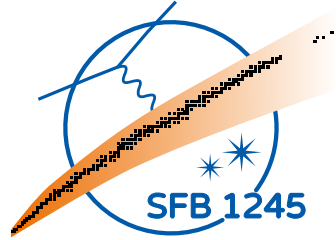




LOEWE

Exzellente Forschung für
Hessens Zukunft



TECHNISCHE
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AB INITIO TECHNIQUES IN NUCLEAR THEORY

Lotta Jokiniemi (she/her)

Institut für Kernphysik, Theoriezentrum, TU Darmstadt

École Joliot Curie – Saint Pierre d'Oléron, France, 2026

OUTLINE FOR THE LECTURES

Lecture 1

Introduction to ab initio nuclear theory

Lecture 2

From nuclear forces to nuclear properties

Lecture 3

From weak interactions to nuclear observables

Lecture 4

Nuclear probes of physics beyond the standard model

LECTURE 1

- **Introduction**

Nuclear many-body problem. What is ab initio in nuclear physics?

- **Short reminder of quantum many-body physics**

Single-particle bases. Slater determinants. Second quantization.

- **Nuclear many-body Hamiltonian**

Nuclear force. Chiral effective field theory.

INTRODUCTION

CHART OF NUCLIDES



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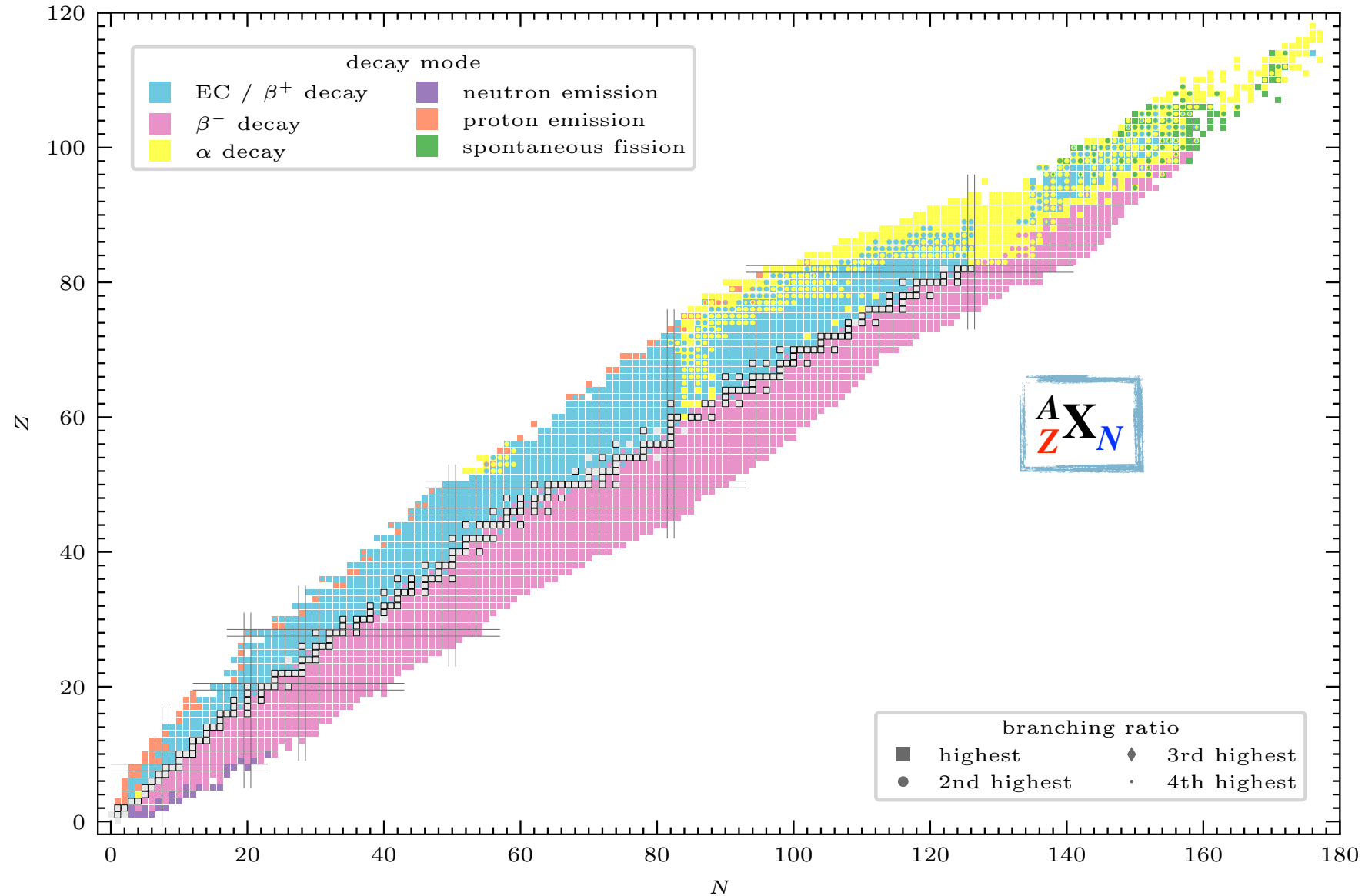


Figure courtesy of Catharina Brase

CHART OF NUCLIDES

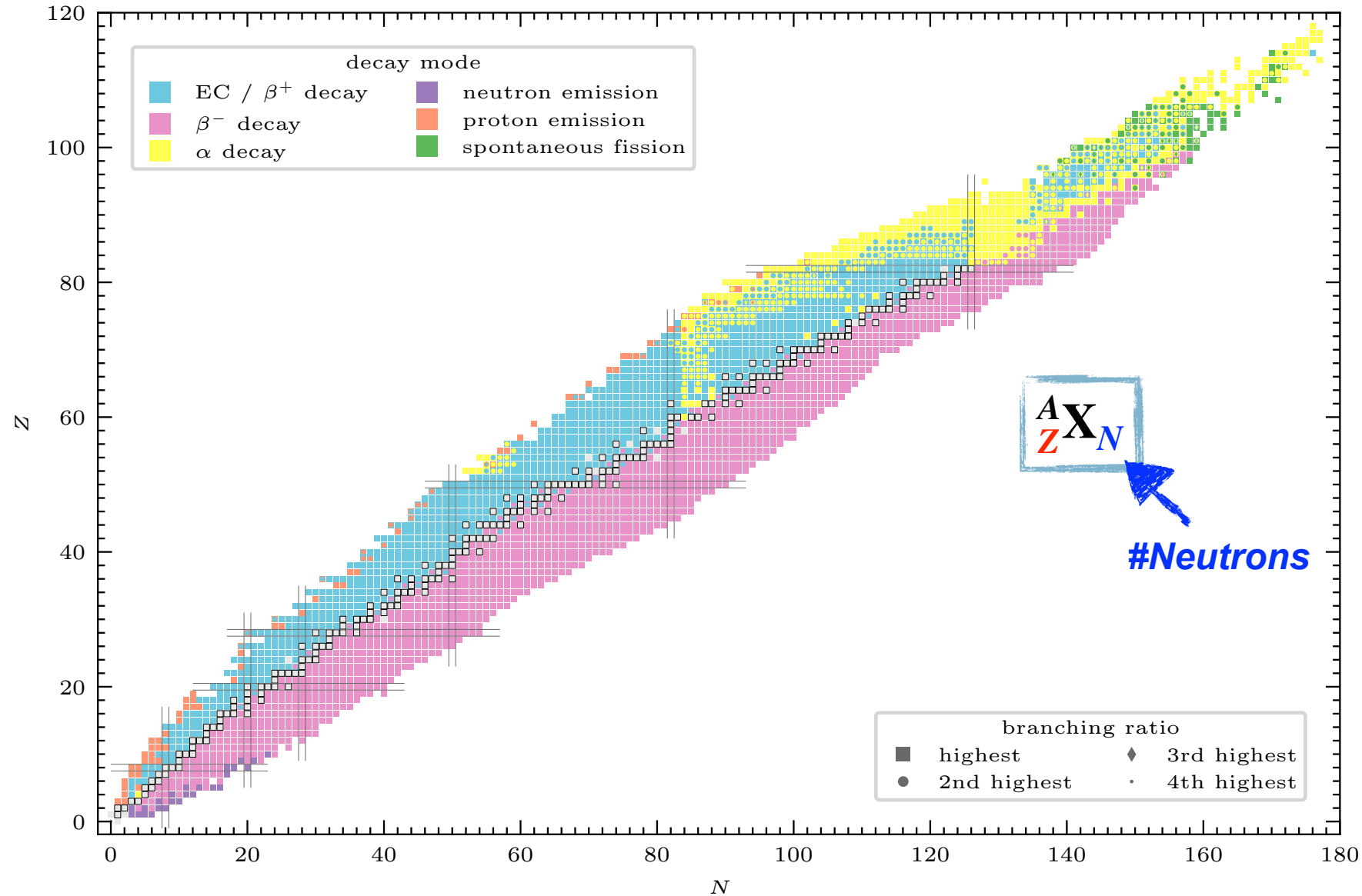


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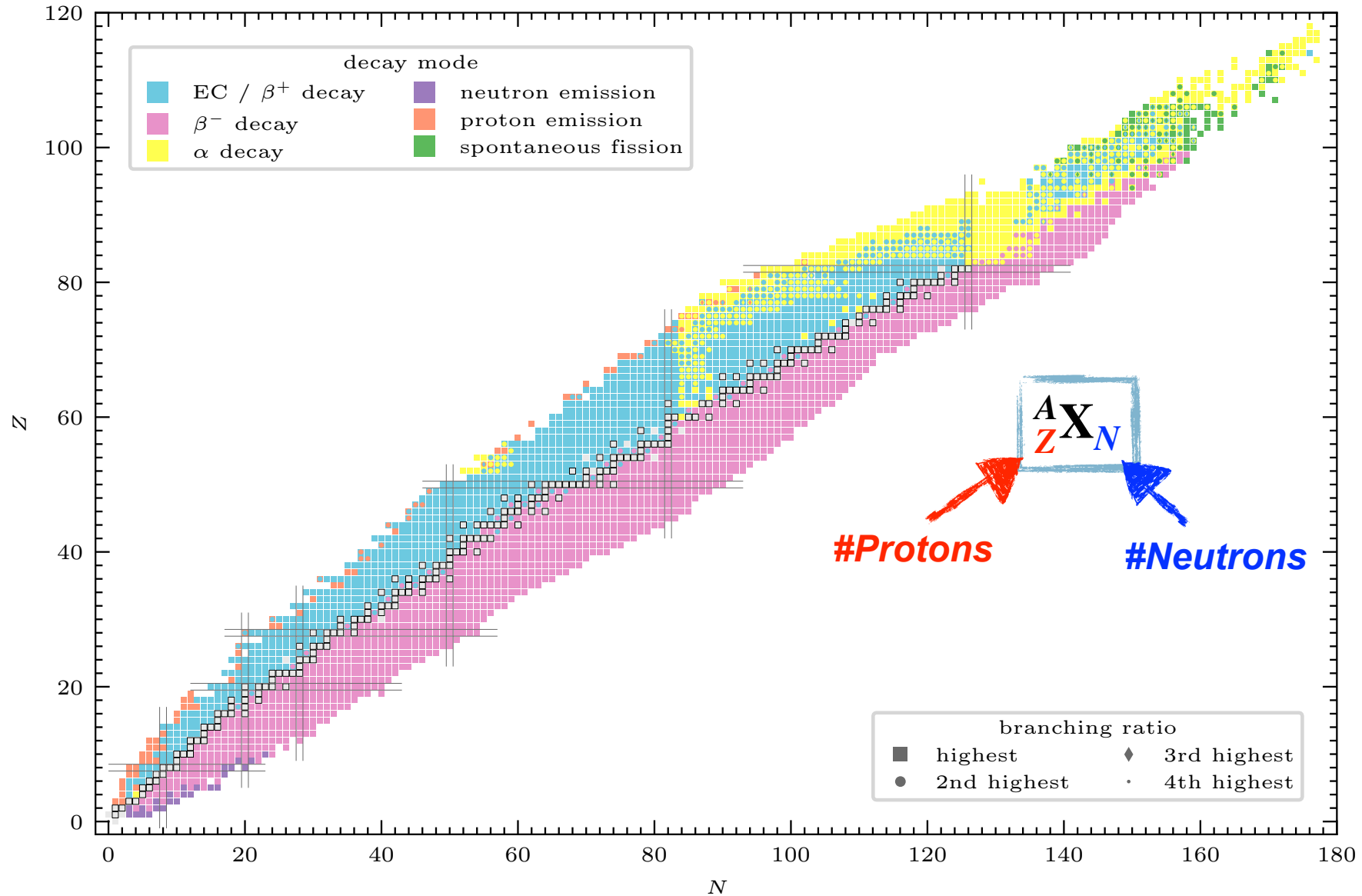


Figure courtesy of Catharina Brase

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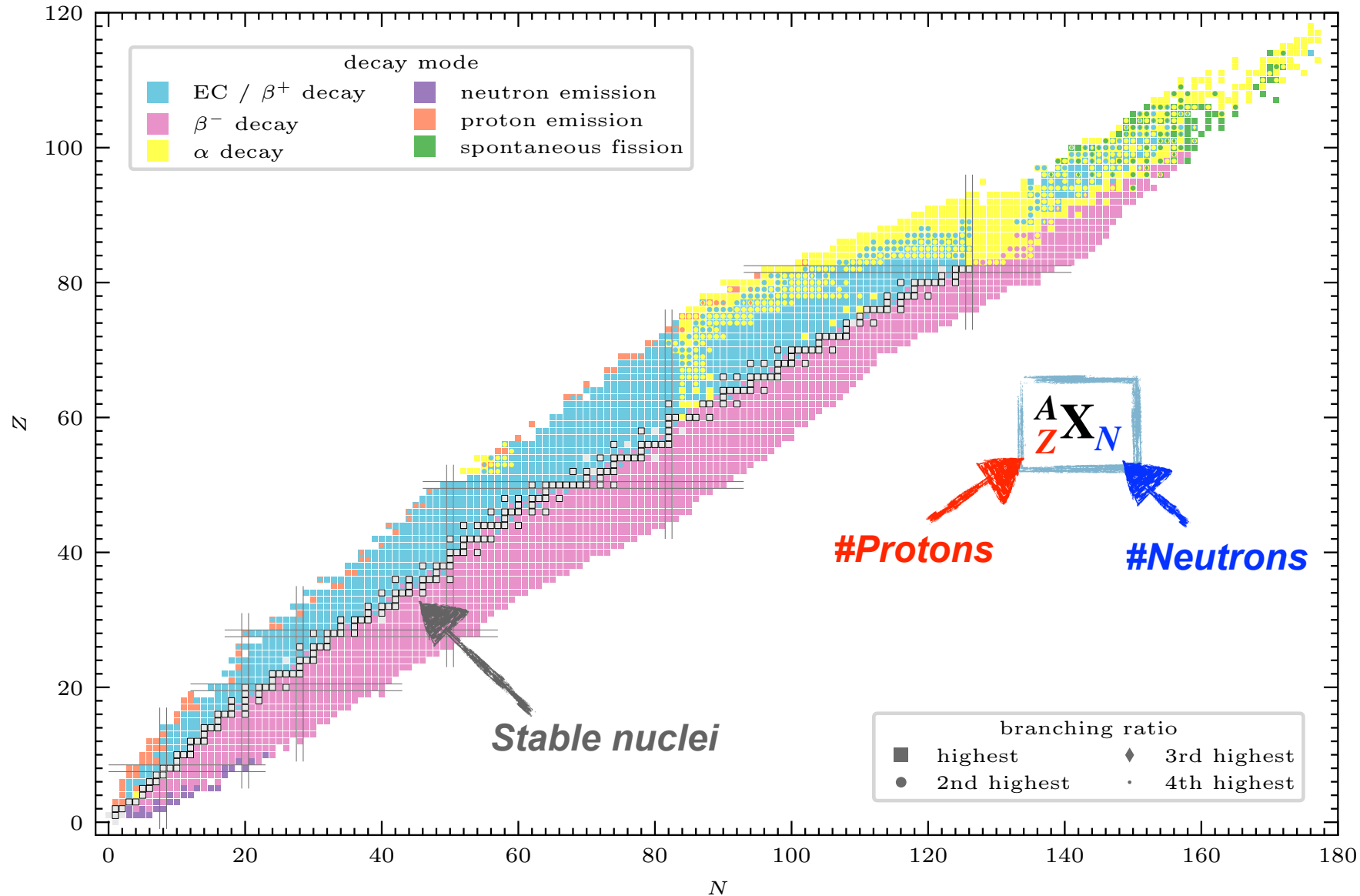


Figure courtesy of Catharina Brase

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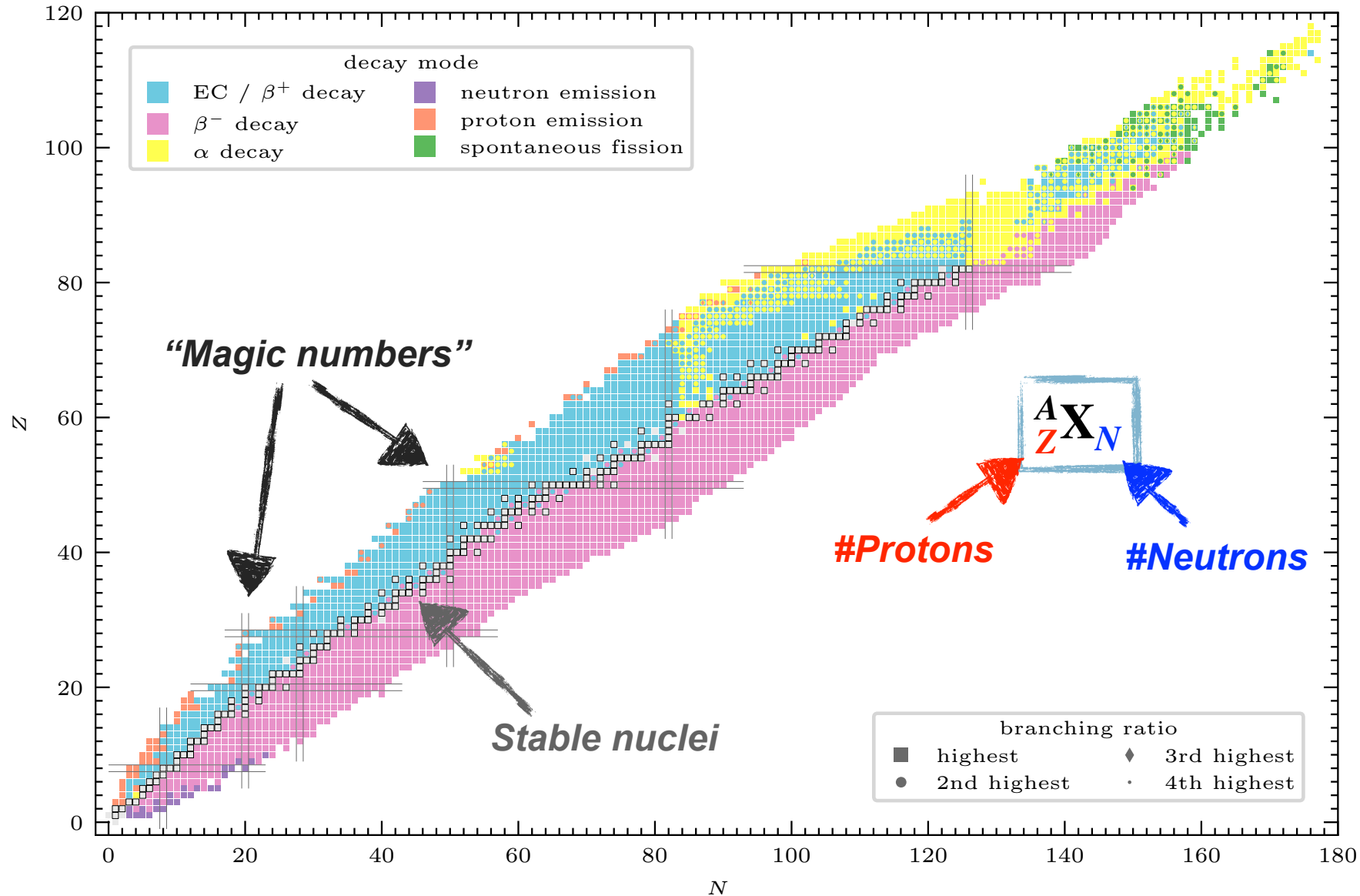


Figure courtesy of Catharina Brase

CHART OF NUCLIDES



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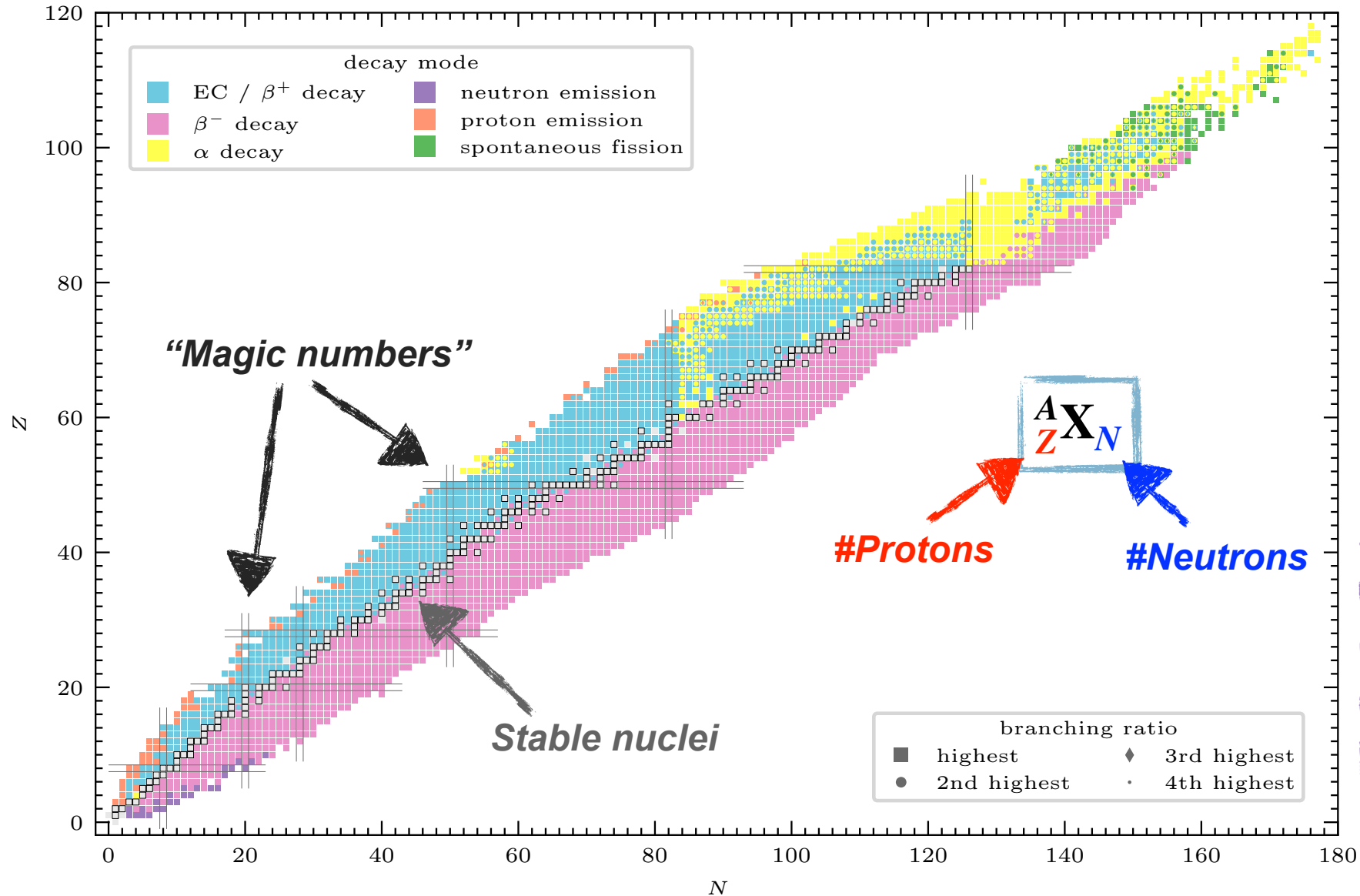
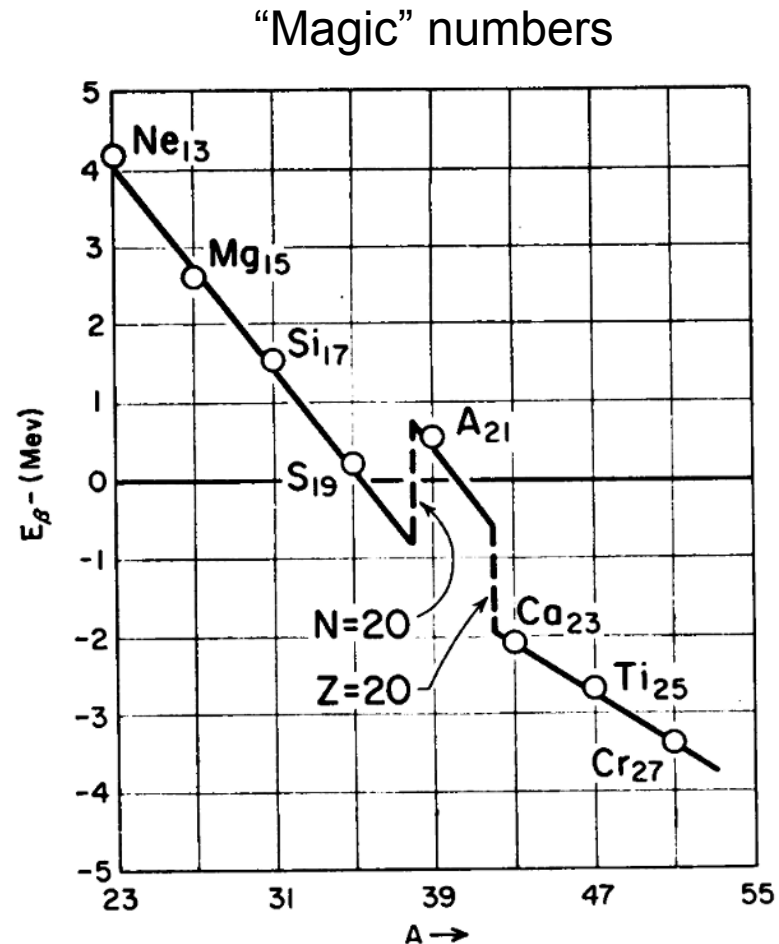
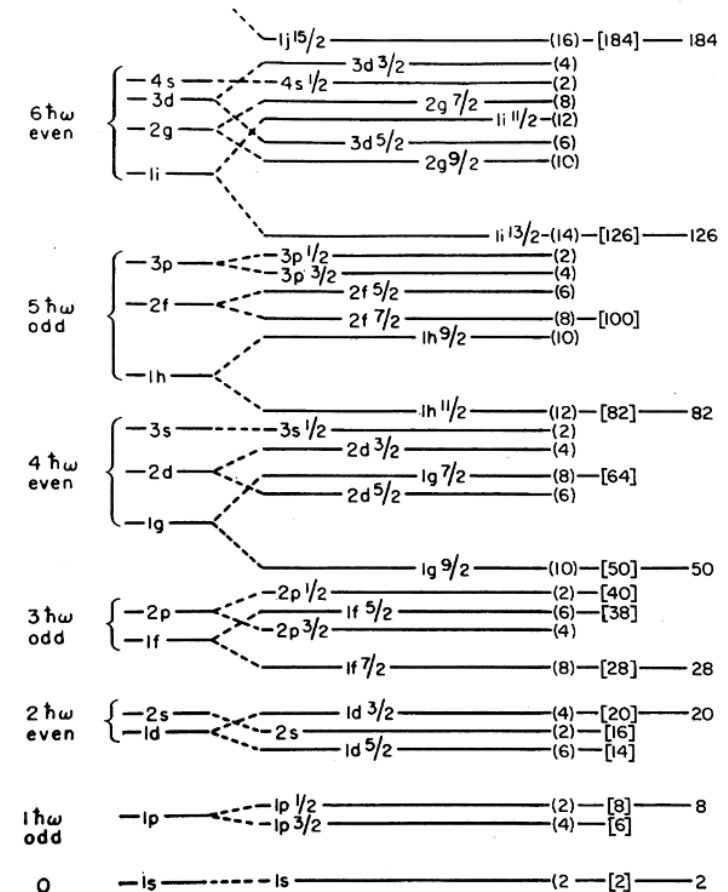


Figure courtesy of Catharina Brase

PHENOMENOLOGICAL METHODS BASED ON OBSERVATIONS



Nuclear shell model

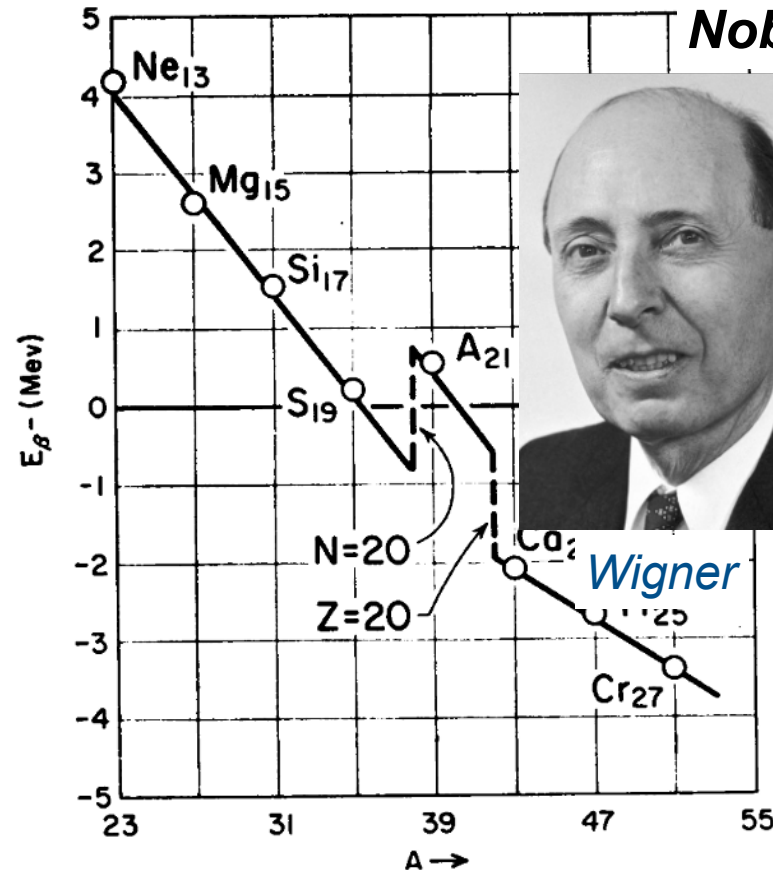


M. Göppert-Mayer, Science 145, 999 (1964)

PHENOMENOLOGICAL METHODS BASED ON OBSERVATIONS



“Magic” numbers



Nobel Prize in Physics 1963



Wigner

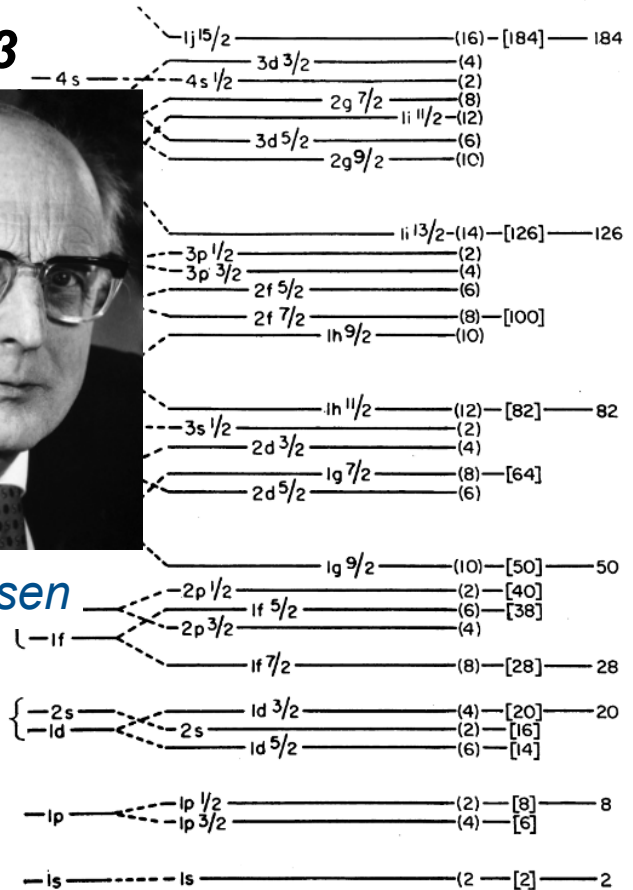


Göppert-Mayer



Jensen

Nuclear shell model



M. Göppert-Mayer, *Science* 145, 999 (1964)

PHENOMENOLOGICAL METHODS BASED ON OBSERVATIONS

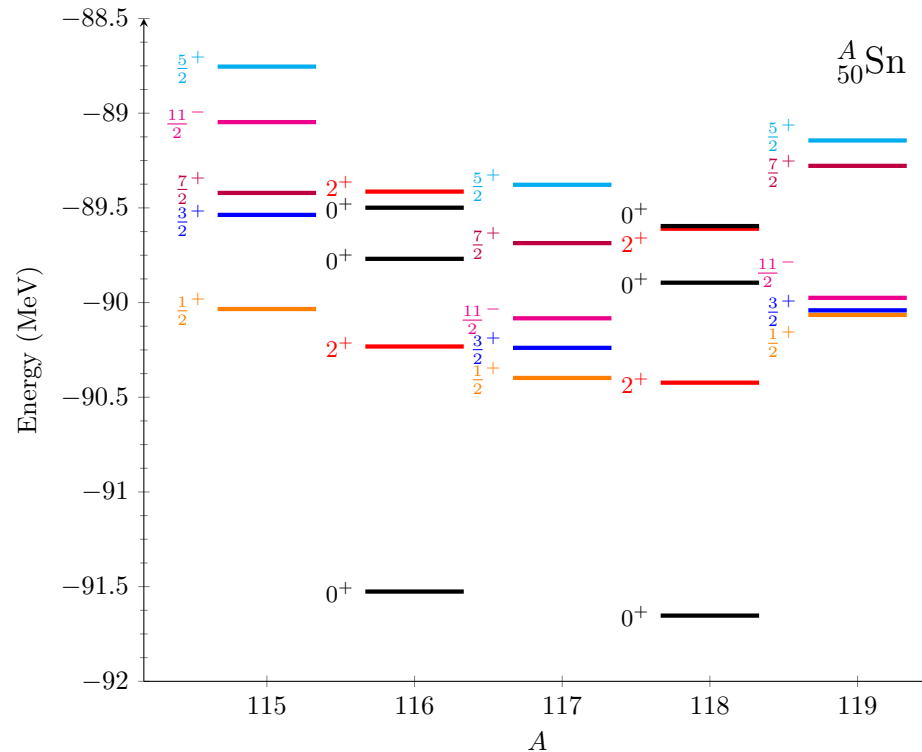


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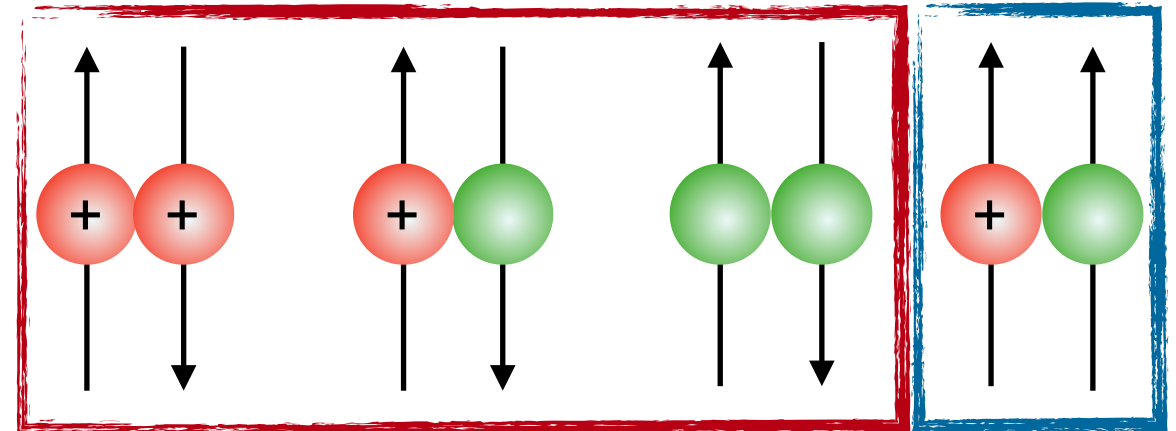
Remember:

