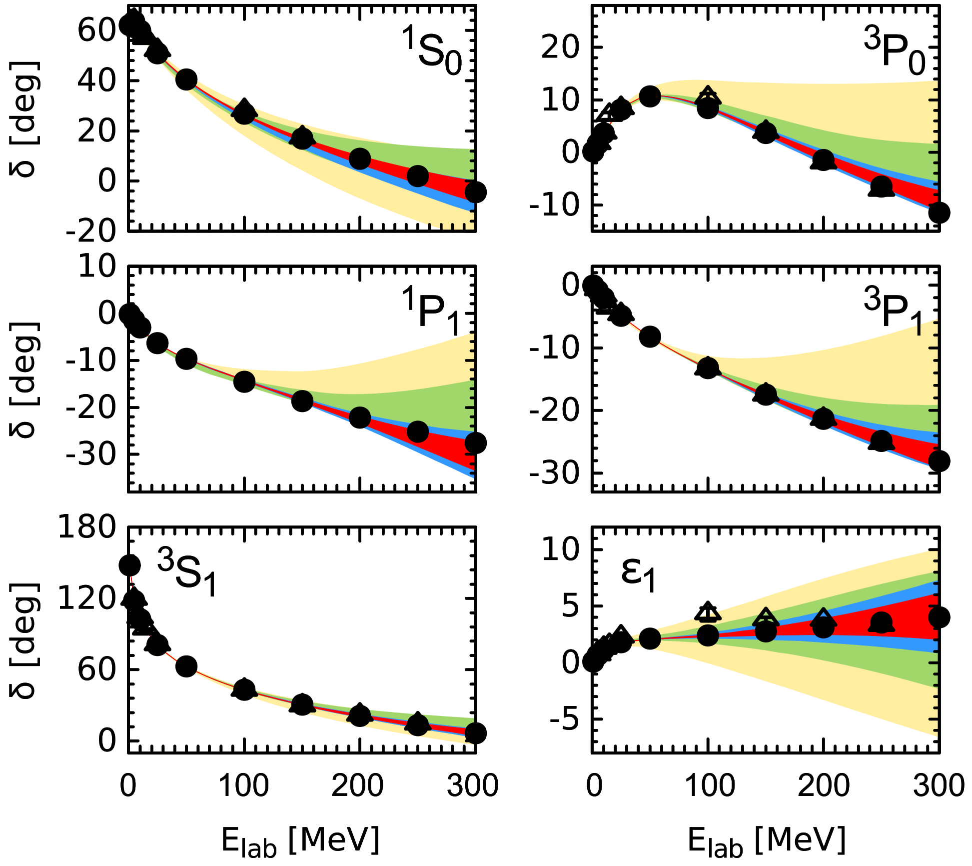
○ Estimate of error from $(Q/M)^{\nu+1}$

○ Proliferation of terms → convergence?

Chiral effective field theory

- Chiral EFT: a **systematic** framework to construct *A*N interactions (*A*=2, 3, …)
- Main features:
  - High-energy physics unresolved → **soft potentials** → improved many-body convergence
  - Many-body forces and currents consistently derived
  - A **theoretical error** can be, in principle, assigned to each order in the expansion





