

# *Ab initio nuclear structure*

— From QCD to many-body observables —

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*Aussois Winter School*

December 8th, 2021



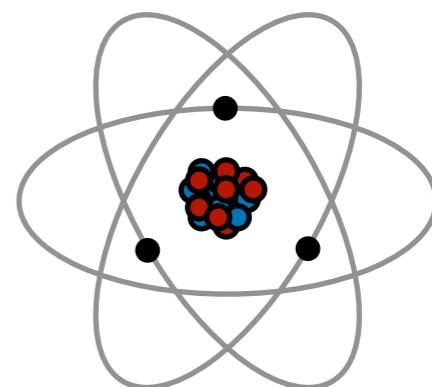
TECHNISCHE  
UNIVERSITÄT  
DARMSTADT



**Alexander Tichai**

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Technische Universität Darmstadt



# What is ‘*Ab initio*’ ... ?

***Ab initio*** (‘From scratch’)

Solve the nuclear many-body problem in  
a systematically improvable way

$$H |\Psi_n\rangle = E_n |\Psi_n\rangle$$

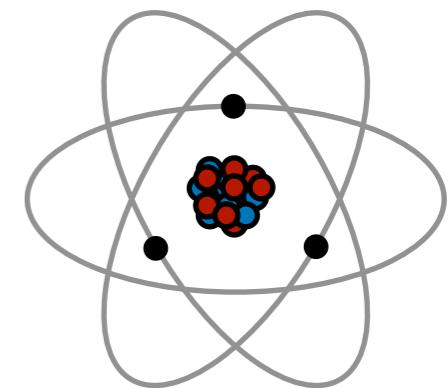
$\triangleq$

**Use of controlled expansions**

**QCD**

(Quantum chromodynamics)

**Nuclear observables**



**... and other things!**

**Basis convergence**

**Many-body solution**

**RG transformation**

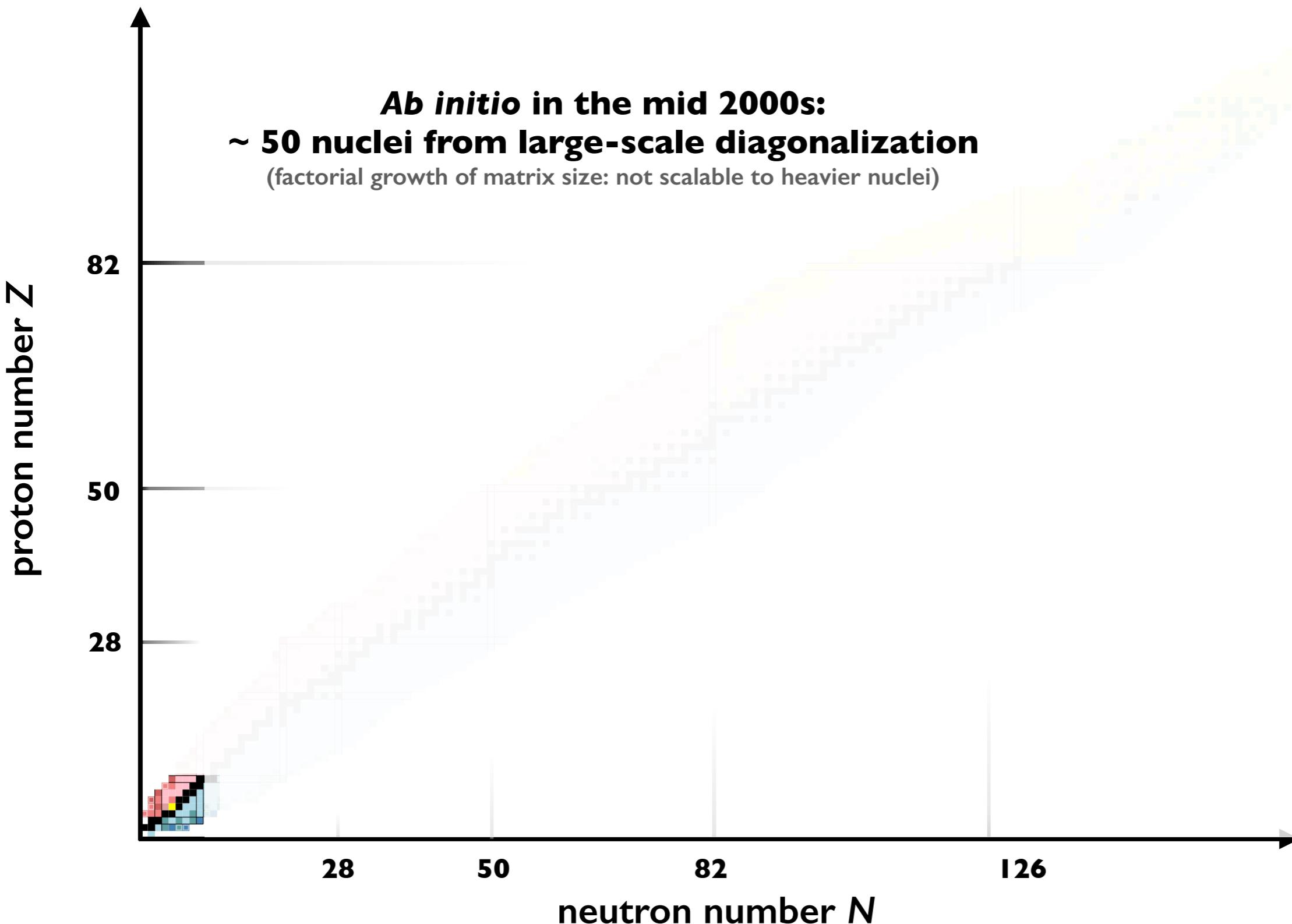
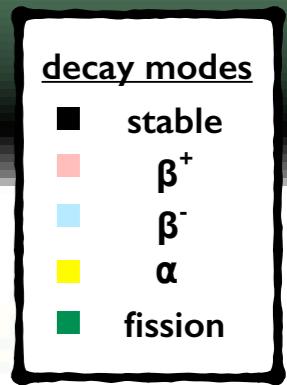
**Interaction model**

**Regularisation**

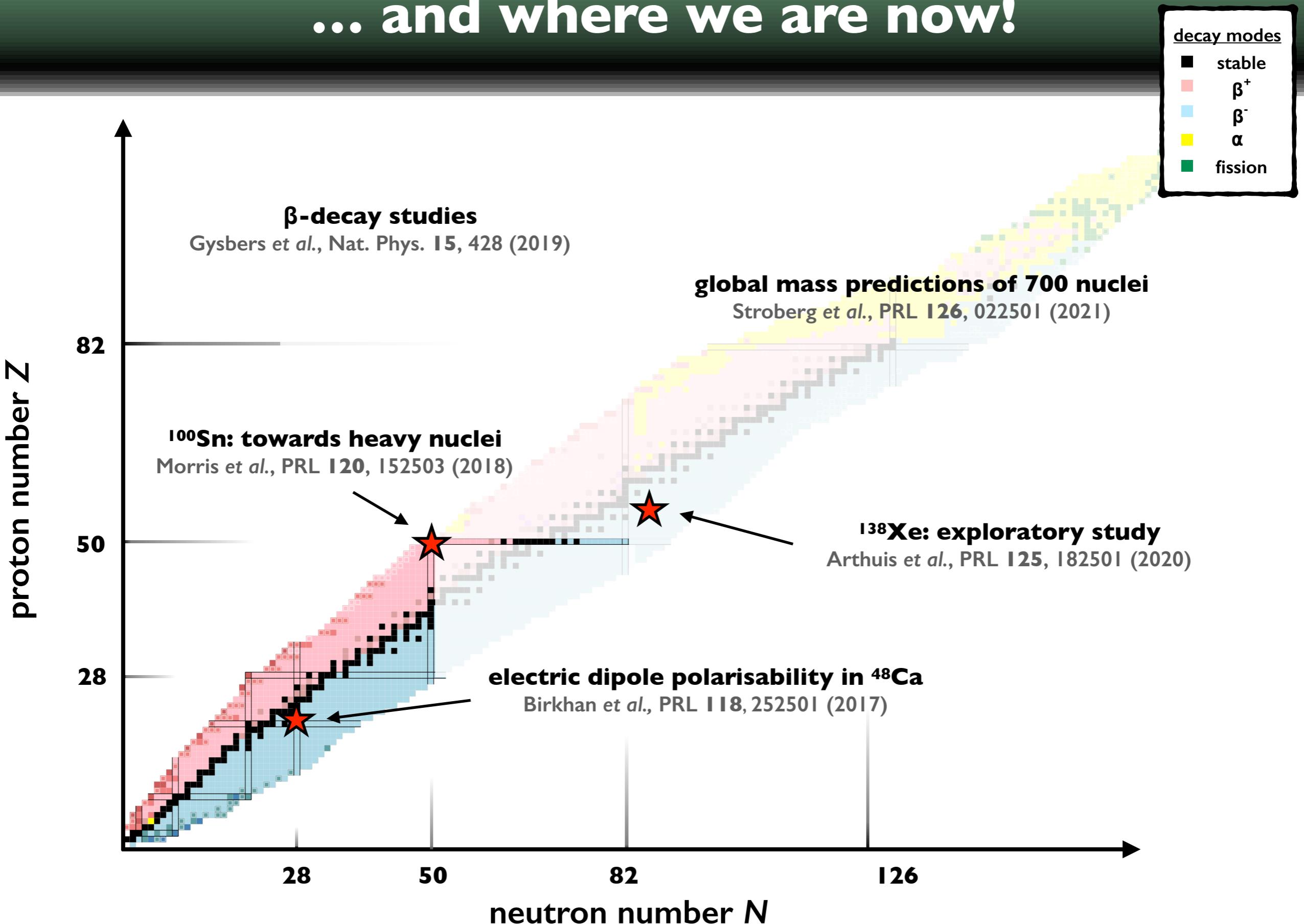
**Approximations**

**Effective field theory**

# ... what it was ...



# ... and where we are now!



# Controlled expansions

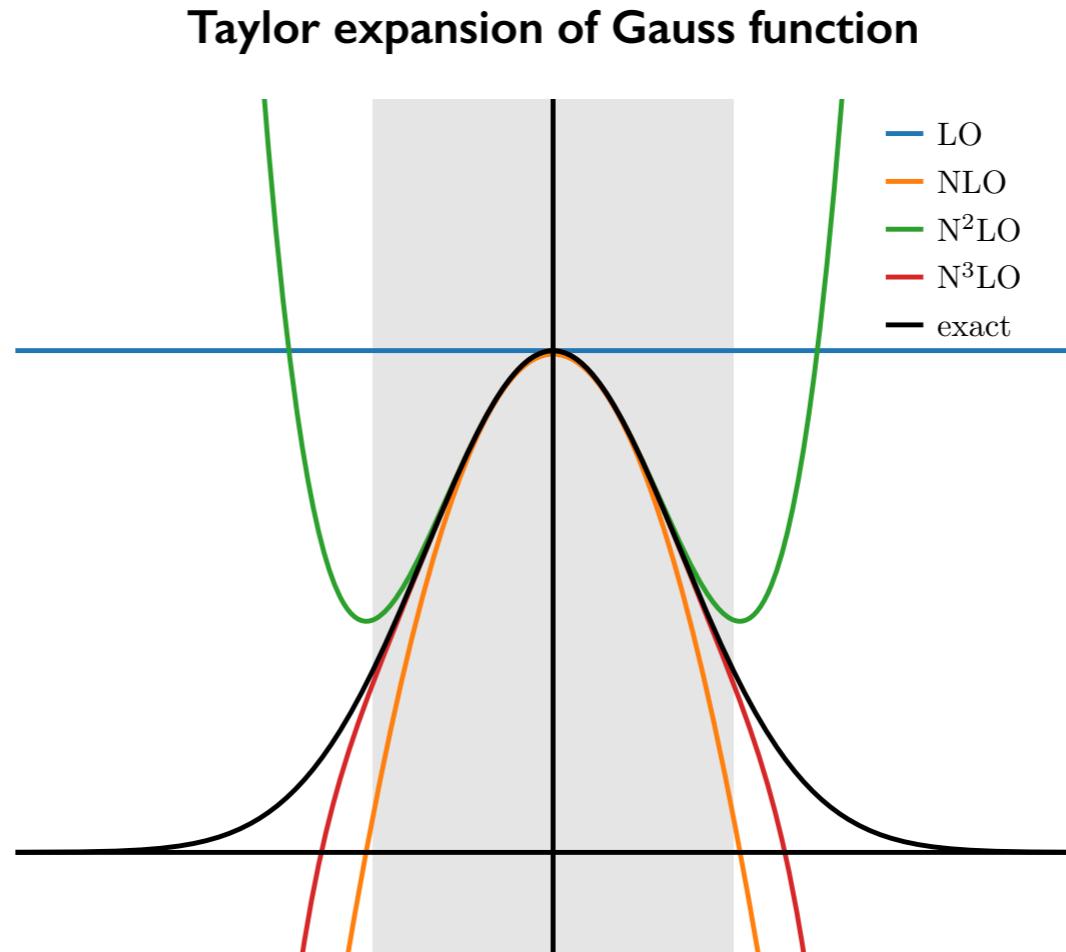
$$f_{\text{exact}} = e^{-x^2}$$

$$f_{\text{LO}} = 1$$

$$f_{\text{NLO}} = 1 - x^2$$

$$f_{\text{N}^2\text{LO}} = 1 - x^2 + \frac{1}{2}x^4$$

$$f_{\text{N}^3\text{LO}} = 1 - x^2 + \frac{1}{2}x^4 - \frac{1}{6}x^6$$



- **Leading-order approximation:** simple to obtain but poor accuracy
- **Higher-order corrections:** refinement of description but evaluation more complex
- **Choice of reference point sets range of validity of the expansion**
- **Symmetries of exact solution** can be inherited by the approximation scheme

# Overview

Part I

## Nuclear interactions

*'From effective field theories to uncertainty quantification'*

Part II

## Many-body theory

*'From brute-force diagonalization to scalable expansion schemes'*

Part III

## Emerging frontiers

*'A (personal) perspective on computational challenges'*

# Part I

# Nuclear interactions

**From effective field theories to uncertainty quantification**

# The strong interaction

- Dynamics of quarks and gluons is fully encoded in the **QCD Lagrangian**

$$\mathcal{L}_{\text{QCD}} = \bar{q} \left( i \gamma_\mu D^\mu - M \right) q - \frac{1}{4} G_{\mu\nu}^a G^{a,\mu\nu}$$