Neutron: $t = \frac{1}{2}, t_z = \frac{1}{2}$

Proton: $t = \frac{1}{2}, t_z = -\frac{1}{2}$



Nucleon pairing



$T = 1, J = 0$

$T = 0, J > 0$

PHENOMENOLOGICAL METHODS BASED ON OBSERVATIONS

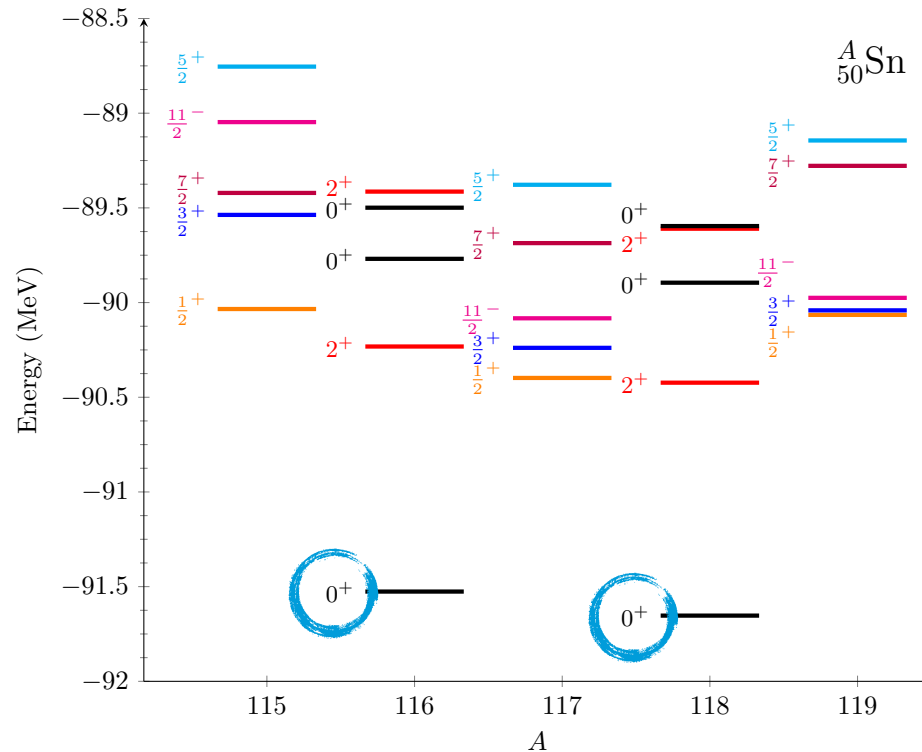


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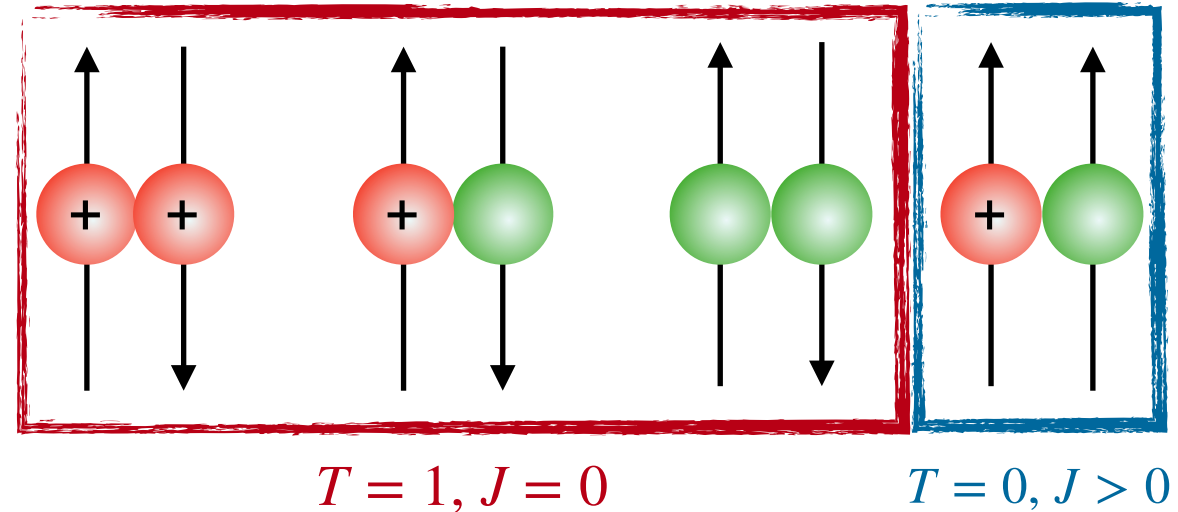
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Nucleon pairing



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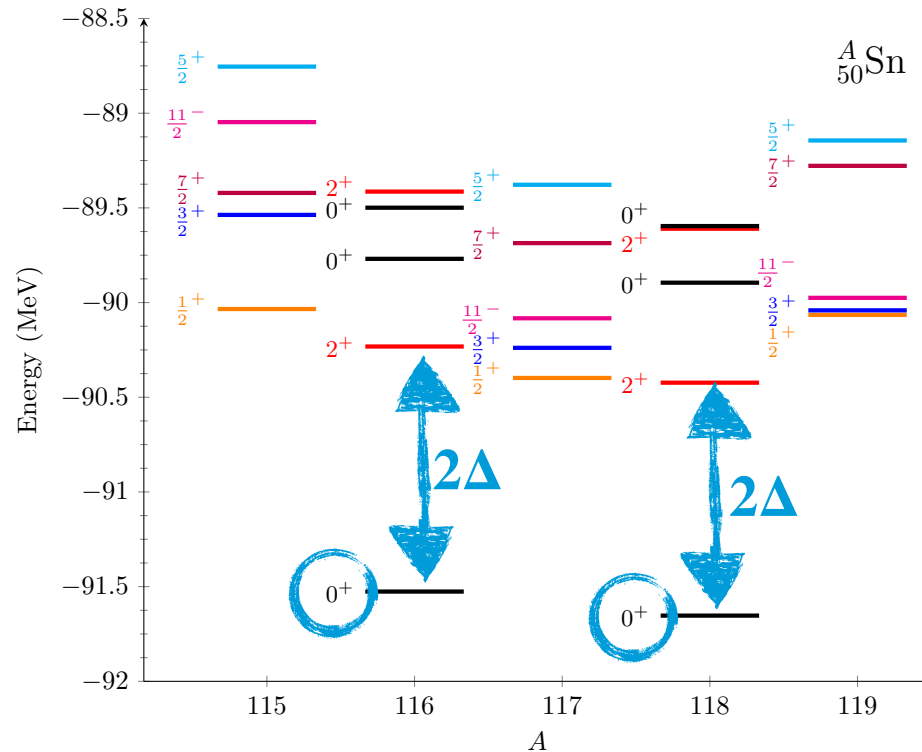


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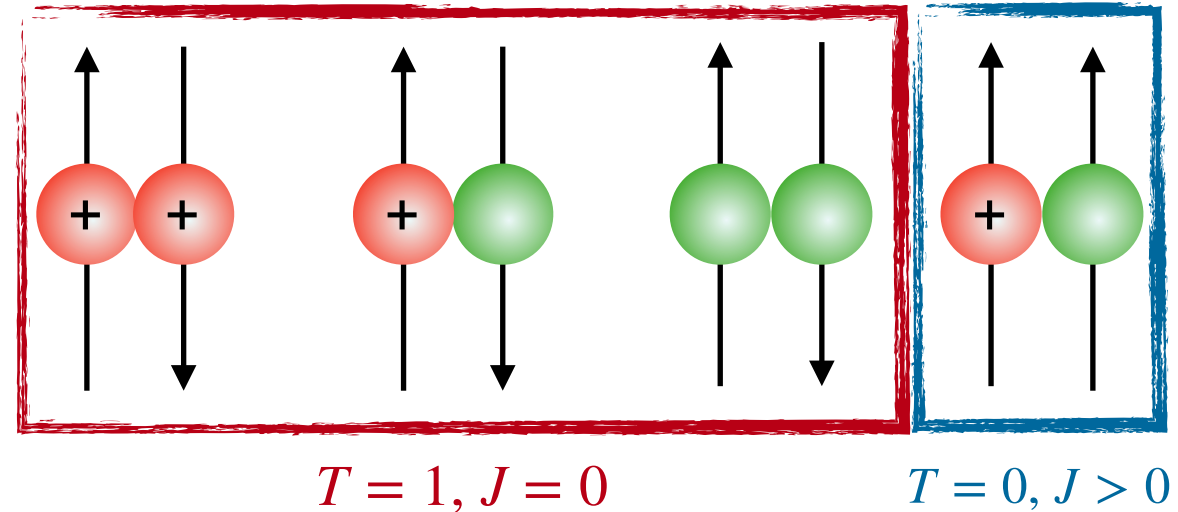
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Nucleon pairing



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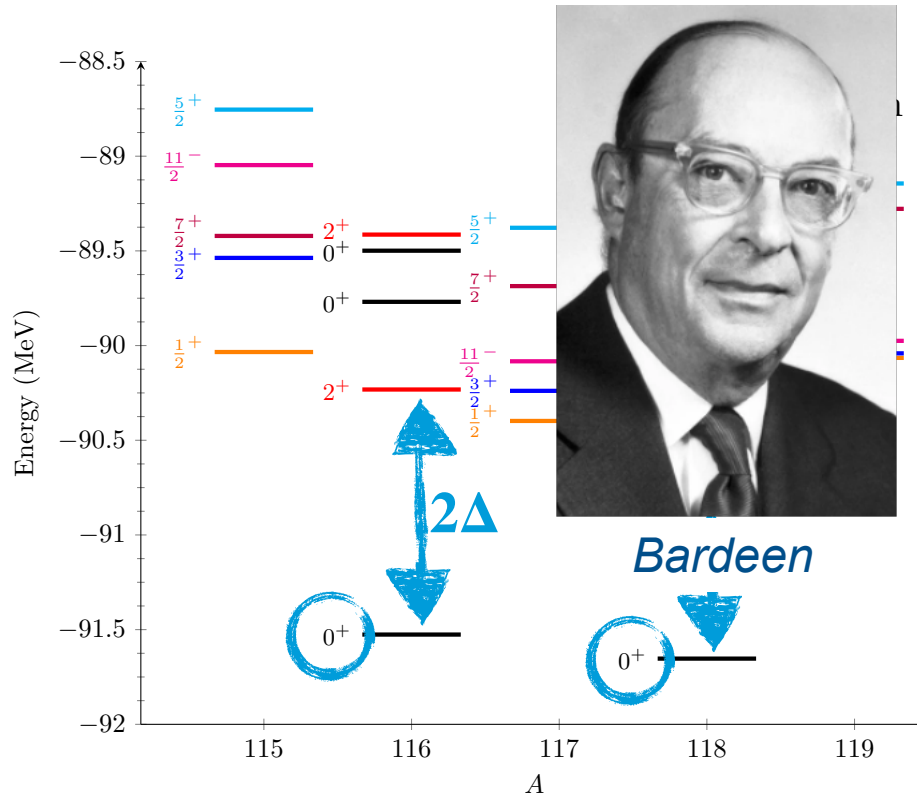
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Nobel Prize in Physics 1972

Remember:

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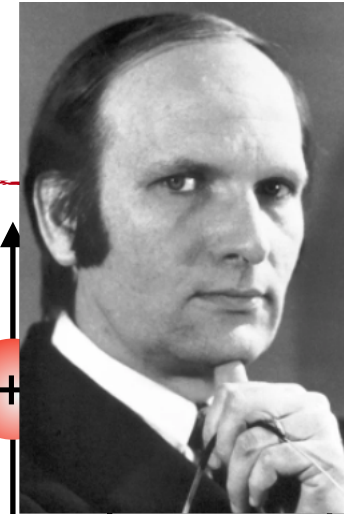
Proton: $t = \frac{1}{2}, t_z = -\frac{1}{2}$



Cooper



Bardeen



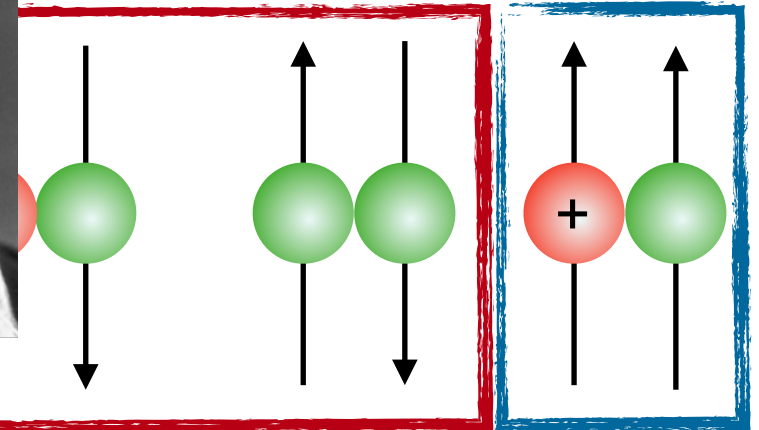
Schrieffer



Nucleon pairing

$T = 1, J = 0$

$T = 0, J > 0$



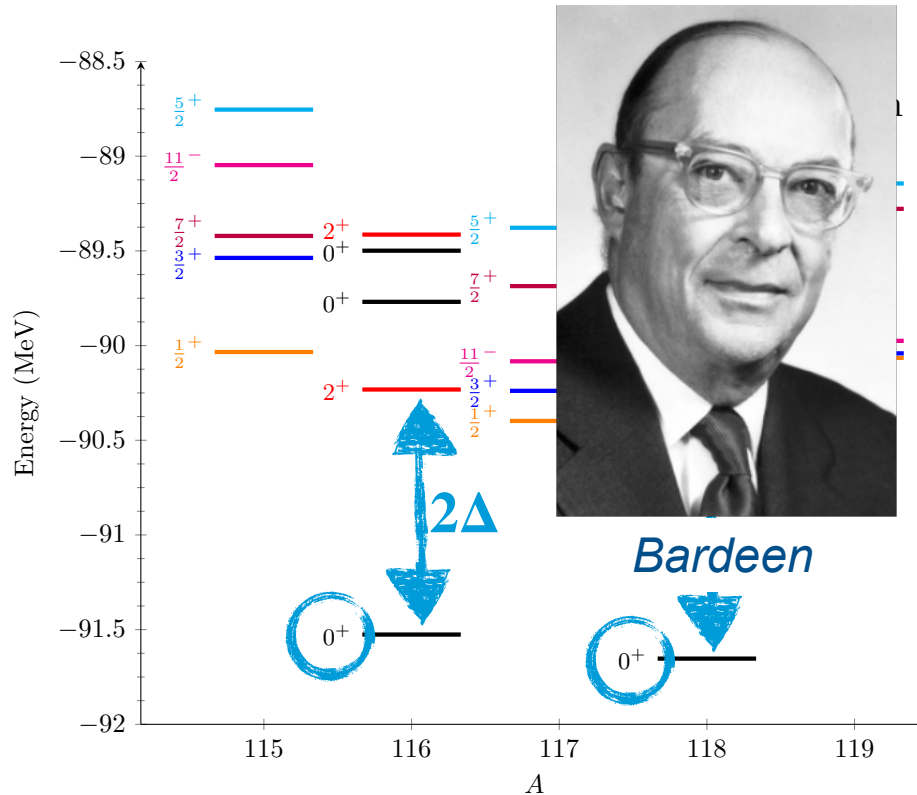
PHENOMENOLOGICAL METHODS BASED ON OBSERVATIONS

Nobel Prize in Physics 1972

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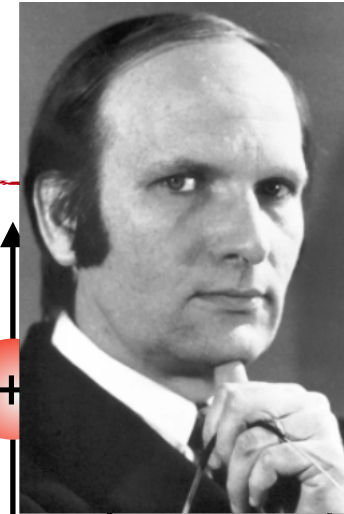
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Bardeen

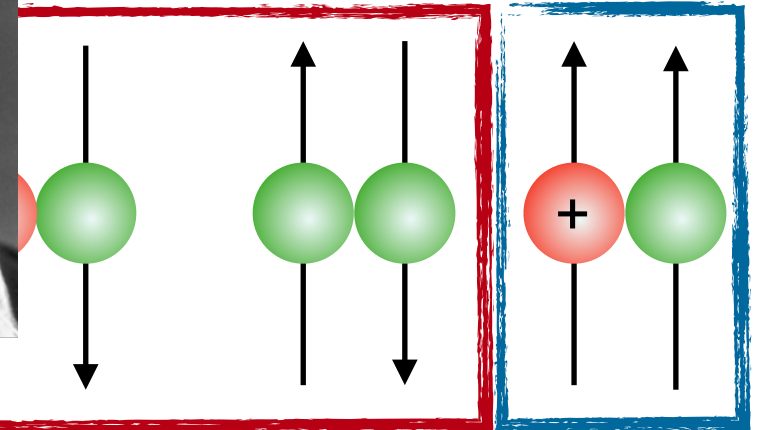


Cooper



Schrieffer

Nucleon pairing



$T = 1, J = 0$

$T = 0, J > 0$

→ **BCS theory for nuclei**

→ **Quasiparticle random-phase approximation, ...**

AB INITIO (LAT. FROM THE BEGINNING) NUCLEAR THEORY

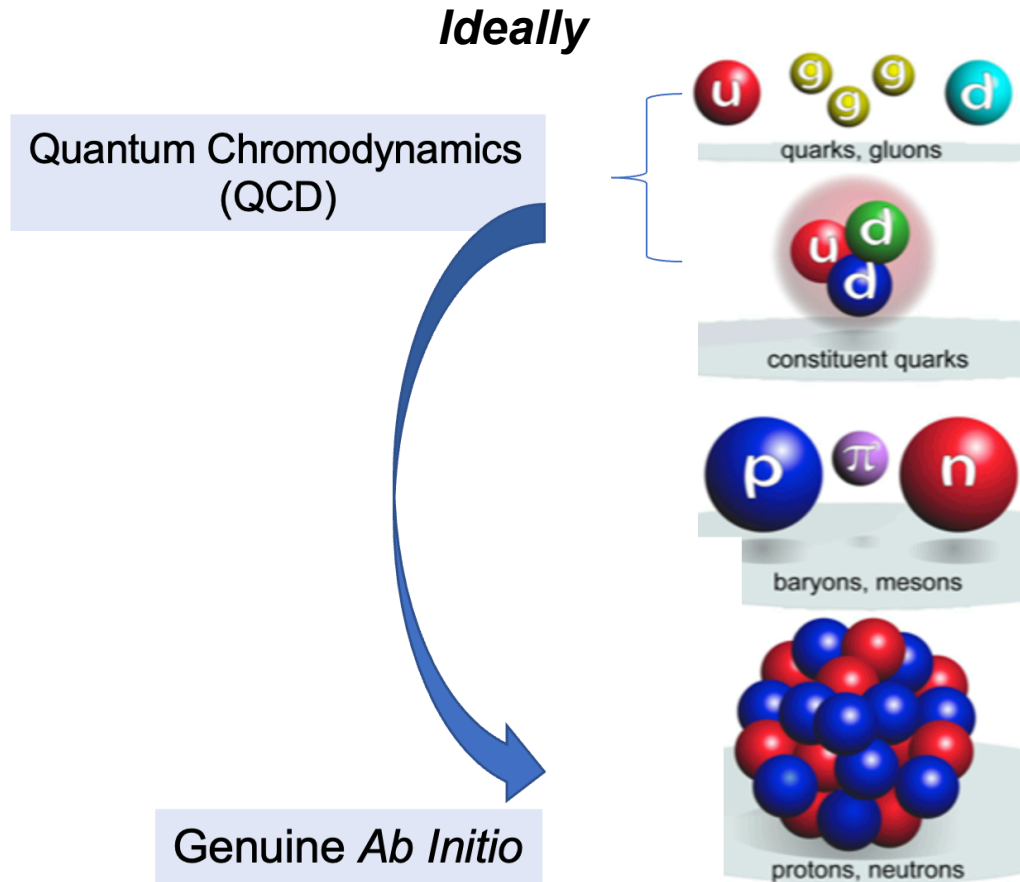


Figure courtesy of P. Navrátil

AB INITIO (LAT. FROM THE BEGINNING) NUCLEAR THEORY

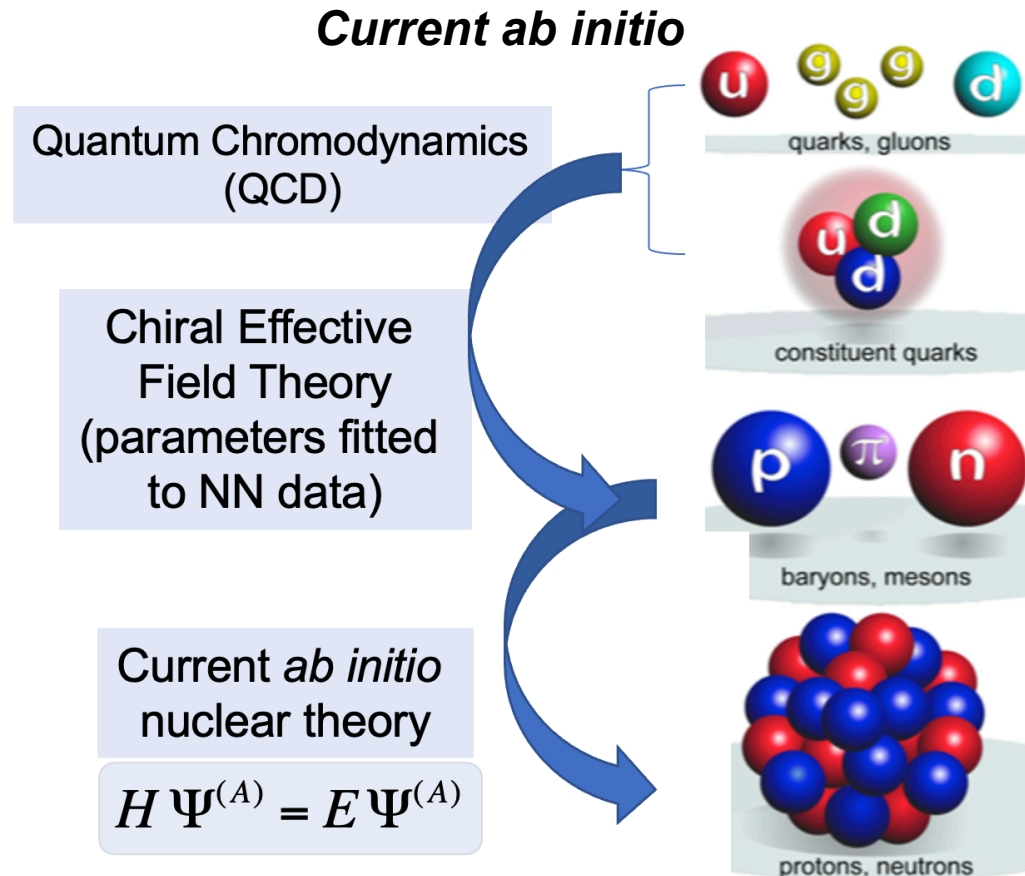


Figure courtesy of P. Navrátil

AB INITIO (LAT. FROM THE BEGINNING) NUCLEAR THEORY

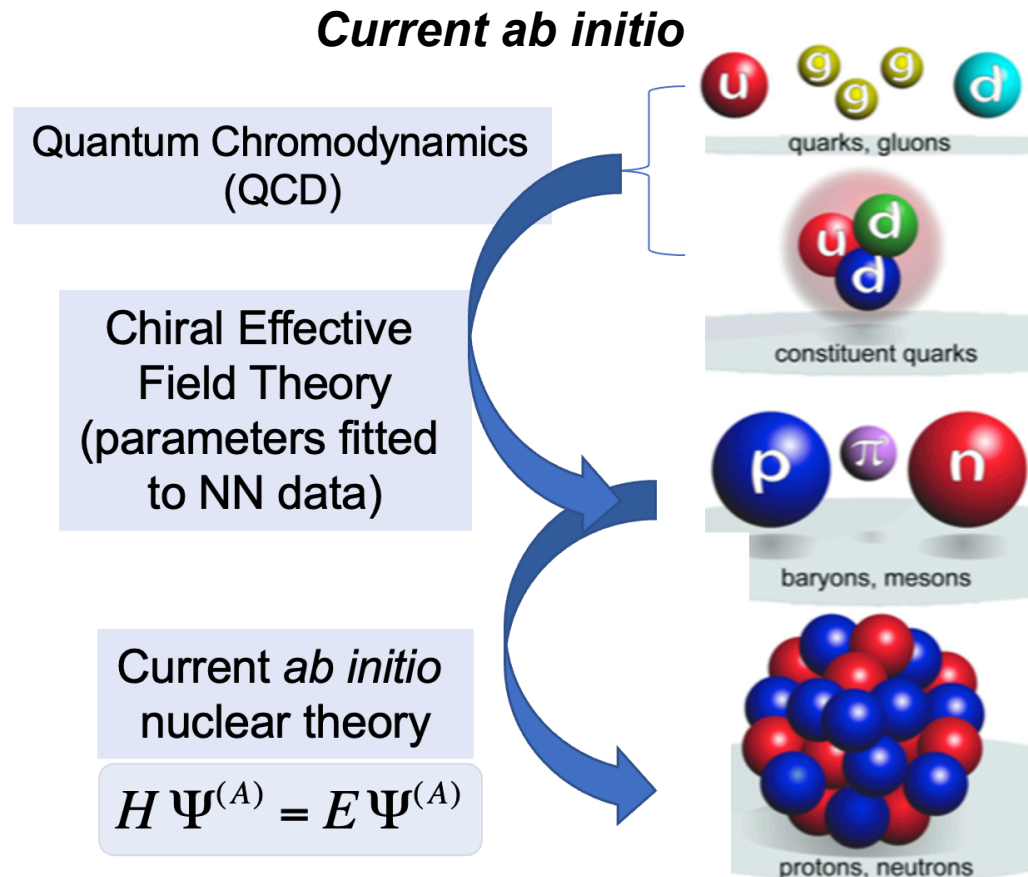


Figure courtesy of P. Navrátil

Chiral expansion of nuclear forces

	NN	3N	4N
LO (Q/Λ_χ) ⁰			
NLO (Q/Λ_χ) ²			
NNLO (Q/Λ_χ) ³			
N ³ LO (Q/Λ_χ) ⁴			

H. Hergert, *Front. Phys.* 8 (2020)

AB INITIO (LAT. FROM THE BEGINNING) NUCLEAR THEORY

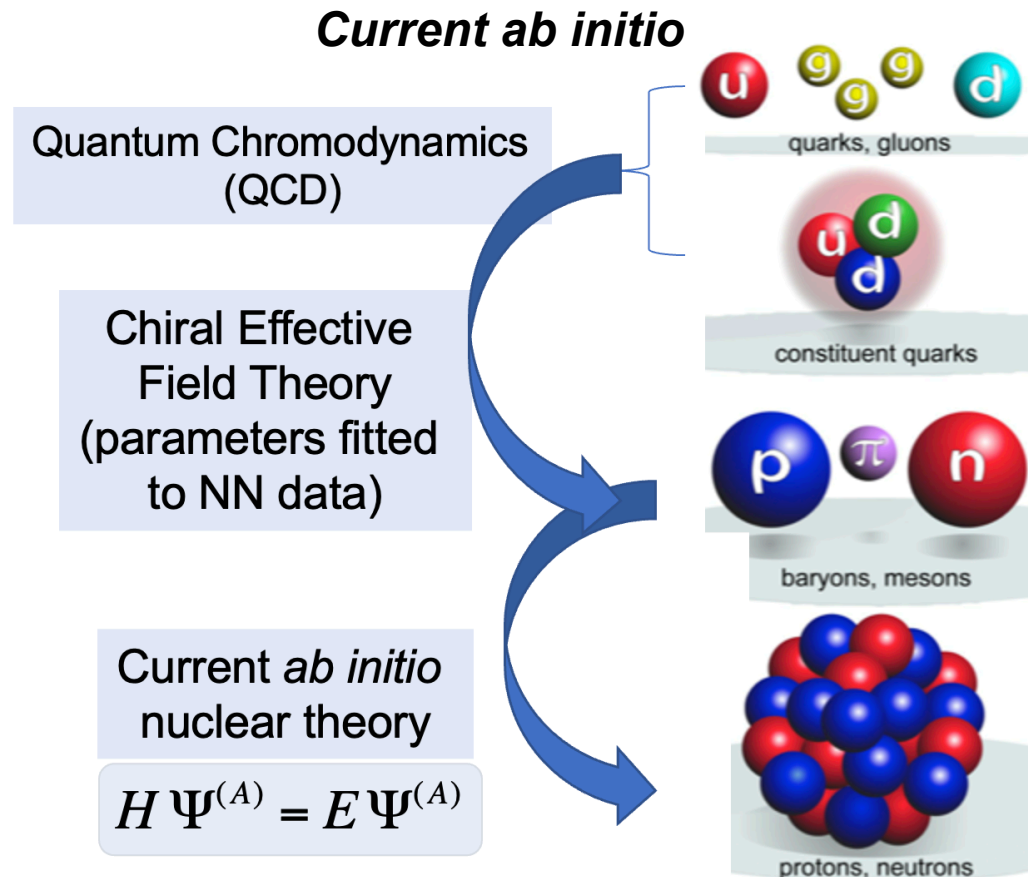


Figure courtesy of P. Navrátil

Chiral expansion of nuclear forces

	NN	3N	4N
LO (Q/Λ_χ) ⁰		$H = T + V^{\text{NN}} + V^{\text{3N}} + \dots$	
NLO (Q/Λ_χ) ²			
NNLO (Q/Λ_χ) ³			
N ³ LO (Q/Λ_χ) ⁴			

H. Hergert, *Front. Phys.* 8 (2020)

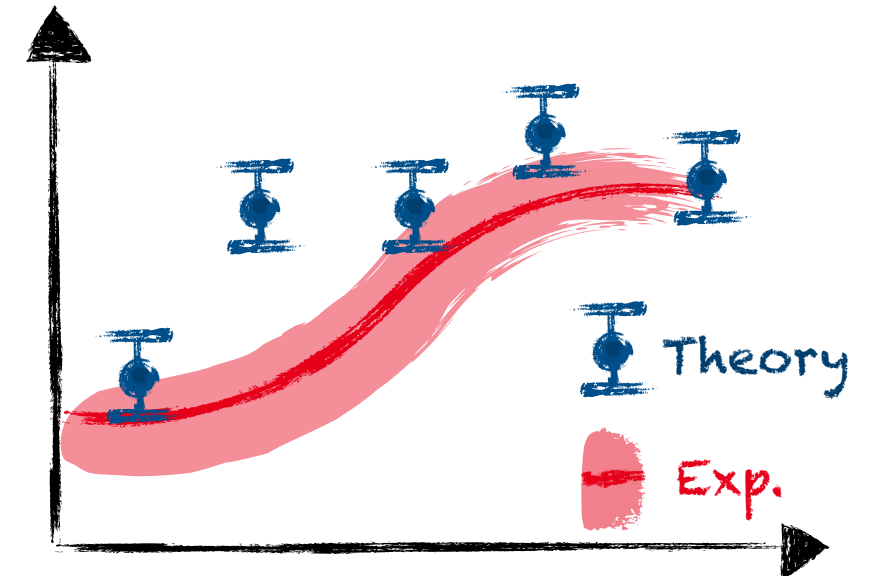
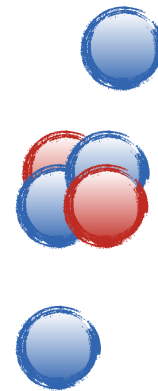
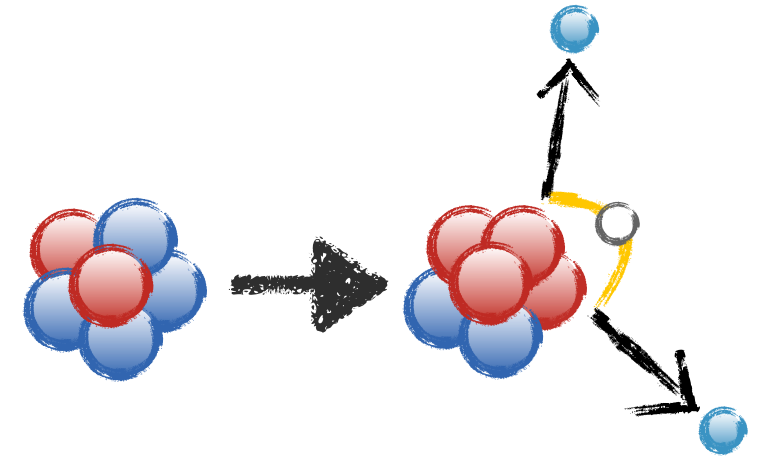


AB INITIO (LAT. FROM THE BEGINNING) NUCLEAR THEORY

*“... we interpret the **ab initio** method to be a **systematically improvable** approach for **quantitatively** describing nuclei using the **finest resolution scale possible** while **maximizing its predictive capabilities**”*

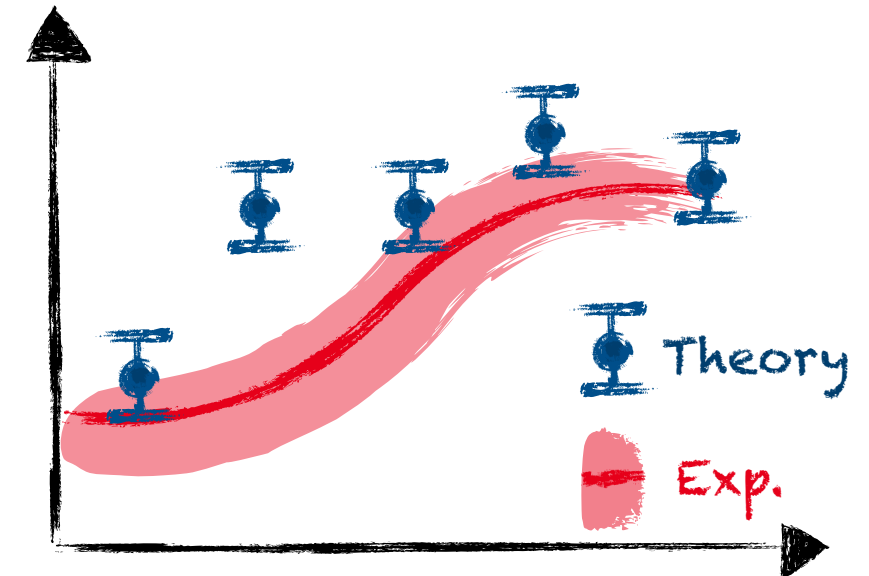
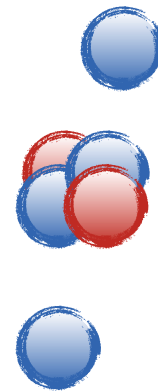
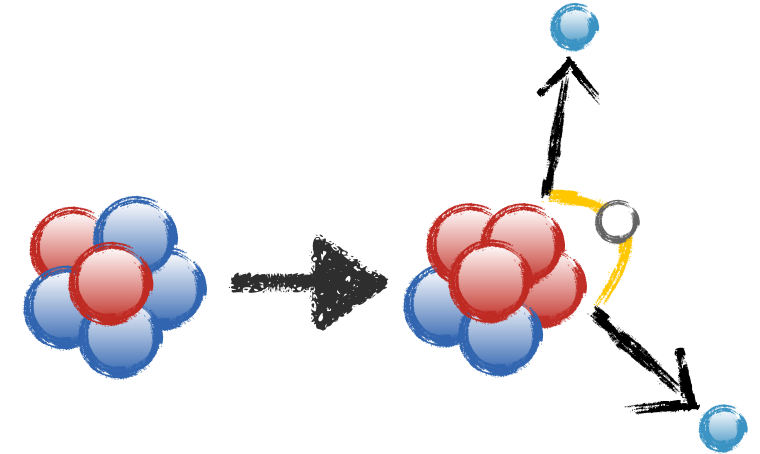
Ekström, Forssén, Hagen, Jansen, Jiang, and Papenbrock, Front. Phys. 11, 1129094 (2023)

WHY AB INITIO?



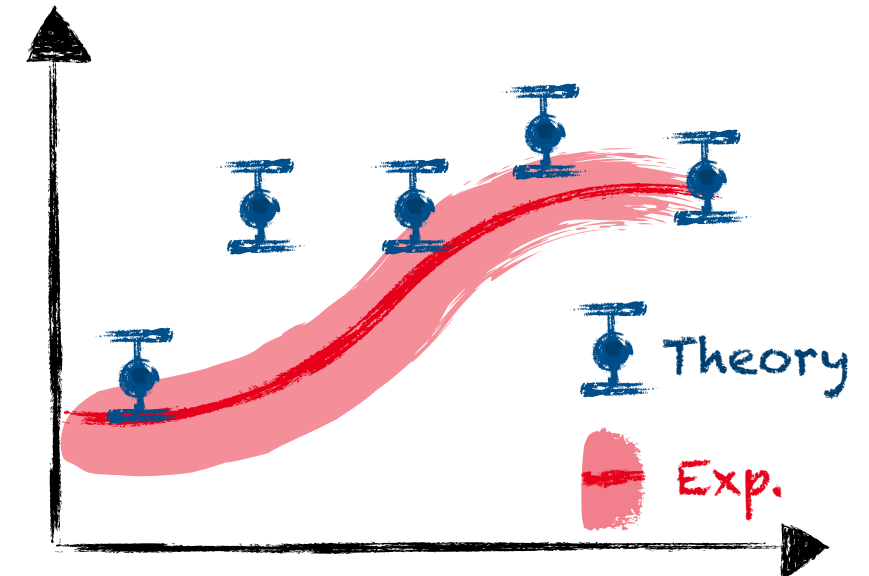
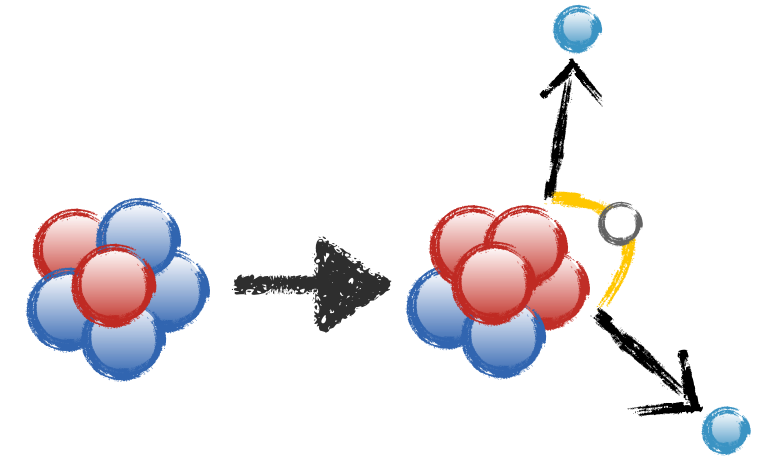
WHY AB INITIO?

- Goal: *Predictive* theory for structure and reactions of nuclei



WHY AB INITIO?