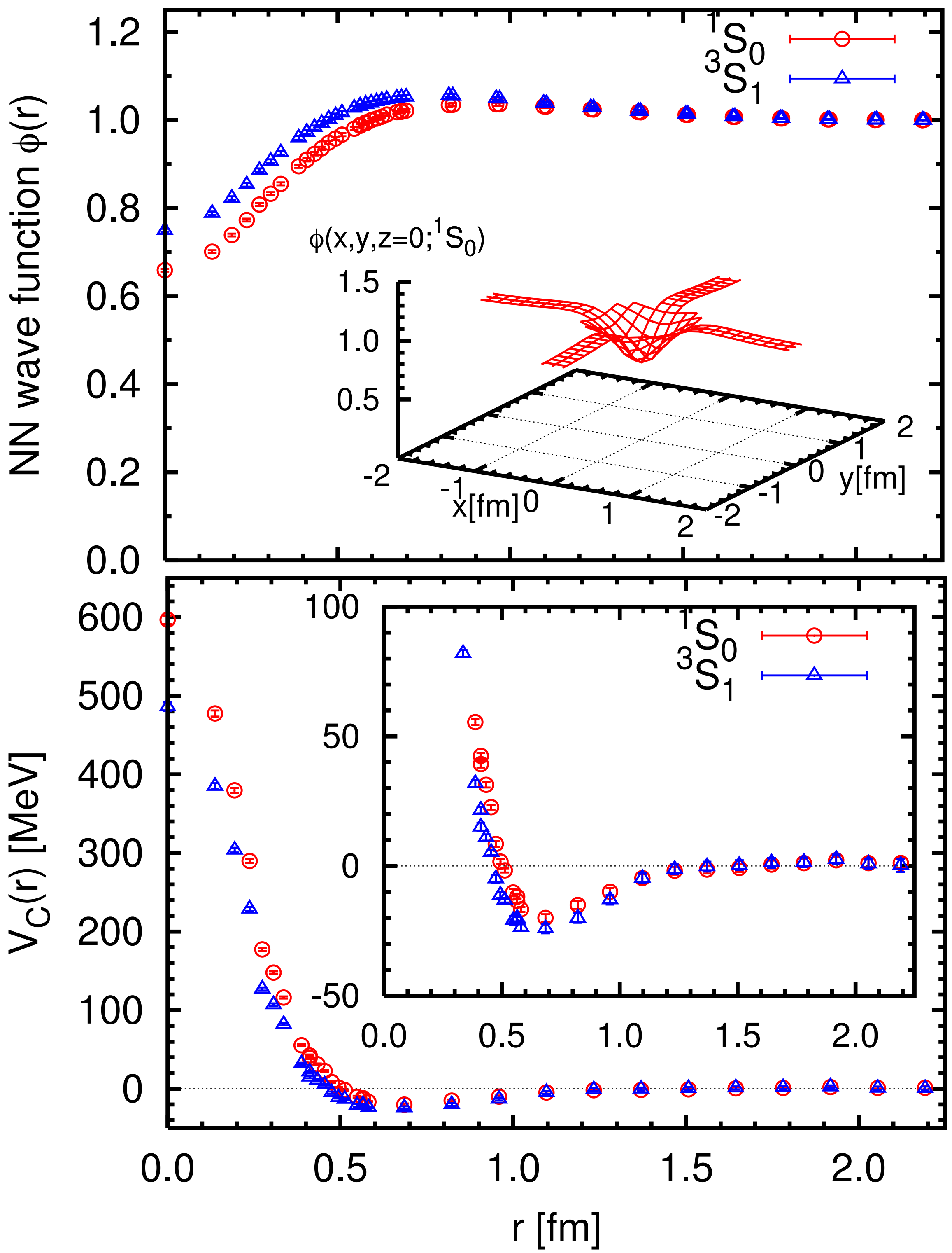
[Epelbaum *et al.* 2015]

➪ Ideally: apply to the many-nucleon system (and propagate the theoretical error)

Potentials from lattice QCD

- First attempts to extract a nucleon-nucleon potential from lattice QCD calculations

[Ishii *et al.* 2007]



- **Technique**
  - Compute NN wave function on the lattice
  - Invert Schrödinger equation

- **Advantages**
  - Connects to a more fundamental level
  - Does not rely on experimental data
  - Can be extended to baryon-baryon interactions

- **Difficulties**
  - Only schematic results so far
    - Unphysical pion masses
    - Model dependent extraction
  - Very complicated to extend to three-body forces

References

- **S. Weinberg**, Phys. Lett. B **251** 288 (1990) & Nucl. Phys. B **363** 3 (1991)
    - *Founding work on EFT for nuclear physics*
- **U. van Kolck**, arXiv:1902.03141 (2019)
    - *“Les Houches” lectures on EFT for nuclear physics*
- **E. Epelbaum *et al.***, Rev. Mod. Phys. **81** 1773 (2009)
    - *Review on nuclear forces derived within chiral EFT*
- **H.-W. Hammer *et al.***, Rev. Mod. Phys. **92** 025004 (2020)
    - *Review on nuclear effective field theories (including - but not only - chiral EFT)*
- **U. van Kolck**, Front. in Phys. **8** 79 (2020)
    - *Review on the problem of renormalisation of chiral nuclear forces*
- **N. Ishii *et al.***, Phys. Rev. Lett. **99** 022001 (2007); **S. Aoki *et al.***, Prog. Theor. Phys. **123** 89 (2010)
    - *Article and review on nuclear forces from lattice QCD*
- **V. Somà**, Eur. Phys. J. Plus **133** 434 (2018)
    - *Pedagogical (very) brief history of nuclear interactions*