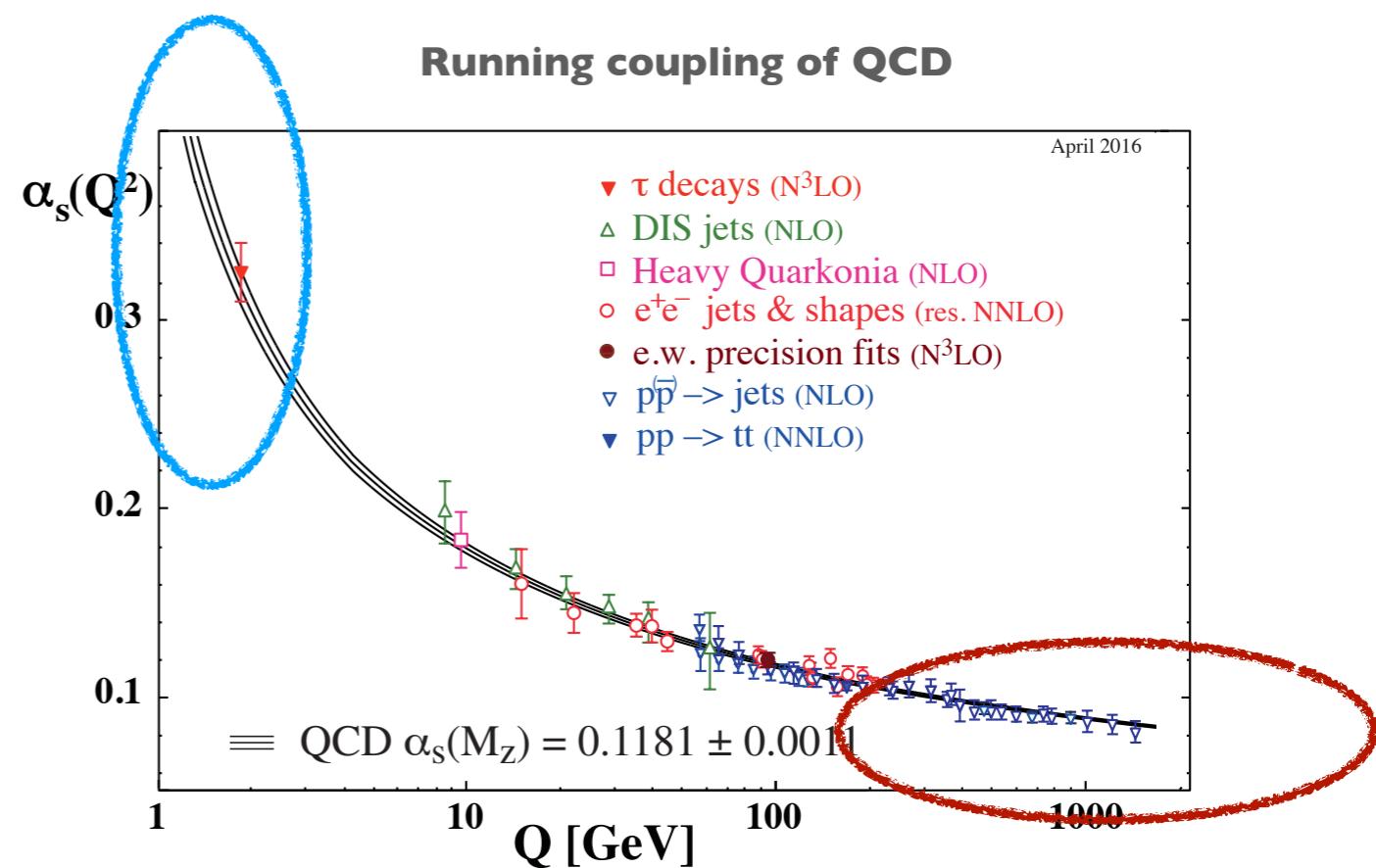
- Asymptotic freedom:** quarks interact weakly and QCD is perturbative at high energies

→ perturbative QCD (pQCD)

$$O = O^{(0)} + \alpha_s O^{(1)} + \alpha_s^2 O^{(2)} + \dots$$

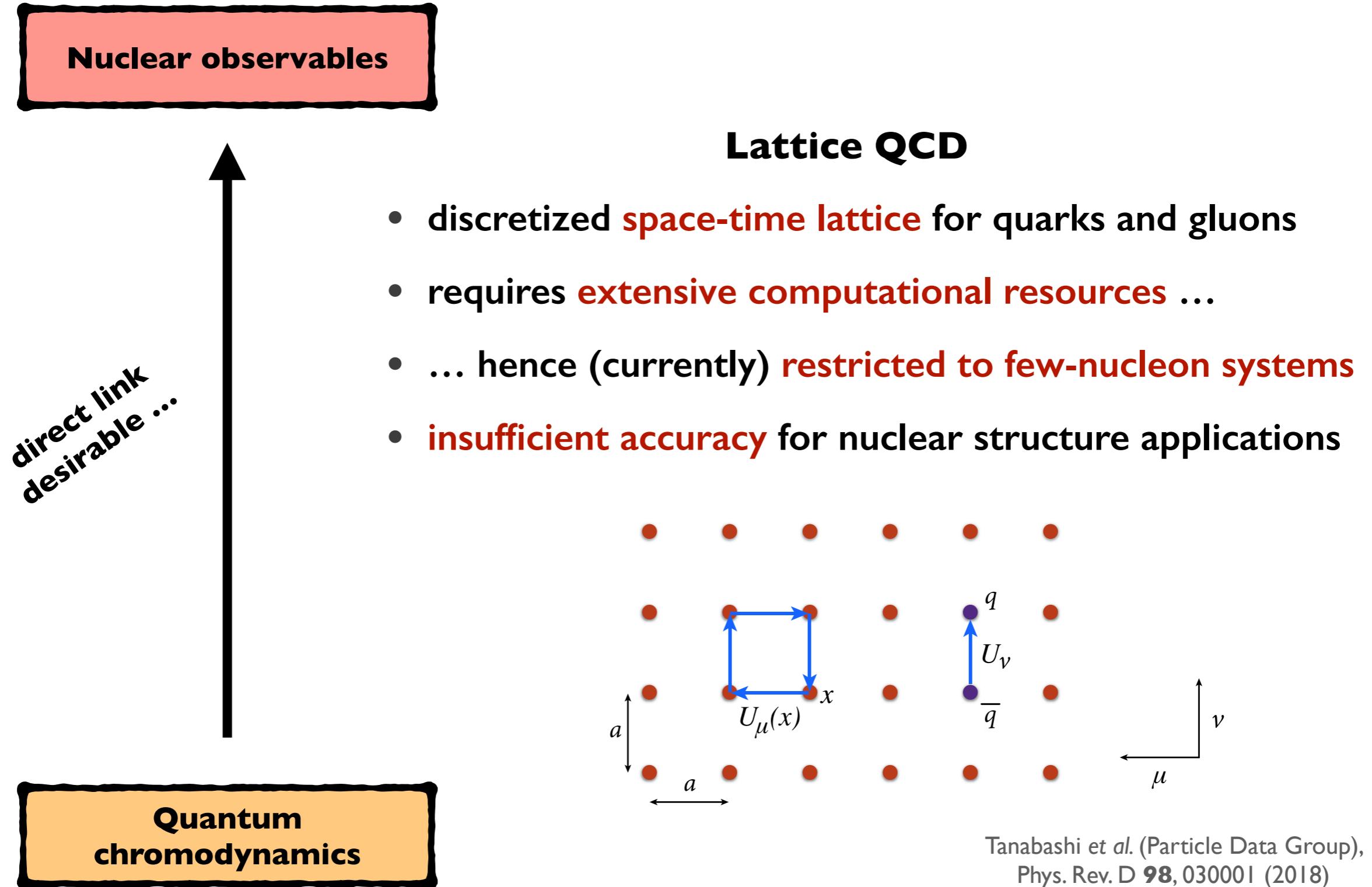
- Confinement:** quarks interact strongly and QCD is highly non-perturbative at low energies

→ Lattice QCD



Tanabashi et al. (Particle Data Group),  
Phys. Rev. D **98**, 030001 (2018)

# From QCD to nuclear observables

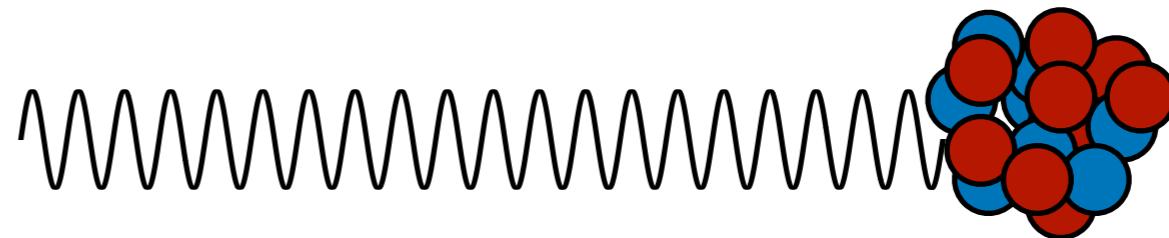


# The role of resolution

- High-energy probes **resolve the nucleon substructure**, i.e., quarks and gluons

high energy/short wavelength

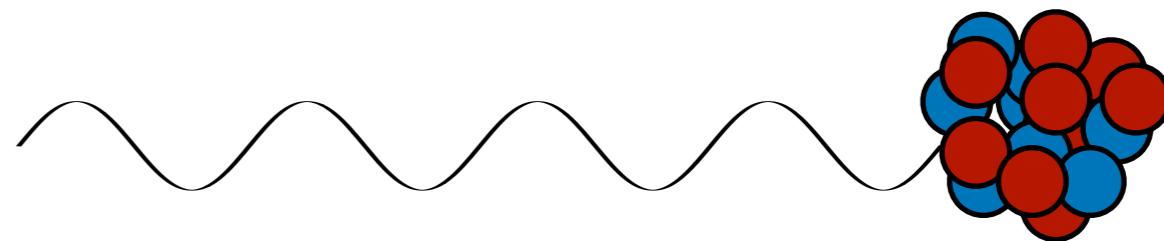
$$\lambda \ll R$$



- Low-energy probes do **NOT** resolve the nucleon substructure

low energy/long wavelength

$$\lambda \gg R$$



- Replace the fine details (quarks and gluons) by simpler objects

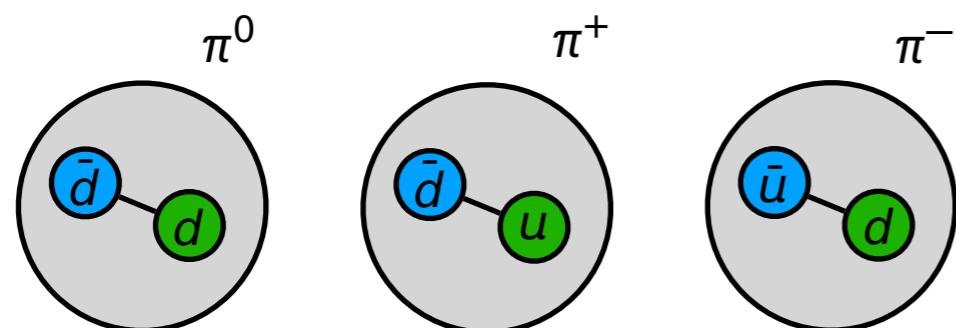


**EFT**  
(effective field theory)

- Use **degrees of freedom** that are relevant in low-energy regime

# Chiral effective field theory

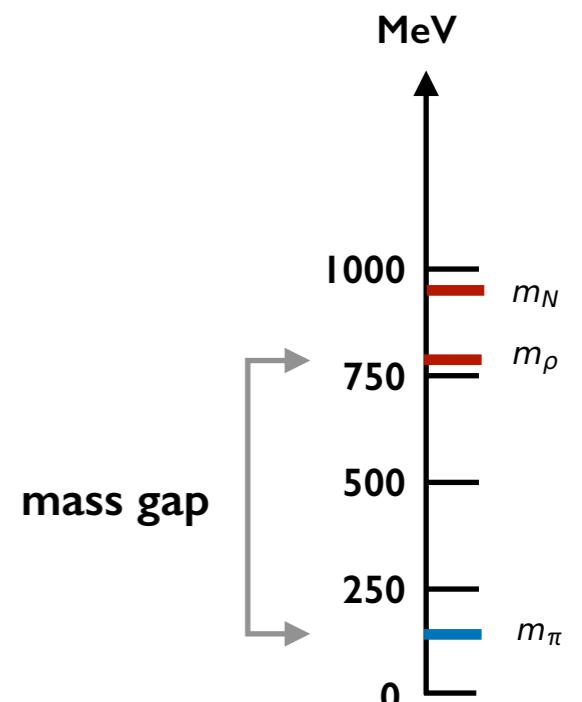
- Identify **effective degrees of freedom** in low-energy domain: **nucleons** and **pions**



schematic picture of the pion multiplet

$$m_{\pi^\pm} \approx 139.57 \text{ MeV}$$
$$m_{\pi^0} \approx 134.98 \text{ MeV}$$

- Pions mediate the strong interaction at long distances
- Expansion parameter from separation of scales at low energies

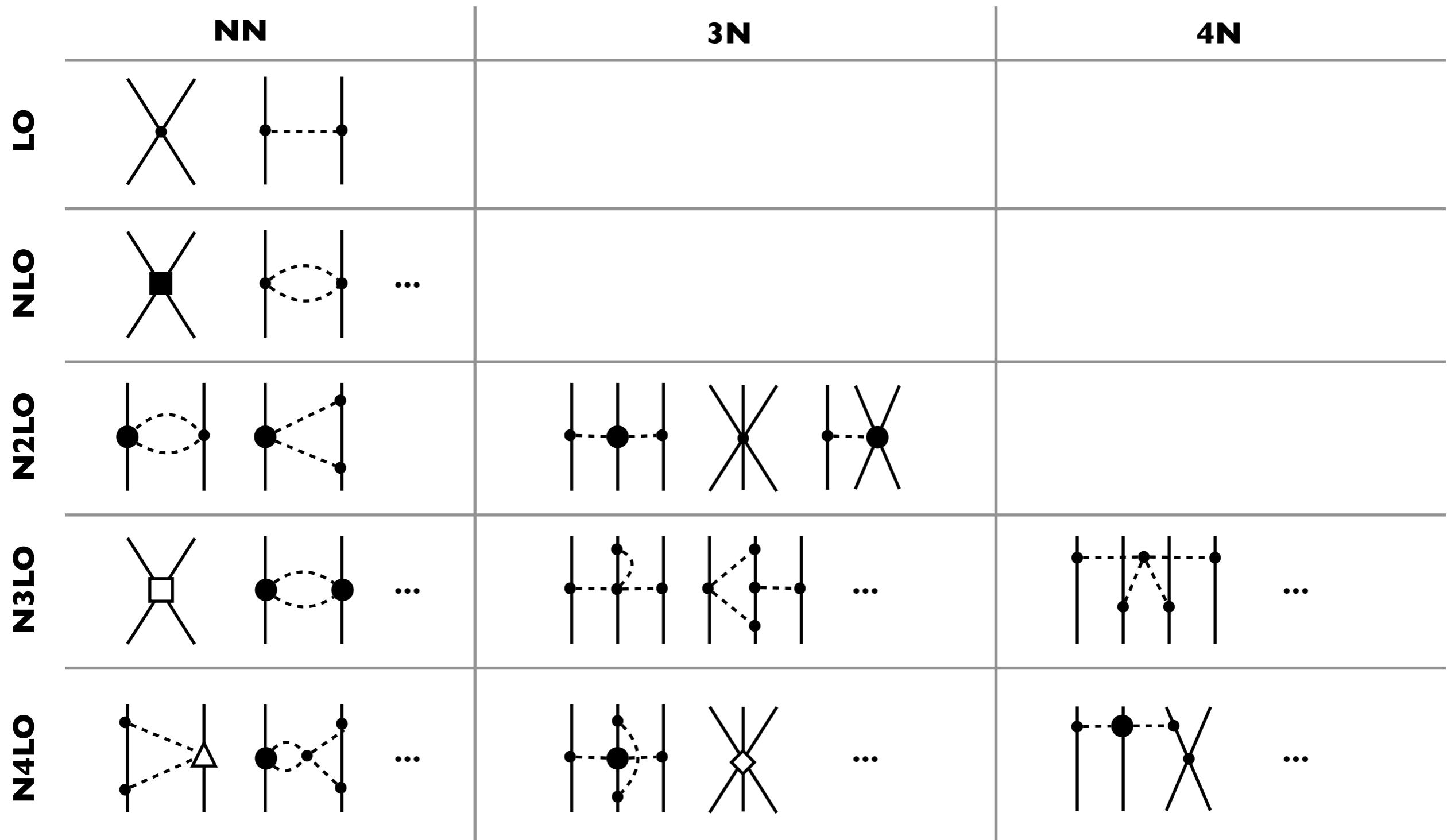
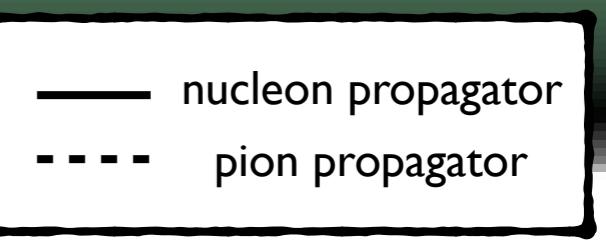