- Goal: *Predictive* theory for structure and reactions of nuclei
- Needed for:
 - Tests of **fundamental symmetries**
 - Predictions for **beyond-standard model processes**
 - Physics of **exotic nuclei**
 - **Uncertainty quantification**



NUCLEAR MANY-BODY PROBLEM

$$H^{(A)}\Psi_n^{(A)} = E_n \Psi_n^{(A)}$$

Nuclear Hamiltonian

$$H^{(A)} = \sum_{i=1}^A \frac{p_i^2}{2m} + \sum_{i<j=1}^A V^{NN}(x_i - x_j) + \left(\sum_{i<j<k=1} V^{3N} + \dots \right)$$

NUCLEAR MANY-BODY PROBLEM

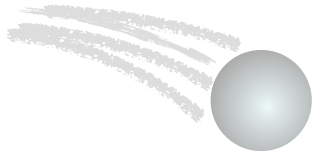


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*Kinetic energy
of a nucleon*



NUCLEAR MANY-BODY PROBLEM

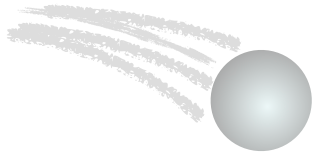


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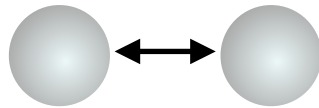
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*Kinetic energy
of a nucleon*



*Interaction between
two nucleons*



NUCLEAR MANY-BODY PROBLEM

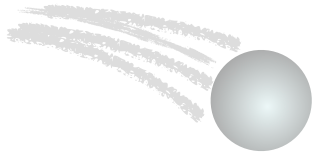


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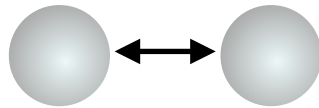
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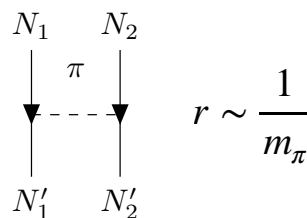
*Kinetic energy
of a nucleon*



*Interaction between
two nucleons*



(Pion exchange)



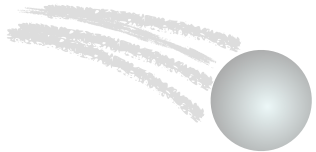
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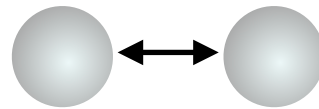
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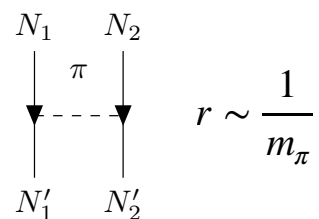
*Kinetic energy
of a nucleon*



*Interaction between
two nucleons*

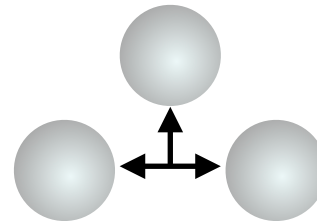


(Pion exchange)



$$r \sim \frac{1}{m_\pi}$$

*Interaction between
three nucleons*



NUCLEAR MANY-BODY PROBLEM



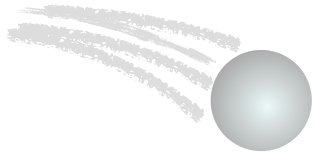
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Eigenstate

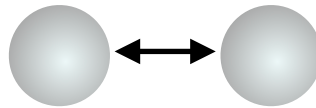
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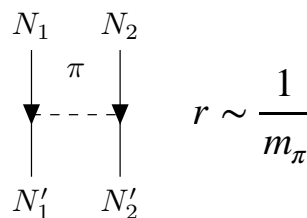
*Kinetic energy
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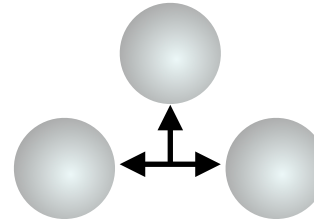
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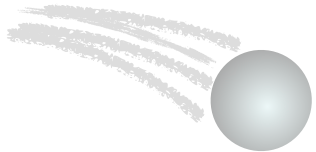
Eigenstate

Eigenenergy

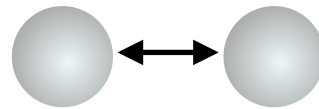
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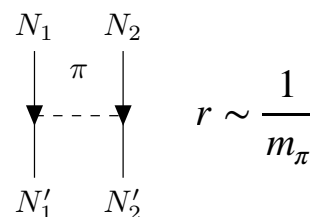
*Kinetic energy
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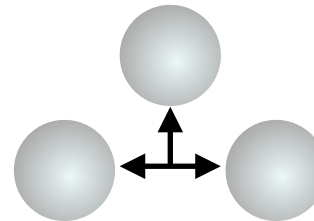
*Interaction between
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NUCLEAR MANY-BODY PROBLEM

$$H^{(A)} \Psi_n^{(A)} = E_n \Psi_n^{(A)}$$

Eigenstate

Eigenenergy

Groundstate: lowest eigenstate

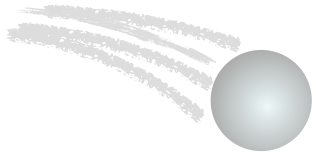
Bound state: $E_n - E_{\text{breakup}} < 0$

Scattering state: $E_n - E_{\text{breakup}} > 0$

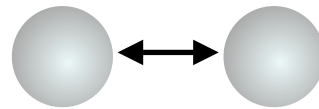
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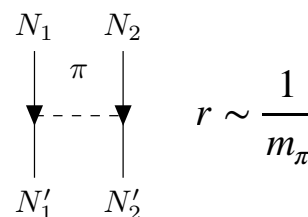
Kinetic energy
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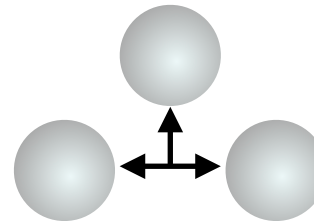
Interaction between
two nucleons



(Pion exchange)



Interaction between
three nucleons



NUCLEAR MANY-BODY PROBLEM

$$H^{(A)} \Psi_n^{(A)} = E_n \Psi_n^{(A)}$$

Eigenstate

Eigenenergy

Groundstate: lowest eigenstate

Bound state: $E_n - E_{\text{breakup}} < 0$

Scattering state: $E_n - E_{\text{breakup}} > 0$

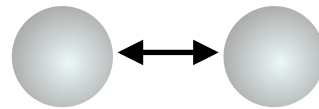
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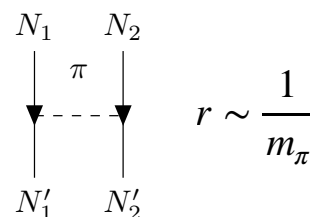
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of a nucleon



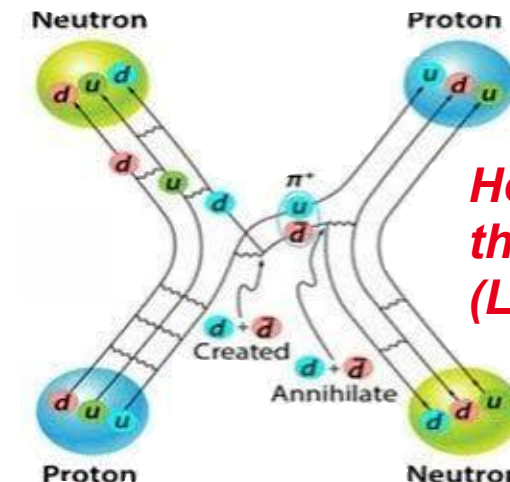
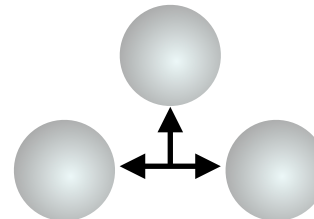
Interaction between
two nucleons



(Pion exchange)



Interaction between
three nucleons



**How to model
the nuclear force?
(Lecture 1)**

medium.com/@mohamedkefw

NUCLEAR MANY-BODY PROBLEM

$$H^{(A)} \Psi_n^{(A)} = E_n \Psi_n^{(A)}$$

Eigenstate

Eigenenergy

Groundstate: lowest eigenstate

Bound state: $E_n - E_{\text{breakup}} < 0$

Scattering state: $E_n - E_{\text{breakup}} > 0$

Nuclear Hamiltonian

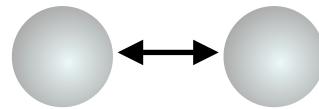
$$H^{(A)} = \sum_{i=1}^A \frac{p_i^2}{2m} + \sum_{i<j=1}^A V^{NN}(x_i - x_j) + \left(\sum_{i<j<k=1}^A V^{3N} + \dots \right)$$

*How to describe the
many-body states?
(Lecture 2)*

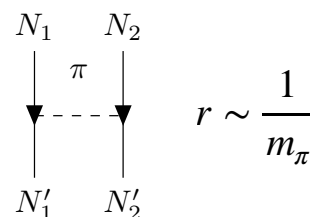
Kinetic energy
of a nucleon



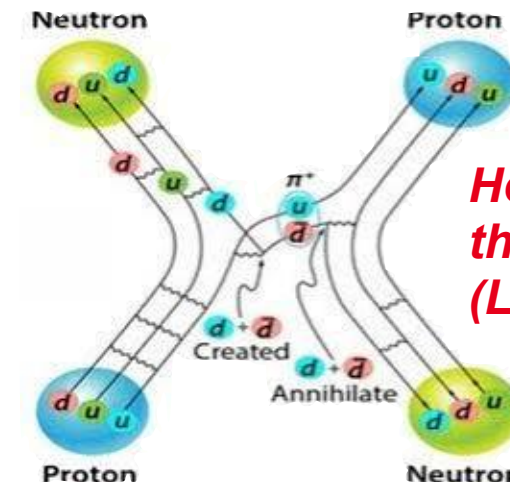
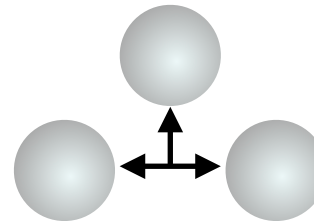
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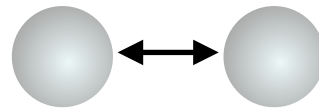
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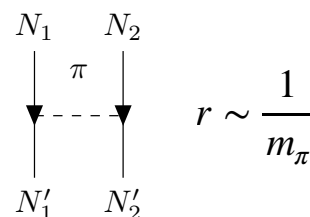
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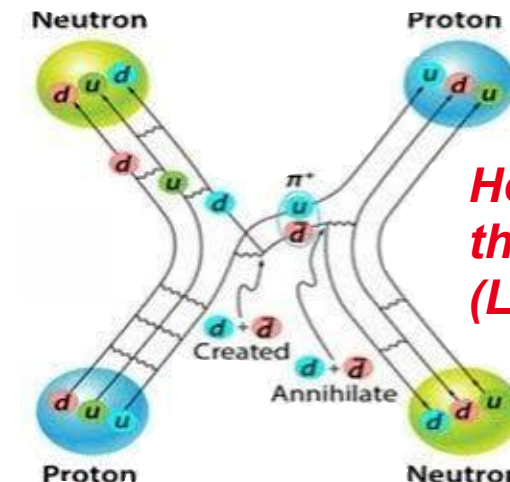
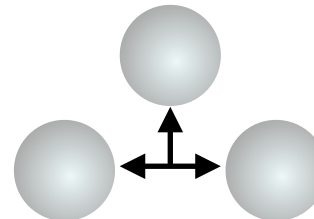


(Pion exchange)



$$r \sim \frac{1}{m_\pi}$$

Interaction between
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*How to model
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SHORT REMINDER OF QUANTUM MANY-BODY PHYSICS

SINGLE-PARTICLE BASIS

SINGLE-PARTICLE BASIS



- Each A nucleons have **position**, **spin**, and **isospin** degrees of freedom

$$|\alpha_i\rangle = |r_i\rangle \otimes |\sigma_i\rangle \otimes |\tau_i\rangle, \quad i = 1, 2, \dots, A$$

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- Typical basis choice for configuration-space methods (e.g. *shell model*)

$$|r\rangle = |n \, l \, m_l\rangle \quad (\text{e.g. spherical harmonic oscillator})$$

$$|\sigma\rangle = |s = \frac{1}{2}, m_s\rangle \quad (\text{eigenstates of } S^2 \text{ and } S_z \text{ with eigenvalue } s = \frac{1}{2})$$

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- Total angular momentum** from spin-orbit coupling

$$|n(l \frac{1}{2}) j m; \frac{1}{2} m_t\rangle = \sum_{m_l, m_s} (l m_l \frac{1}{2} m_s | j m) |n l m_l\rangle \otimes |\frac{1}{2} m_s\rangle \otimes |\frac{1}{2} m_t\rangle$$

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Clebsh-Gordan coefficient

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Clebsh-Gordan coefficient

- E.g. the spatial representation of $|\alpha\rangle$ in harmonic oscillator basis

$$\langle \mathbf{x} | \alpha \rangle = \phi_\alpha(\mathbf{x}) = g_{n_a l_a}(r) \sum_{m_l m_s} (l m_l \frac{1}{2} m_s | j m) Y_{l m_l}(\Omega) \chi_{\frac{1}{2} m_s}, \quad \chi_{\frac{1}{2} \frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_{\frac{1}{2} -\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

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- Nucleons are **fermions** → many-body states have to be **antisymmetric**

$$|\alpha_1 \dots \alpha_i \dots \alpha_j \dots \alpha_A\rangle = - |\alpha_1 \dots \alpha_j \dots \alpha_i \dots \alpha_A\rangle$$



Pauli Principle

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- A -body basis states expressed as **Slater determinants**

$$|\alpha_1 \alpha_2 \dots \alpha_A\rangle = \frac{1}{\sqrt{A!}} \sum_{\pi} \text{sgn}(\pi) P_{\pi}(|\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \dots \otimes |\alpha_A\rangle) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_{\alpha_1}(x_1) & \dots & \phi_{\alpha_A}(x_1) \\ \vdots & \ddots & \vdots \\ \phi_{\alpha_A}(x_1) & \dots & \phi_{\alpha_A}(x_N) \end{vmatrix}$$

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Permutation

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Signum of permutation *Permutation*

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- Given a complete basis $\{|\alpha\rangle\}$, **Slater determinants form a complete basis of the antisymmetric A -body Hilbert space**

$$\mathcal{H}_A^{\text{as}} \subset \mathcal{H}_A = \underbrace{\mathcal{H}_1 \otimes \mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_1}_{A-1 \text{ times}}$$

$$\mathbf{1} = \sum_{\alpha_1 < \alpha_2 < \dots < \alpha_A} |\alpha_1 \alpha_2 \dots \alpha_A\rangle \langle \alpha_1 \alpha_2 \dots \alpha_A| = \frac{1}{A!} \sum_{\alpha_1 \alpha_2 \dots \alpha_A} |\alpha_1 \alpha_2 \dots \alpha_A\rangle \langle \alpha_1 \alpha_2 \dots \alpha_A|$$

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Hilbert space:

An inner product space, whose associated metric is complete.

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- General antisymmetric state can be **expanded in Slater determinant basis**

$$|\Psi^{(A)}\rangle = \sum_{\alpha_1 < \alpha_2 < \dots < \alpha_A} C_{\alpha_1 \alpha_2 \dots \alpha_A} |\alpha_1 \alpha_2 \dots \alpha_A\rangle$$

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SECOND QUANTIZATION

Tarufi, Perroni, Filippis, <https://arxiv.org/pdf/2507.09229>



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- **Fock space** defined as a direct sum of antisymmetric N -particle Hilbert spaces

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where $n_i \in \{0, 1\}$ is the number of fermions in state $|\alpha_i\rangle$ and $\sum_i n_i = N$

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- **Creation and annihilation operators**

$$a_i^\dagger |n_1, n_2, \dots, n_i, \dots, n_\infty; N\rangle = (-1)^{\sum_{j<i} n_j} (1 - n_i) |n_1, n_2, \dots, 1 + n_i, \dots, n_\infty; N + 1\rangle,$$

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- **Anticommutation relations** $\{a_{\alpha_i}^\dagger, a_{\alpha_i}^\dagger\} = 0, \quad \{a_{\alpha_i}, a_{\alpha_i}\} = 0, \quad \{a_{\alpha_i}, a_{\alpha_j}^\dagger\} = \delta_{\alpha_i \alpha_j}$

SECOND QUANTIZATION: STATES

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SECOND QUANTIZATION: STATES

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- Remember: $a_{\alpha_i}^\dagger |0\rangle = |\alpha_i\rangle$, $a_{\alpha_i} |0\rangle = 0 \rightarrow \langle 0| a_{\alpha_i} = \langle \alpha_i|$, $\langle 0| a_{\alpha_i}^\dagger = 0$

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- A -particle state in $\mathcal{H}_A^{\text{as}}$ can be written as **creation operators acting on vacuum state**

$$|\alpha_1 \alpha_2 \dots \alpha_A\rangle = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \dots a_{\alpha_A}^\dagger |0\rangle$$

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- Alternatively, one can define an A -body **reference state**

$$|\Phi\rangle \equiv |\alpha_1 \alpha_2 \dots \alpha_A\rangle$$

and construct Slater determinants as particle-hole excitations on top of it

$$|\Phi_i^a\rangle = a_{\alpha_a}^\dagger a_{\alpha_i} |\Phi\rangle$$

$$|\Phi_{ij}^{ab}\rangle = a_{\alpha_a}^\dagger a_{\alpha_b}^\dagger a_{\alpha_j} a_{\alpha_i} |\Phi\rangle,$$

index convention: $i, j, k, \dots$: states occupied in the reference state

$a, b, c, \dots$: states unoccupied in the reference state

SECOND QUANTIZATION: OPERATORS

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- Operators can also be expressed in terms of creation and annihilation operators

SECOND QUANTIZATION: OPERATORS



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Tarufi, Perroni, Filippis, <https://arxiv.org/pdf/2507.09229>

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- Note:** we will make use of the second quantization later in the lectures

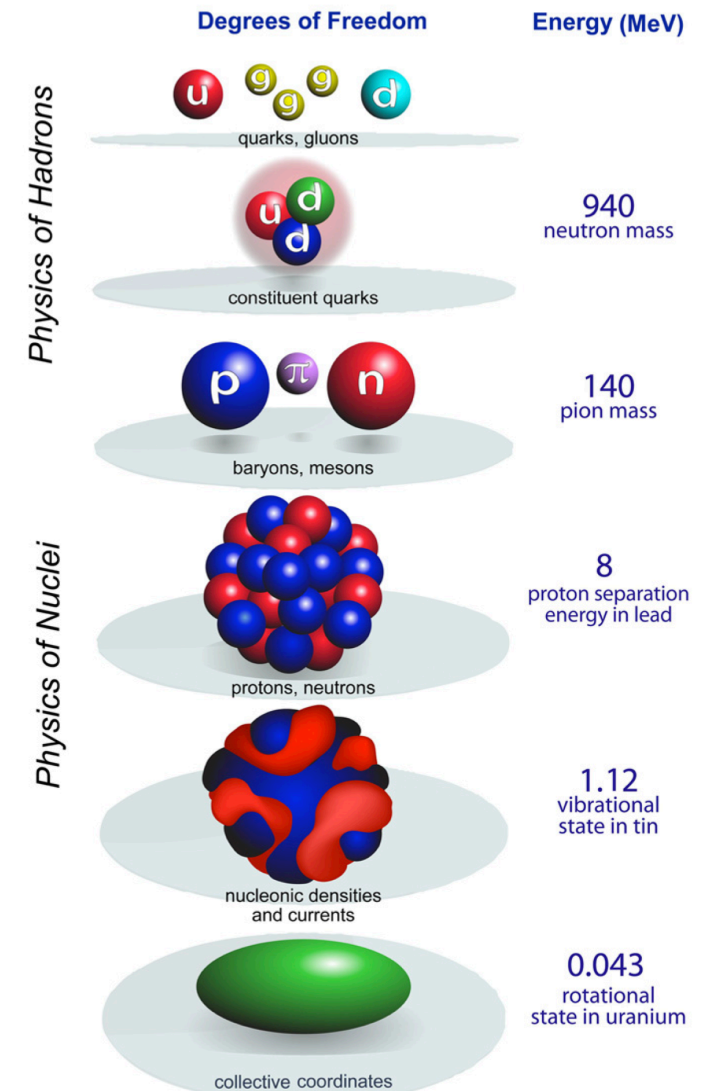


NUCLEAR MANY-BODY HAMILTONIAN

FROM QCD TO NUCLEI



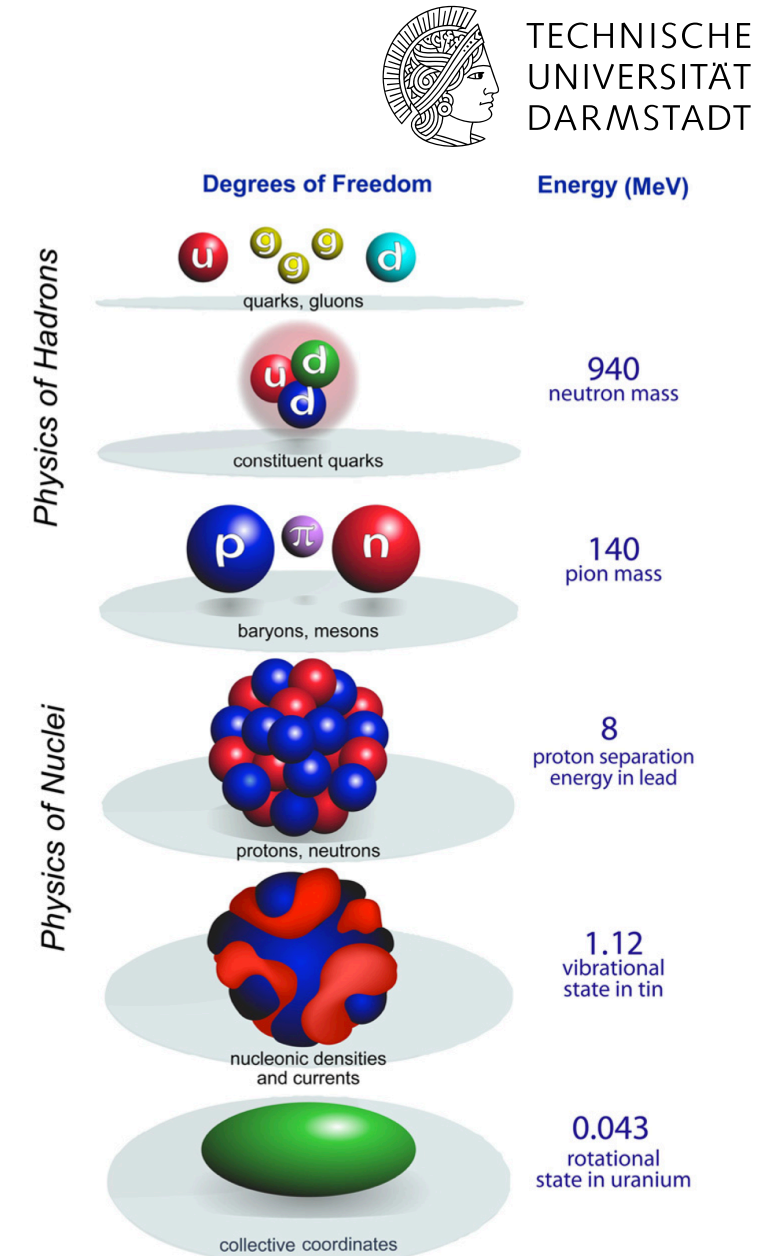
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Furnstahl, Hebeler, Rep. Prog. Phys. 76, 126301 (2013)

FROM QCD TO NUCLEI

- Different energy scales:



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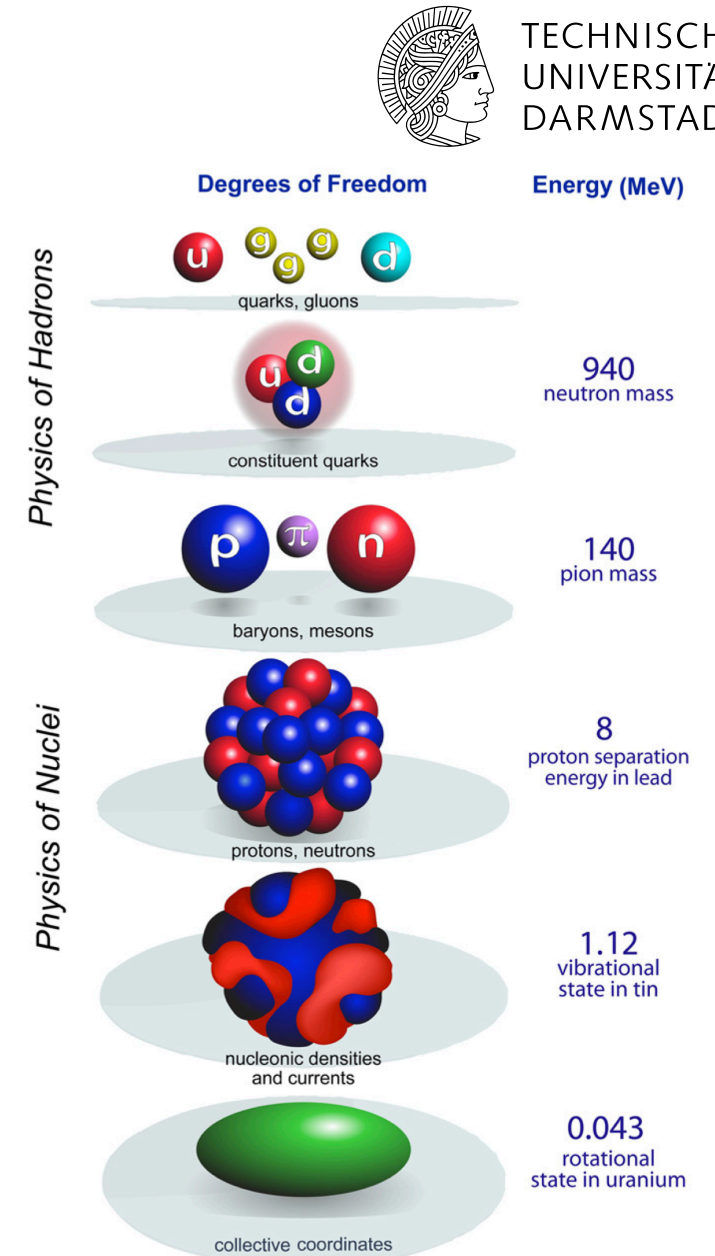
FROM QCD TO NUCLEI



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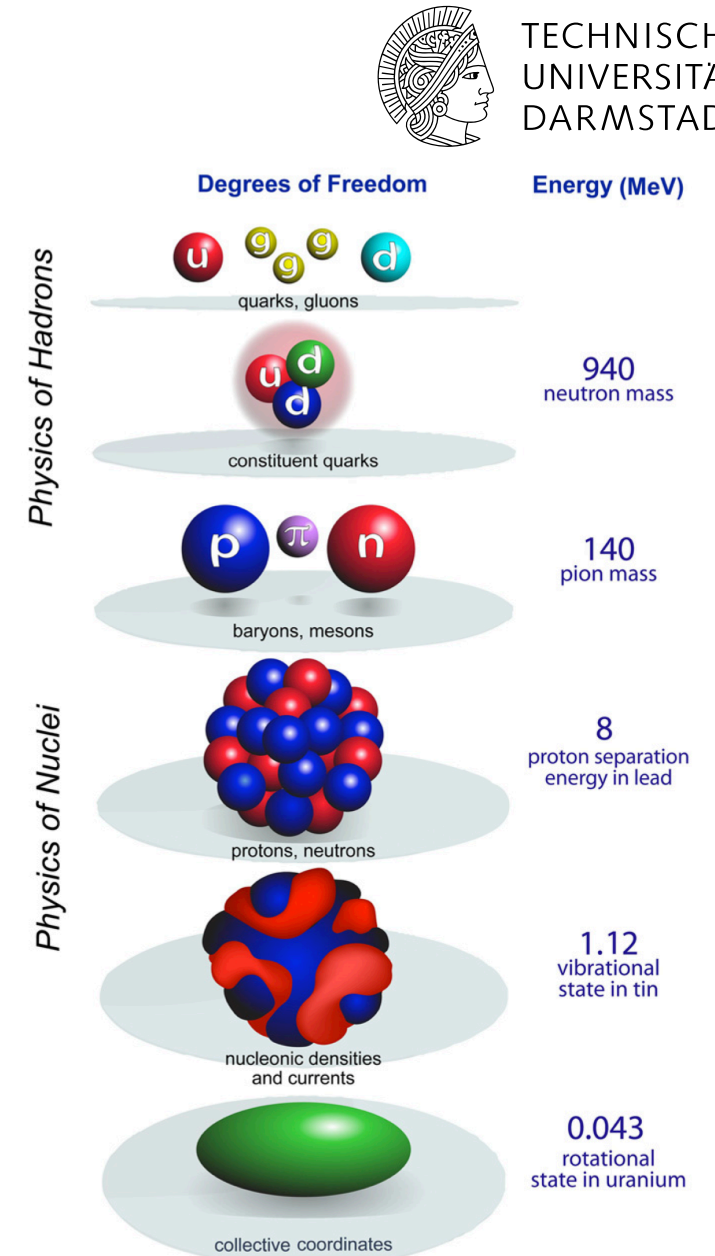
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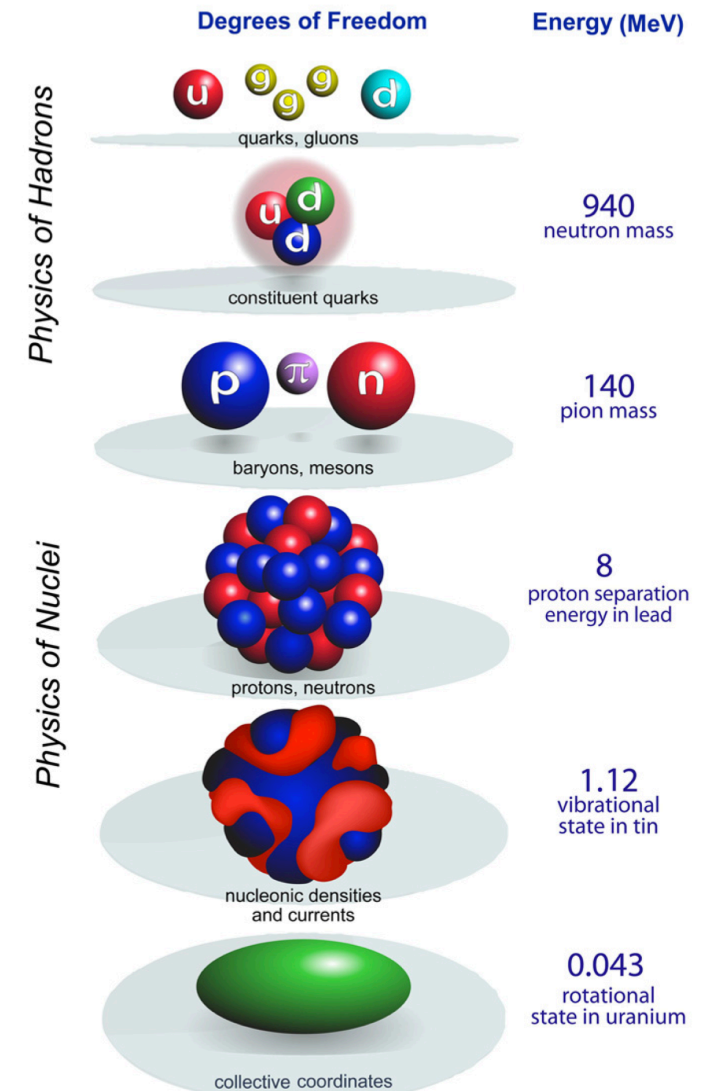
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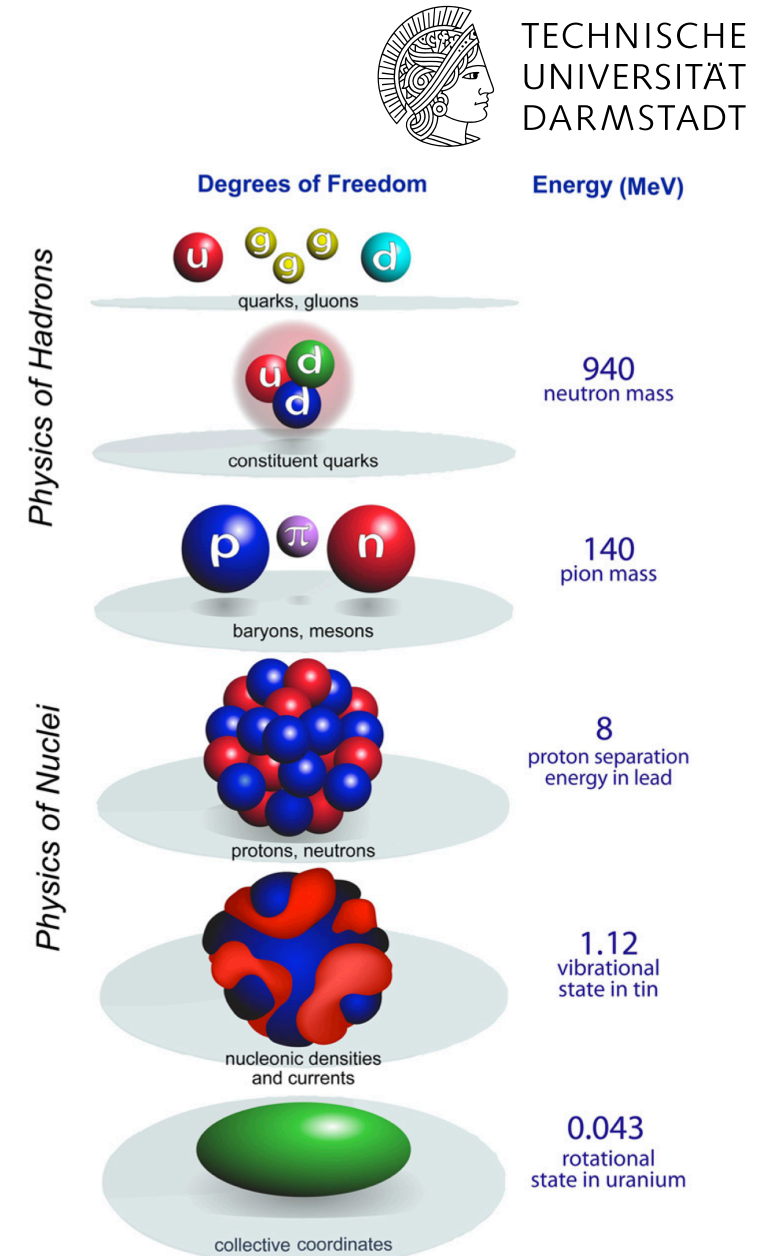
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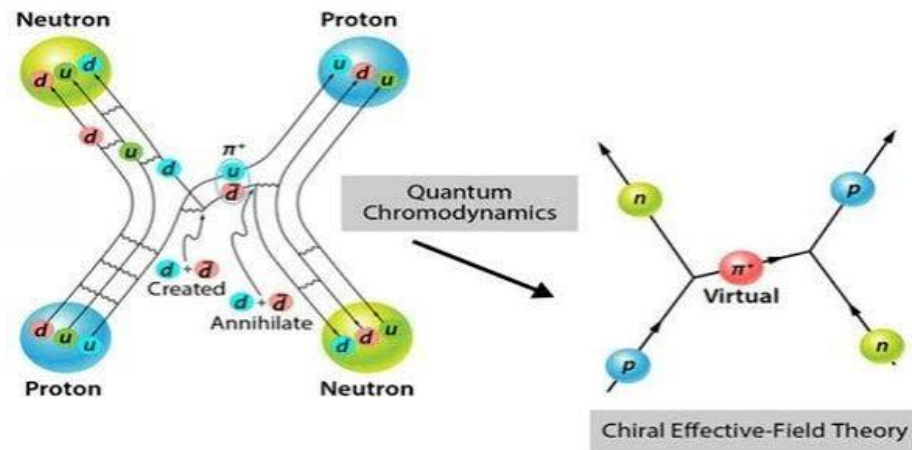
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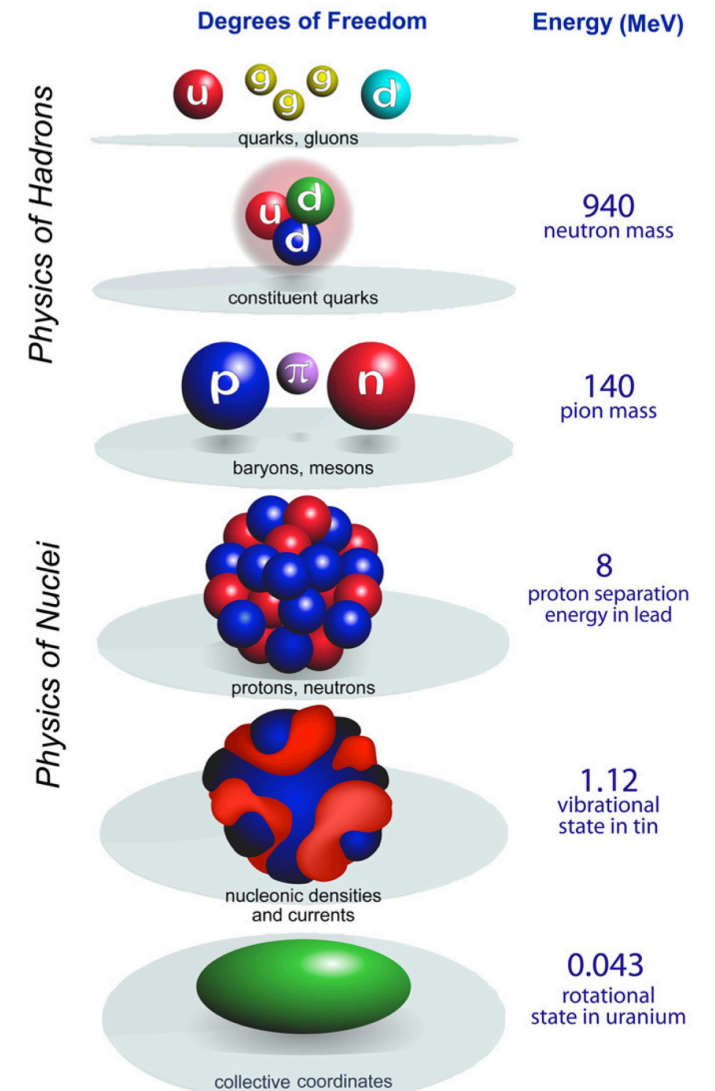