$$\frac{Q}{\Lambda}$$

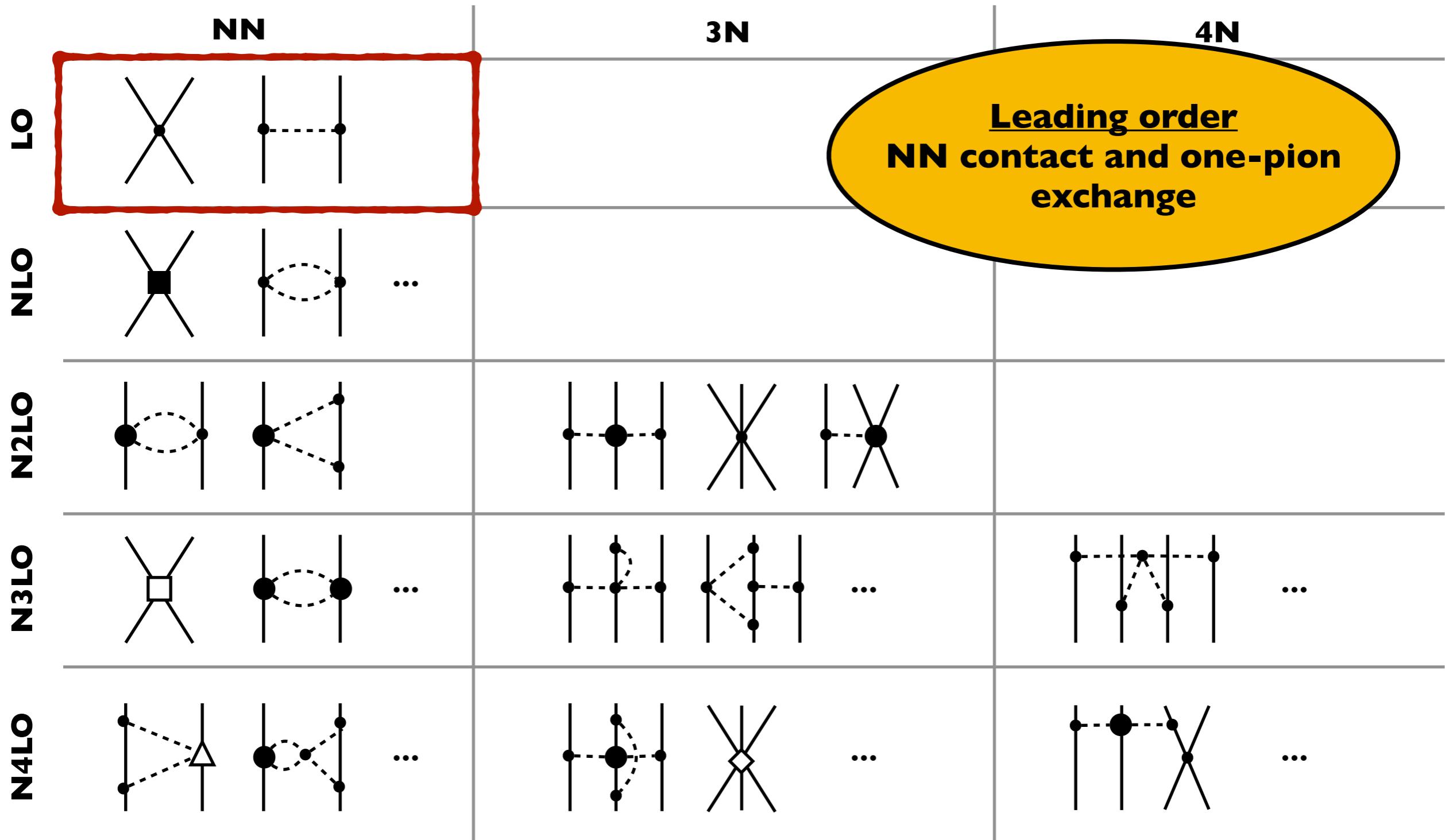
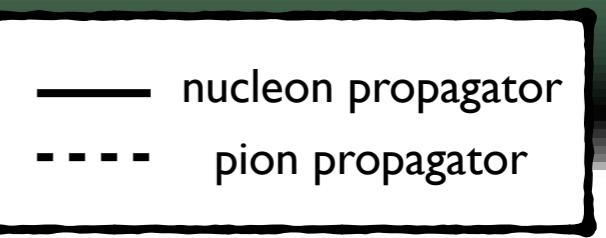
'soft scale'  
(typical momentum/pion mass) →  $\frac{Q}{\Lambda}$  ← 'hard scale'  
(breakdown of the theory)

- High-energy physics captured by a few **short-range couplings** (LECs)
- Systematically improvable theory with **prediction** of higher-body operators

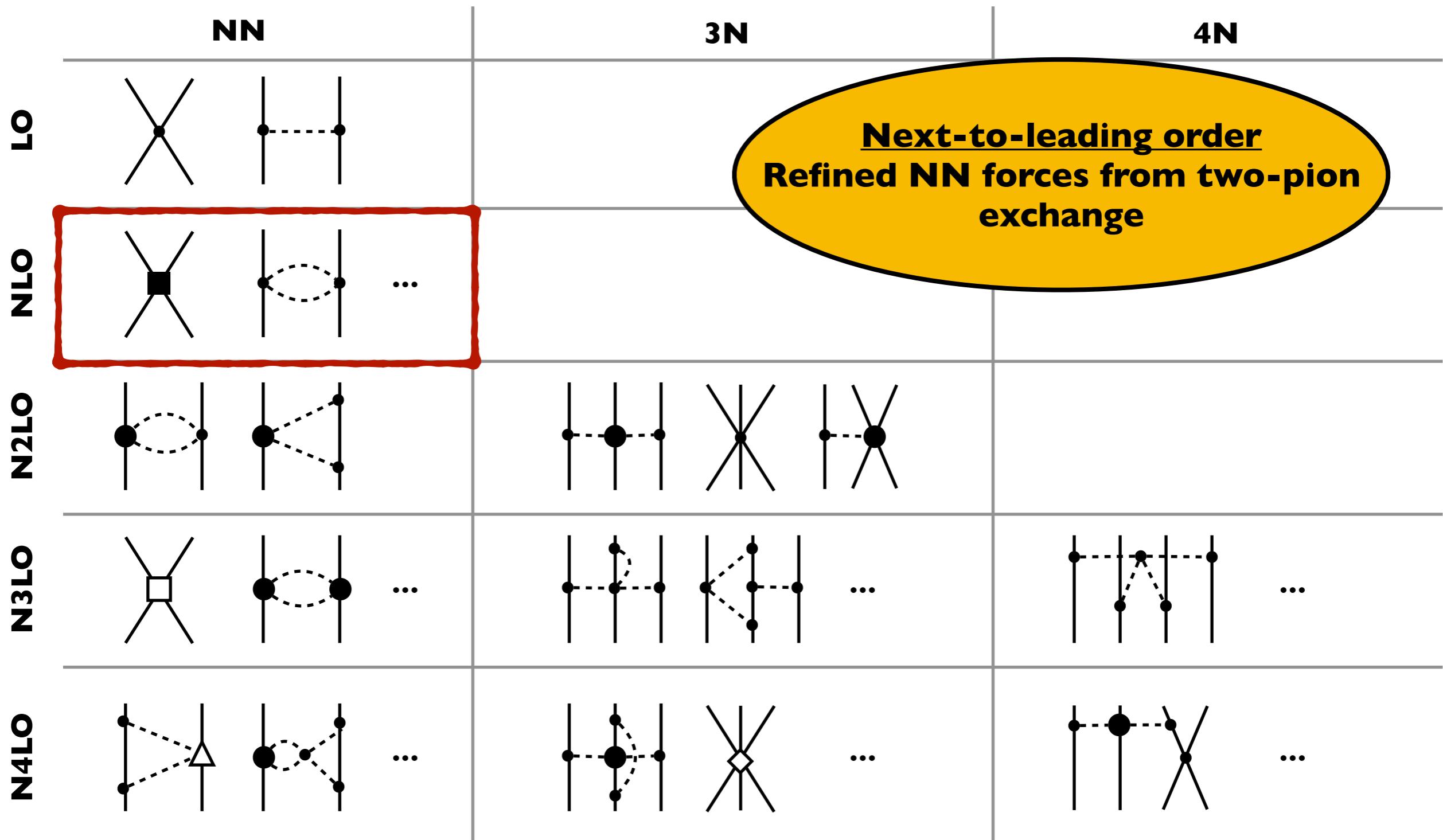
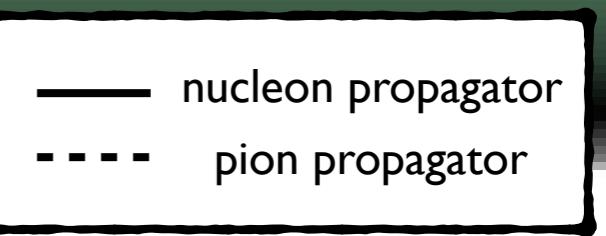
# Power counting



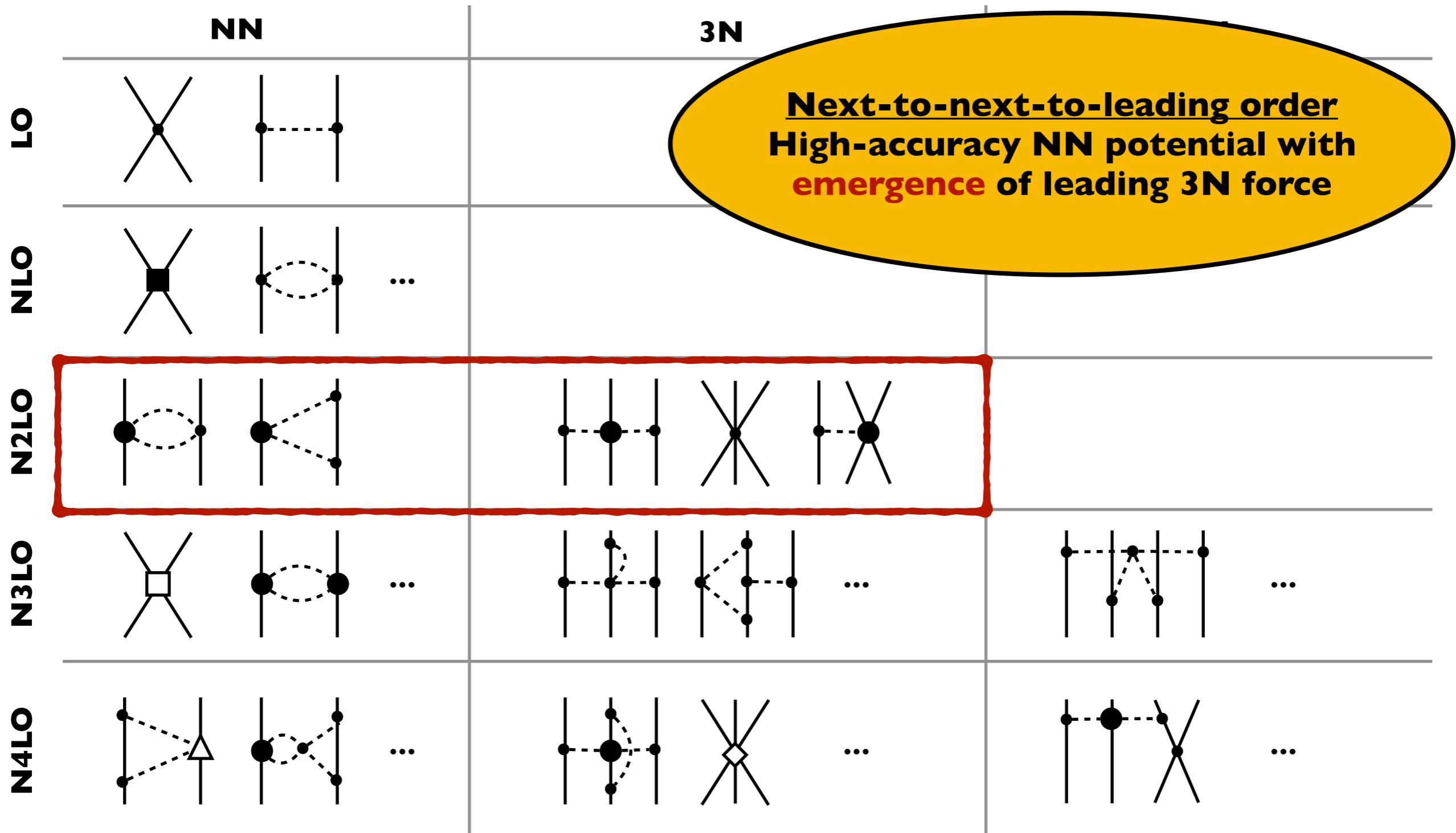
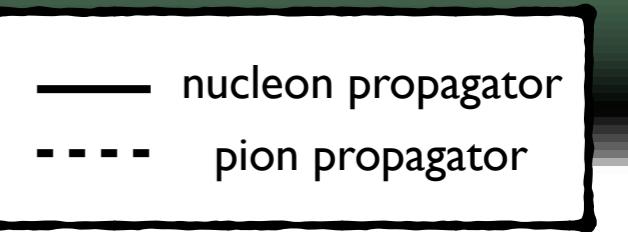
# Power counting



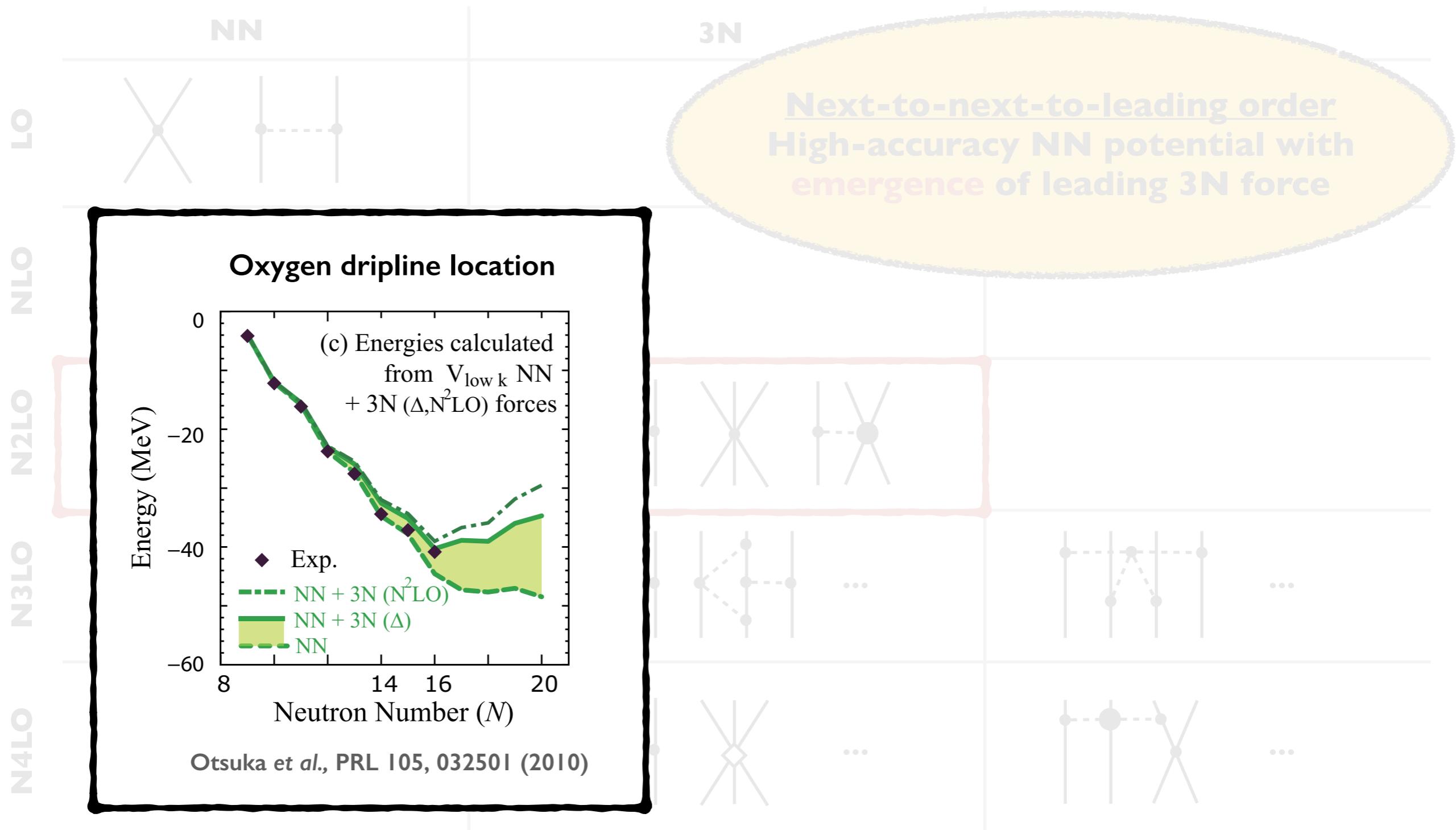
# Power counting



# Power counting



# Power counting



# The nuclear potential

Machleidt, Entem,  
Phys. Rept. 503 (2011) 1-75

- Nuclear interaction consists of **complicated operator structure**

angular momentum  
 $L$  not conserved!