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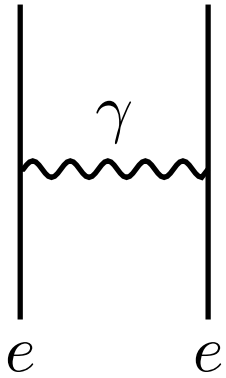
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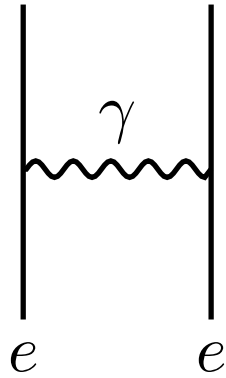
Electromagnetic interaction



- **Infinite range**
 - Exchange of a **massless particle**

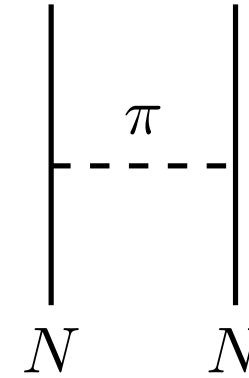
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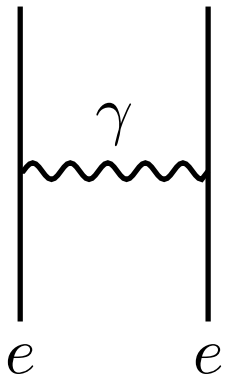
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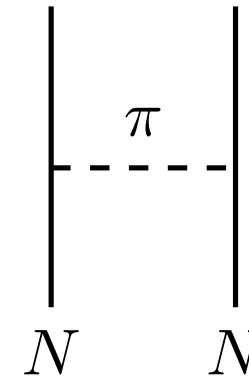
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Nucleon-nucleon interaction



**One-pion-exchange
(OPE) potential**



Yukawa



**Nobel Prize
in Physics
1949**

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CHIRAL SYMMETRIES



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Bernard, Kaiser, Meißner, Int. J Mod. Phys. 4, 193-475 (1995); Ecker, <https://arxiv.org/abs/hep-ph/9805500>; Pich, <https://arxiv.org/abs/1804.05664>

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- Which is symmetric under unitary transformations $U_L, U_R \in SU(2)$ in the flavour space

$$q_L \rightarrow U_L(x)q_L = \exp(-i\boldsymbol{\theta}_L \cdot \boldsymbol{\tau})q_L, \quad q_R \rightarrow U_R(x)q_R = \exp(-i\boldsymbol{\theta}_R \cdot \boldsymbol{\tau})q_R$$

CHIRAL SYMMETRY BREAKING



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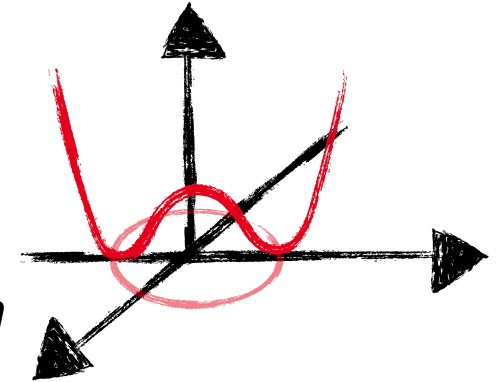
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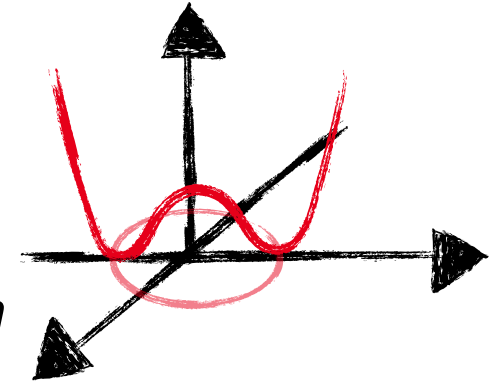
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CHIRAL EFFECTIVE FIELD THEORY

Weinberg, Physica A 96, 327-340 (1979); Pich, <https://arxiv.org/abs/1804.05664>



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 - Write down the **most general Lagrangian**

$$\mathcal{L}_{\text{eff}} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{\pi N} + \mathcal{L}_{NN} + \dots$$

consistent with chiral symmetry

CHIRAL EFFECTIVE FIELD THEORY



Weinberg, *Physica A* 96, 327-340 (1979); Pich, <https://arxiv.org/abs/1804.05664>

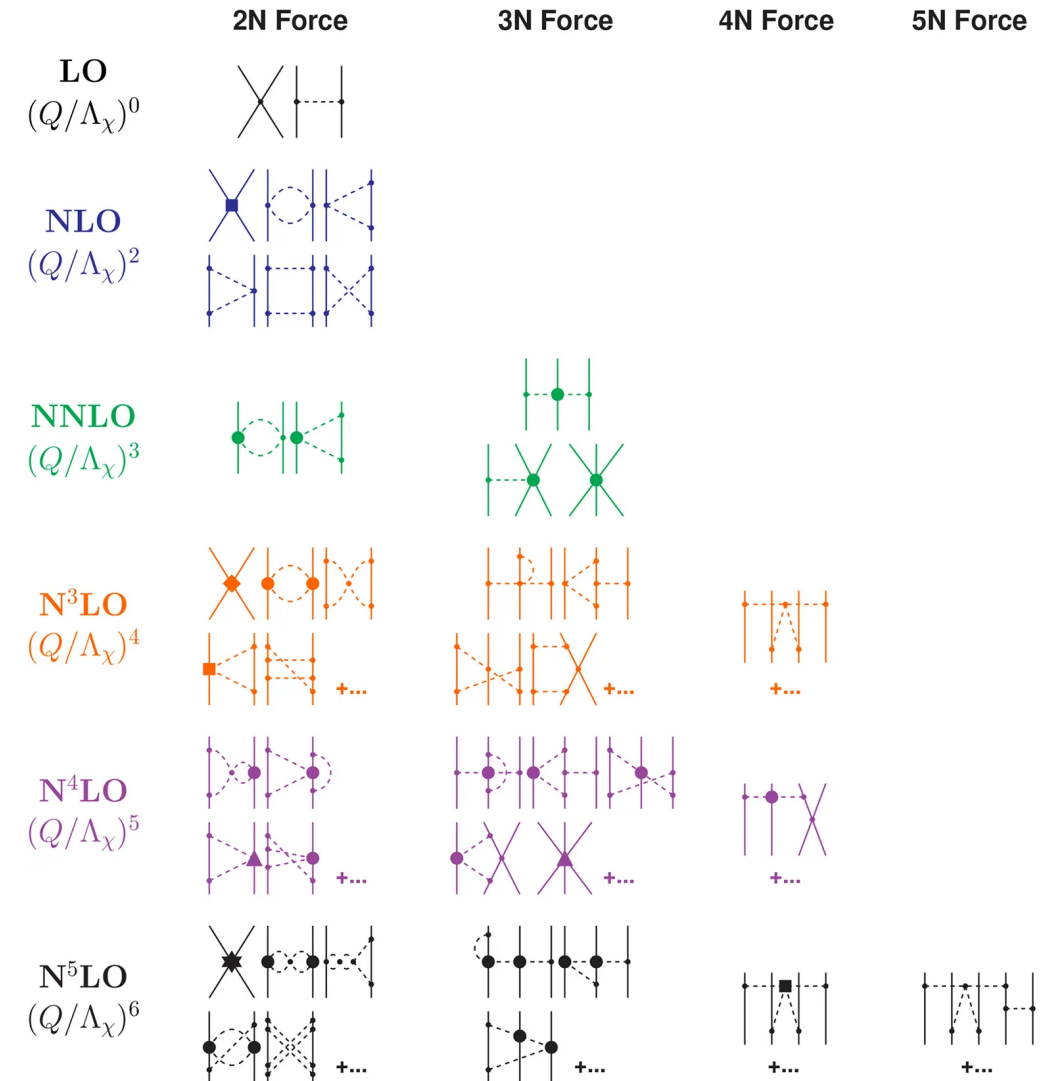
- Use **effective field theory** to analyze the low-energy dynamics of QCD
 - Identify relevant **degrees of freedom** (π , p , n) and their **transformation under the chiral group**
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$$\mathcal{L}_{\text{eff}} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{\pi N} + \mathcal{L}_{NN} + \dots$$
consistent with chiral symmetry
 - Order interactions and amplitudes according to a **power counting scheme**

CHIRAL EXPANSION OF NUCLEAR FORCES

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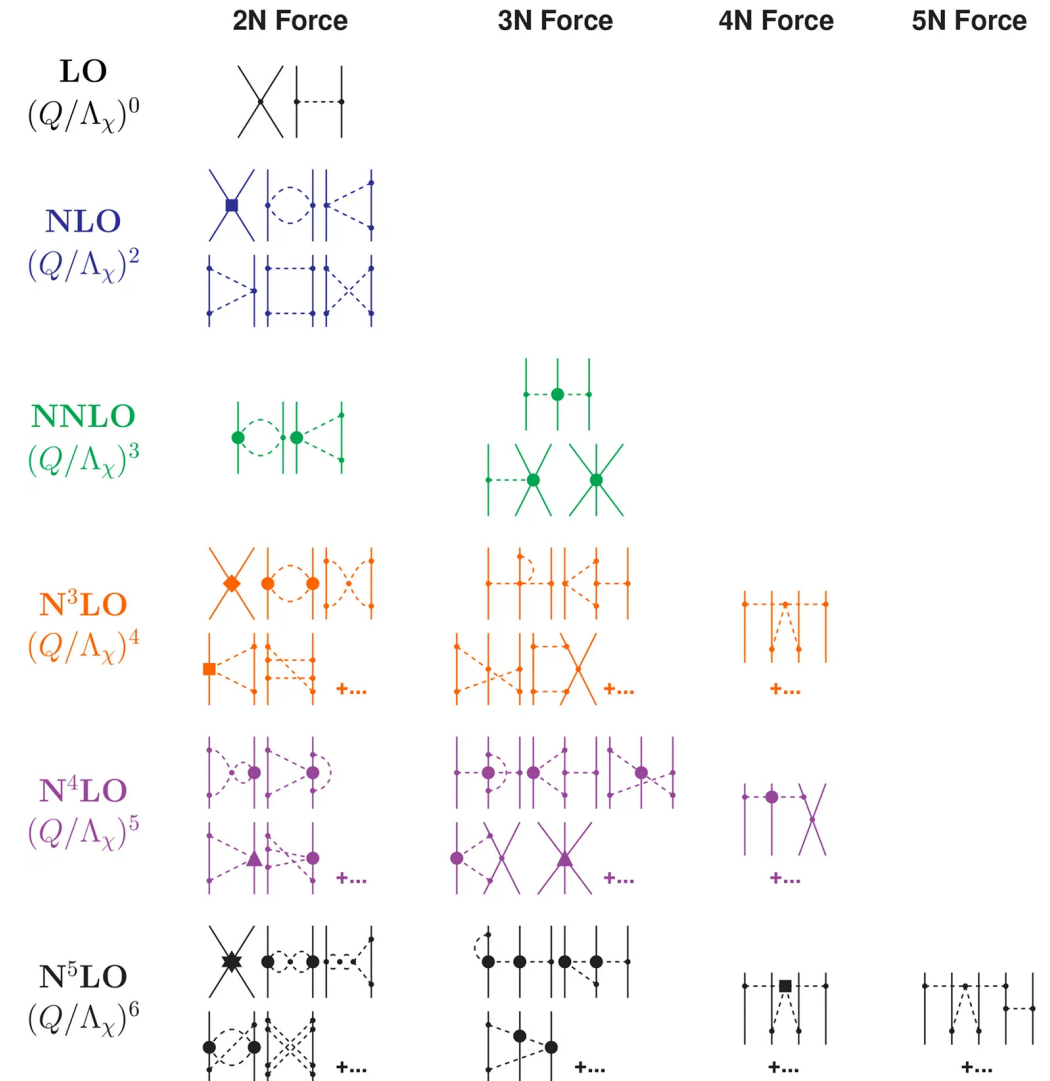


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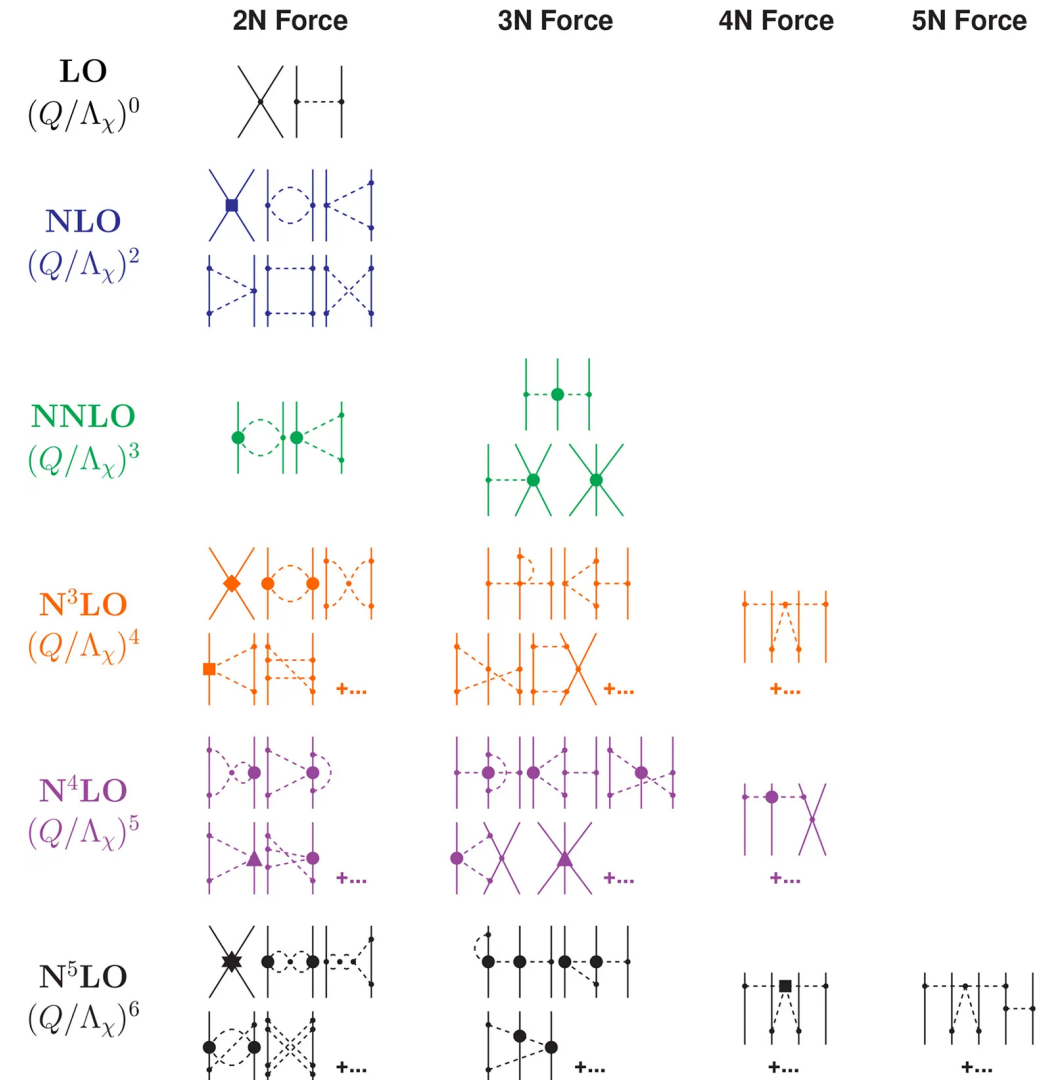
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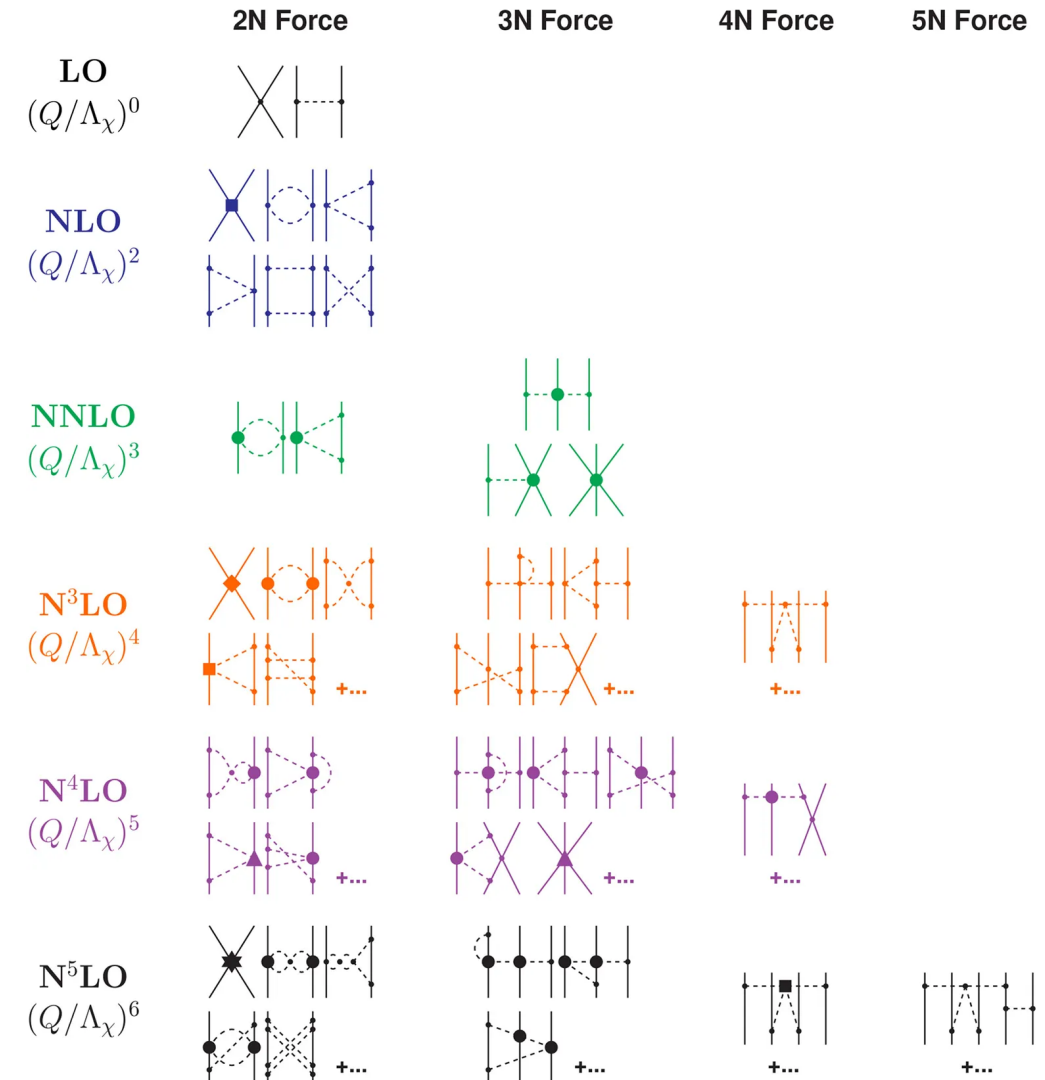
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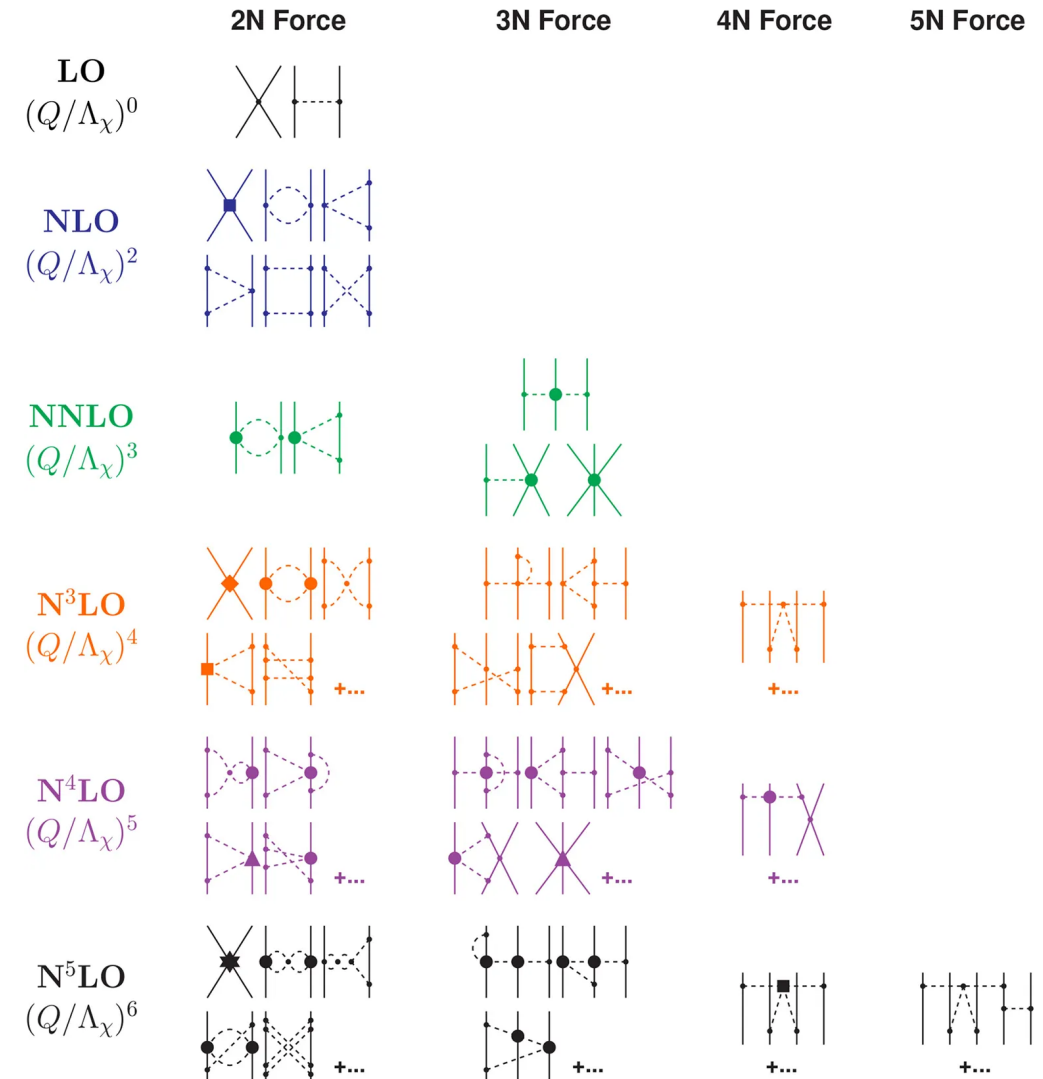
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$$Q \sim m_\pi \sim 138 \text{ MeV}$$

$$\Lambda_\chi \sim 1 \text{ GeV}$$

$$\rightarrow (Q/\Lambda_\chi) \sim 0.1$$



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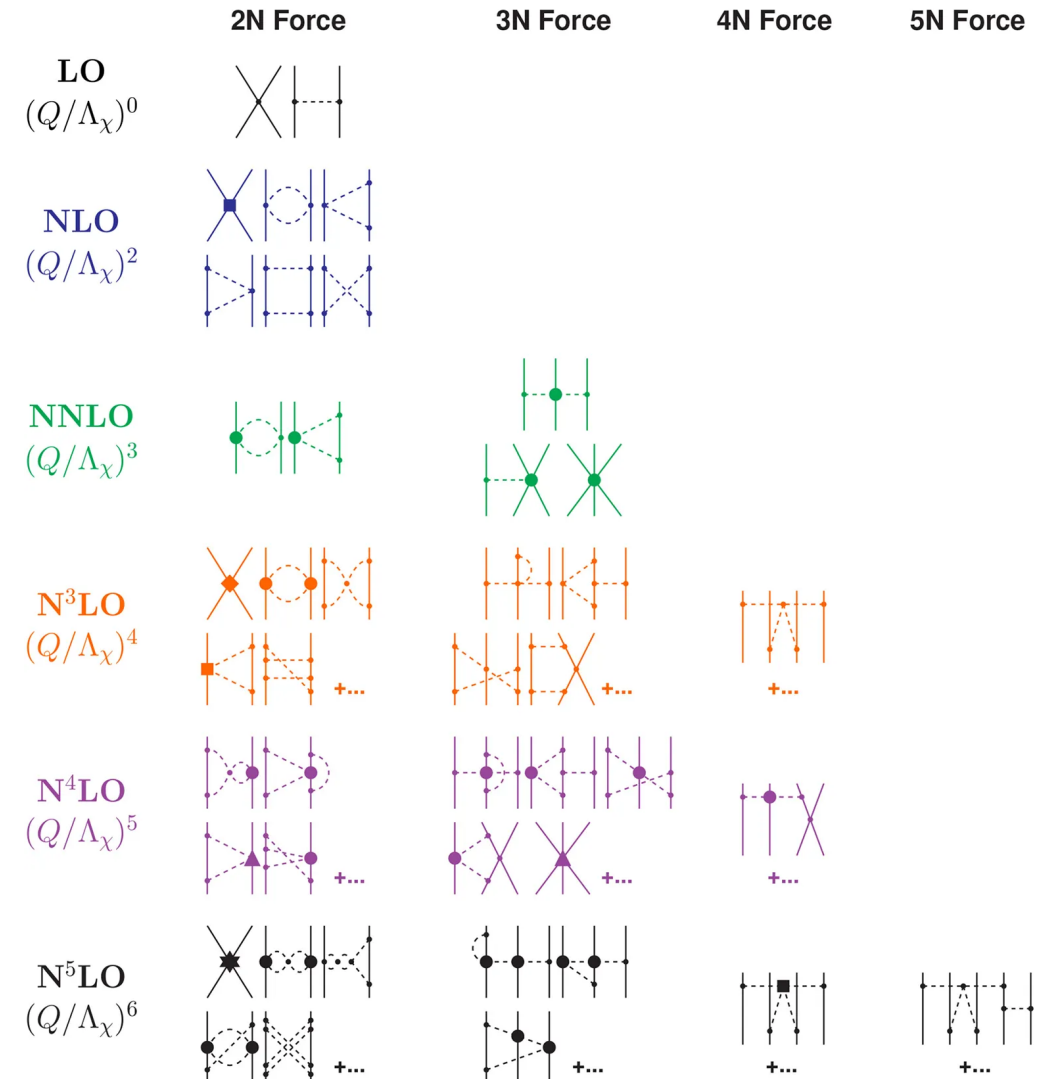
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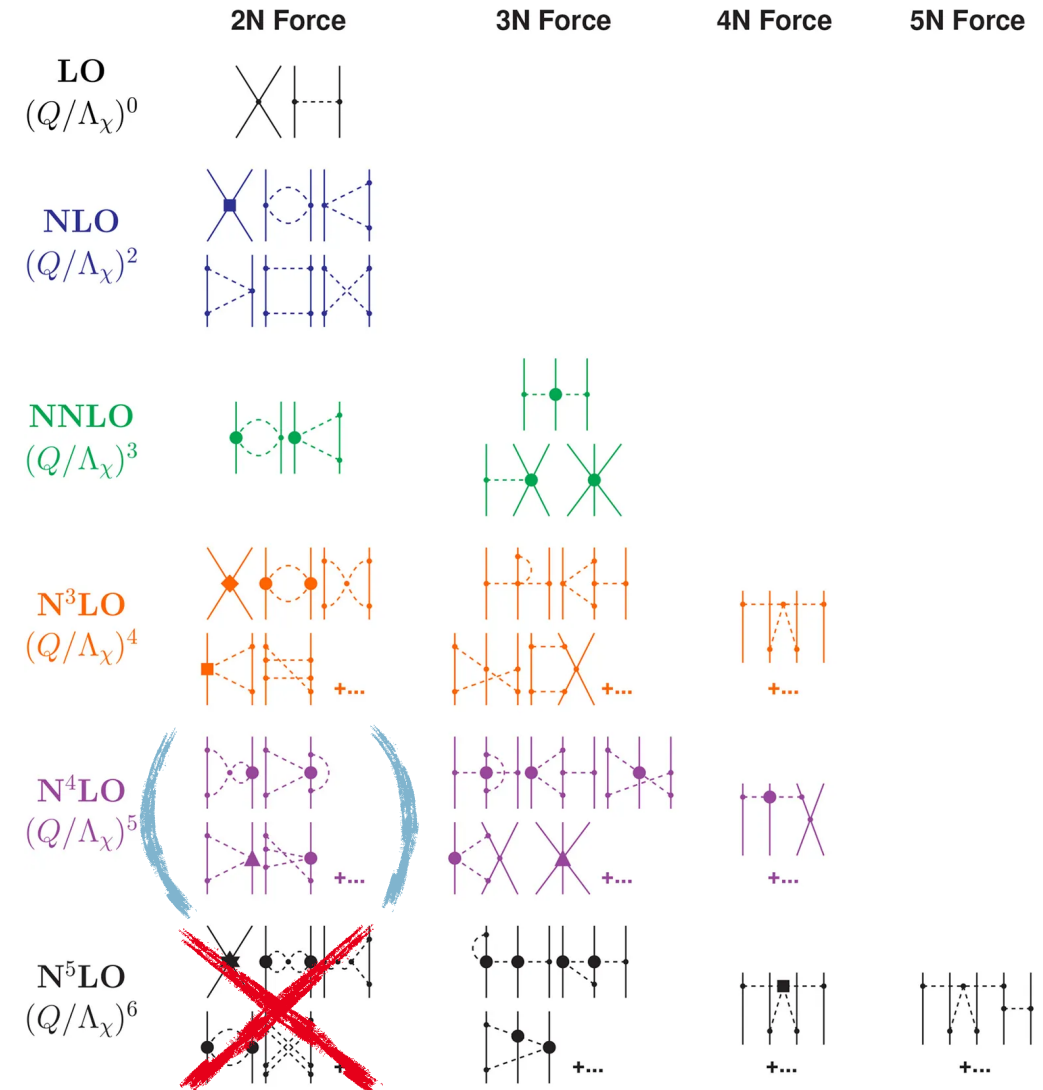
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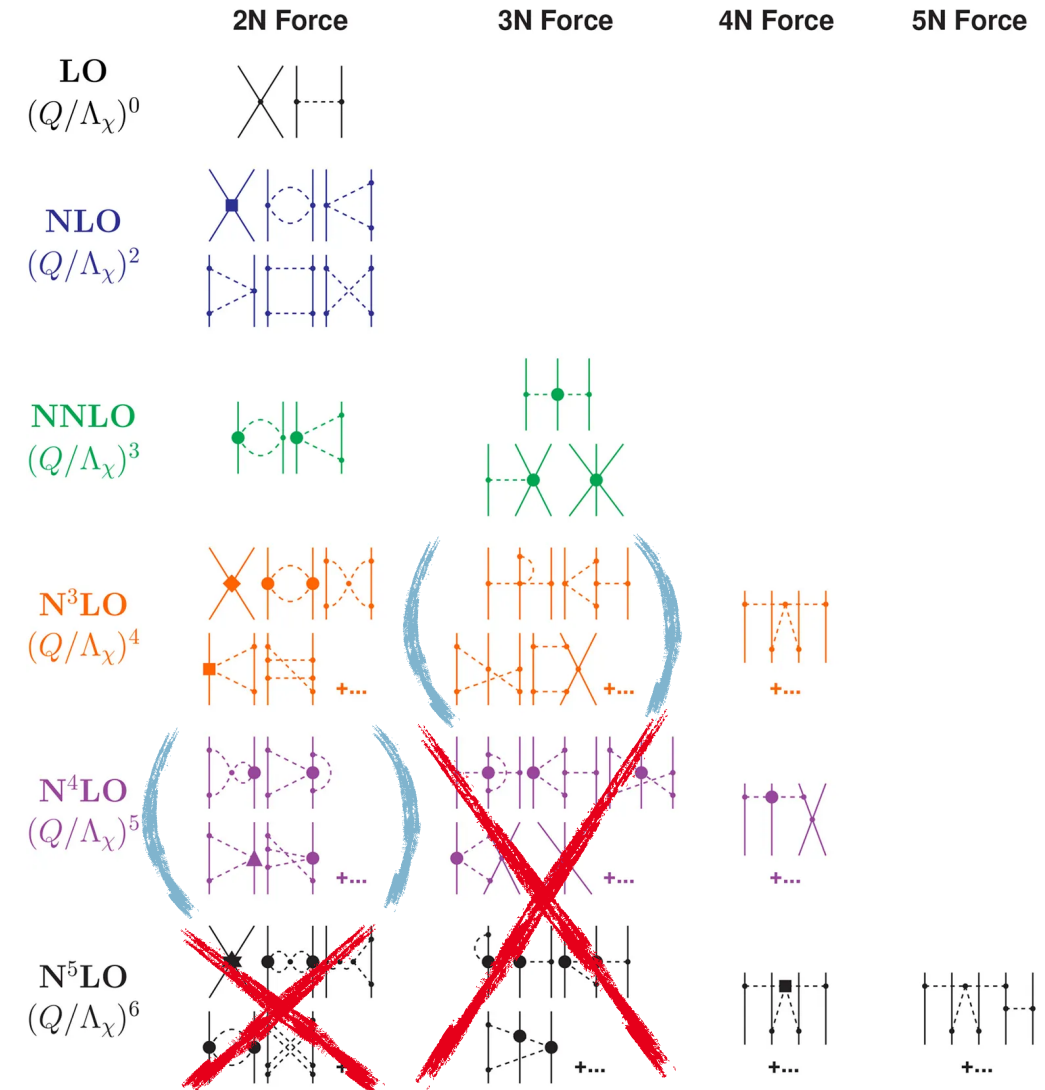
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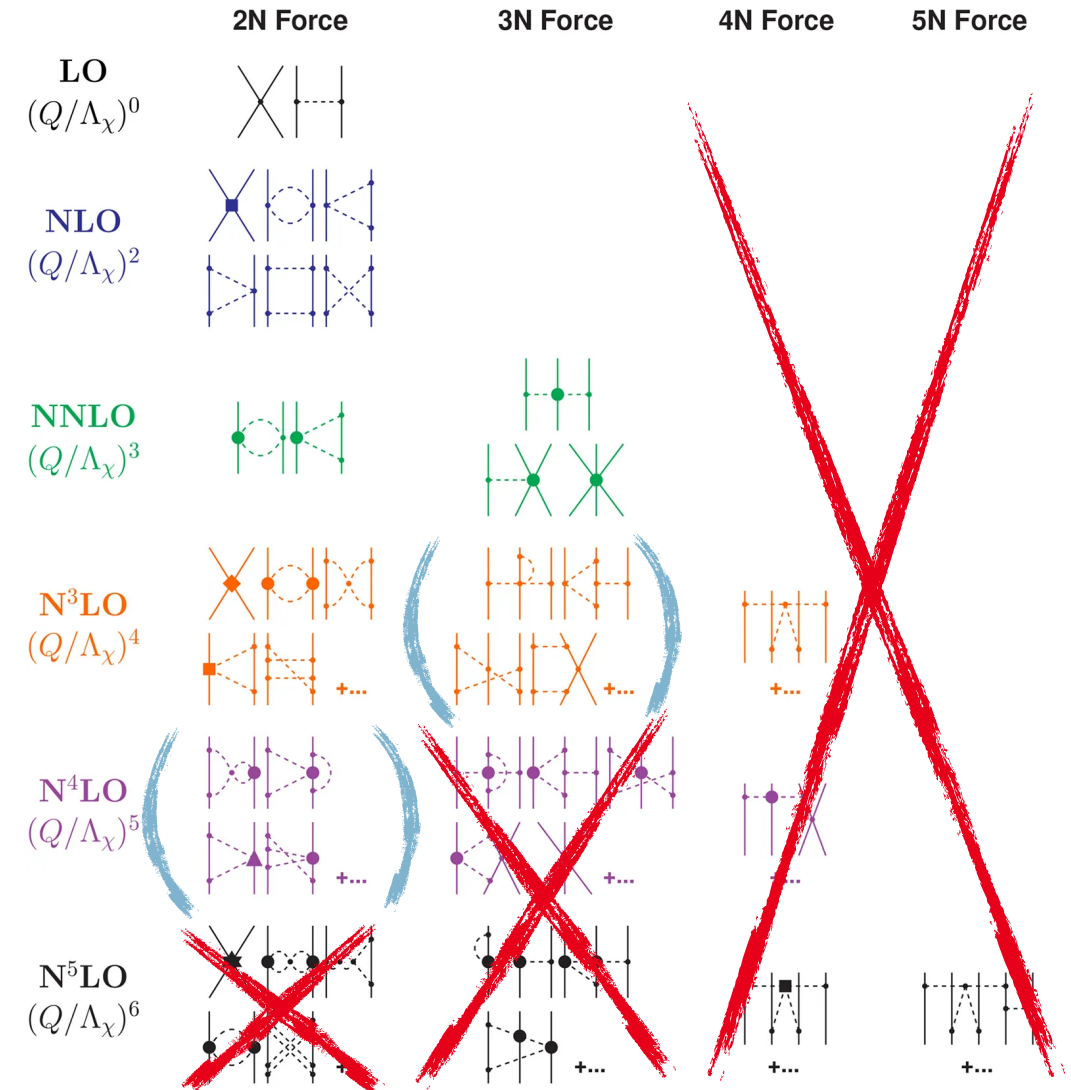
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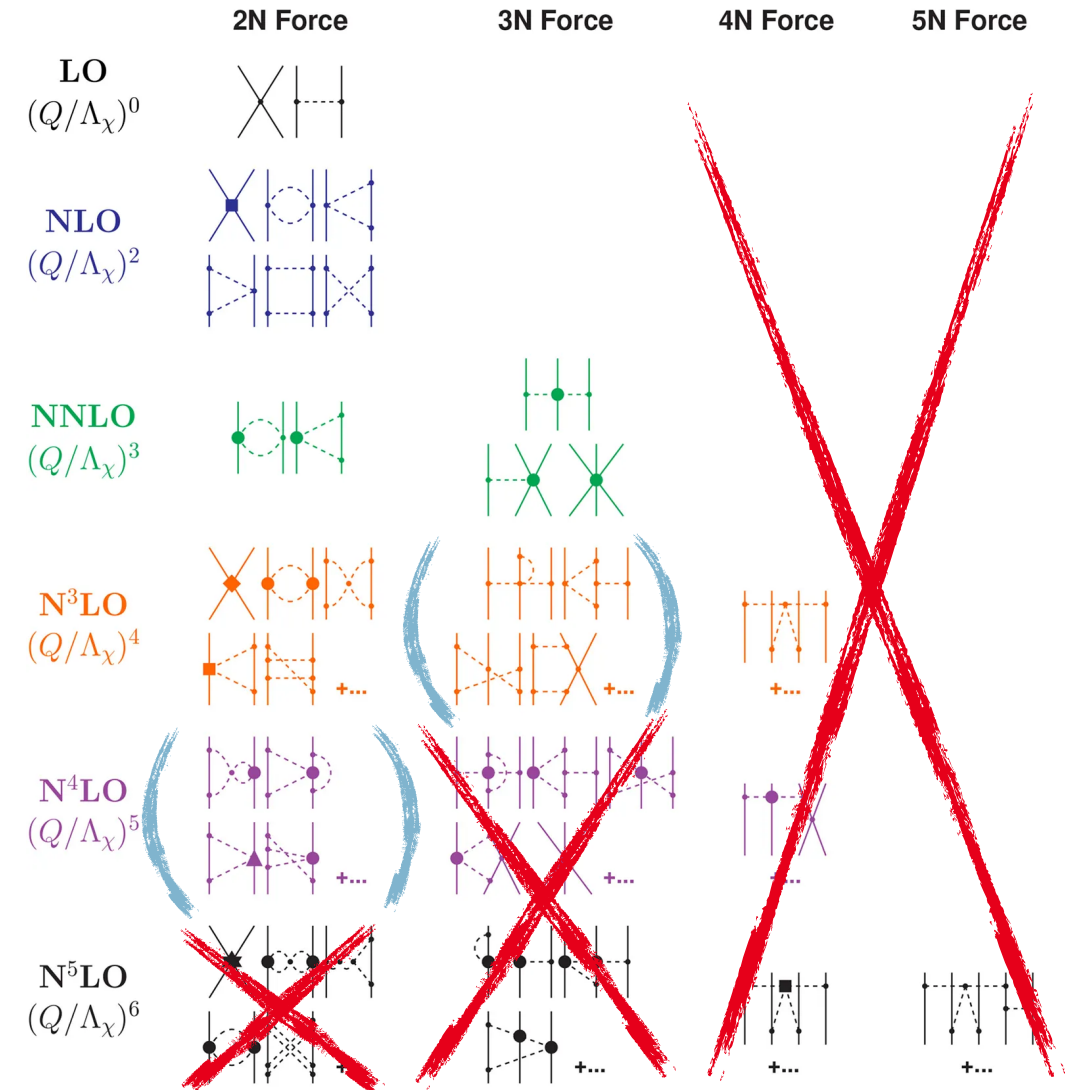
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- **Next order gives an estimate for the error of the truncation:** $(Q/\Lambda_\chi)^{\nu+1}$