$$V_{\text{nucl.}} = V_{\text{central}} + V_{\text{spin-orbit}} + V_{\text{tensor}} + \dots$$

$\frac{3}{r^2}(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2$

↑  
 $\propto \vec{L} \cdot \vec{S}$

- Example: simple central component from **long-range pion exchange**

$$V_{\text{Yukawa}}(r) = \frac{e^{-mr}}{r}$$

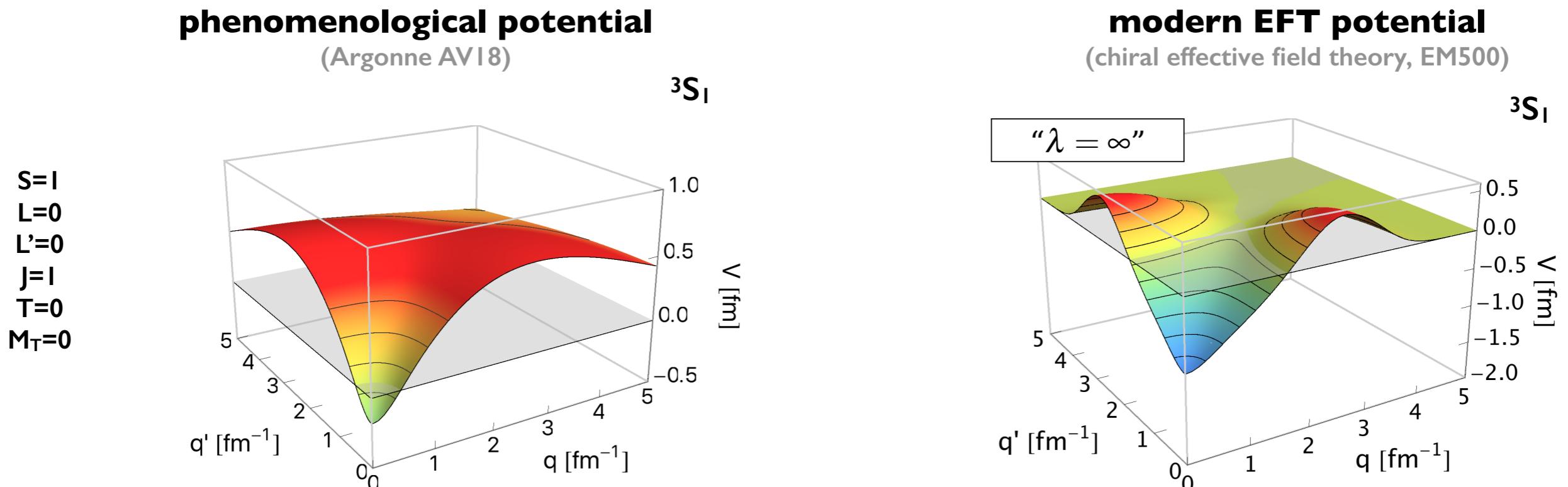
- Incorporate all operator structures consistent with **symmetry principles**

$$\{(\vec{\sigma}_1 \cdot \vec{\sigma}_2), (\vec{\tau}_1 \cdot \vec{\tau}_2), \dots\}$$

- Matrix elements in terms of **momentum and angular-momentum eigenstates**  
(partial-wave decomposition)

$$\langle q'(L'S)J; TM_T | V_{\text{NN}} | q(LS)J; TM_T \rangle$$

# Matrix elements



Hergert et al., arXiv: 1612.08315

- before 2000s: *ad hoc postulation* of operator structure based on symmetries
  - high-precision potentials but uncertainty quantification complicated
- since 2000s: *emergence* of operator structure from low-energy EFT expansion

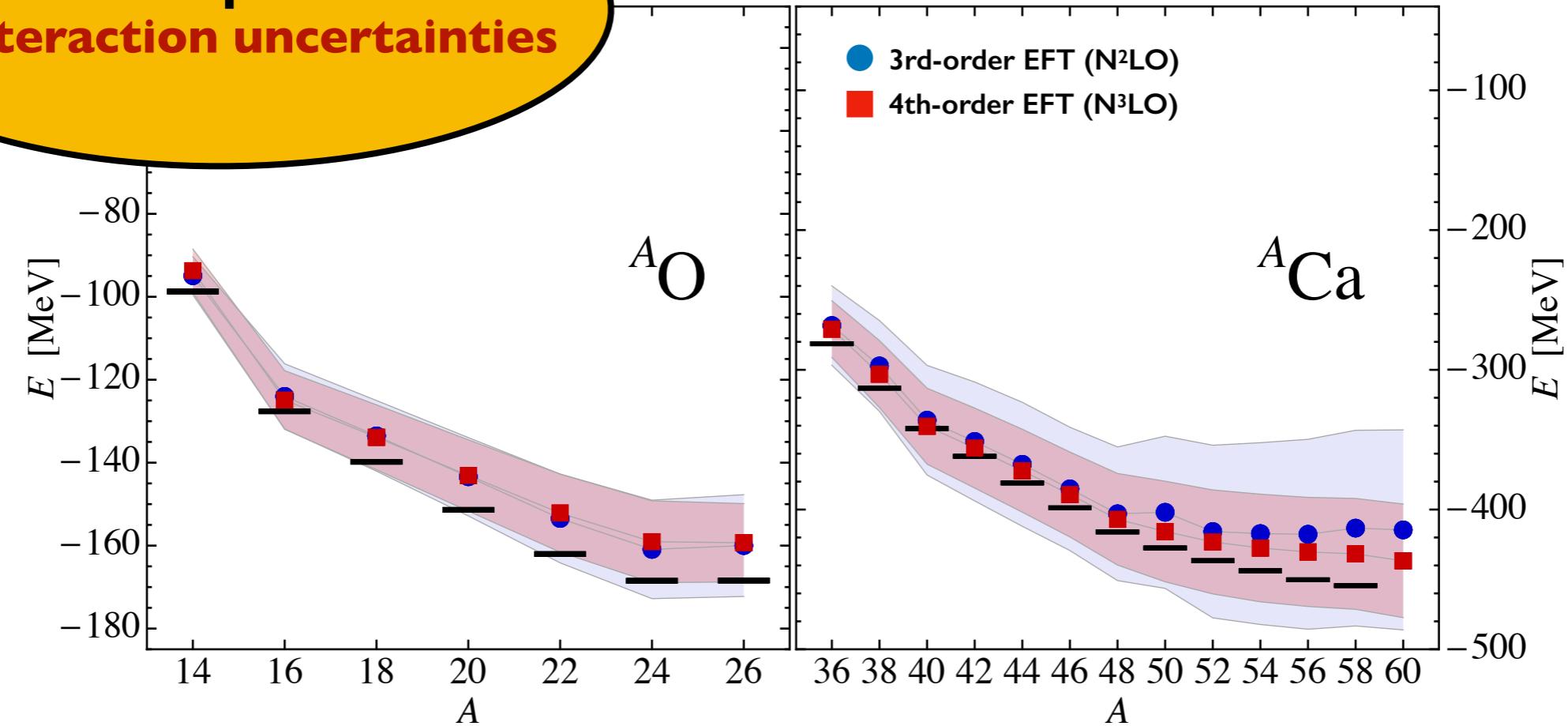
# Uncertainty quantification

Interaction

Hüther et al.,  
PLB 808, 135651 (2020)

EFT enables quantification  
of interaction uncertainties

Tichai, Roth, Duguet,  
Front. Phys. 8:164 (2020)

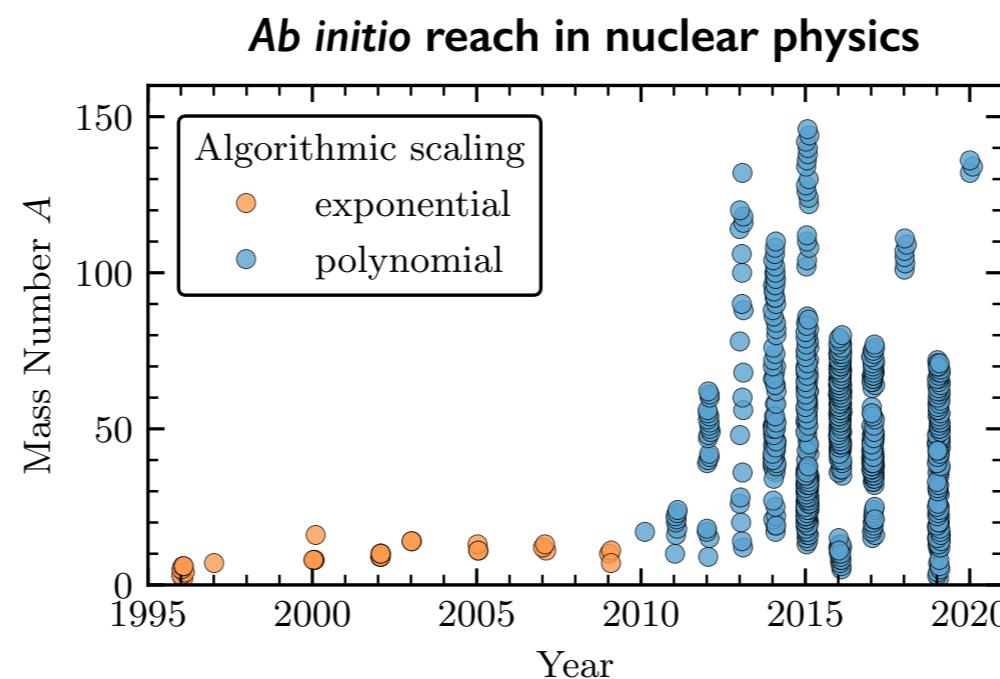


- Error bands correspond to **interaction uncertainty** from EFT expansion
- Higher orders in EFT expansion yield reduced uncertainties

# Part II

# Many-body theory

**From brute-force diagonalization to scalable expansion schemes**



# Configuration interaction

- Goal: solve the non-relativistic **Schrödinger equation** for given nuclear Hamiltonian

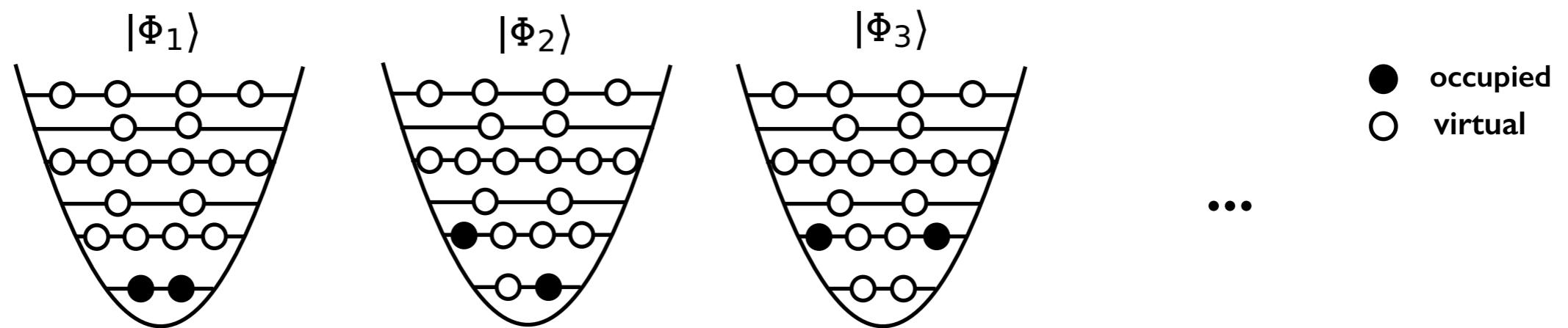
$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

chiral EFT input    many-body wave function                                  nuclear binding energy

- **Brute-force solution:** pick a matrix representation in  $A$ -body Hilbert space and diagonalize

$$H_{IJ} \equiv \langle \Phi_I | H | \Phi_J \rangle \quad \mathcal{B} \equiv \{ |\Phi_1\rangle, \dots, |\Phi_N\rangle \} \quad \xleftarrow{\text{Slater determinants}}$$

- **Many-body states** from filling single-particle states in an independent-particle model



- **Computational challenge:** there are a lot of different many-body states contributing ...