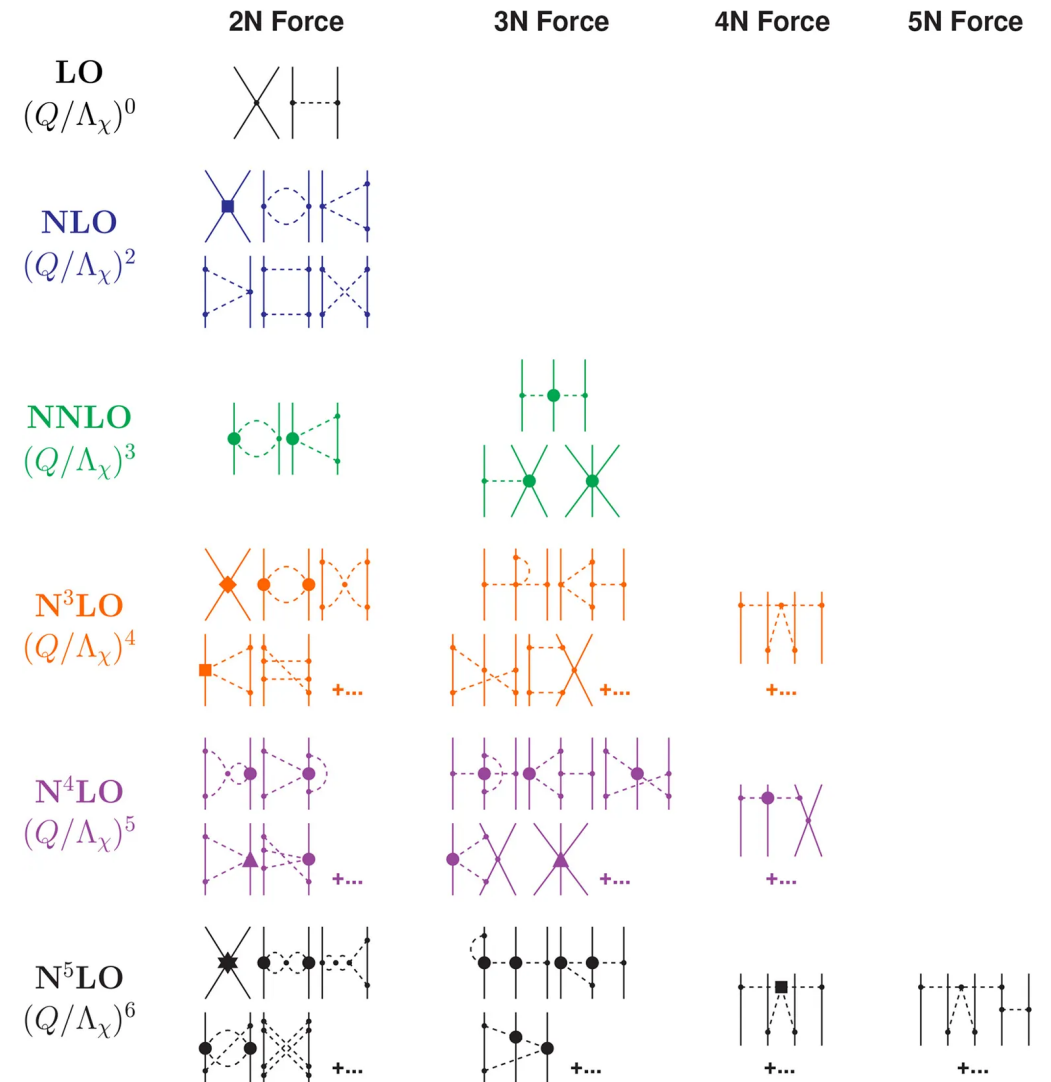
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POWER COUNTING

Weinberg, *Physica A* 96, 327-340 (1979)



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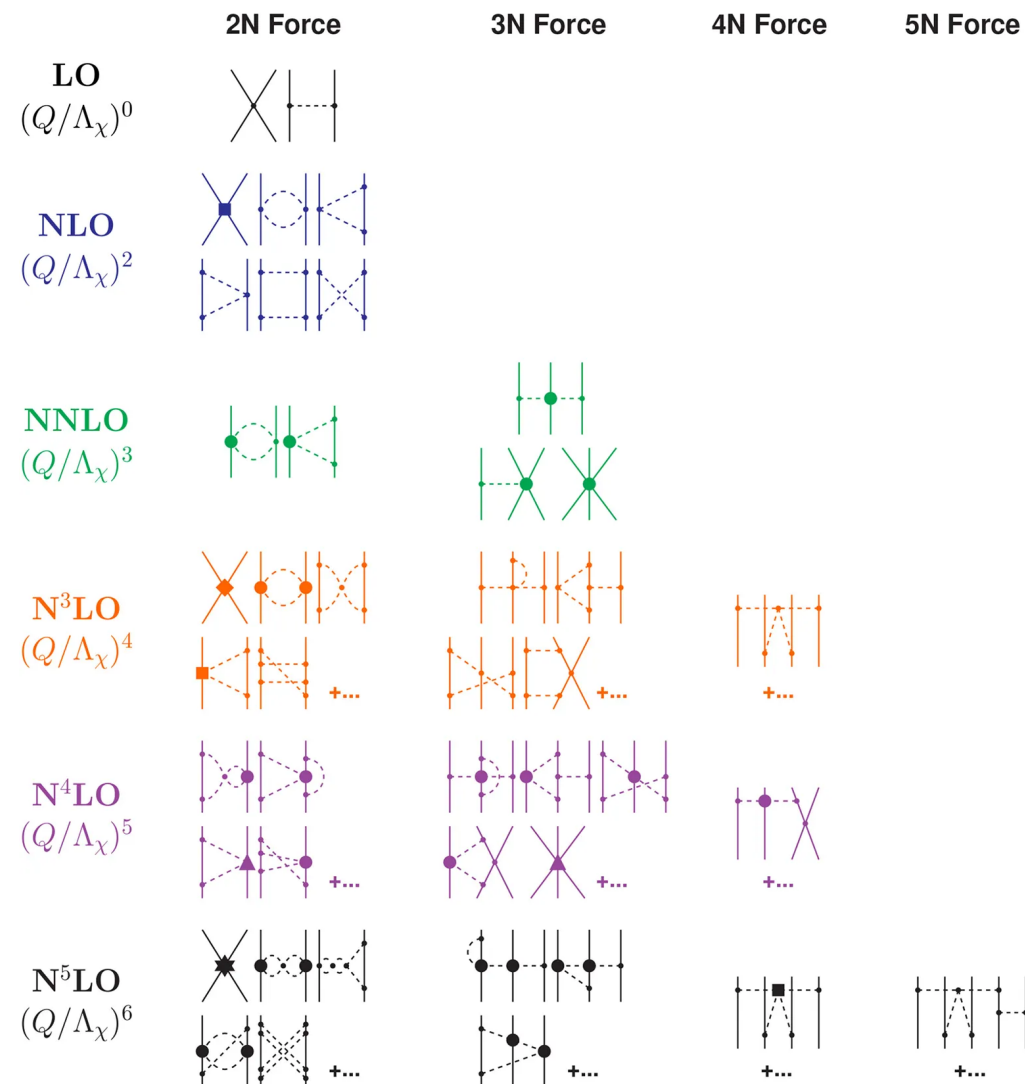
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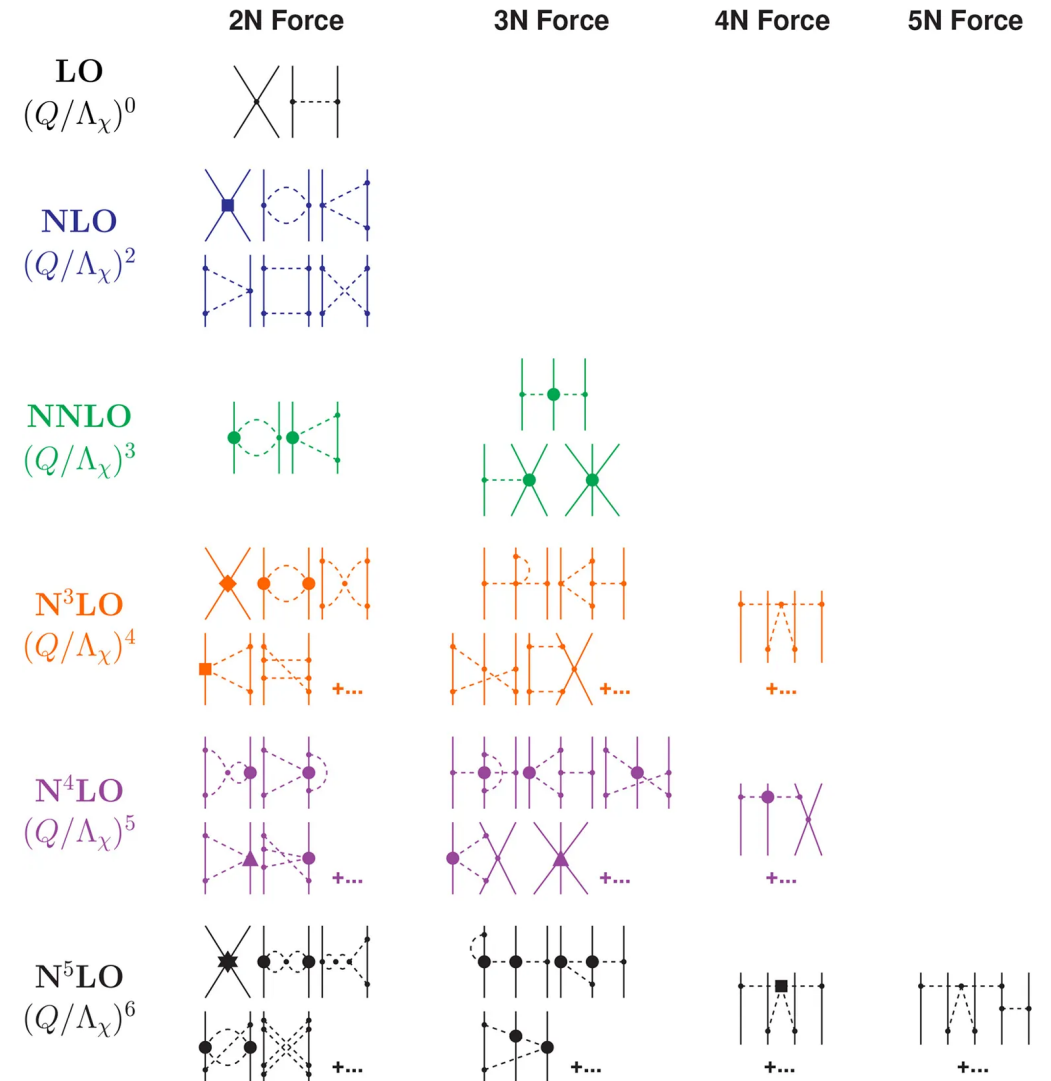
Pion propagator: Q^{-2}

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Four-momentum integration $(\int d^4p)$: Q^4



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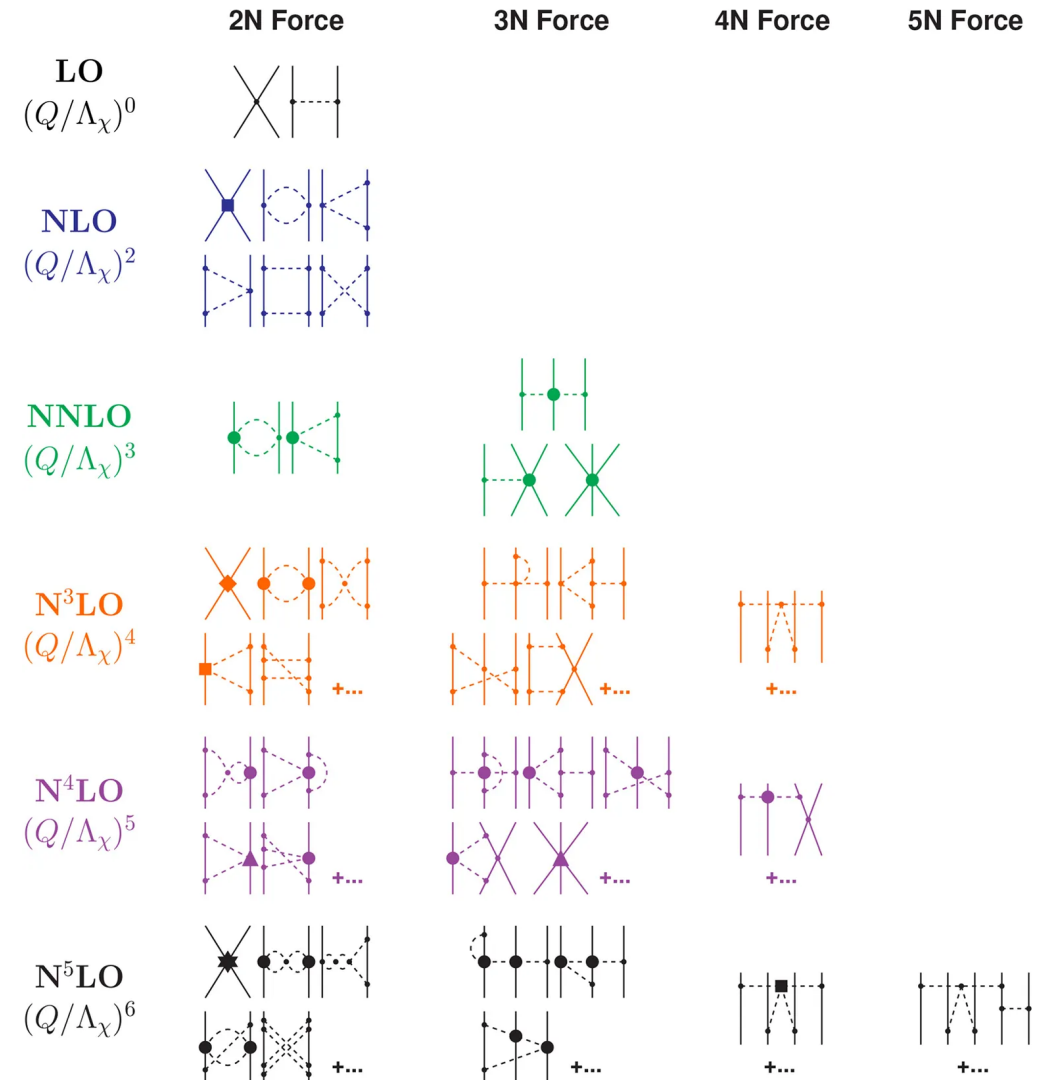
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$$\nu = -2 + 2A - 2C + 2L + \sum_i \Delta_i, \quad \Delta_i \equiv d_i + \frac{n_i}{2} - 2$$



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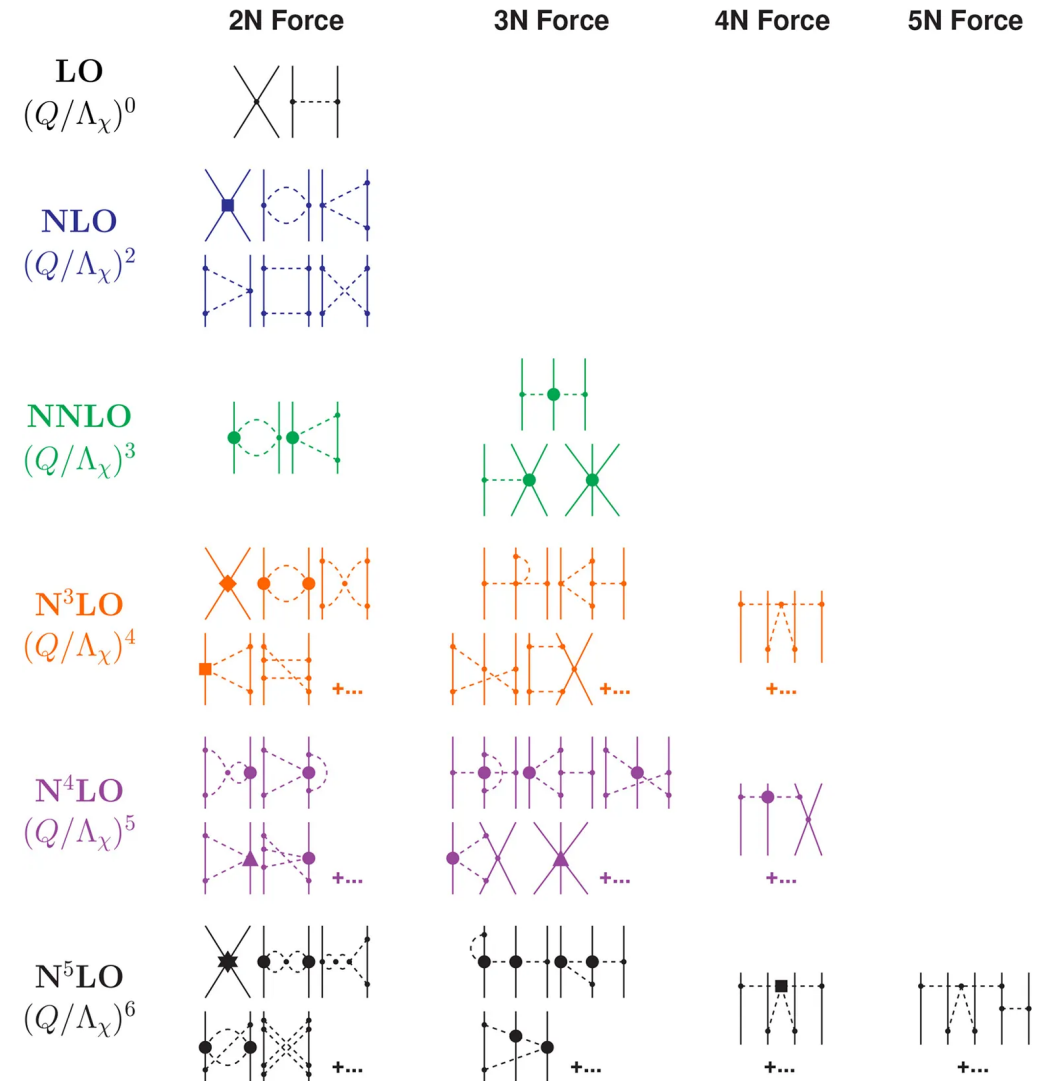
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(mN : $2N, 3N, \dots$)



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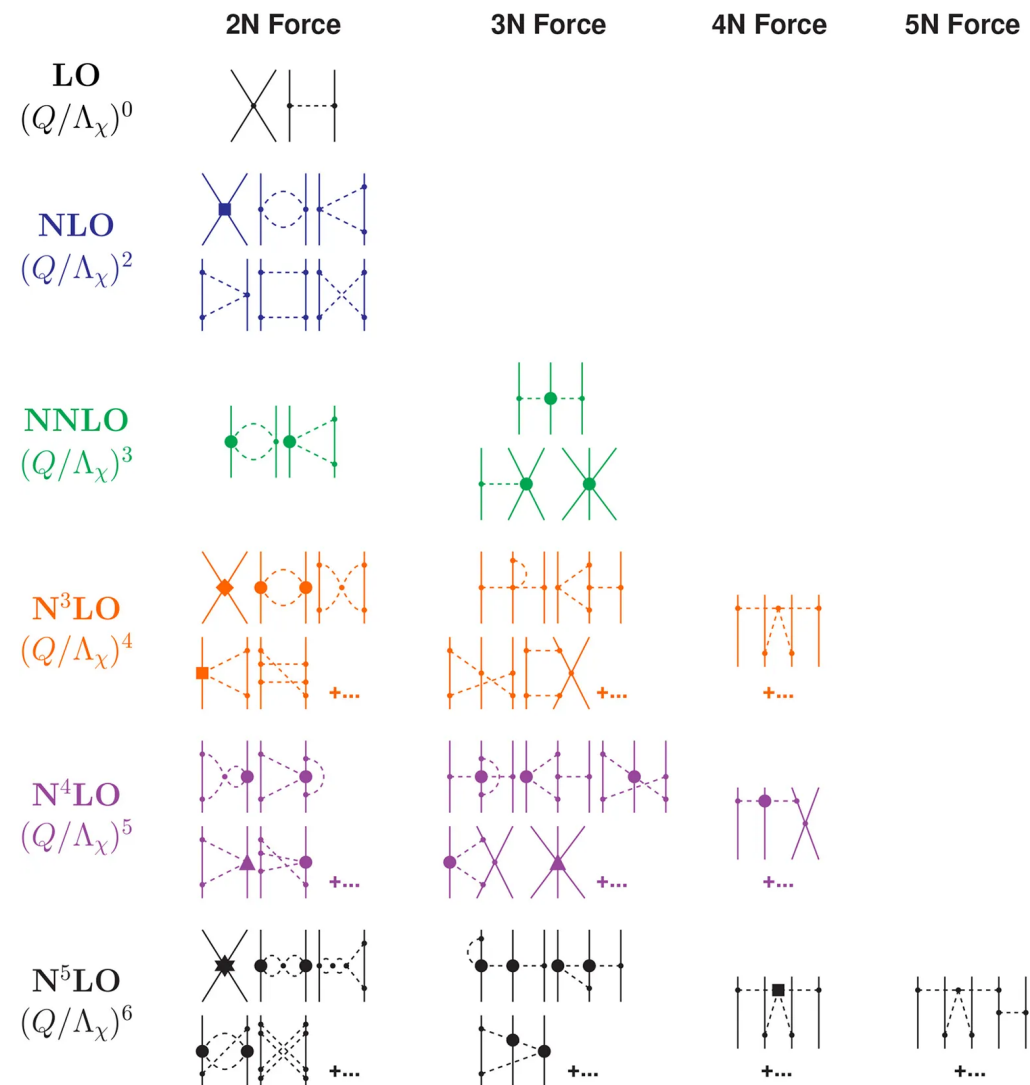
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#Loops

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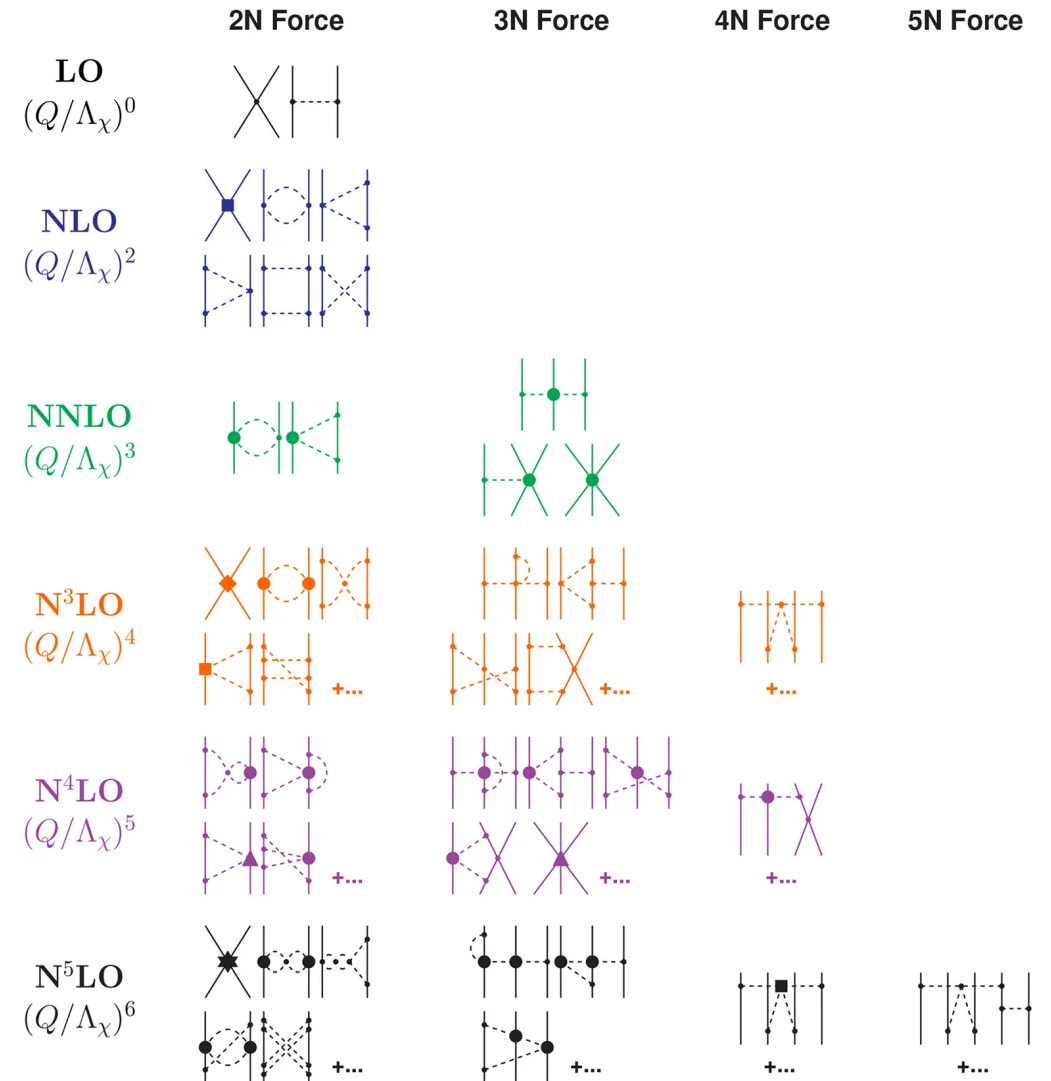
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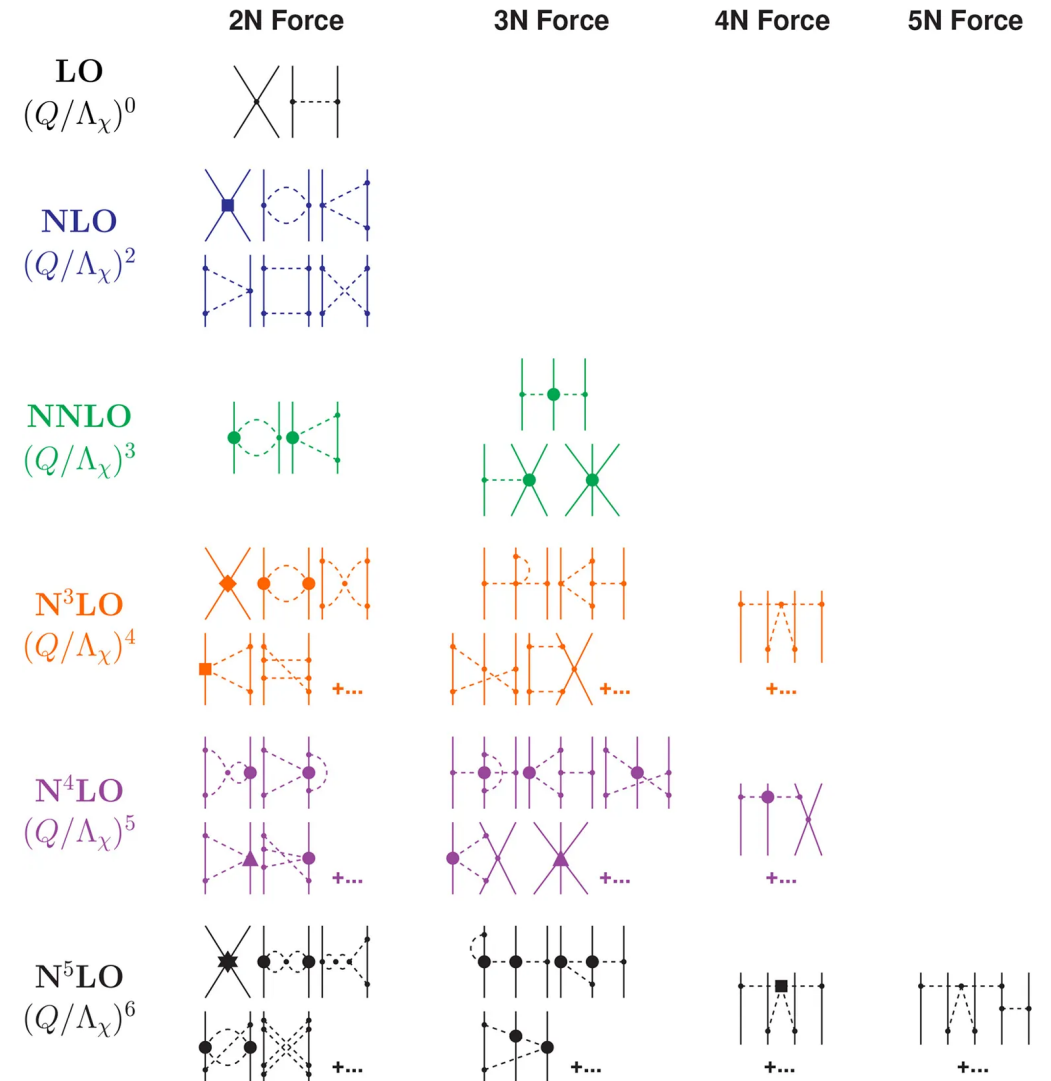
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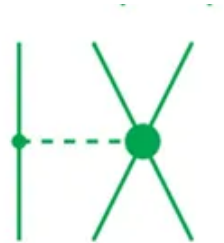
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Vertex indices

	•	●	■	▲	◆	★
Δ_i	0	1	2	3	4	6

Examples:



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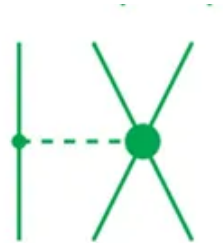
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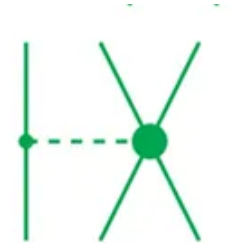
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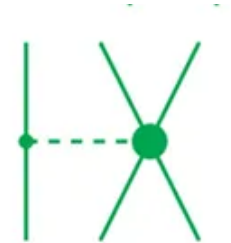
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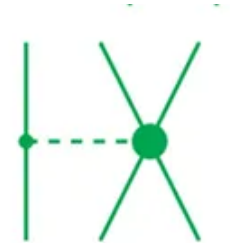
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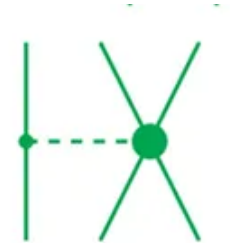
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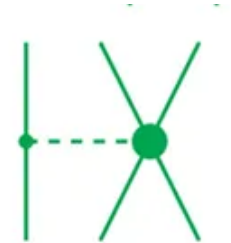
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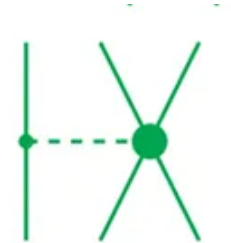
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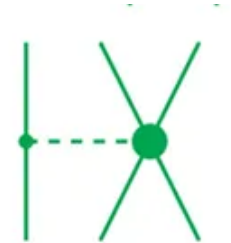
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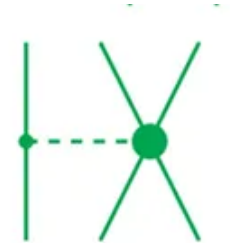
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$$\rightarrow \nu = 0 \text{ (LO)}$$

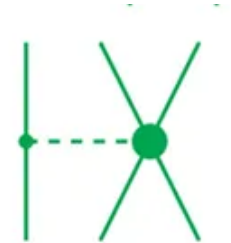


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POWER COUNTING: EXAMPLES

- Power of a connected irreducible A -nucleon diagram:

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- $\Delta_i \equiv d_i + \frac{n_i}{2} - 2$

Vertex indices

	•	●	■	▲	◆	★
Δ_i	0	1	2	3	4	6

Examples:



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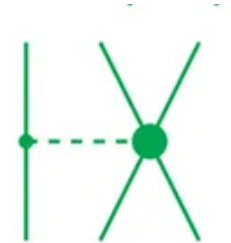
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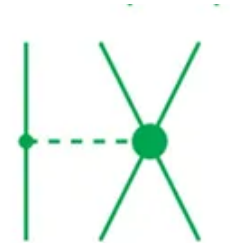
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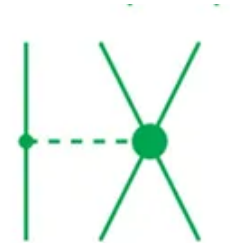
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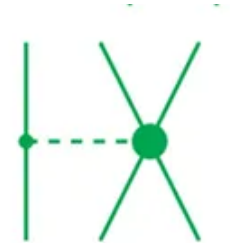
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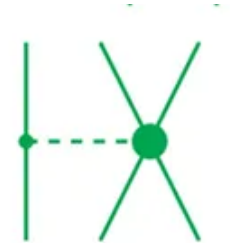
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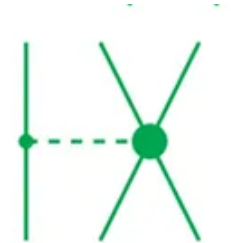
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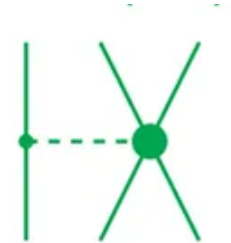
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LEADING-ORDER NN POTENTIAL

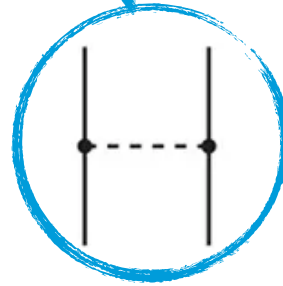


$$V_{\text{LO}}^{NN} = V_{1\pi} + V_{\text{ct}}^{(0)} = -\frac{g_A^2}{4F_\pi^2} \tau_1 \cdot \tau_2 \frac{\boldsymbol{\sigma}_1 \cdot \mathbf{q} \boldsymbol{\sigma}_2 \cdot \mathbf{q}}{q^2 + m_\pi^2} + C_S + C_T \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$$

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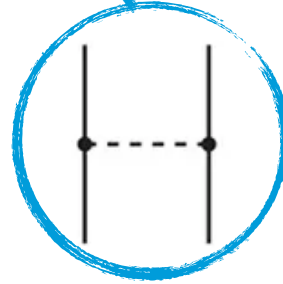
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Axial-vector coupling constant: $g_A \sim 1.29$

Pion decay constant: $F_\pi \sim 92 \text{ MeV}$

Momentum exchange: $\mathbf{q} = \mathbf{p}' - \mathbf{p}$

$\boldsymbol{\tau}$, $\boldsymbol{\sigma}$ isospin and spin operators



LEADING-ORDER NN POTENTIAL



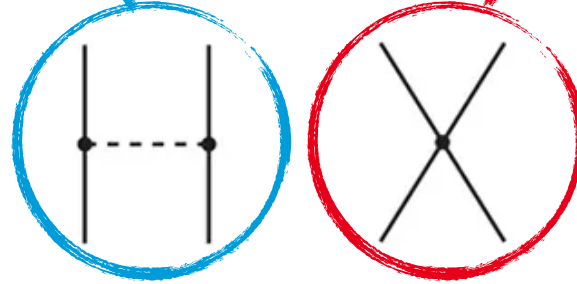
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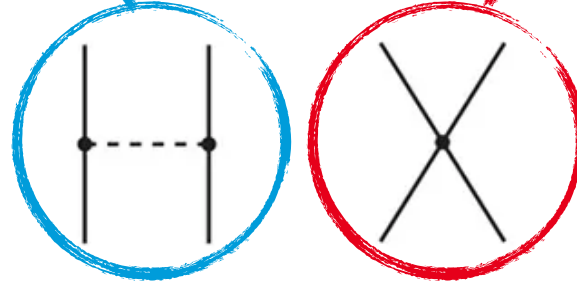


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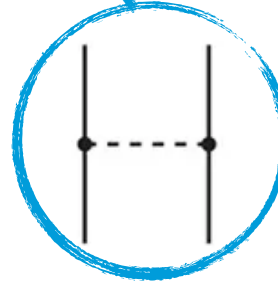
C_S , C_T low-energy
constants (LECs)
fitted to NN data

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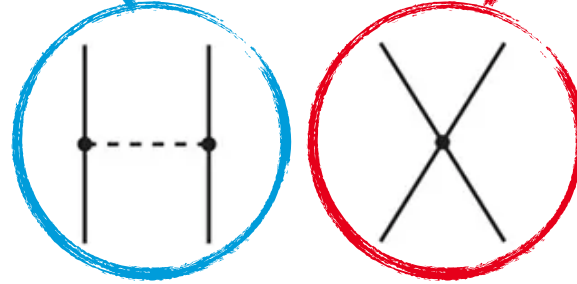
- Where does the **charge-dependence** enter (positively charged protons vs neutral neutrons)?