# A non-scalable solution

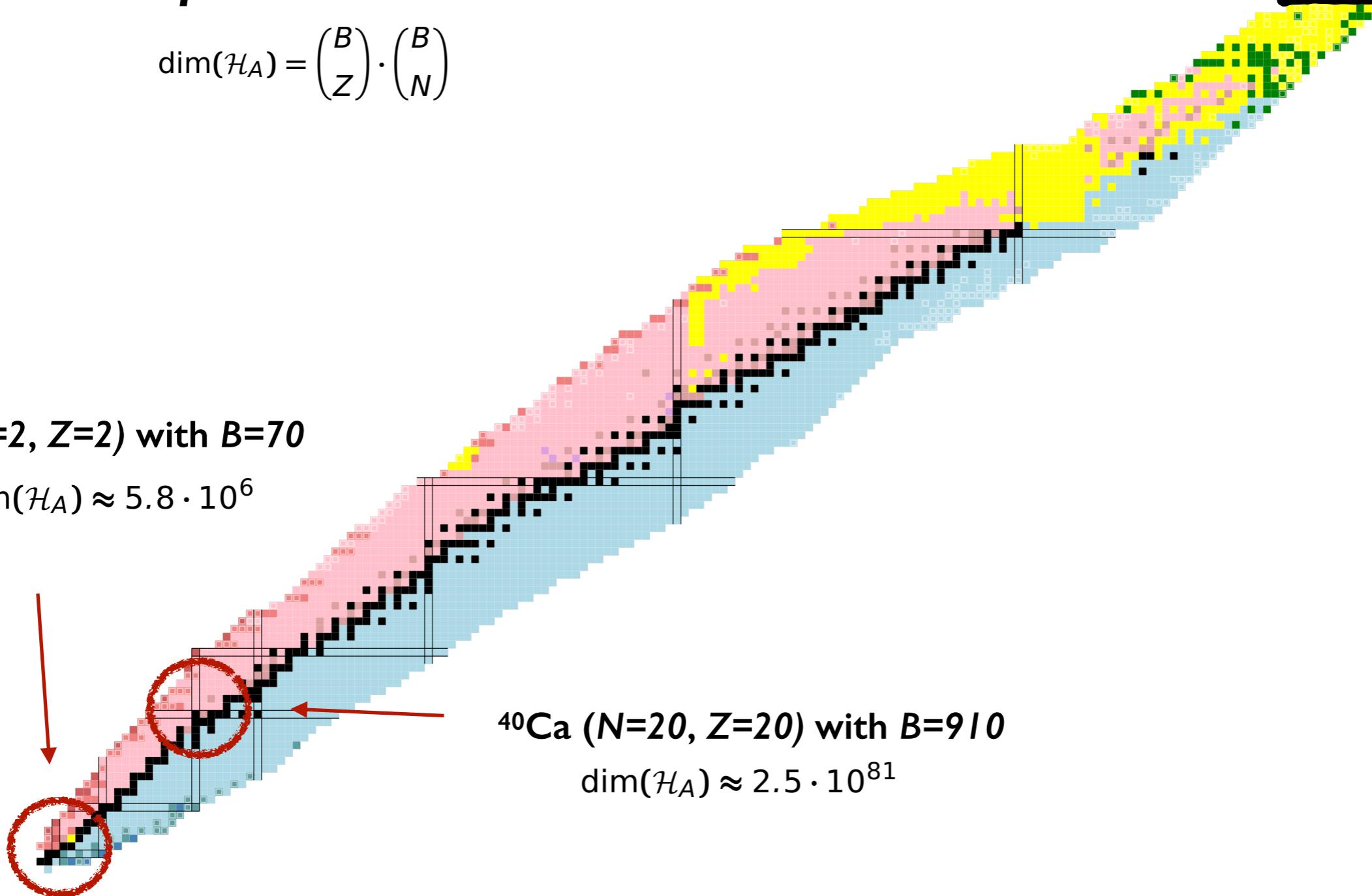
**Setting**  
Z protons  
N neutrons  
B orbits

**'Exponential wall'**

$$\dim(\mathcal{H}_A) = \binom{B}{Z} \cdot \binom{B}{N}$$

${}^4\text{He}$  ( $N=2$ ,  $Z=2$ ) with  $B=70$

$$\dim(\mathcal{H}_A) \approx 5.8 \cdot 10^6$$

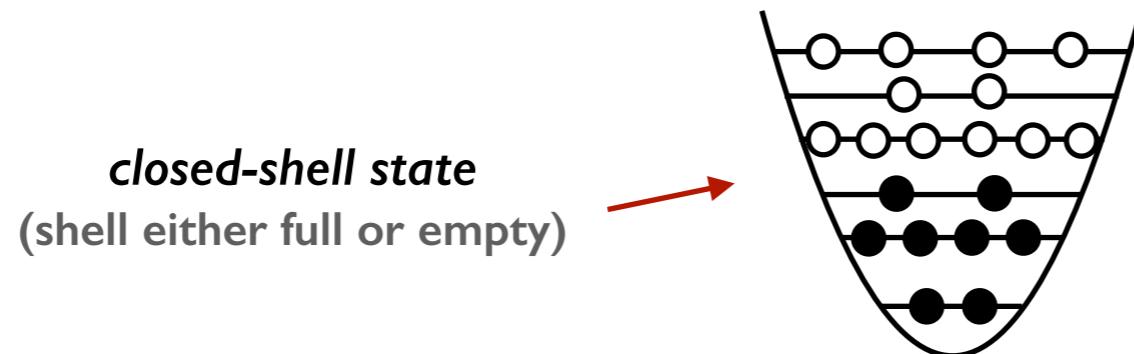


# Towards medium-mass systems

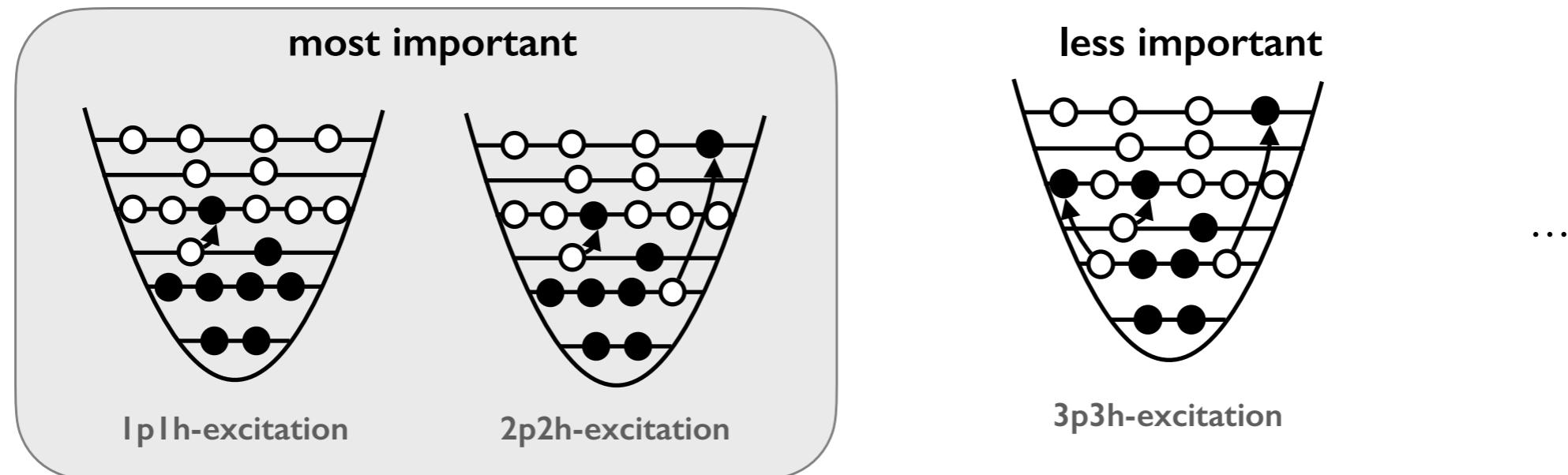
- Crucial observation: the exact wave function is **dominated by very few configurations**

$$|\Psi_{\text{exact}}\rangle = \sum_I c_I |\Phi_I\rangle \quad \text{with} \quad \sum_I c_I^2 = 1$$

- **Reference state:** identify the most important configuration and expand around it



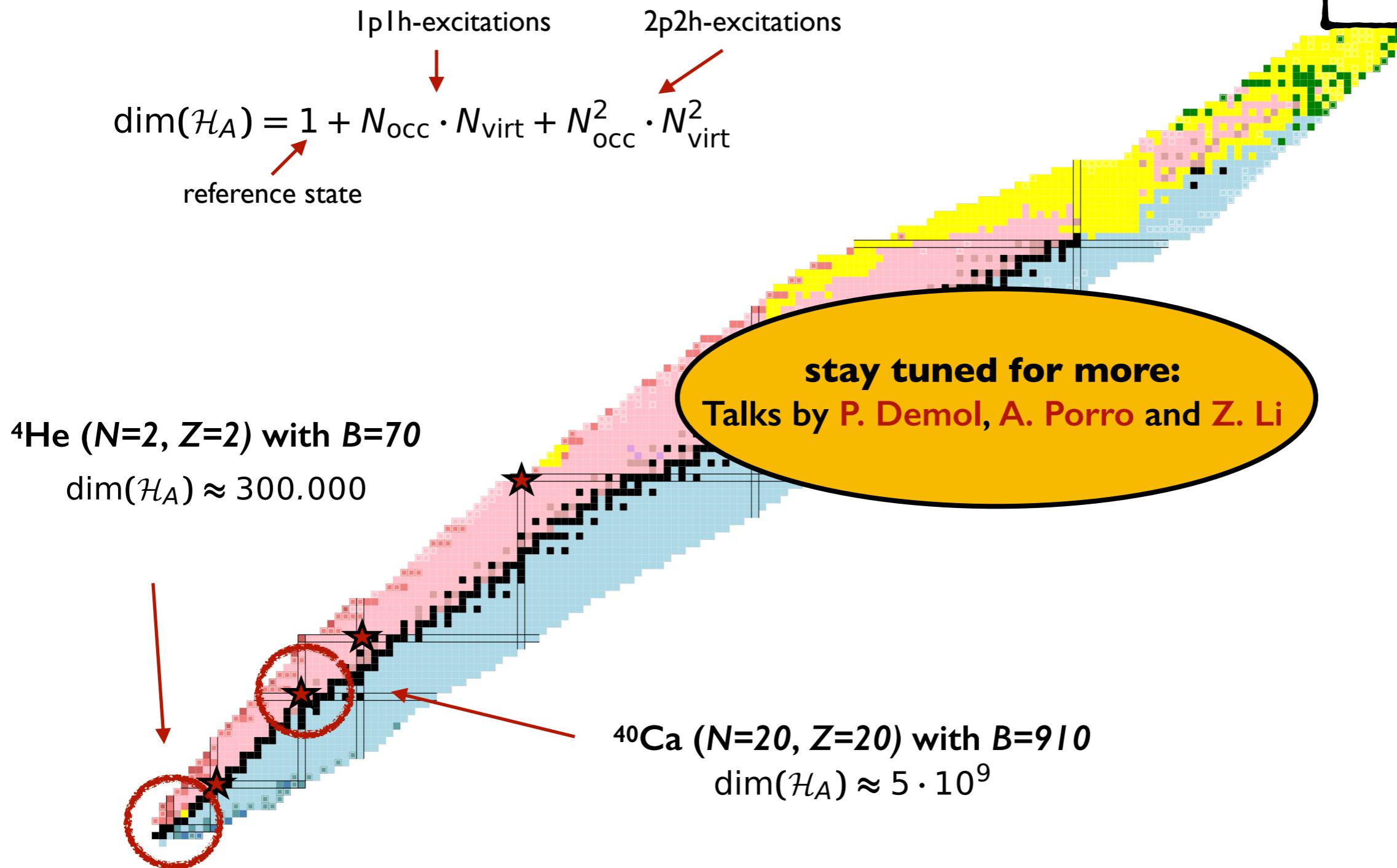
- **Hierarchy of importance of many-body configurations** in terms of excitation level



# Expansion techniques

**Setting**  
Z protons  
N neutrons  
B orbits

polynomial in system size!



# ‘Standard’ perturbation theory

- Divide the full many-body problem into an **unperturbed part** and a **perturbation**

$$H_\lambda = H_0 + \lambda H_1 \quad \text{with} \quad H_0|\Phi\rangle = E^{(0)}|\Phi\rangle$$

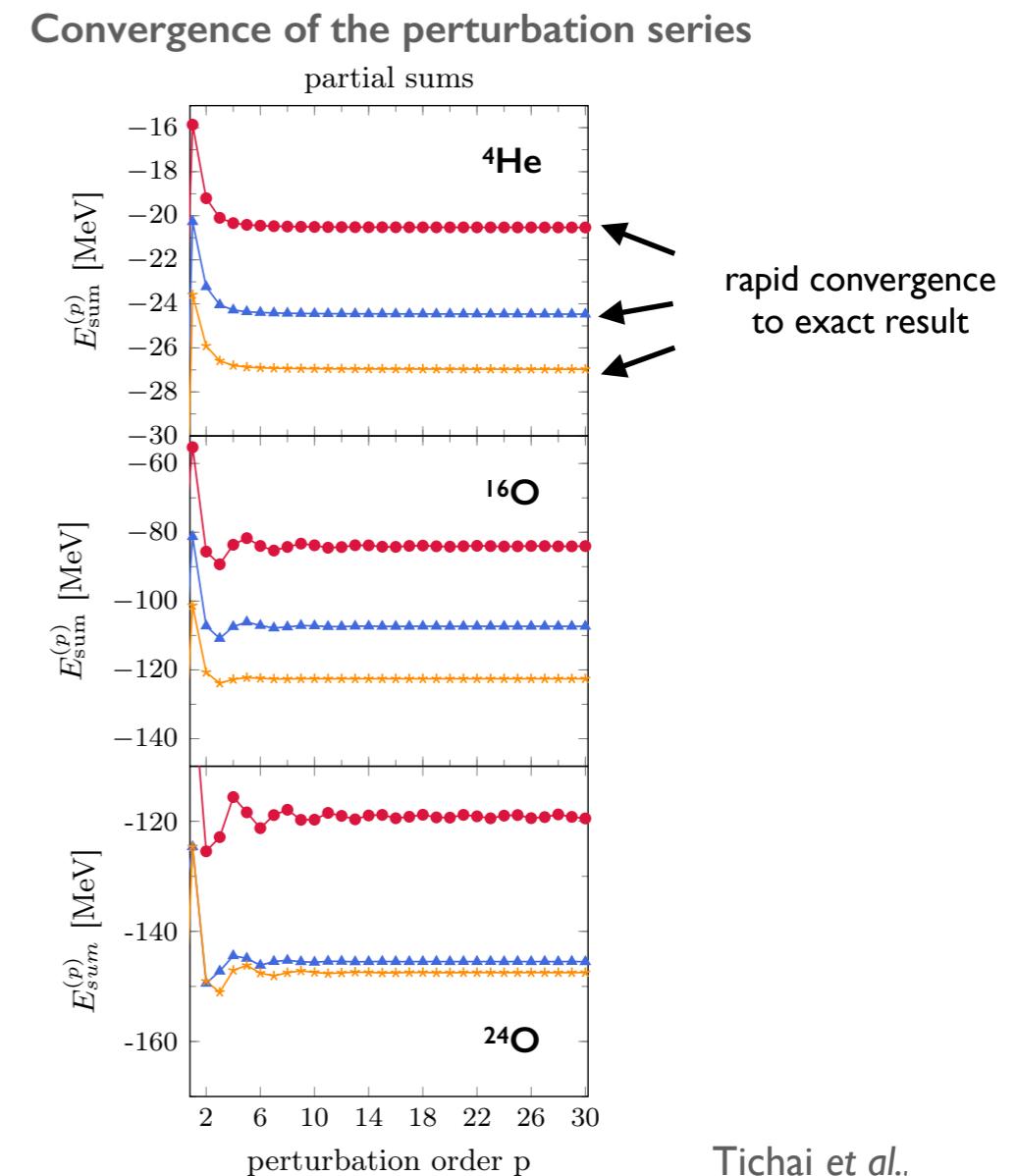
- Perturbative expansion: **power-series ansatz**

$$E_{\text{exact}} = E^{(0)} + E^{(1)} + E^{(2)} + E^{(3)} + \dots$$

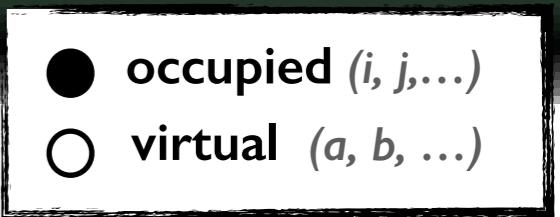
- Evaluation of corrections supported by **diagrammatic techniques** (Feynman diagrams)
- Mean-field reference state (Hartree-Fock) captures bulk part of nuclear observable

**defines the leading order!**

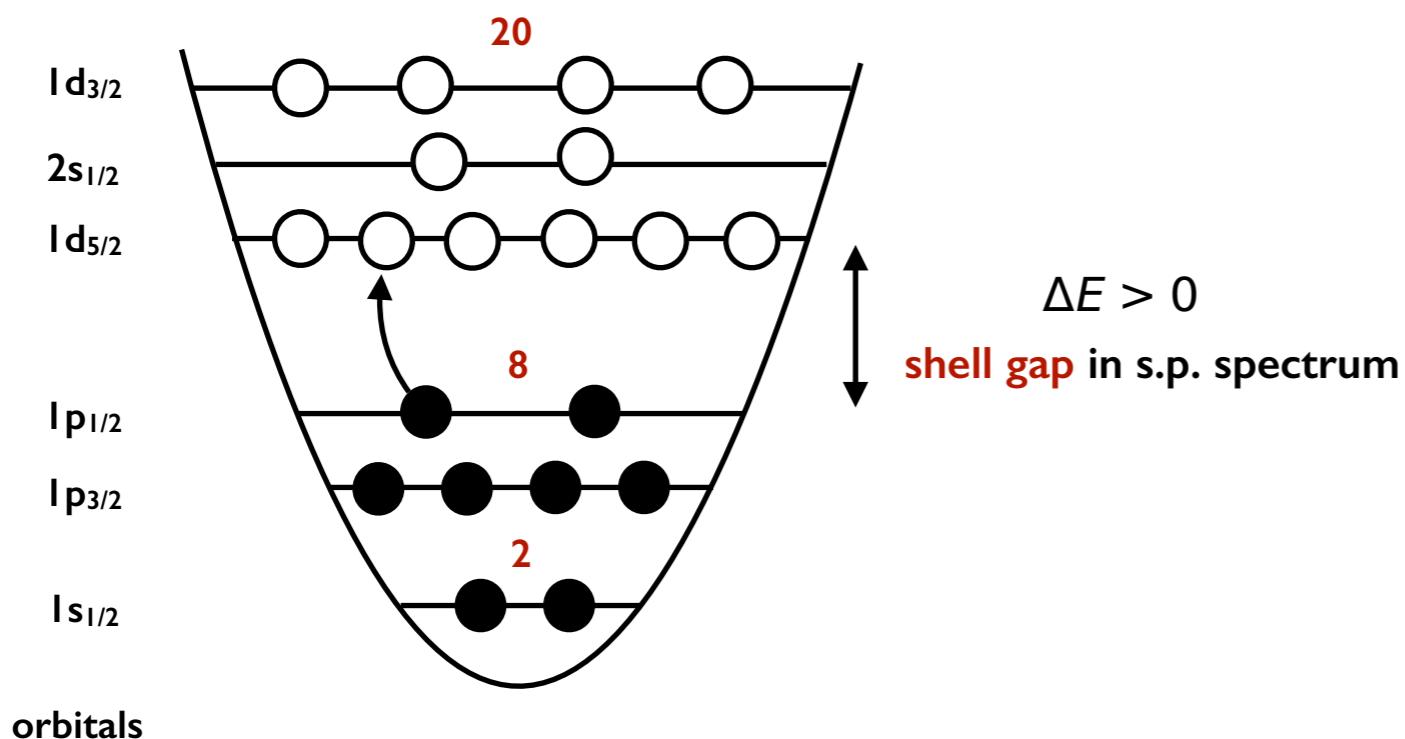
- Rationale: standard perturbation theory is **well under control in closed-shell systems**



# Closed-shell nuclei



$^{16}\text{O}$  neutron states



Non-degenerate with respect  
to particle-hole excitations

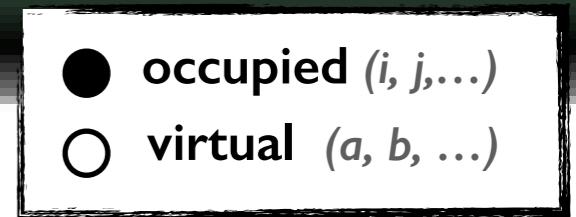


Occupation numbers:  
zero (○) or one (●)

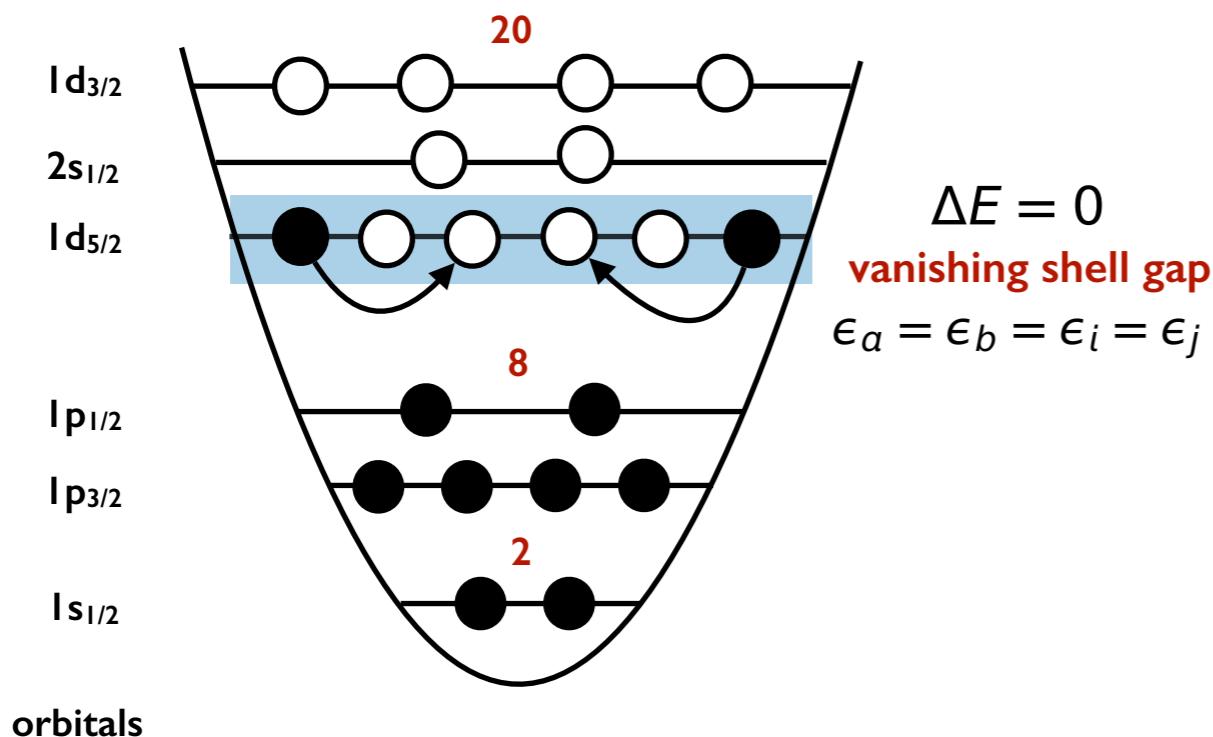
Perturbation theory well-defined

$$E^{(2)} = \frac{1}{4} \sum_{abij} \frac{H_{abij} H_{ijab}}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$$

# Open-shell nuclei



$^{18}\text{O}$  neutron states



Appearance of fractional occupation numbers in valence shell ( $1d_{5/2}$ )

Degenerate with respect to particle-hole excitations

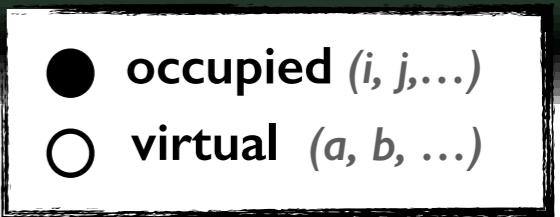


Perturbation theory degenerate

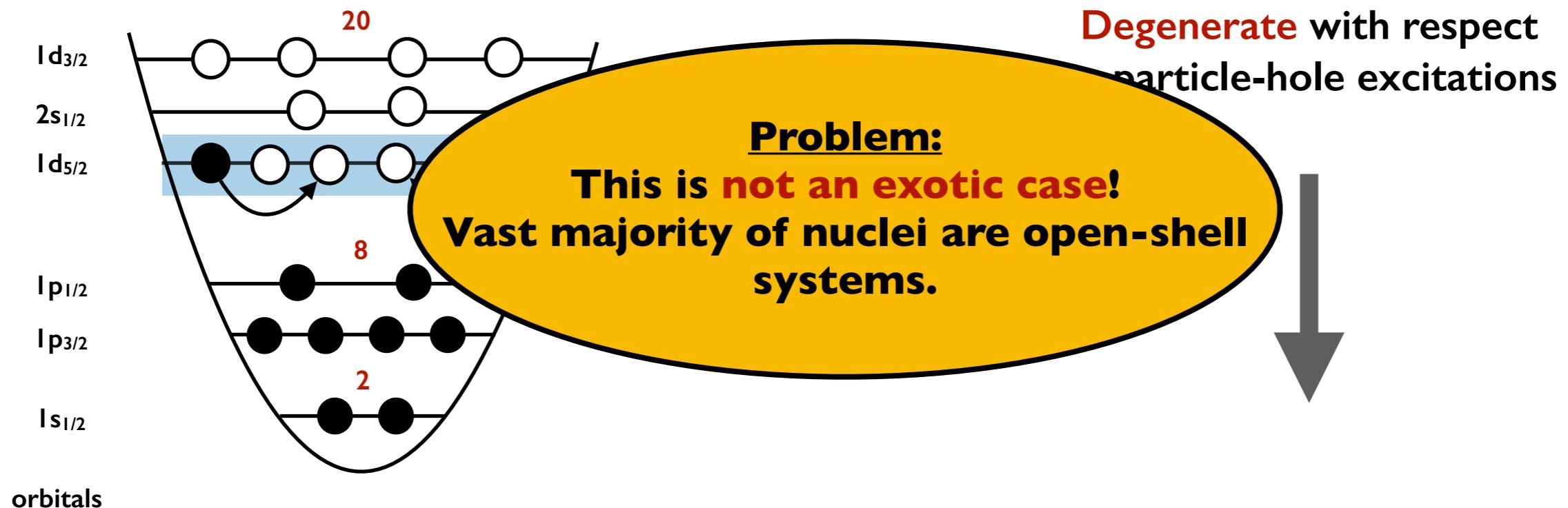
$$E^{(2)} = \frac{1}{4} \sum_{abij} \frac{H_{abij} H_{ijab}}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$$

Division by zero!

# Open-shell nuclei



$^{18}\text{O}$  neutron states



Appearance of fractional occupation numbers in valence shell ( $1d_{5/2}$ )

Perturbation theory degenerate

$$E^{(2)} = \frac{1}{4} \sum_{abij} \frac{H_{abij} H_{ijab}}{\epsilon_i + \epsilon_j - \epsilon_a - \epsilon_b}$$

Division by zero!

# Bogoliubov many-body perturbation theory

- **Symmetry breaking:** choose reference state with lower symmetry than Hamiltonian

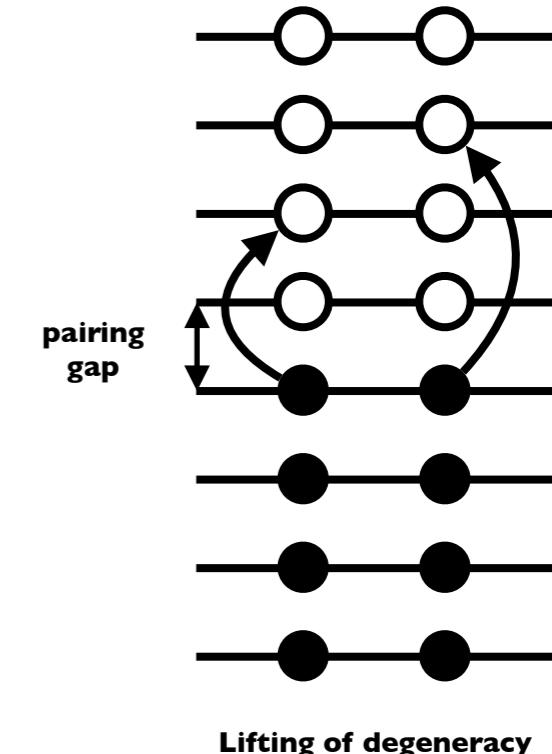
$$\hat{A}|\Phi\rangle \neq A_0|\Phi\rangle \quad \text{but} \quad \langle\Phi|\hat{A}|\Phi\rangle = A_0$$

- **Introduction of Bogoliubov quasi-particles**

$$\beta_k^\dagger = \sum_p (U_{pk} c_p^\dagger + V_{pk} c_p) \quad \beta_k = \sum_p (U_{pk}^* c_p + V_{pk}^* c_p^\dagger)$$

- **Pairing correlations included in reference state**

Hartree-Fock-Bogoliubov solution  $\longrightarrow |\Phi\rangle = \mathcal{C} \prod_k \beta_k |0\rangle$



- Comparison of formalism: why does it help in practice?

## ‘Standard’ MBPT

$$E^{(2)} = -\frac{1}{4} \sum_{abij} \frac{H_{abij} H_{ijab}}{\epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j}$$

All  $E_k > 0$   
(no degeneracy possible!)

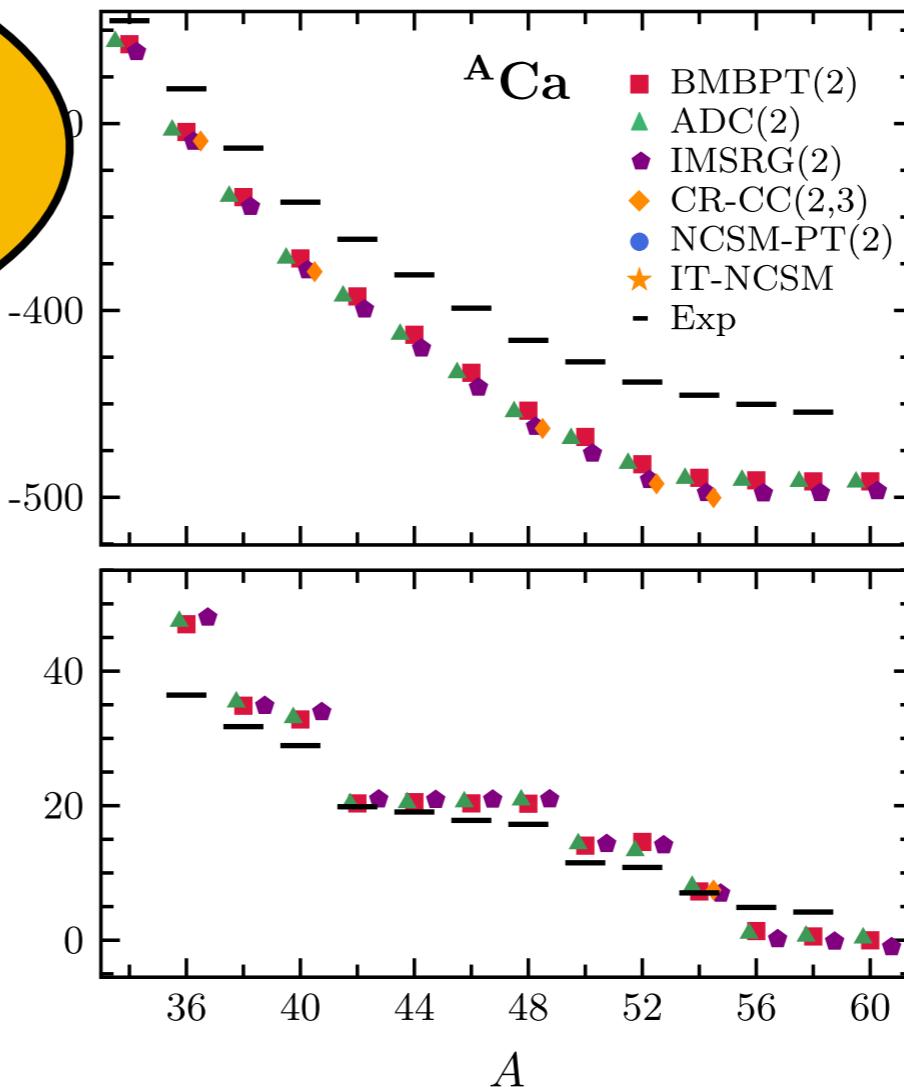
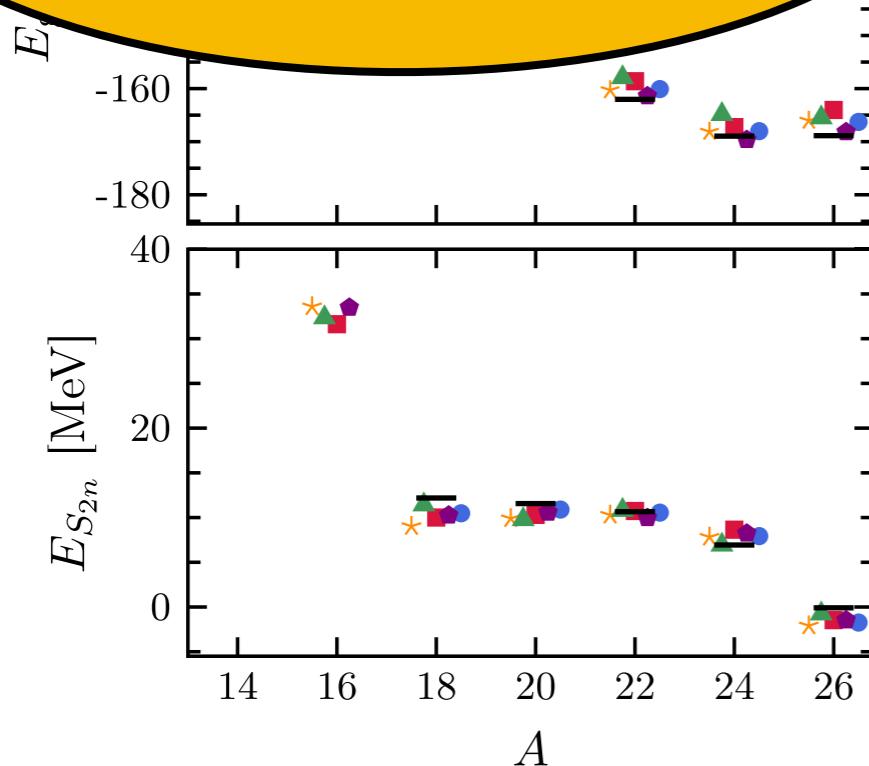
## Bogoliubov MBPT

$$E^{(2)} = -\frac{1}{24} \sum_{k_1 k_2 k_3 k_4} \frac{\Omega_{k_1 k_2 k_3 k_4}^{40} \Omega_{k_1 k_2 k_3 k_4}^{04}}{E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}}$$