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C_S , C_T low-energy
constants (LECs)
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- Where does the **charge-dependence** enter (positively charged protons vs neutral neutrons)?
- Charge dependence taken into account in the pion-exchange terms:

$$V_{1\pi}^{(pp)}(\mathbf{p}, \mathbf{p}') = V_{1\pi}^{(nn)}(\mathbf{p}, \mathbf{p}') = V_{1\pi}(m_{\pi^0})$$

$$V_{1\pi}^{(np)}(\mathbf{p}', \mathbf{p}) = -V_{1\pi}(m_{\pi^0}) + (-1)^{I+1} 2V_{1\pi}(m_{\pi^\pm})$$

REGULATORS

Entem, Machleidt, Nosyk, Phys. Rev. C 96, 024004 (2017)



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REGULATORS

Entem, Machleidt, Nosal, Phys. Rev. C 96, 024004 (2017)



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- The potential satisfies the non-relativistic **Lippmann-Schwinger equation**

$$\hat{T}(\mathbf{p}', \mathbf{p}) = \hat{V}(\mathbf{p}', \mathbf{p}) + \int d^3\mathbf{p}'' \hat{V}(\mathbf{p}', \mathbf{p}'') \frac{M_N}{p^2 - p''^2 + i\epsilon} \hat{T}(\mathbf{p}'', \mathbf{p}),$$

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- Need to introduce a **regulator**

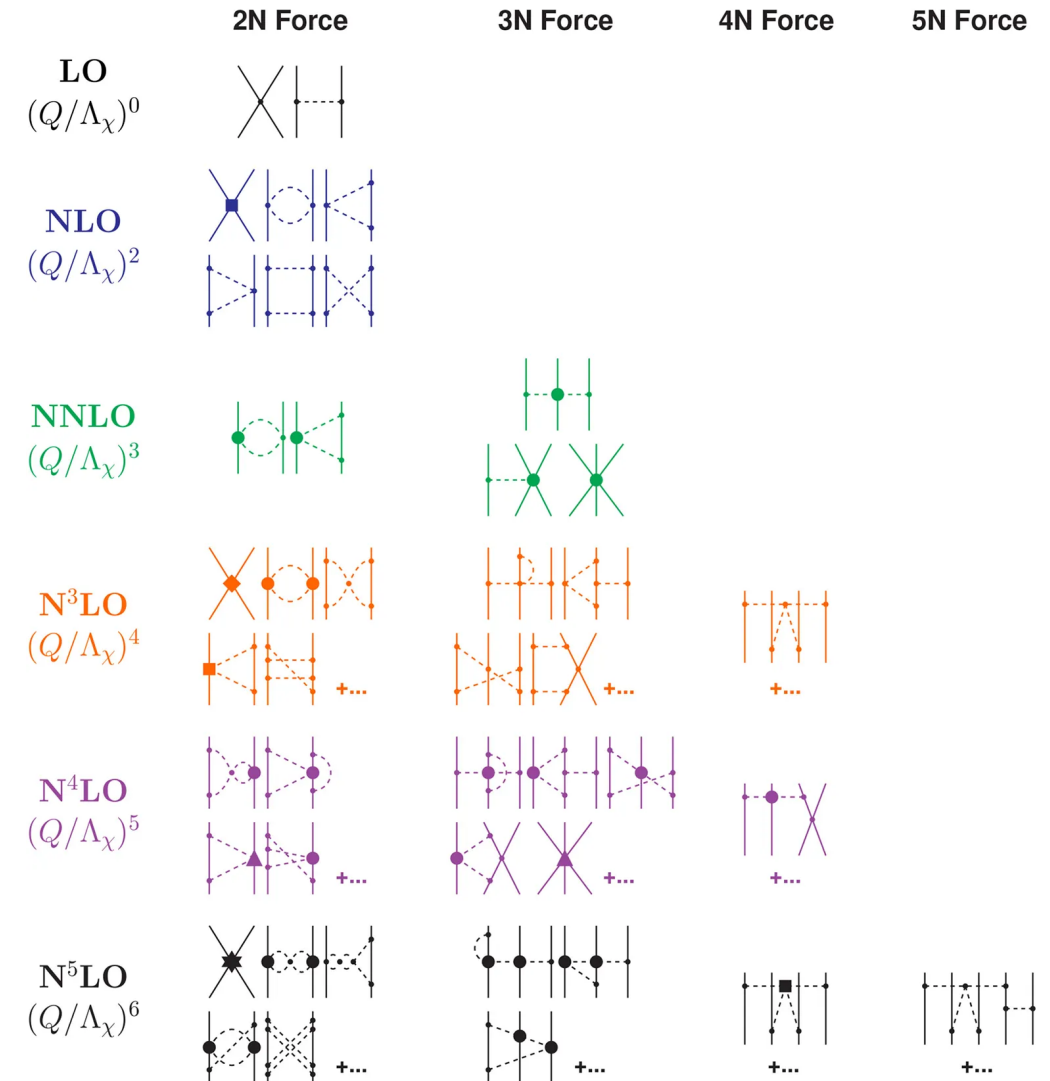
$$\hat{V}(\mathbf{p}', \mathbf{p}) \rightarrow e^{-(p'/\Lambda)^{2n}} \hat{V}(\mathbf{p}', \mathbf{p}) e^{-(p/\Lambda)^{2n}} \approx \hat{V}(\mathbf{p}', \mathbf{p}) \left(1 - \left[\left(\frac{p'}{\Lambda} \right)^{2n} + \left(\frac{p}{\Lambda} \right)^{2n} \right] + \dots \right),$$

where typically $n = 2$ and $\Lambda \in \{450 \text{ MeV} \dots 550 \text{ MeV}\}$

THE LOW-ENERGY CONSTANTS



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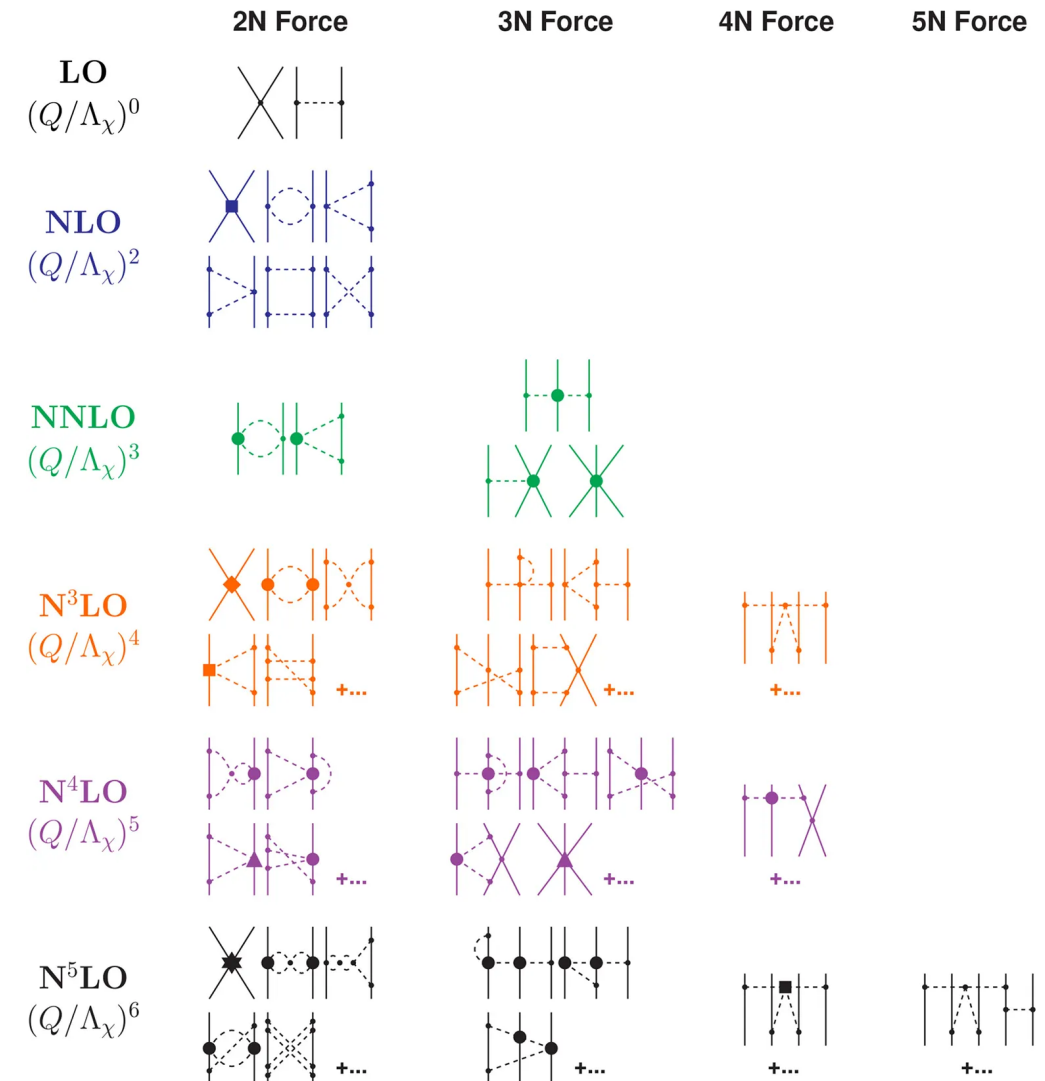


Entem, Machleidt, Nosyk, *Phys. Rev. C* 96, 024004 (2017)

THE LOW-ENERGY CONSTANTS



- High-energy dynamics of the QCD (heavy-meson exchange) integrated out in χ EFT absorbed in the so-called **low-energy constants**

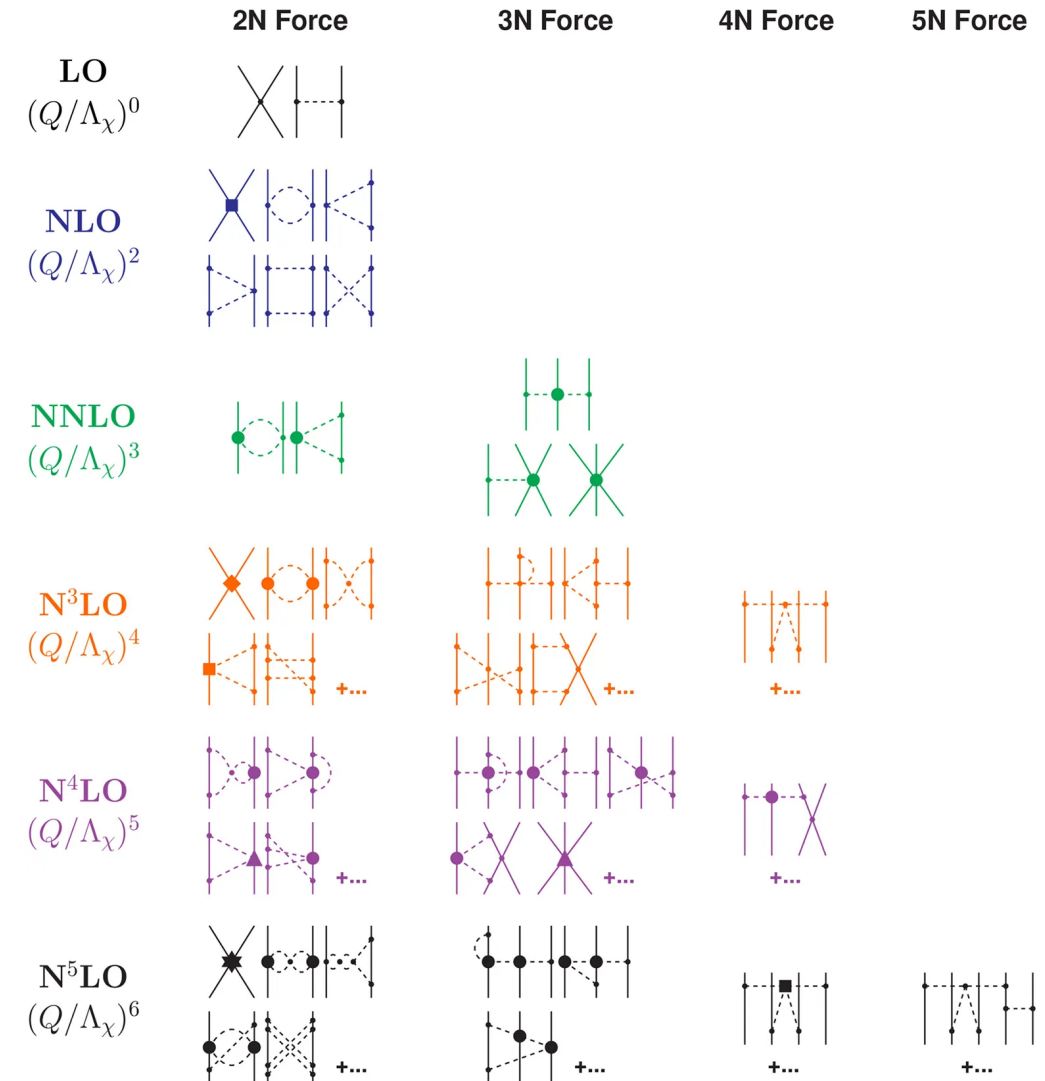


Entem, Machleidt, Nosyk, *Phys. Rev. C* 96, 024004 (2017)

THE LOW-ENERGY CONSTANTS



- **High-energy dynamics of the QCD**
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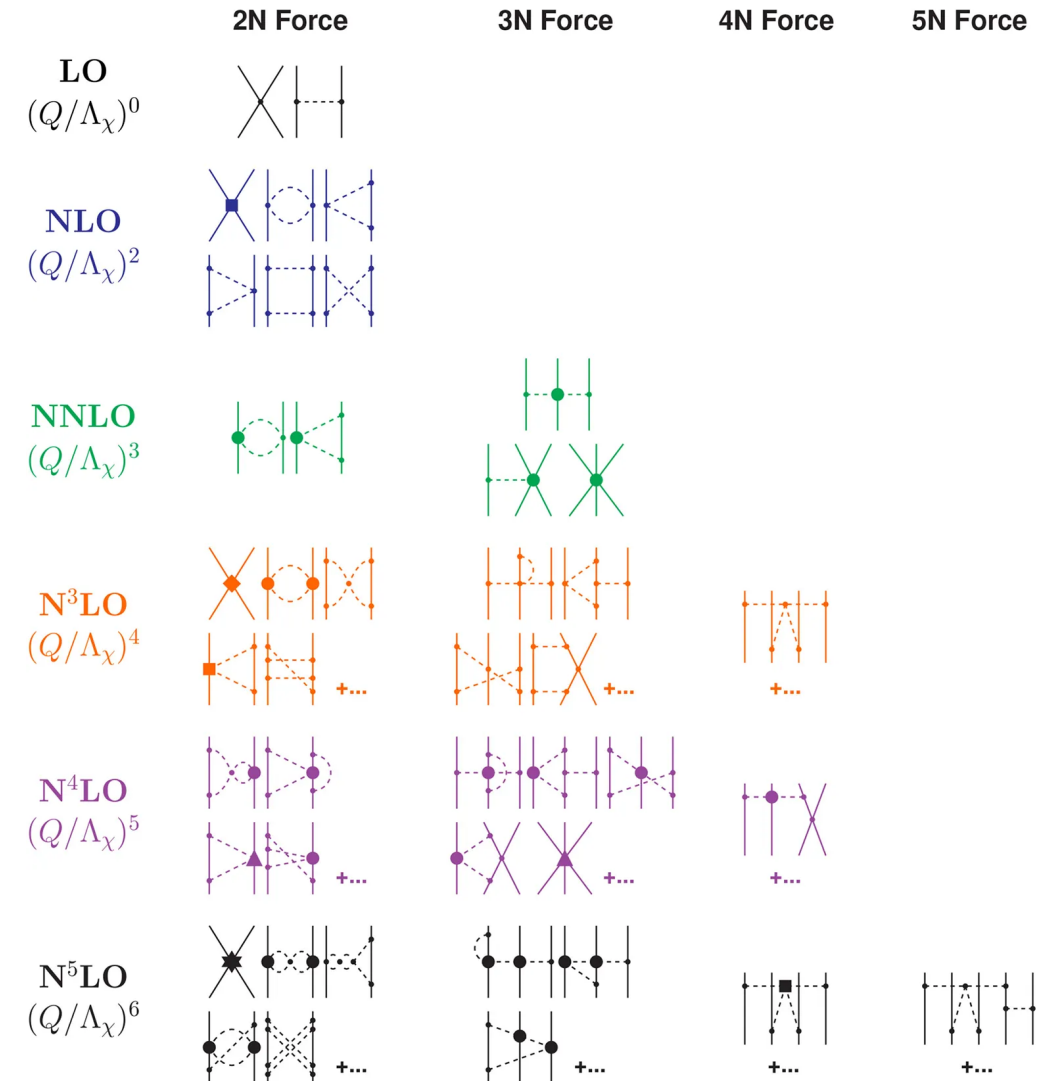


Entem, Machleidt, Nosyk, *Phys. Rev. C* 96, 024004 (2017)

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- Ideally, they would be computed with
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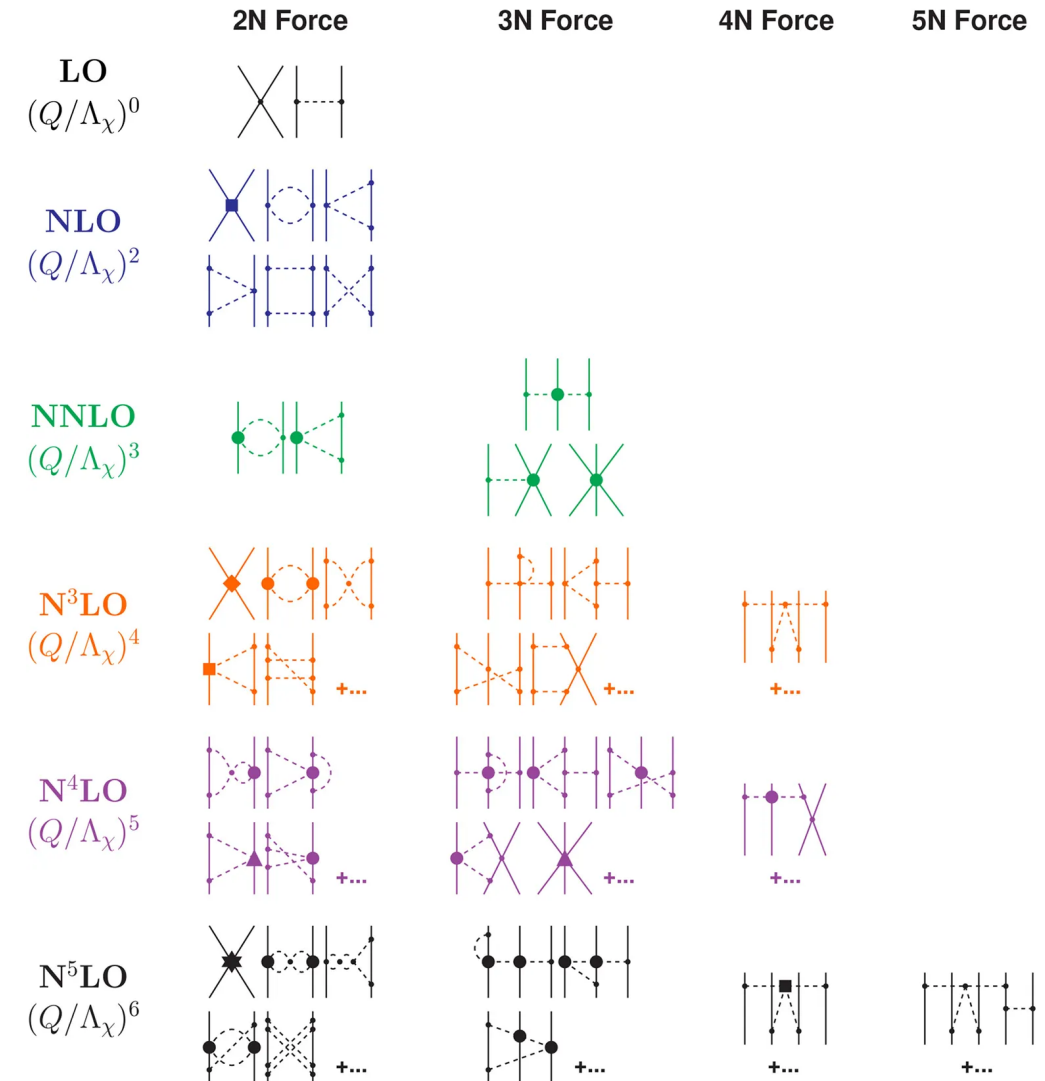


Entem, Machleidt, Nosyk, *Phys. Rev. C* 96, 024004 (2017)

THE LOW-ENERGY CONSTANTS



- **High-energy dynamics of the QCD** (heavy-meson exchange) integrated out in χ EFT absorbed in the so-called **low-energy constants**
- **Unknown couplings**
- Ideally, they would be computed with lattice QCD
- Currently, they are **fitted to experimental data**



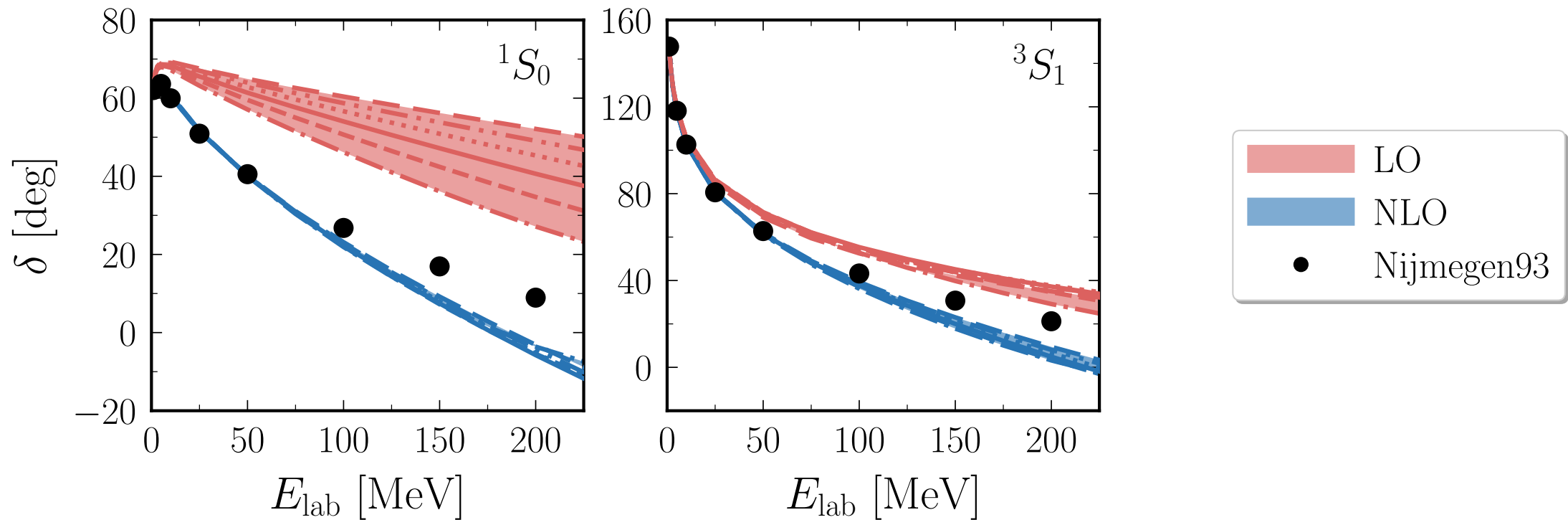
Entem, Machleidt, Nosyk, *Phys. Rev. C* 96, 024004 (2017)

FITTING THE LOW-ENERGY CONSTANTS



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To few-nucleon data (nucleon-nucleon, pion-nucleon scattering)



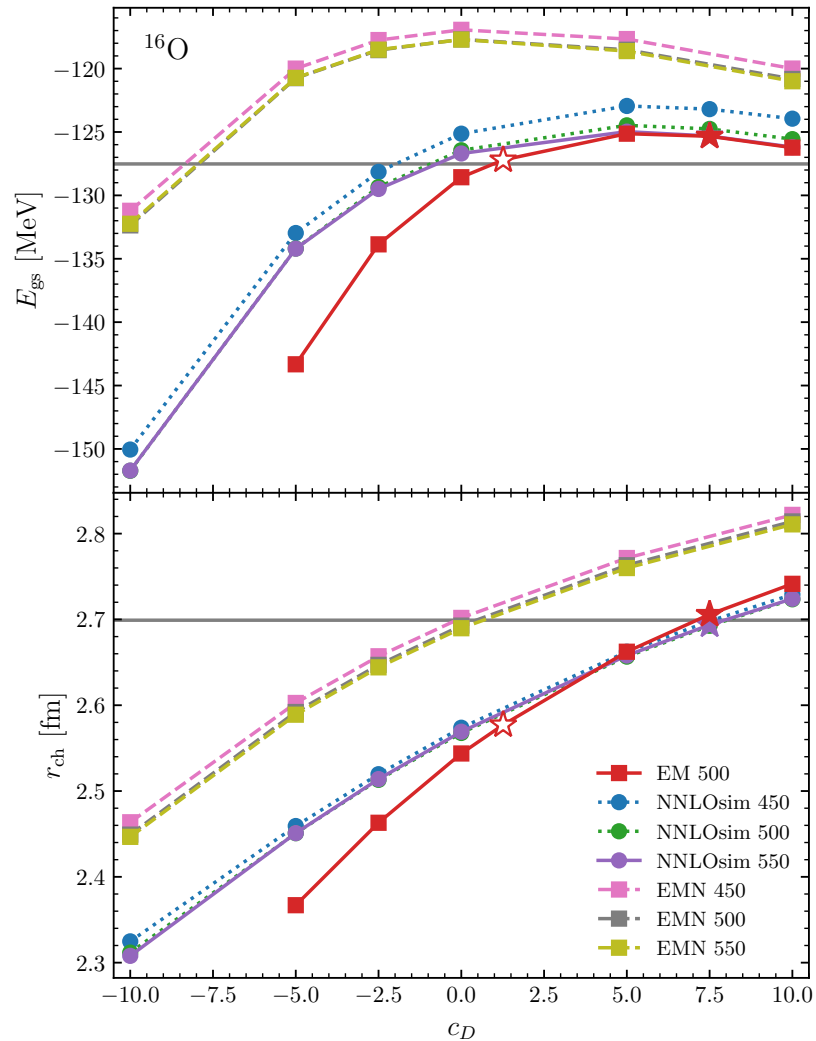
Ren, Epelbaum, Gegelia, Phys.Rev.C 113, 034002 (2026)

FITTING THE LOW-ENERGY CONSTANTS



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To selected nuclear data (ground-state energies and radii of light nuclei)



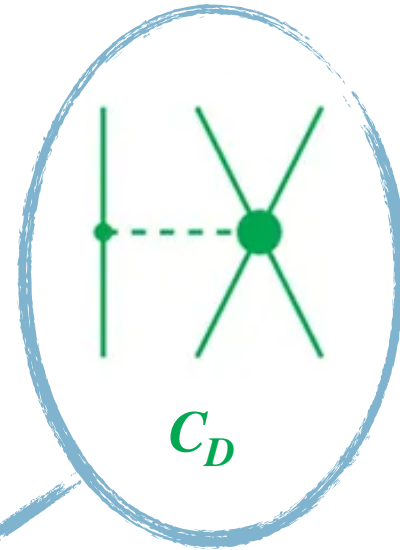
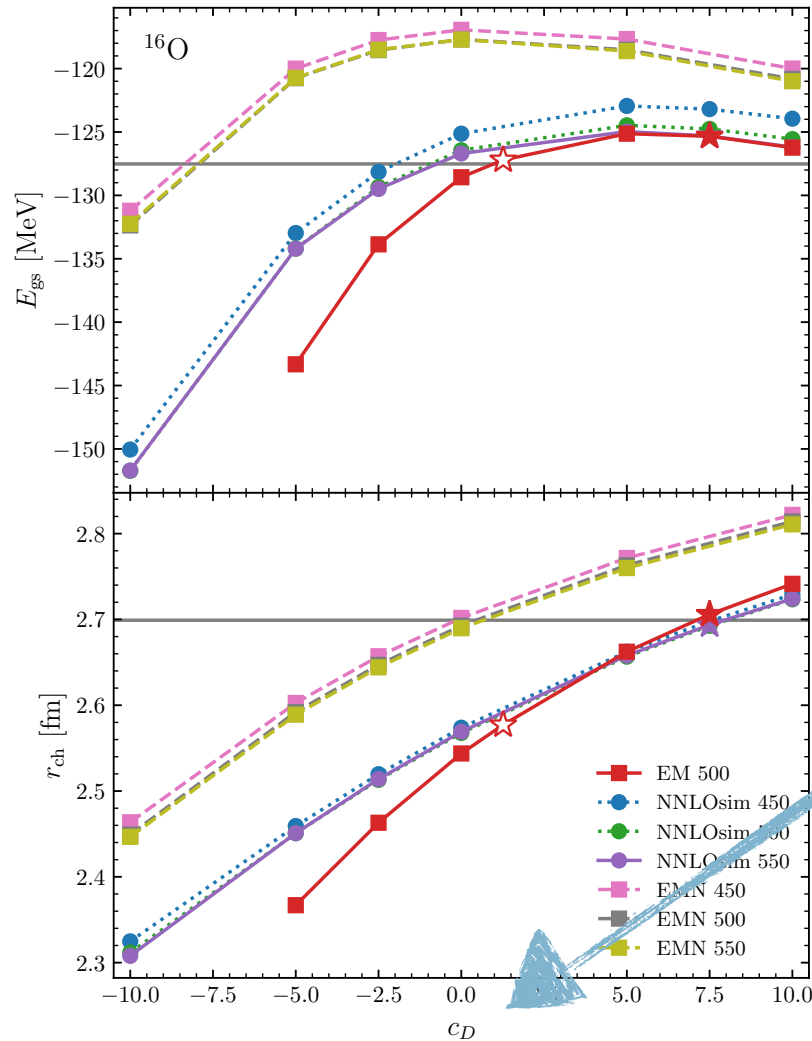
Arthuis, Hebeler, Schwenk,
Eur. Phys. J. A 62, 156 (2026)

FITTING THE LOW-ENERGY CONSTANTS



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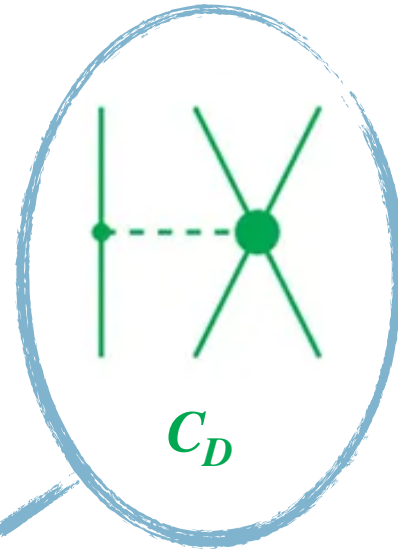
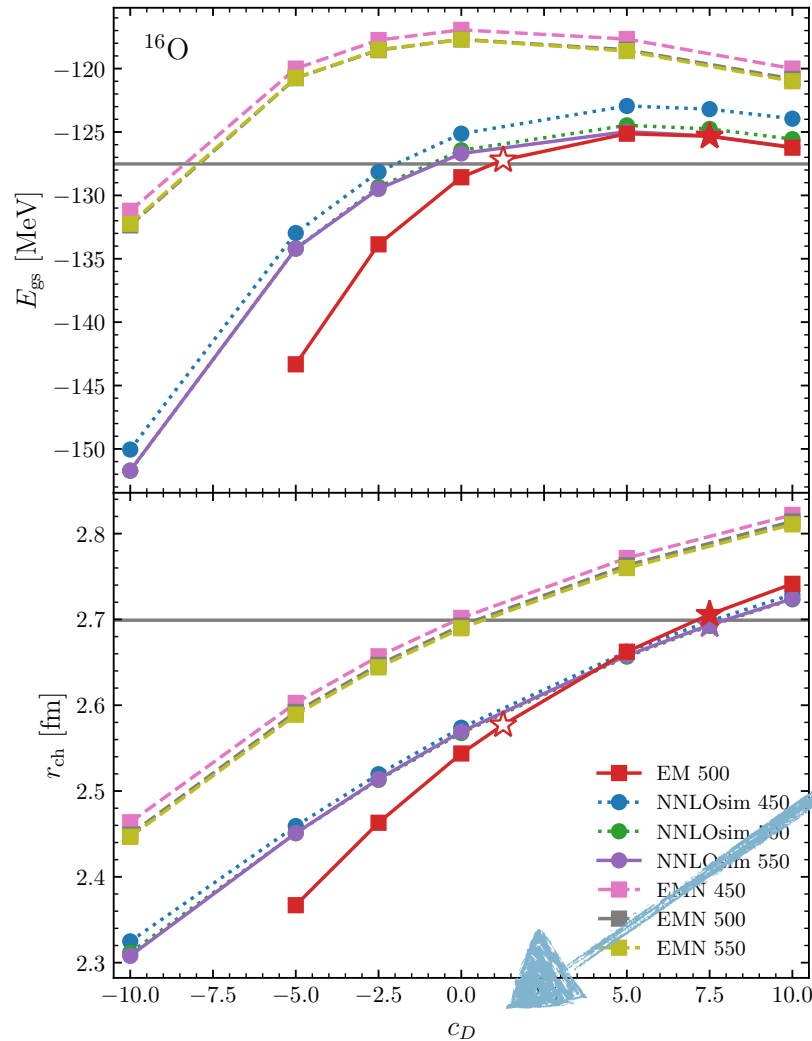
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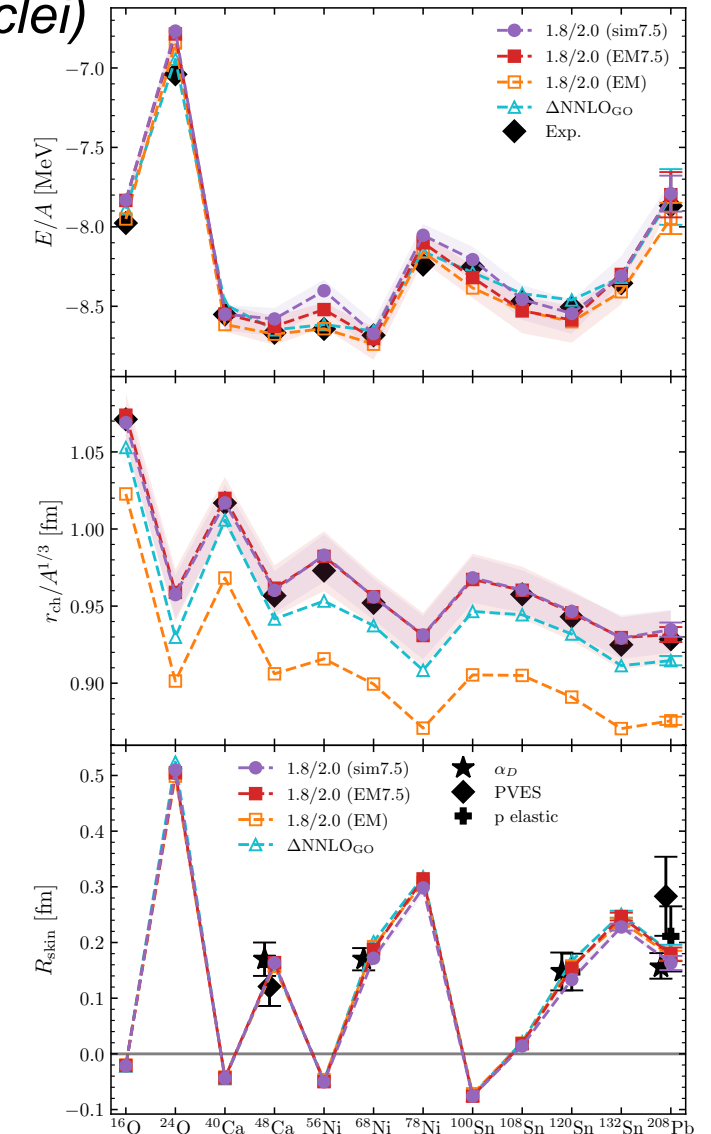


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Arthuis, Hebeler, Schwenk,
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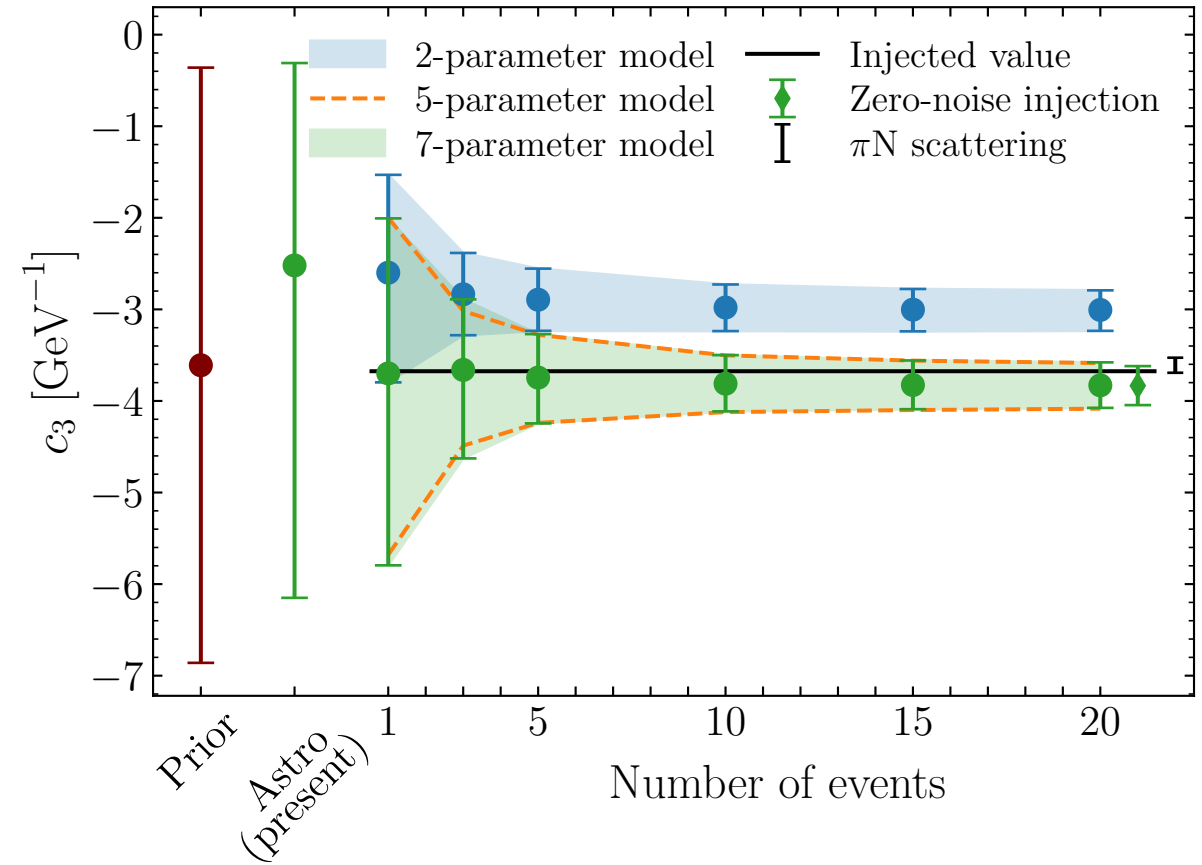
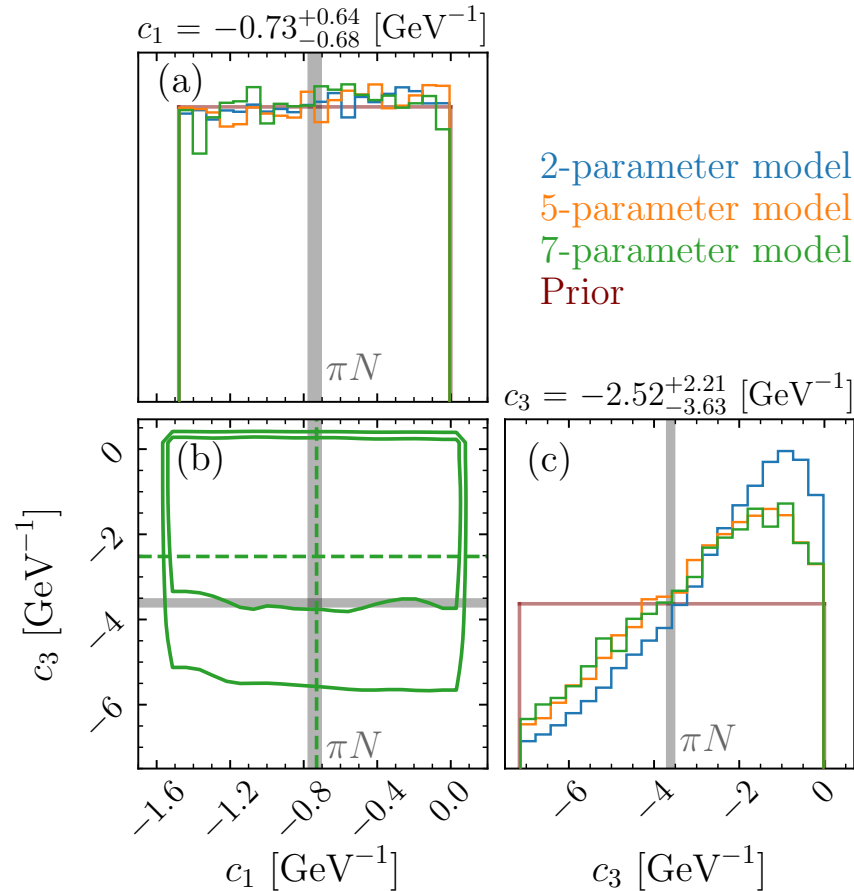


FITTING THE LOW-ENERGY CONSTANTS



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To nuclear matter (astrophysical neutron-star observations)



Somasundaram, Svensson, De, Deneris, Dietz, Landry, Schwenk, Tews, *Nat. Commun.* 16, 9819 (2025)

TAKE-HOME MESSAGES

- *Ab initio* (or first principles) nuclear theory is based nuclear interactions derived from chiral effective field theory
- Chiral effective field theory is a low-energy framework of quantum chromodynamics, where the degrees of freedom are nucleons and pions
- Chiral effective field theory generates two-nucleon, three-nucleon, and multi-nucleon forces on an equal footing
- Diagrams contributing to the forces can be systematically arranged by importance using power counting
- The systematic expansion allows for uncertainty quantification
- Low-energy constants need to be fitted to experimental data

UP NEXT

Lecture 2 *From nuclear forces to nuclear properties*



OUTLINE

Lecture 1

Introduction to ab initio nuclear theory

Lecture 2

From nuclear forces to nuclear properties

Lecture 3

From weak interactions to nuclear observables

Lecture 4

Nuclear probes of physics beyond the standard model

LECTURE 2

- **Introduction**

Nuclear many-body problem. What is ab initio in nuclear physics?

- **Short reminder of quantum many-body physics**

Particle-hole representation. Wick's theorem. Normal-ordering. Unitary transformations.

- **Different ab initio many-body techniques**

Summary of many-body techniques for very light, light and medium-heavy to heavy nuclei.

NUCLEAR MANY-BODY PROBLEM

$$H^{(A)} \Psi_n^{(A)} = E_n \Psi_n^{(A)}$$

Eigenstate

Eigenenergy

Groundstate: lowest eigenstate

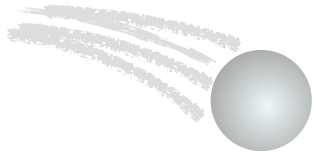
Bound state: $E_n - E_{\text{breakup}} < 0$

Scattering state: $E_n - E_{\text{breakup}} > 0$

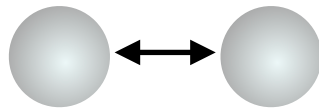
Nuclear Hamiltonian

$$H^{(A)} = \sum_{i=1}^A \frac{p_i^2}{2m} + \sum_{i<j=1}^A V^{NN}(\mathbf{x}_i - \mathbf{x}_j) + \left(\sum_{i<j<k=1}^A V^{3N} \right)$$

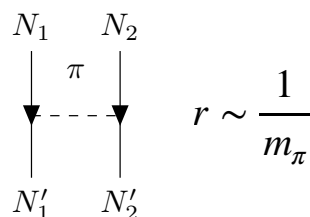
Kinetic energy
of a nucleon



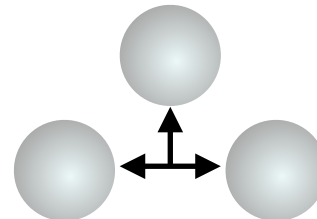
Interaction between
two nucleons



(Pion exchange)

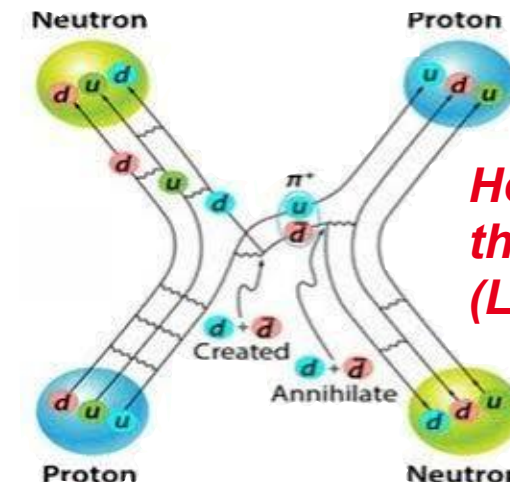


Interaction between
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*How to describe the
many-body states?
(Lecture 2)*

*How to solve the
nuclear many-body
problem? (Lecture 2)*



*How to model
the nuclear force?
(Lecture 1)*

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NUCLEAR MANY-BODY PROBLEM

Spatial, spin and isospin
degrees of freedom:

$$\mathbf{x}_i \equiv \{\mathbf{r}_i, \sigma_i, \tau_i\}$$

$$H^{(A)} \Psi_n^{(A)} = E_n \Psi_n^{(A)}$$

Eigenstate

Eigenenergy

Groundstate: lowest eigenstate

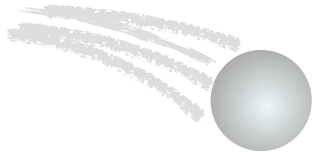
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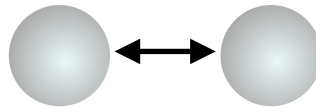
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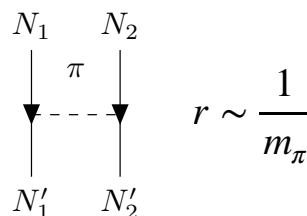
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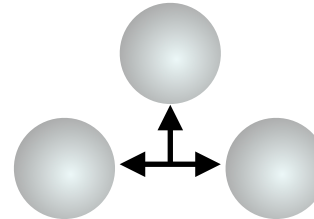
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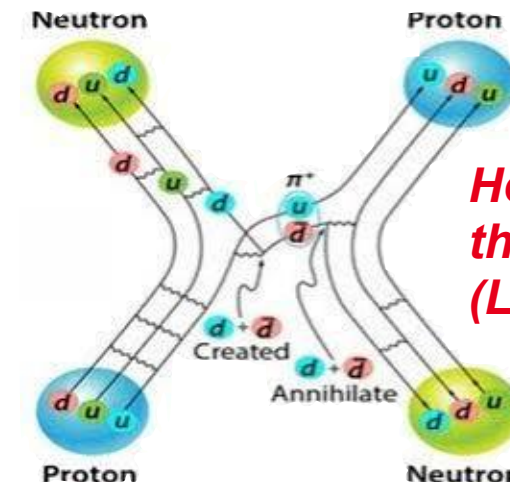


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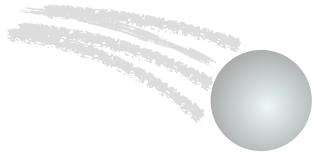
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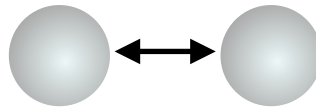
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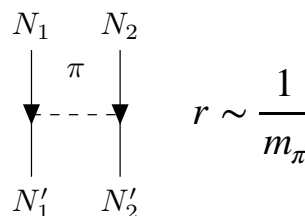
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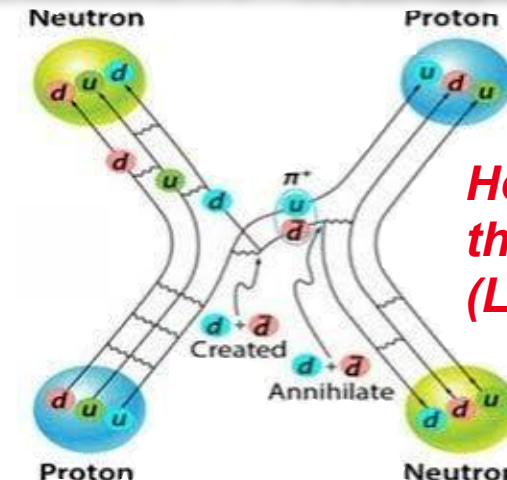
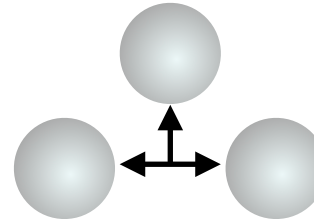
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MORE MANY-BODY QUANTUM MECHANICS

PARTICLE-HOLE REPRESENTATION



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Reminder from previous lecture:

PARTICLE-HOLE REPRESENTATION



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Reminder from previous lecture:

- Defining a **reference state**

$$|\Phi\rangle \equiv |\alpha_1\alpha_2\dots\alpha_A\rangle = a_1^\dagger a_2^\dagger \dots a_A^\dagger |0\rangle$$

PARTICLE-HOLE REPRESENTATION



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$$|\Phi\rangle \equiv |\alpha_1\alpha_2\dots\alpha_A\rangle = a_1^\dagger a_2^\dagger \dots a_A^\dagger |0\rangle$$

- One can construct **arbitrary Slater determinants as particle-hole excitations** on top of a reference state $|\Phi\rangle$ as

$$|\Phi_i^a\rangle = a_a^\dagger a_i |\Phi\rangle$$

$$|\Phi_{ij}^{ab}\rangle = a_a^\dagger a_b^\dagger a_j a_i |\Phi\rangle,$$

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- Here I have introduced the short-hand notations $a_p^\dagger \equiv a_{\alpha_p}^\dagger$ and $a_p \equiv a_{\alpha_p}$

index convention: $i, j, k, \dots$: states occupied in the reference state

$a, b, c, \dots$: states unoccupied in the reference state

$p, q, r, \dots$: any state

NORMAL ORDERING

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- Defining property: **expectation value with the reference state vanishes**
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Signum of the needed permutation

- To normal order with respect to an A -body reference state, we can use the anticommutation rules of the creation and annihilation operators, or **Wick's theorem**

WICK'S THEOREM

Suhonen, "From Nucleons to Nucleus: concepts of microscopic nuclear theory" (2007)



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WICK'S THEOREM

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- A product of creation and annihilation operators $A_i \in \{a_i^\dagger, a_i\}$ can be expressed as

$$\begin{aligned} & A_1 A_2 \dots A_n \\ &= \{A_1 A_2 \dots A_n\} + \sum_{(ij)} \{A_1 \dots \overbrace{A_i \dots A_j} \dots A_n\} + \sum_{(ij)(kl)} \{A_1 \dots \overbrace{A_i \dots A_k \dots A_j \dots A_l} \dots A_n\} + \dots \end{aligned}$$

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#Crossings of contractions

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NORMAL ORDERING: A-BODY REFERENCE

Djärv et al., Phys. Rev. C 104, 024324 (2021)



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- One can **normal order the Hamiltonian w.r.t. a reference state** $|\Phi\rangle = a_{\alpha_1}^{\dagger} \dots a_{\alpha_A}^{\dagger} |0\rangle$ using the **contraction rules**

$$\overline{a_{\alpha}^{\dagger} a_{\beta}} \equiv \langle \Phi | a_{\alpha}^{\dagger} a_{\beta} | \Phi \rangle = \dots = \begin{cases} \delta_{\alpha\beta}, & \text{if } \alpha, \beta \in \{\alpha_1, \dots, \alpha_A\} \\ 0, & \text{otherwise} \end{cases}$$

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Reminder:

$$\overline{AB} \equiv AB - \{AB\}$$

$$\langle 0 | \{ \dots \} | 0 \rangle$$

$$\rightarrow \langle 0 | AB | 0 \rangle = \langle 0 | \overline{AB} | 0 \rangle + \langle 0 | \{AB\} | 0 \rangle = \langle 0 | \overline{AB} | 0 \rangle = \overline{AB}$$

NORMAL ORDERING: A-BODY REFERENCE



Djärv et al., Phys. Rev. C 104, 024324 (2021)

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NORMAL-ORDERED TWO-BODY APPROXIMATION (NO2B)



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Hagen et al., Phys. Rev. C 76, 034302 (2007); Roth et al., Phys. Rev. Lett. 109, 052501 (2012); Djärv et al., Phys. Rev. C 104, 024324 (2021)

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$$V_{3N} = \frac{1}{6} \sum_{\alpha, \beta, \gamma \in \mathcal{R}} \langle \alpha\beta\gamma | \bar{v}^{3N} | \alpha\beta\gamma \rangle + \frac{1}{2} \sum_{\alpha\alpha'} \sum_{\beta, \gamma \in \mathcal{R}} \langle \alpha\beta\gamma | \bar{v}_{3N} | \alpha'\beta\gamma \rangle \{a_{\alpha}^{\dagger} a_{\alpha'}\} + \frac{1}{4} \sum_{\alpha\beta\alpha'} \sum_{\gamma \in \mathcal{R}} \langle \alpha\beta\gamma | \bar{v}^{3N} | \alpha'\beta'\gamma \rangle \{a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\beta'} a_{\alpha'}\} + \frac{1}{36} \sum_{\alpha\beta\gamma\alpha'\beta'\gamma'} \langle \alpha\beta\gamma | \bar{v}^{3N} | \alpha'\beta'\gamma' \rangle \{a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma}^{\dagger} a_{\gamma'} a_{\beta'} a_{\alpha'}\}$$

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States in the reference state *States outside the reference state*

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- Normal-ordered two-body approximation:** Approximate the full three-nucleon force taking the normal-ordered two-body terms

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 - Significantly reduce computational cost and storage**

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- Any antisymmetric state can be expanded as Slater determinants

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- To describe short-range correlations, one needs a superposition of Slater determinants

UNITARY TRANSFORMATIONS

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 - Improve the convergence of the many-body calculations by transforming the Hamiltonian into a (band/block) diagonal form
 - Preserve the physics of the initial Hamiltonian and observables

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- **Unitary transformations conserve the eigenenergies** (spectrum) of the initial Hamiltonian: acting with a unitary operator U satisfying $\mathbf{1} = U^\dagger U = UU^\dagger$ on both sides of the Schrödinger equation, we get

$$\begin{aligned} H|\Psi\rangle &= E|\Psi\rangle \quad \parallel U^\dagger \times \\ U^\dagger H|\Psi\rangle &= EU^\dagger|\Psi\rangle \\ \underbrace{U^\dagger H U U^\dagger}_{\equiv \tilde{H}}|\Psi\rangle &= E \underbrace{U^\dagger}_{\equiv |\tilde{\Psi}\rangle}|\Psi\rangle \\ \rightarrow \tilde{H}|\tilde{\Psi}\rangle &= E|\tilde{\Psi}\rangle \end{aligned}$$

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 \rightarrow \tilde{H}|\tilde{\Psi}\rangle &= E|\tilde{\Psi}\rangle
 \end{aligned}$$

- **Unitary transformations also preserve expectation values of operators** (observables)

$$\langle \Psi | \mathcal{O} | \Psi' \rangle = \langle \underbrace{\Psi |}_{{=}\langle \tilde{\Psi} |} \underbrace{U U^\dagger \mathcal{O} U U^\dagger}_{{=}\tilde{\mathcal{O}}} \underbrace{|\Psi' \rangle}_{{=}| \tilde{\Psi}' \rangle} \rangle = \langle \tilde{\Psi} | \tilde{\mathcal{O}} | \tilde{\Psi}' \rangle$$

SIMILARITY RENORMALIZATION GROUP (SRG)

Bogner, Furnstahl, Perry, Phys. Rev. C 75, 061001(R) (2007)



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- ***Continuous unitary transformation to pre-diagonalize the Hamiltonian with respect to a given basis***



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$$H_\alpha = U_\alpha^\dagger H U_\alpha \quad \mathcal{O}_\alpha = U_\alpha^\dagger \mathcal{O} U_\alpha$$

- **Differentiate both sides** with respect to α

$$\begin{aligned} \frac{d}{d\alpha} H_\alpha &= \left(\frac{d}{d\alpha} U_\alpha^\dagger \right) H U_\alpha + U_\alpha^\dagger H \left(\frac{d}{d\alpha} U_\alpha \right) \\ &= \left(\frac{d}{d\alpha} U_\alpha^\dagger \right) U_\alpha U_\alpha^\dagger H U_\alpha + U_\alpha^\dagger H U_\alpha U_\alpha^\dagger \left(\frac{d}{d\alpha} U_\alpha \right) \\ &= \left(\frac{d}{d\alpha} U_\alpha^\dagger \right) U_\alpha H_\alpha + H_\alpha U_\alpha^\dagger \left(\frac{d}{d\alpha} U_\alpha \right) \end{aligned}$$

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- Differentiating both sides of the unitary condition $1 = U_\alpha^\dagger U_\alpha$, we get

$$0 = \frac{d}{d\alpha} 1 = \left(\frac{d}{d\alpha} U_\alpha^\dagger \right) U_\alpha + U_\alpha^\dagger \left(\frac{d}{d\alpha} U_\alpha \right) \rightarrow -U_\alpha^\dagger \left(\frac{d}{d\alpha} U_\alpha \right) = \left(\frac{d}{d\alpha} U_\alpha^\dagger \right) U_\alpha$$

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- Define an **antihermitian generator** via

$$\eta_\alpha = -U_\alpha^\dagger \left(\frac{d}{d\alpha} U_\alpha \right) = \left(\frac{d}{d\alpha} U_\alpha^\dagger \right) U_\alpha = -\eta_\alpha^\dagger$$

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$$\frac{d}{d\alpha} H_\alpha = \left(\frac{d}{d\alpha} U_\alpha^\dagger \right) U_\alpha H_\alpha + H_\alpha U_\alpha^\dagger \left(\frac{d}{d\alpha} U_\alpha \right) = \eta_\alpha H_\alpha - H_\alpha \eta_\alpha = [\eta_\alpha, H_\alpha]$$

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- Changing of the Hamiltonian as a function of the flow parameter can be written as the **commutator of the generator with the Hamiltonian**
- This is how we define the **SRG flow equation**

$$\left(\text{think of Heisenberg equation of motion } \frac{dO}{dt} = \frac{i}{\hbar} [H, O] + \frac{\partial O}{\partial t} \right)$$

SIMILARITY RENORMALIZATION GROUP: SUMMARY

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$$H_\alpha = U_\alpha^\dagger H U_\alpha, \quad O_\alpha = U_\alpha^\dagger O U_\alpha$$

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- **Flow equations** for the Hamiltonian, operator and unitary transformation

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- **SRG is a versatile technique:** the physics of the transformation depends on the generator η_α chosen depending on the “pre-diagonalization” we want to achieve

SIMILARITY RENORMALIZATION GROUP: SUMMARY



Bogner, Furnstahl, Perry, Phys. Rev. C 75, 061001(R) (2007)

- **Consistent transformation of the Hamiltonian and operators**

$$H_\alpha = U_\alpha^\dagger H U_\alpha, \quad O_\alpha = U_\alpha^\dagger O U_\alpha$$

- **Flow equations** for the Hamiltonian, operator and unitary transformation

$$\frac{d}{d\alpha} H_\alpha = [\eta_\alpha, H_\alpha], \quad \frac{d}{d\alpha} O_\alpha = [\eta_\alpha, O_\alpha], \quad \frac{d}{d\alpha} U_\alpha = [\eta_\alpha, U_\alpha] = -U_\alpha \eta_\alpha$$

- **SRG is a versatile technique:** the physics of the transformation depends on the generator η_α chosen depending on the “pre-diagonalization” we want to achieve

- **SRG induces higher-body terms, e.g.**

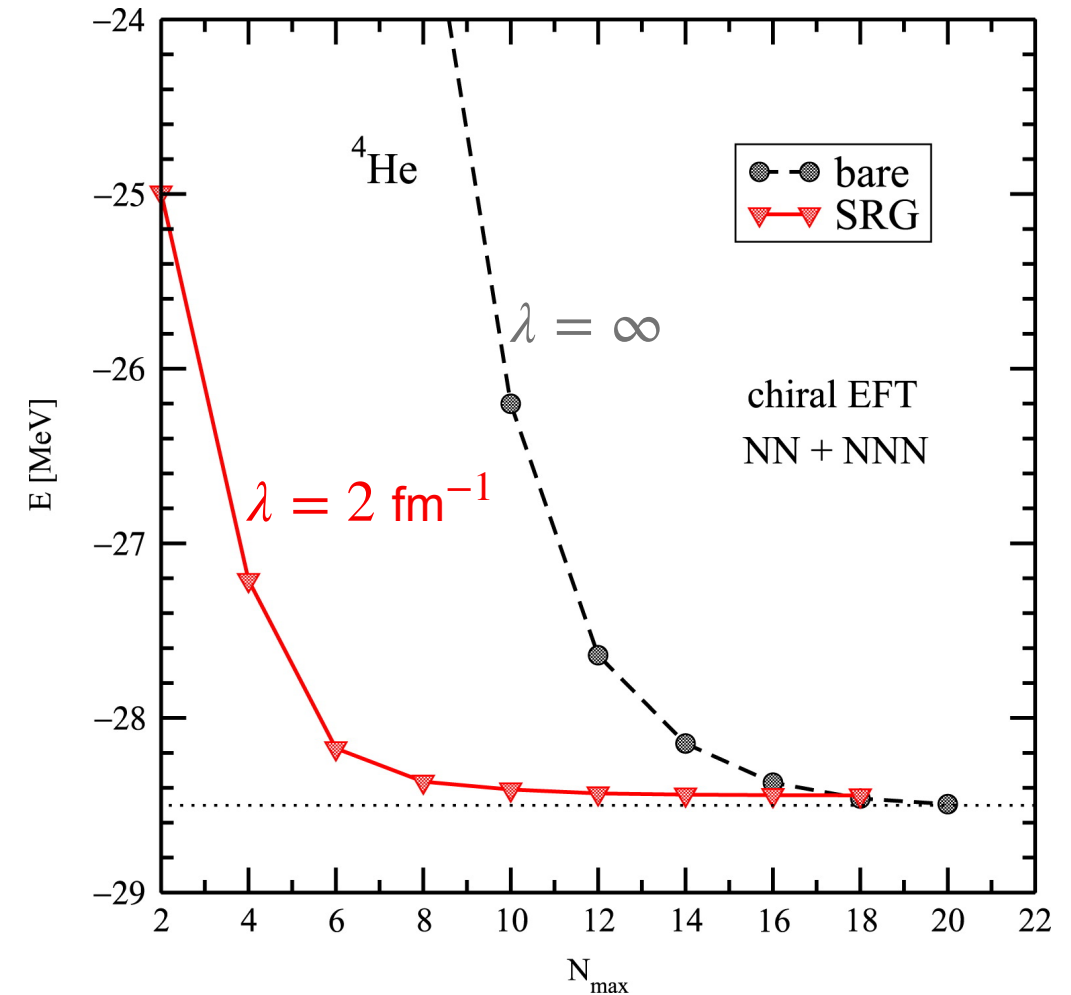
$$O^{1B} \xrightarrow{\text{SRG}} O^{1B} + O^{2B} + O^{3B} + \dots$$

IMPROVED CONVERGENCE WITH SRG EVOLUTION



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Barrett et al., Prog. Part. Nucl. Phys. 69, 131-181 (2013); Jurgenson et al., Phys. Rev. Lett. 103, 082501 (2009)



IMPROVED CONVERGENCE WITH SRG EVOLUTION



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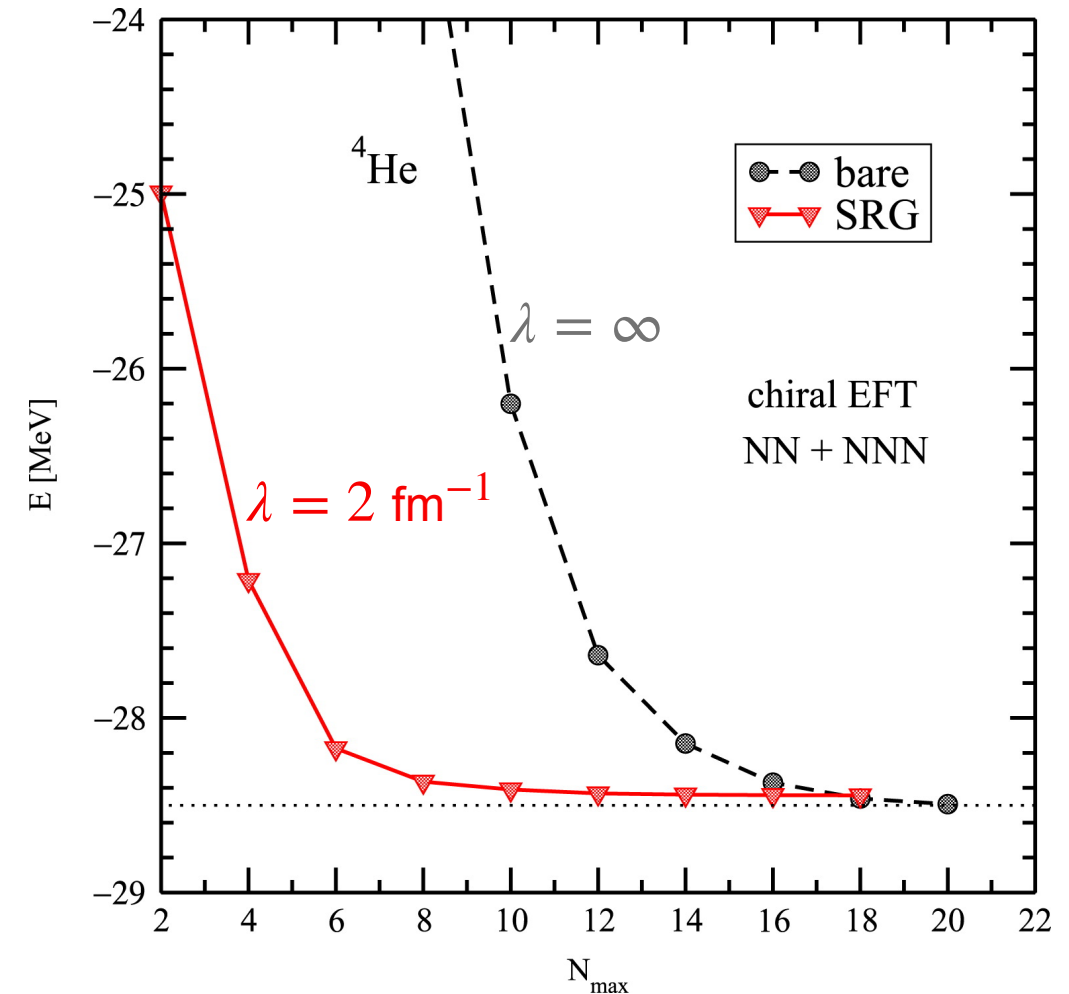
- Flow equation

$$\frac{dH_\lambda}{d\lambda} = [\eta_\lambda, H_\lambda]$$

with the **generator defined with nucleon kinetic energy T ,**

$$\eta_\lambda = -\frac{4}{\lambda^5}[T, H_\lambda]$$

decouple high- and low-momentum parts of H_λ



IMPROVED CONVERGENCE WITH SRG EVOLUTION



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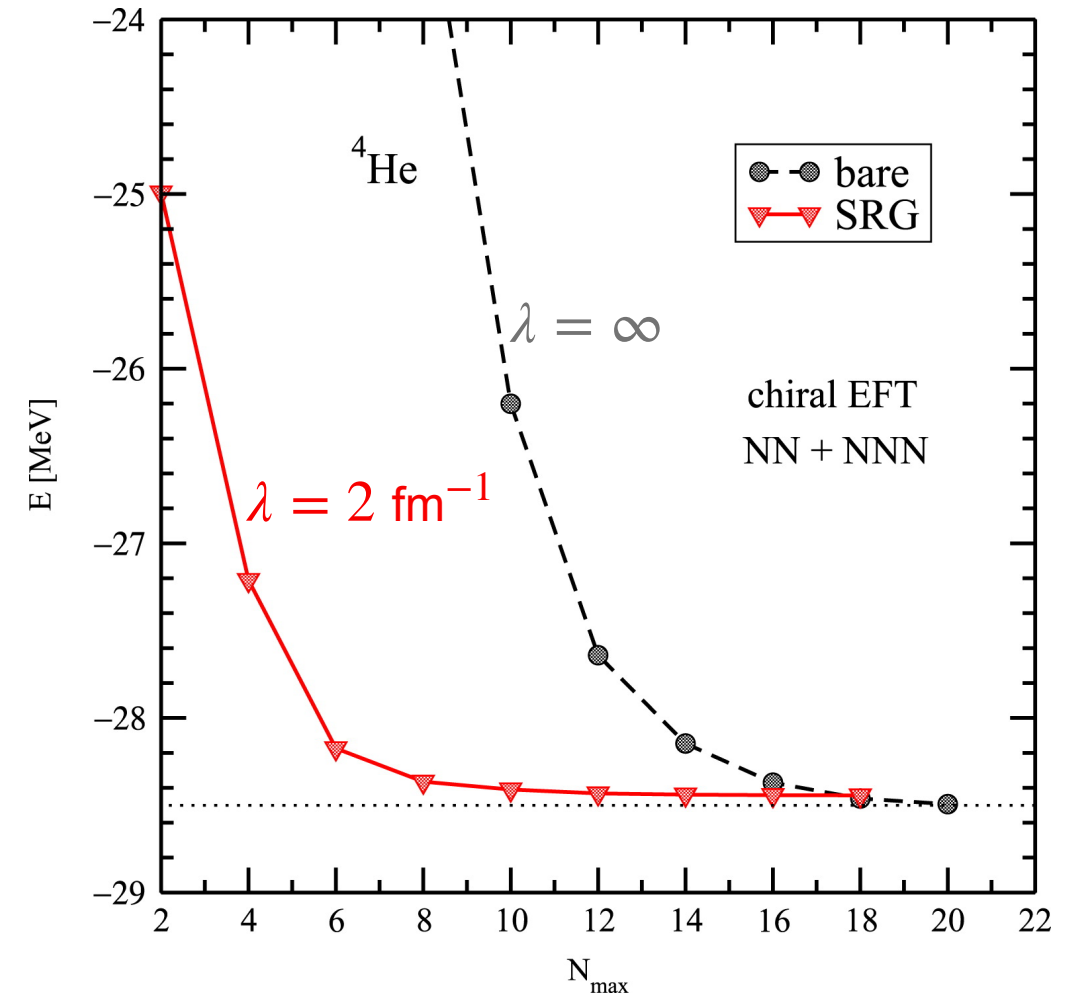
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$$\eta_\lambda = -\frac{4}{\lambda^5}[T, H_\lambda]$$

decouple high- and low-momentum parts of H_λ

- Here λ runs from ∞ to 0; free-space Hamiltonian defined as $H_{\lambda=\infty}$



DIFFERENT AB INITIO MANY-BODY TECHNIQUES

CURRENT REACH OF AB INITIO TECHNIQUES



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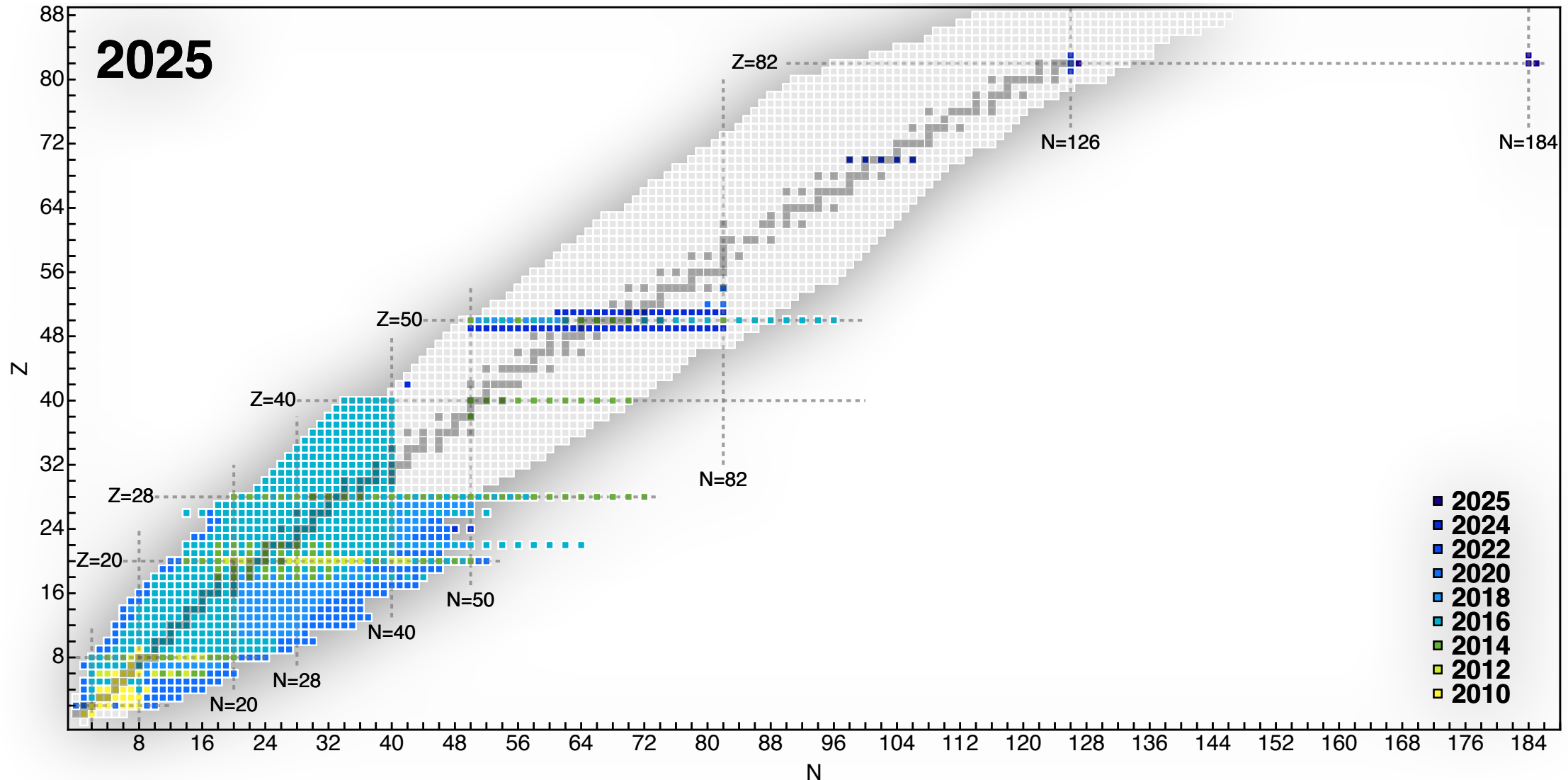