# Medium-mass results

Runtime (in CPU hours)	
NCSM:	20.000
MCPT:	2.000
IMSRG:	1.500
ADC:	400
<b>BMBPT:</b>	< 1

**Be careful:**  
**Deviation from experiment**  
 $\neq$   
**Bad many-body solution**



Tichai et al.,  
PLB **786** 195 (2018)

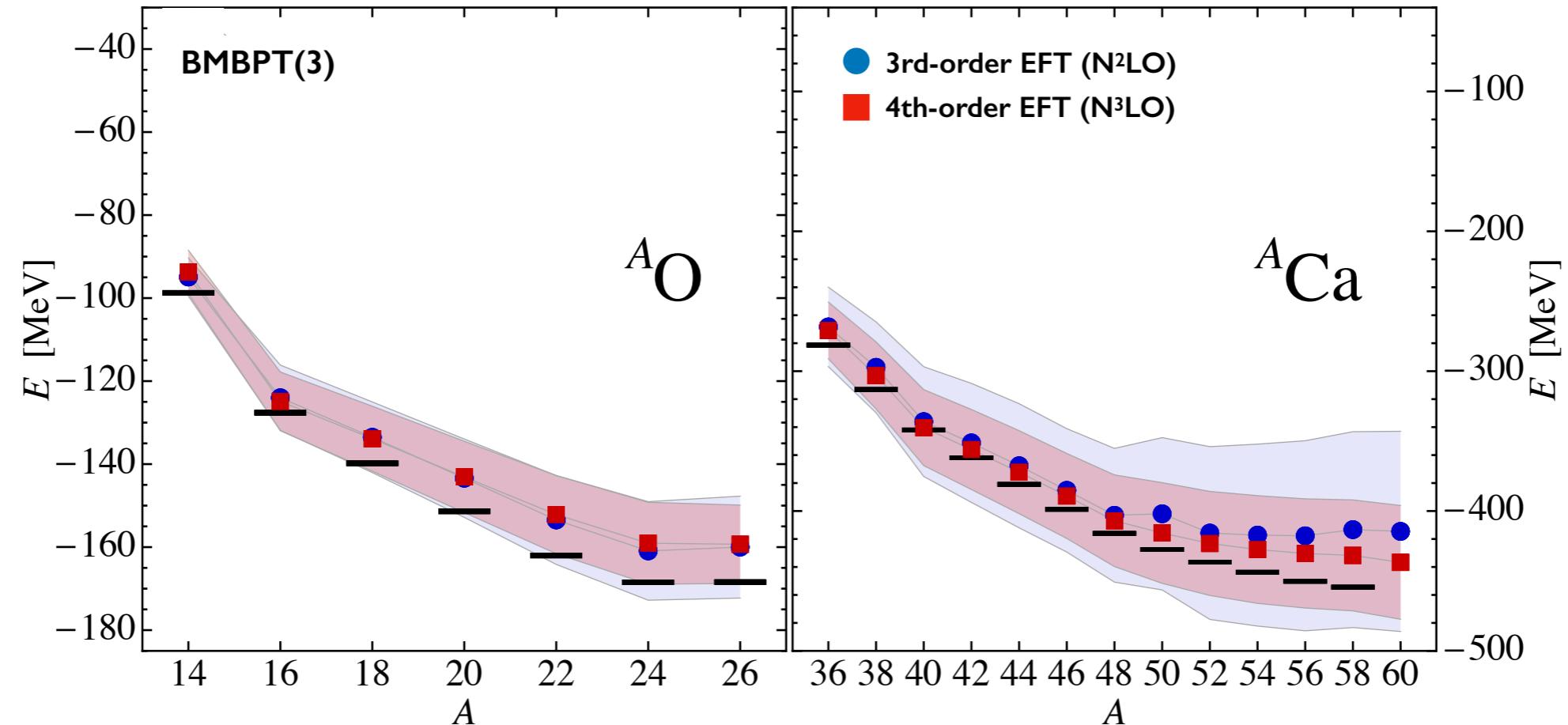
- Excellent agreement of all methods with ‘exact’ results (IT-NCSM)
- Different many-body schemes yield consistent description of open-shell nuclei
- BMBPT is optimal for cheap survey calculations of next-generation chiral Hamiltonians

# New Hamiltonians!

Interaction

Hüther et al.,  
PLB 808, 135651 (2020)

Tichai, Roth, Duguet,  
Front. Phys. 8:164 (2020)

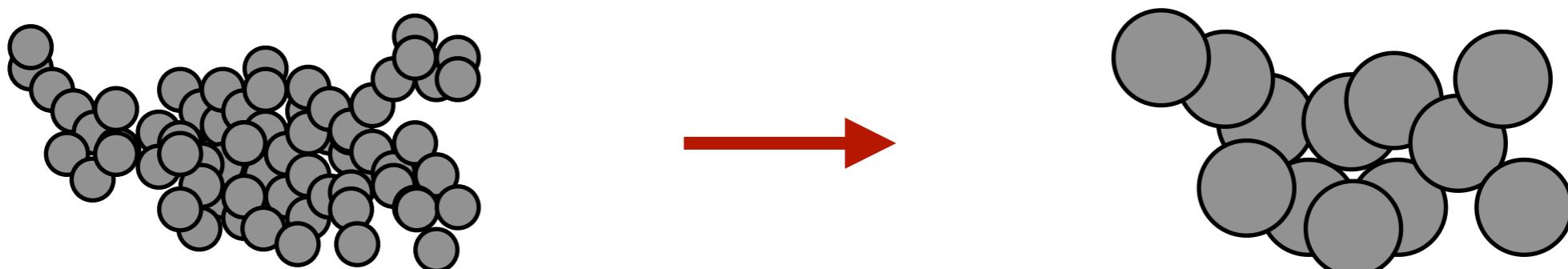


- Inconsistency with experimental data cured with more modern Hamiltonian  
**we used the same many-body formalism!**

# Part III

## Emerging frontiers

**A (personal) perspective on computational challenges**



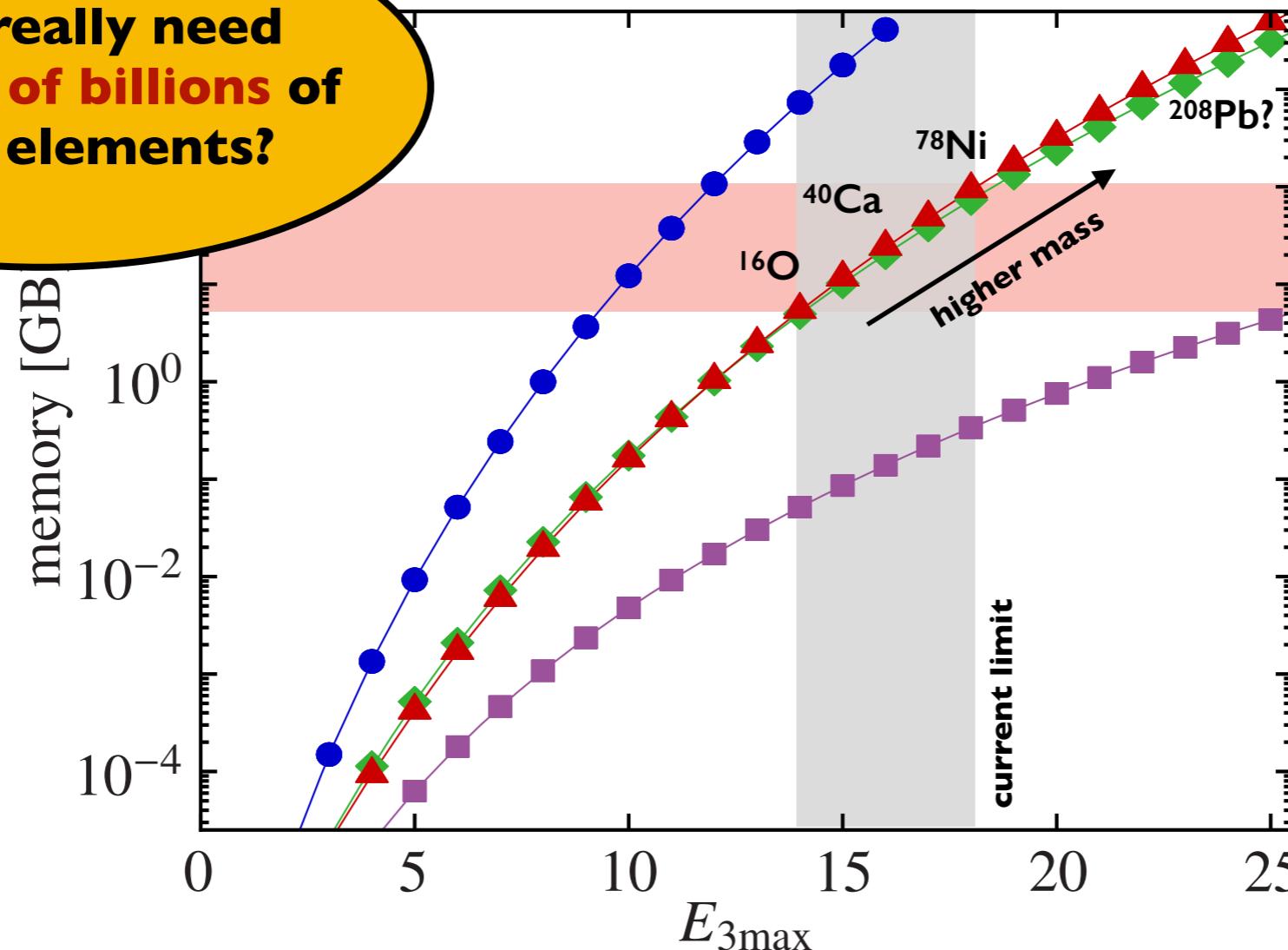
# Three-body matrix elements

**Do we really need  
hundreds of billions of  
matrix elements?**

Roth et al., PRC **90**, 024325 (2014)

**Storage schemes**

- M-scheme
- ▲ J-scheme
- ▼ JT-scheme
- Jacobi basis



← typical HPC limit

see also: Miyagi et al.,  
arXiv:2104.04688 (2021)

- Computational limitations from storage requirements of **three-body operators**

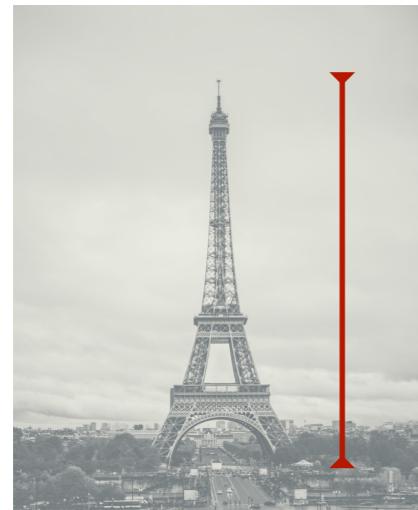
$$\frac{1}{36} \sum_{pqrsstu} V_{pqrsstu}^{3N} c_p^\dagger c_q^\dagger c_r^\dagger c_u c_t c_s$$

# Concepts of data compression

**What is the size of the Eiffel tower?**

**Original picture**

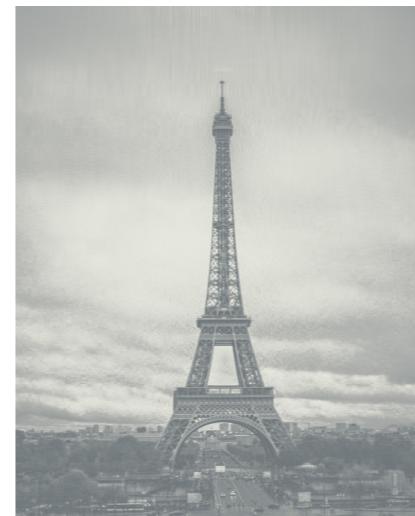
(matrix with entries encoding grey value)



data compression



30 %



9 %



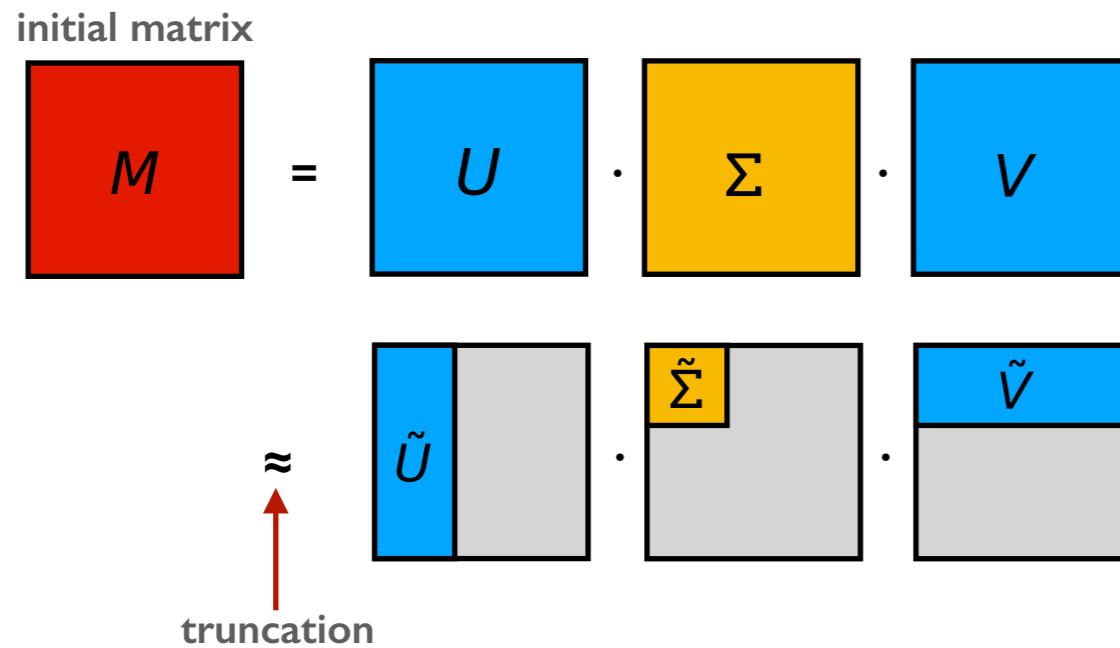
3 %



lack of high-resolution details  
induce small **controllable** error on final quantity

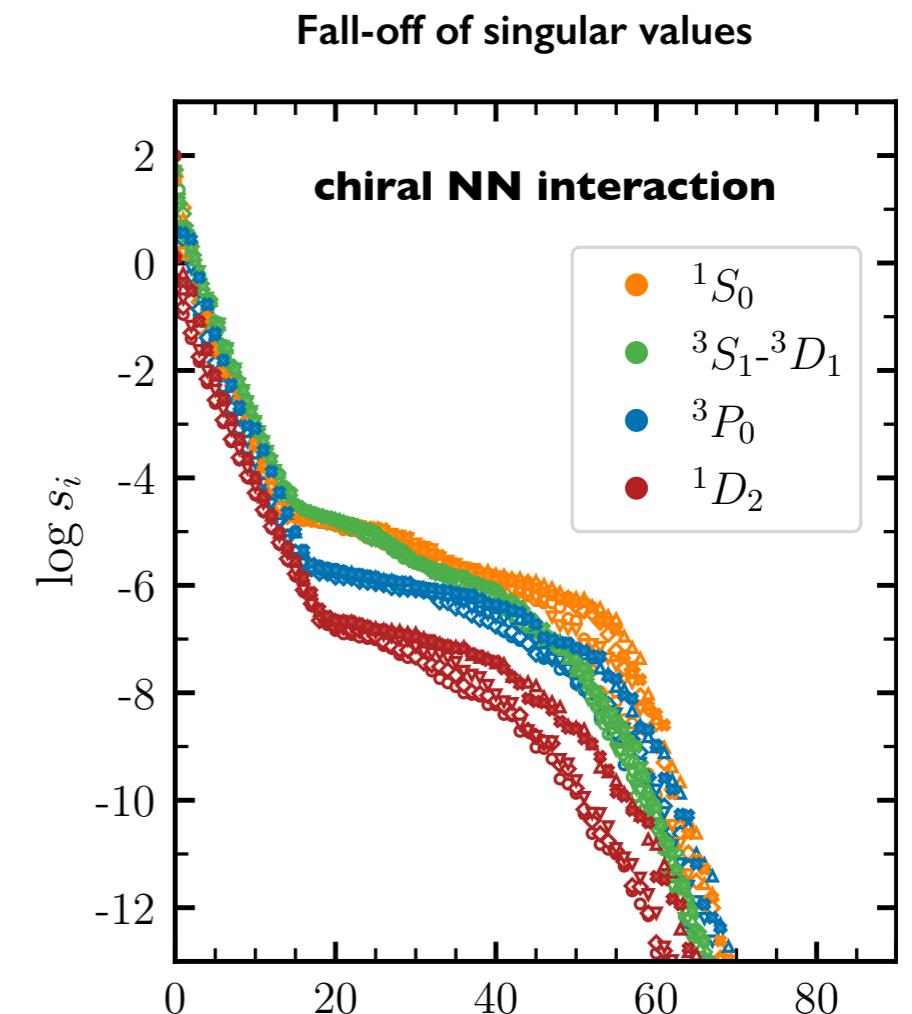
# Matrix decompositions

- Low-rank interaction from **singular-value decomposition (SVD)**



- Keep only **few components** in decomposition
- Exact results are recovered for **infinite rank**
- Rapid suppression of singular values observed

**... but what is the  
impact on observables?**

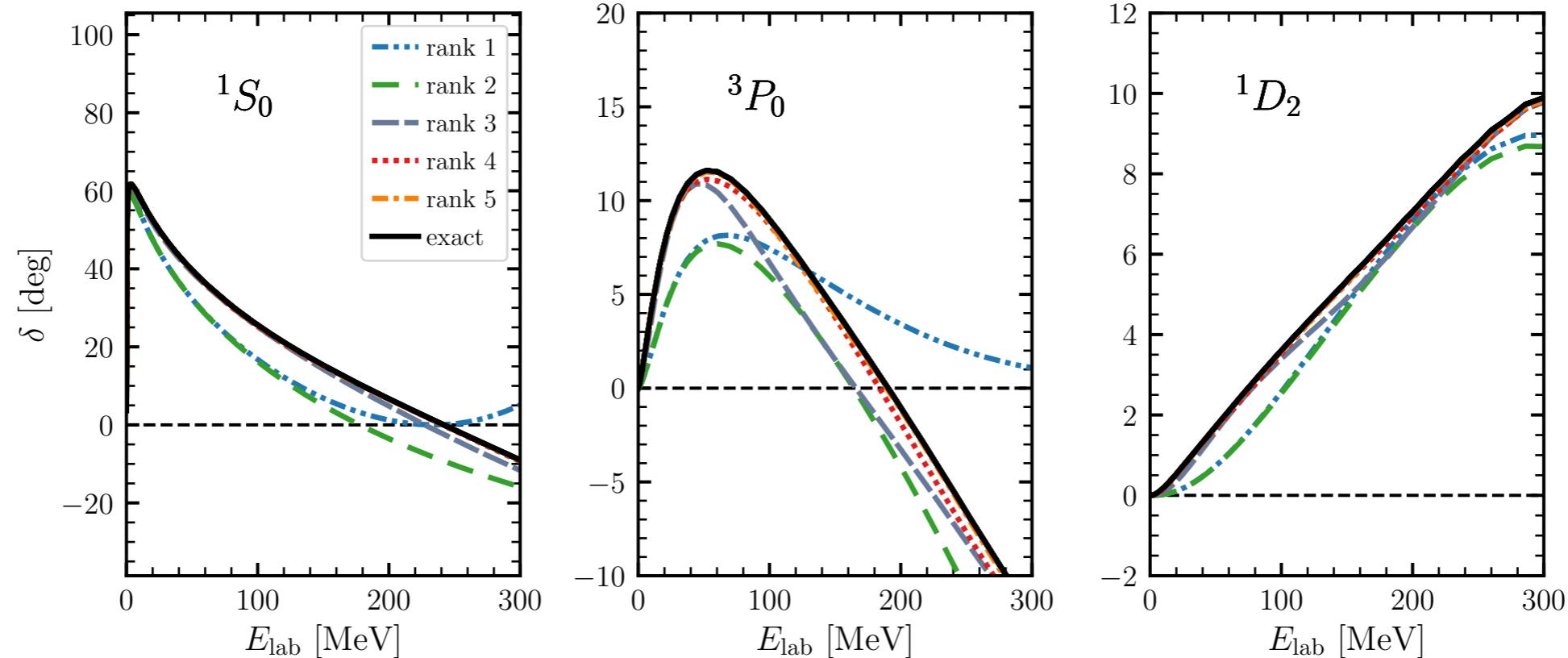


Tichai et al.  
PLB 821, 136623 (2021)

# Two-nucleon phase shifts

Full matrix dimension  
 $N = 100$

Low-energy phase shifts for different low-rank approximations (rank 1-5)



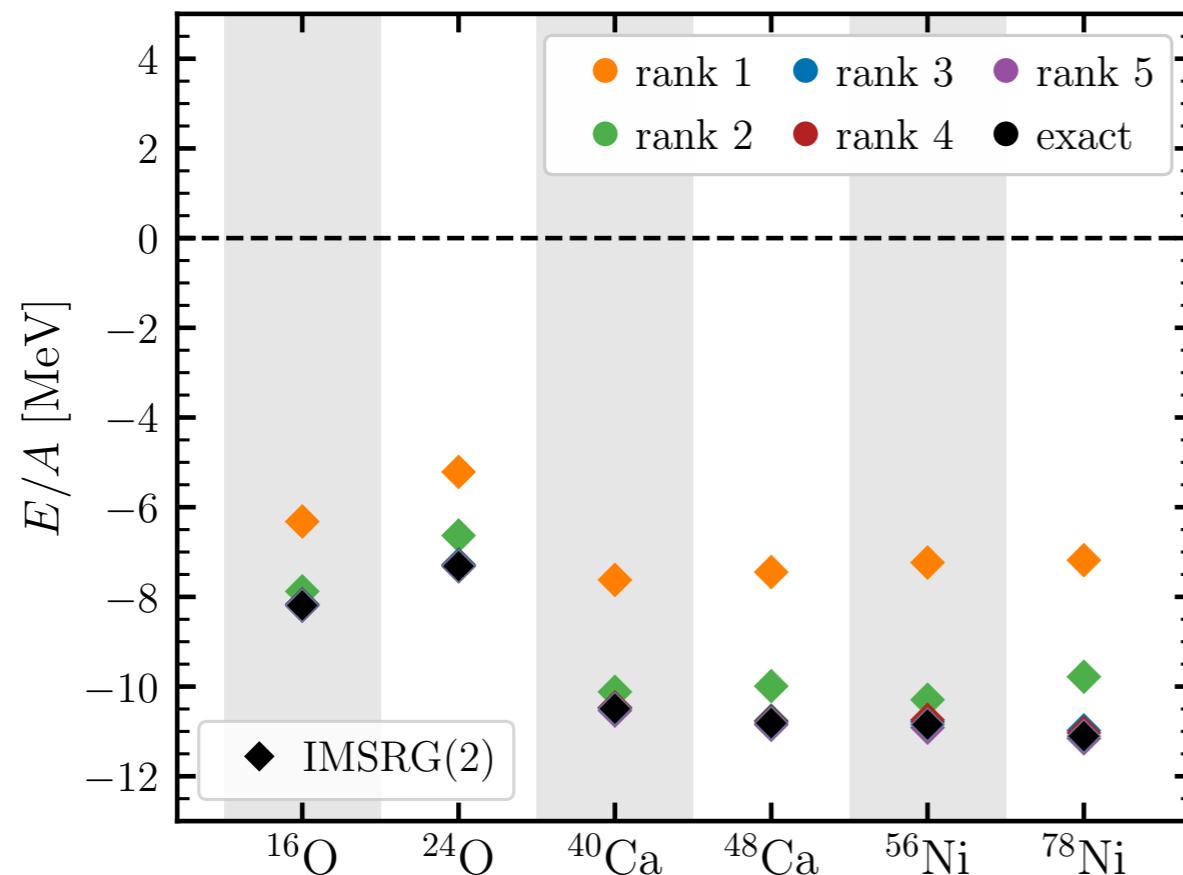
Tichai et al.

PLB 821, 136623 (2021)

- Low-energy phase shifts from Lippmann-Schwinger equation ( $T$  matrix)
- Systematic improvement when including more components in the interactions
- Rank-5 approximation yields (virtually) perfect agreement with exact results

# Many-body applications

Low-rank approximations (rank 1-5) vs. full potential (rank 100)

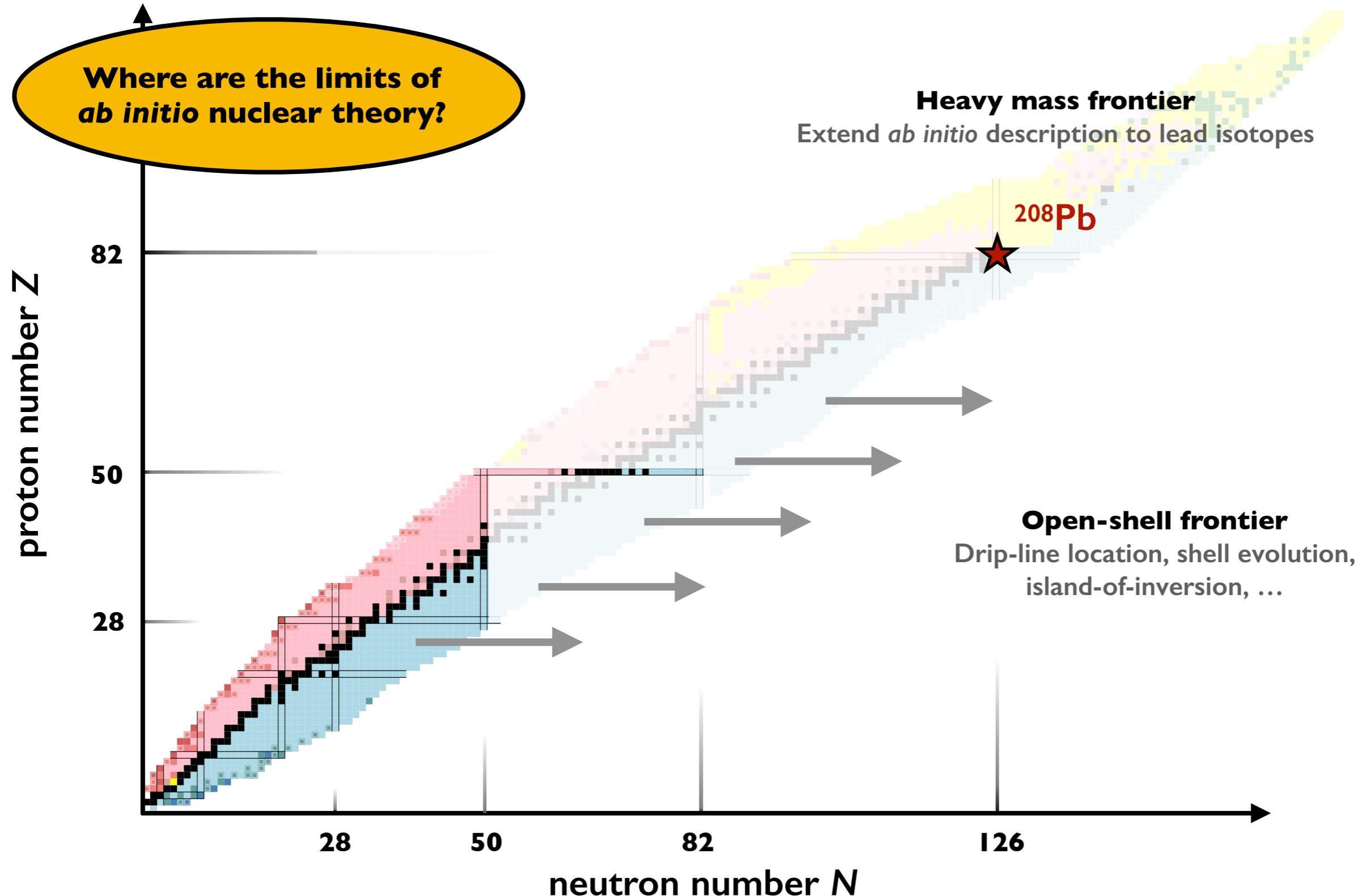


Tichai et al.  
PLB 821, 136623 (2021)

- ***Ab initio workhorse: non-perturbative IMSRG scheme***
- **Systematic convergence of energy per particle with SVD rank**
- **Sub-percent accuracy at SVD-rank 5 at IMSRG(2) truncation level**
- **Quality of low-rank SVD independent of mass number**

**Low-rank SVD**  
Over 99 % accuracy  
with only 5% of information

# Many-body frontiers



# Summary & Outlook

## ***Ab initio nuclear theory***

- ... provides **systematic control** over induced error from approximations
  - ... enables rigorous quantification over uncertainties giving '**theory error bars**'
  - ... therefore has **predictive power** for (yet) unmeasured quantities/systems
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## **Future challenges**

- ... extend description to more **exotic nuclei** and **heavier mass number**
- ... development of statistical toolbox to **quantify many-body uncertainties**
- ... understand and exploit the **true complexity** of the quantum many-body problem

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