Figure courtesy of H. Hergert, adapted from H. Hergert, *Frontiers in Physics* 8, 379 (2020)

CURRENT REACH OF AB INITIO TECHNIQUES



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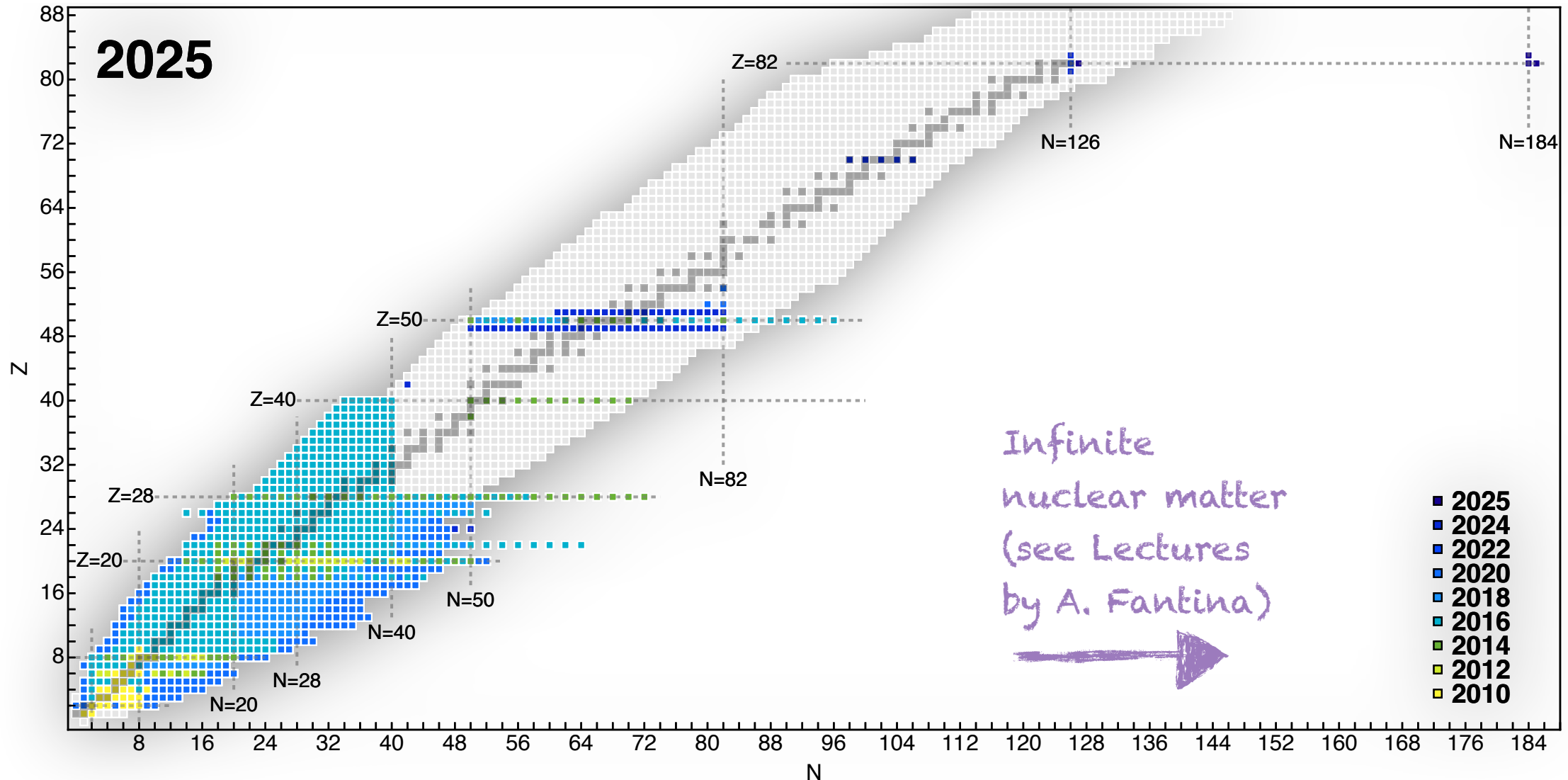
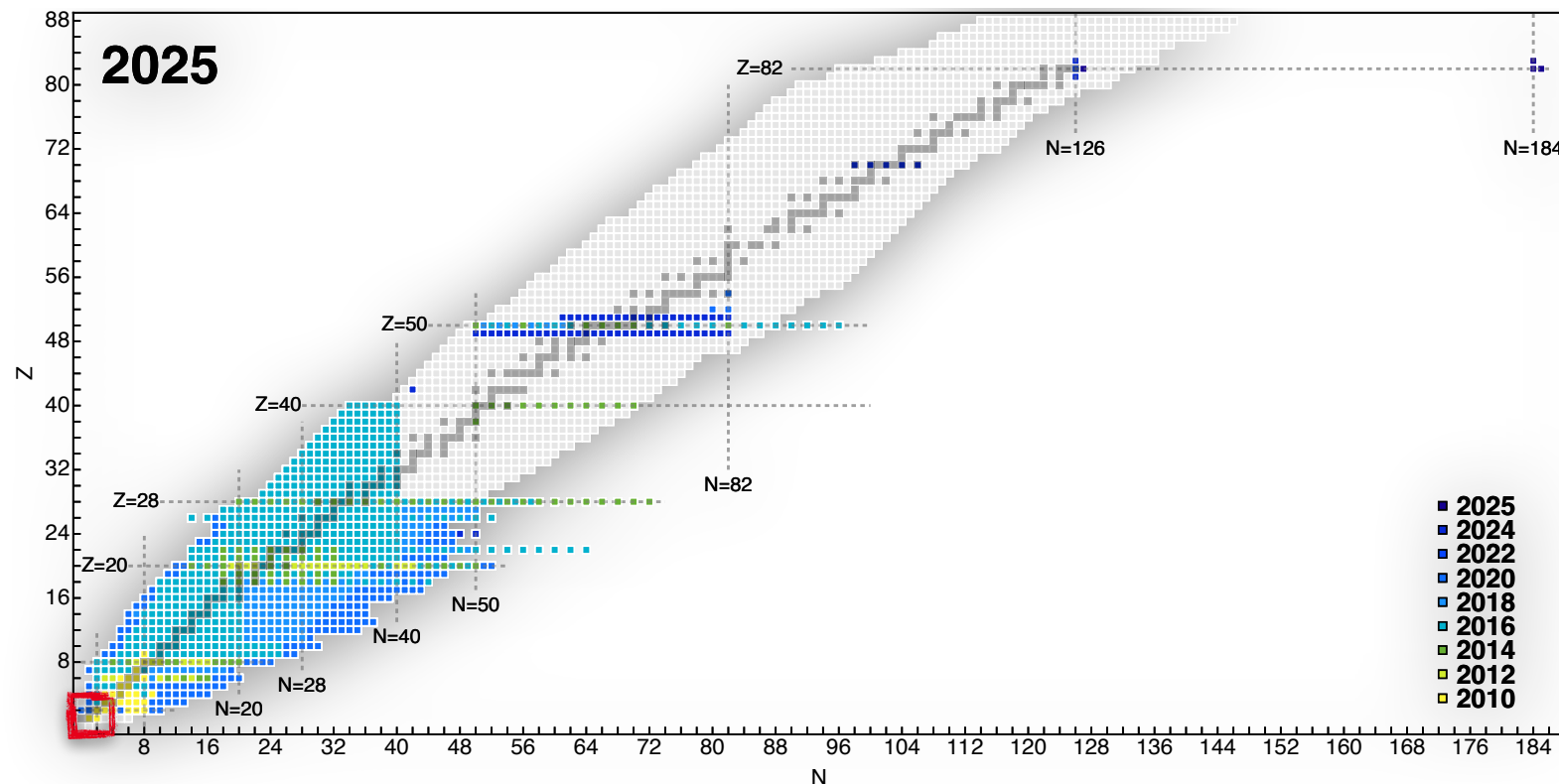


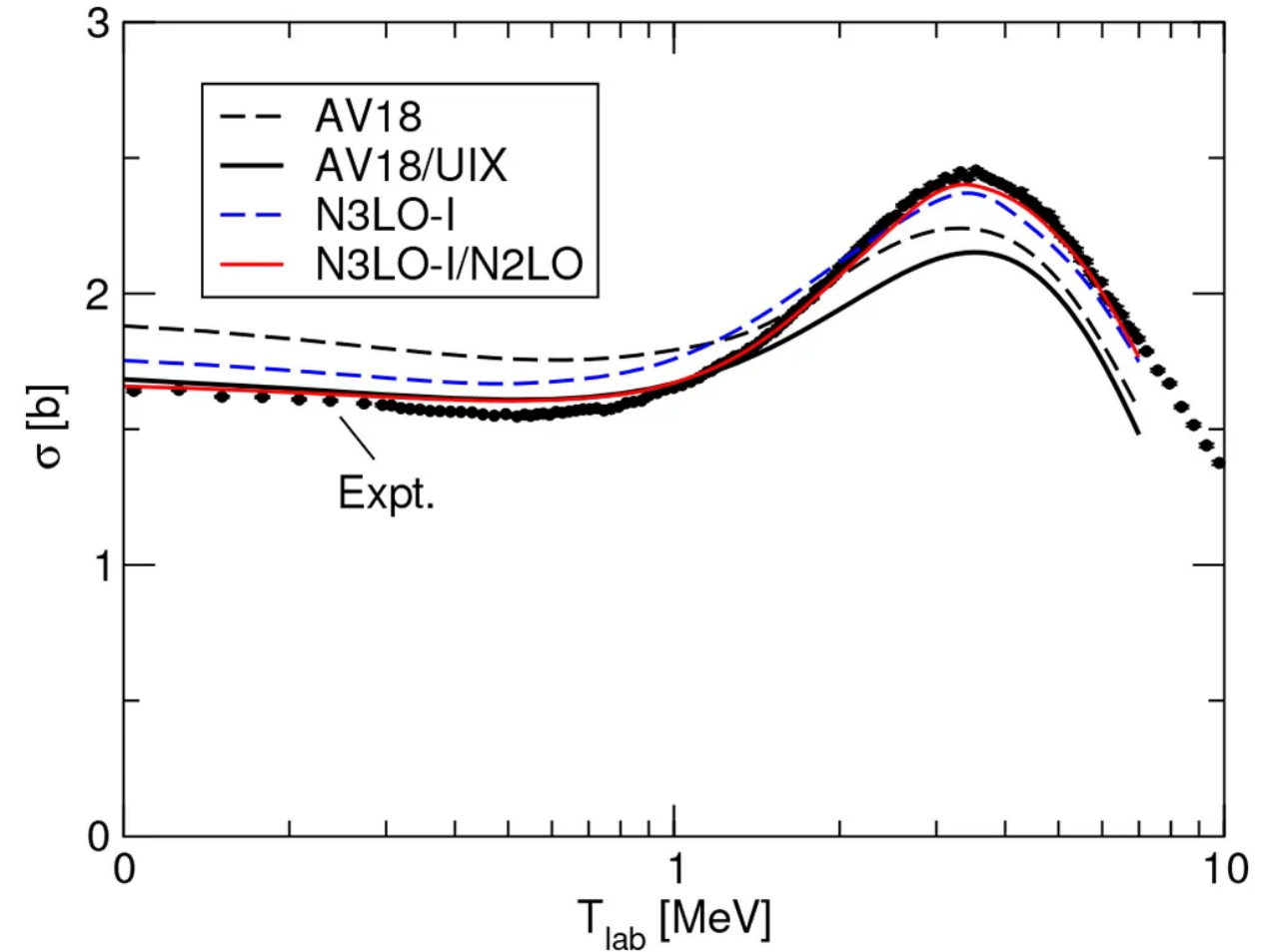
Figure courtesy of H. Hergert, adapted from H. Hergert, *Frontiers in Physics* 8, 379 (2020)



VERY LIGHT NUCLEI ($A \leq 5$)

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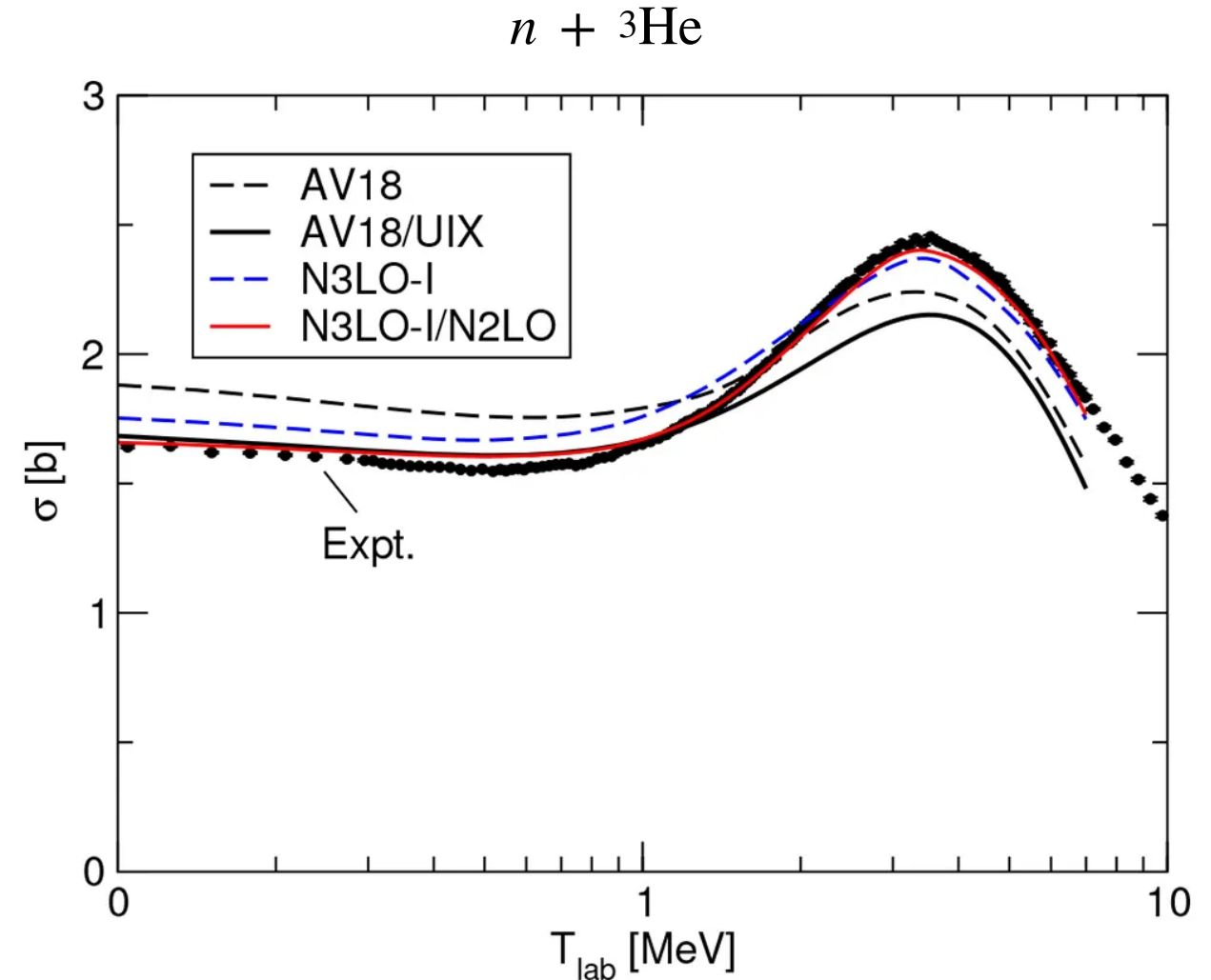
$n + {}^3\text{He}$



Marcucci et al., Front. Phys. 8:69 (2020)

VERY LIGHT NUCLEI ($A \leq 5$)

- Main methods:



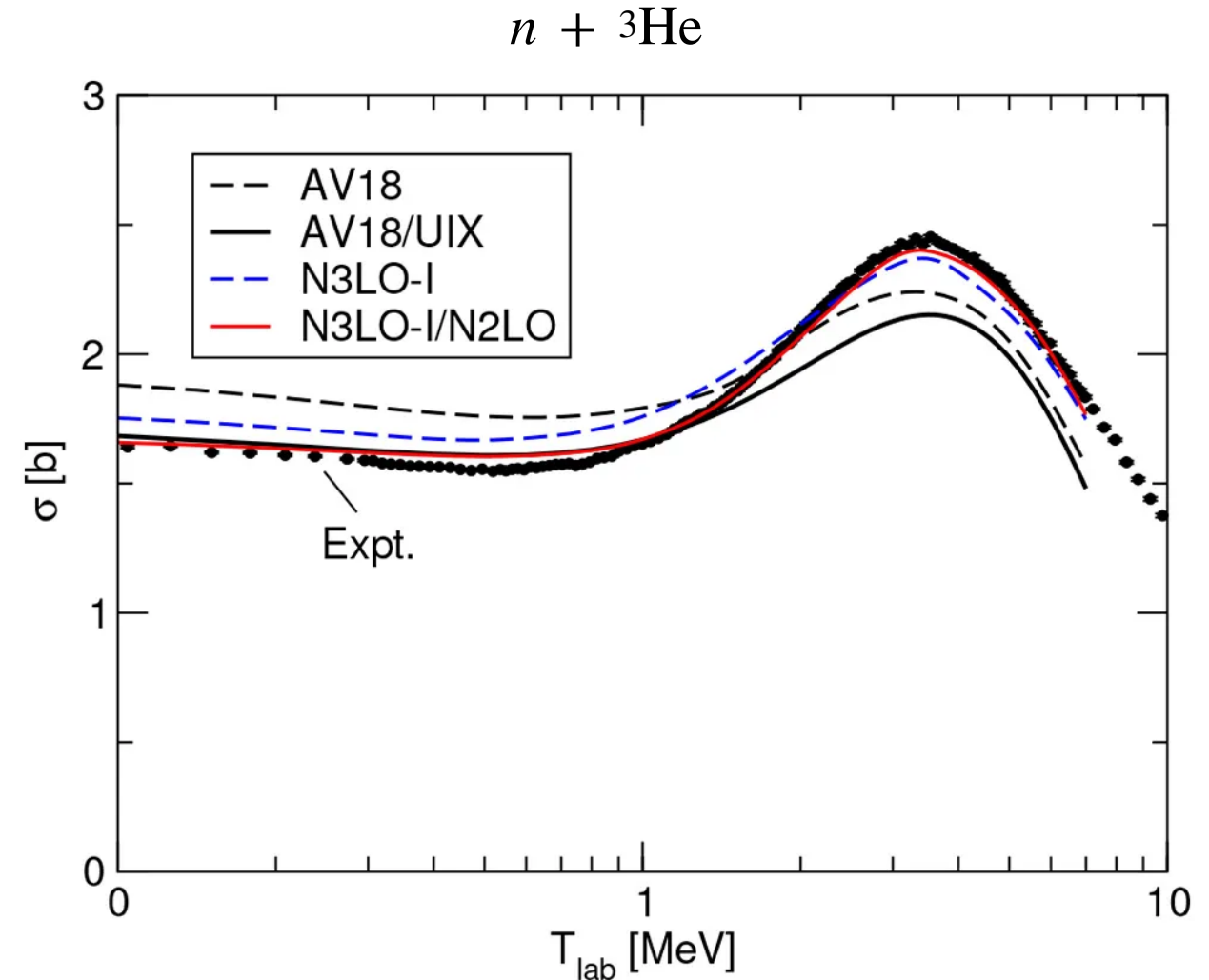
Marcucci et al., Front. Phys. 8:69 (2020)

VERY LIGHT NUCLEI ($A \leq 5$)

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Marcucci et al., Front. Phys. 8:69 (2020)

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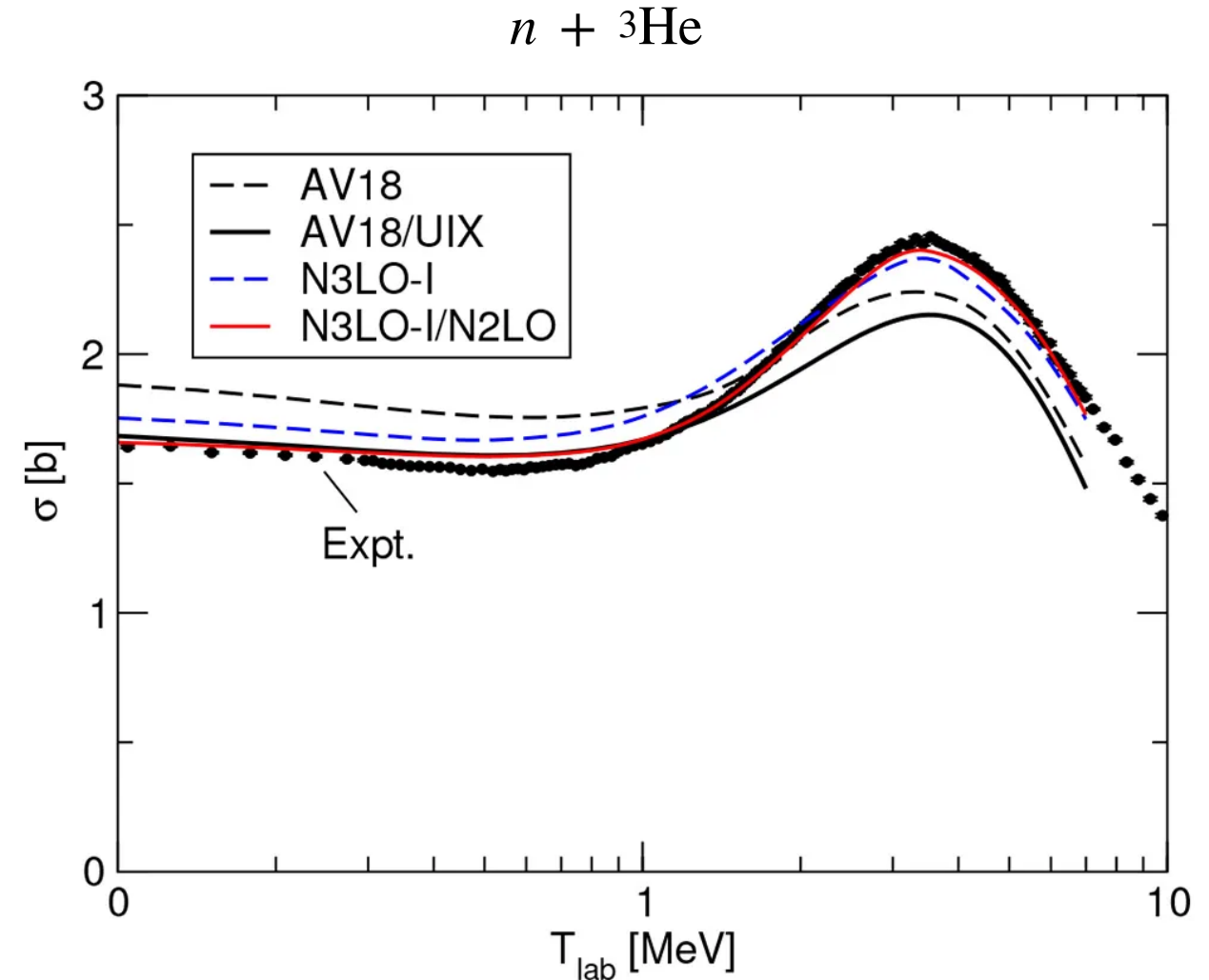
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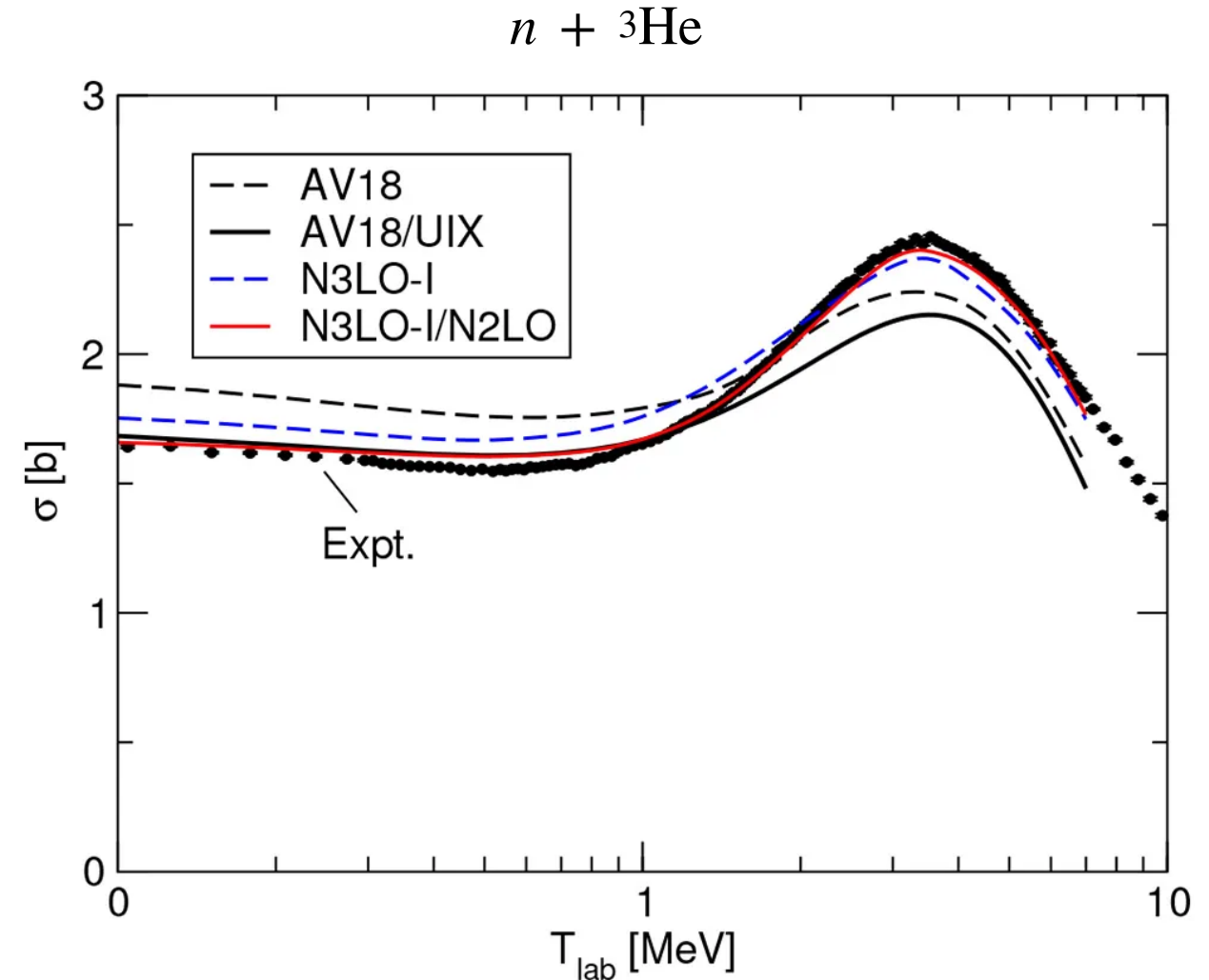
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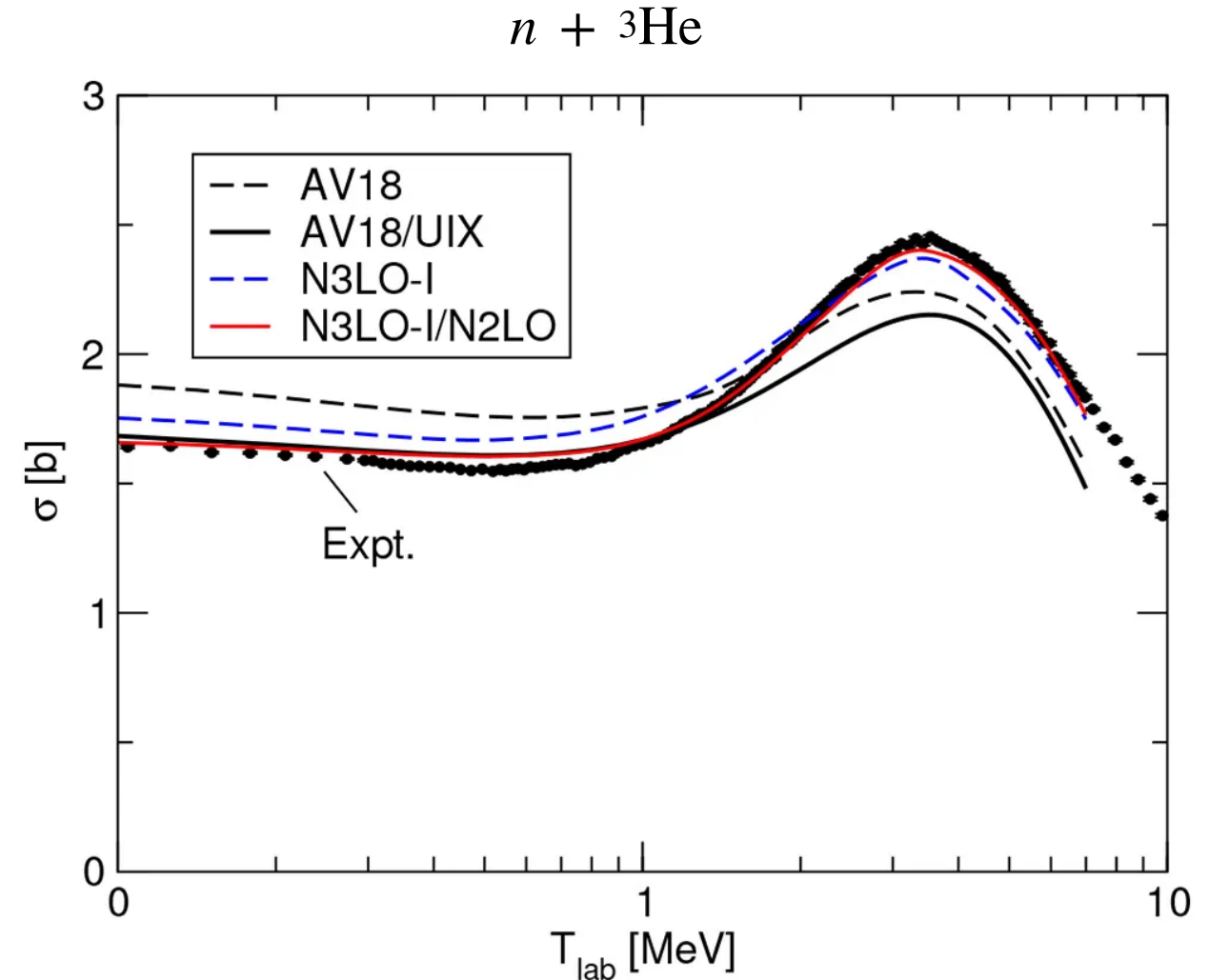
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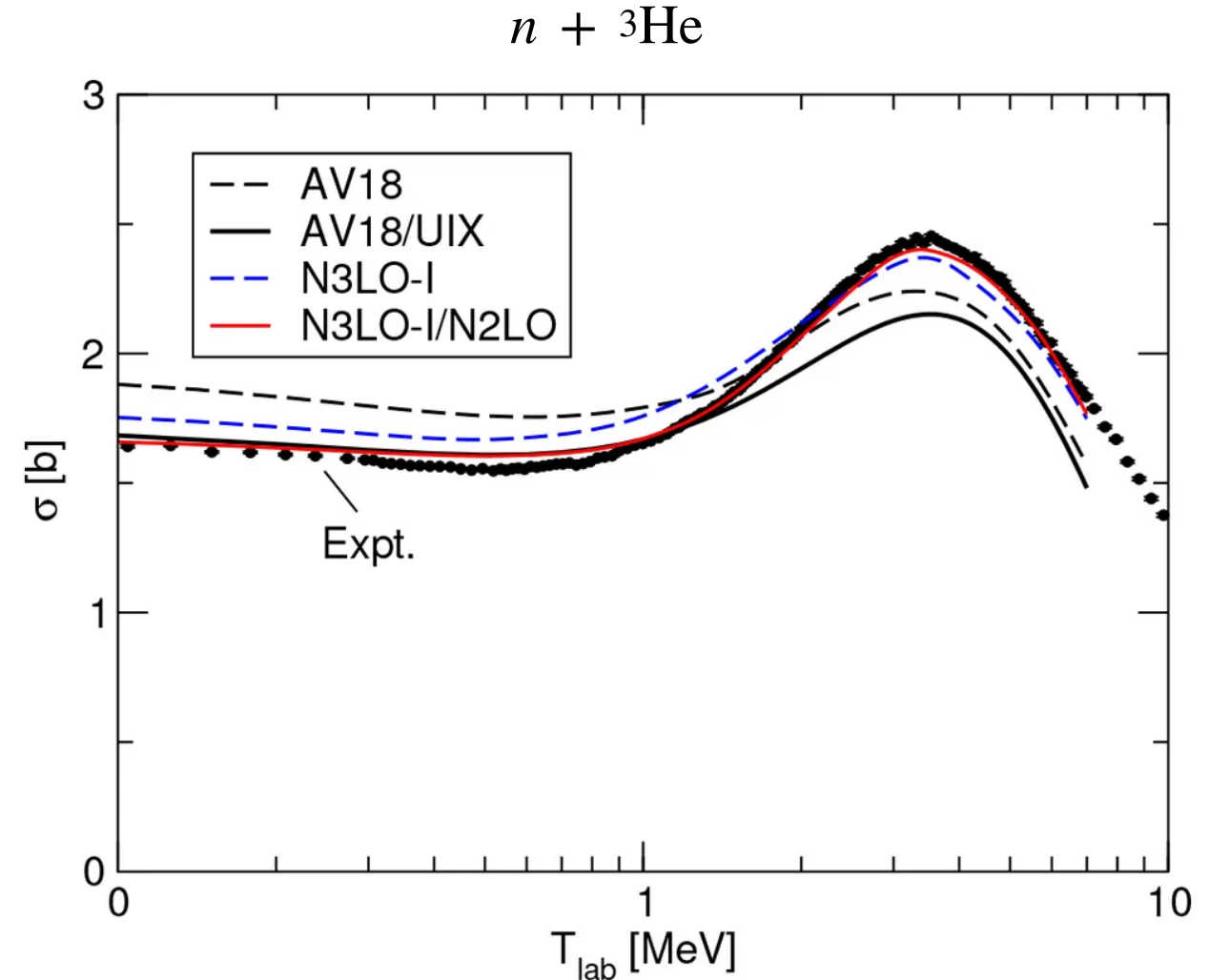
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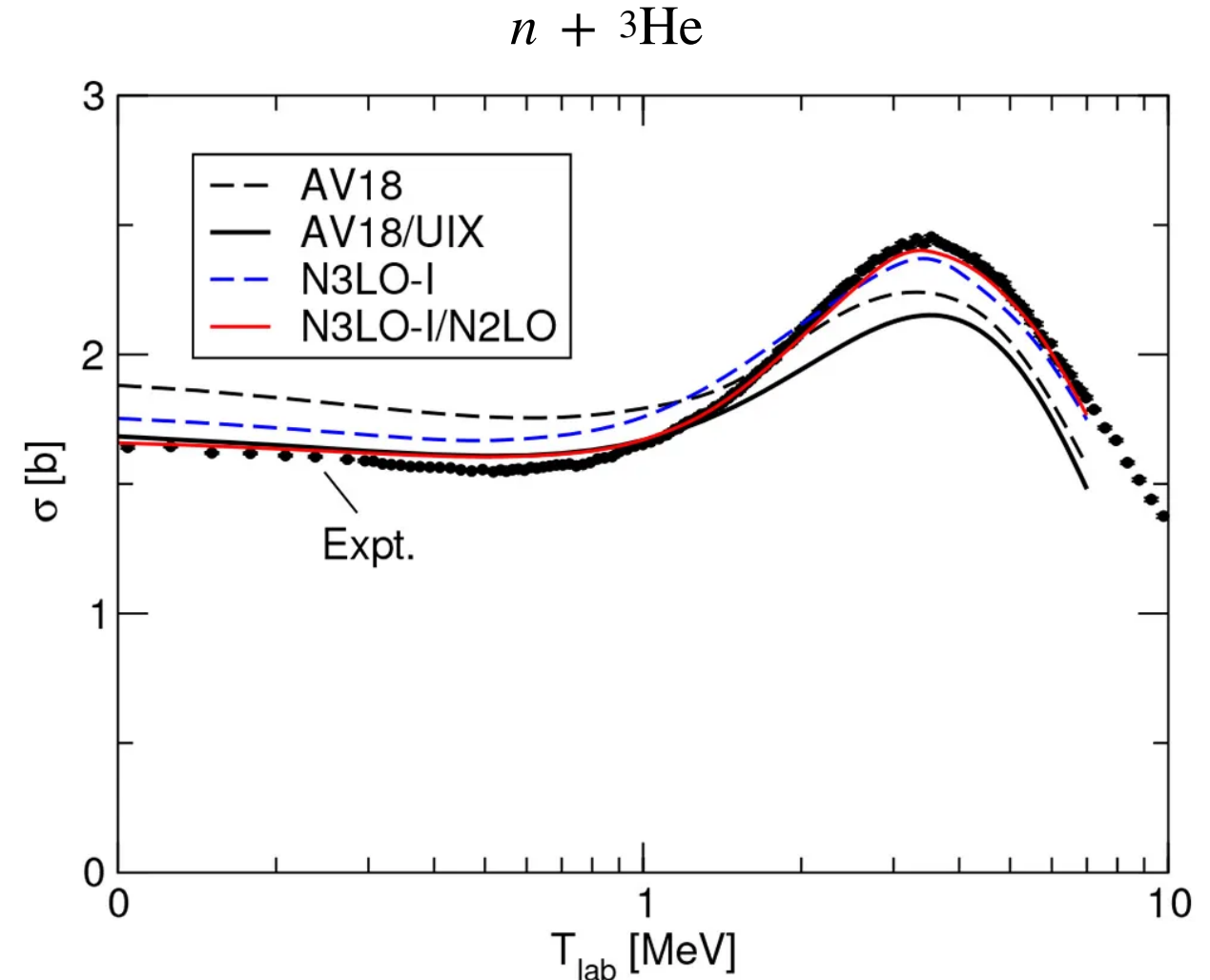
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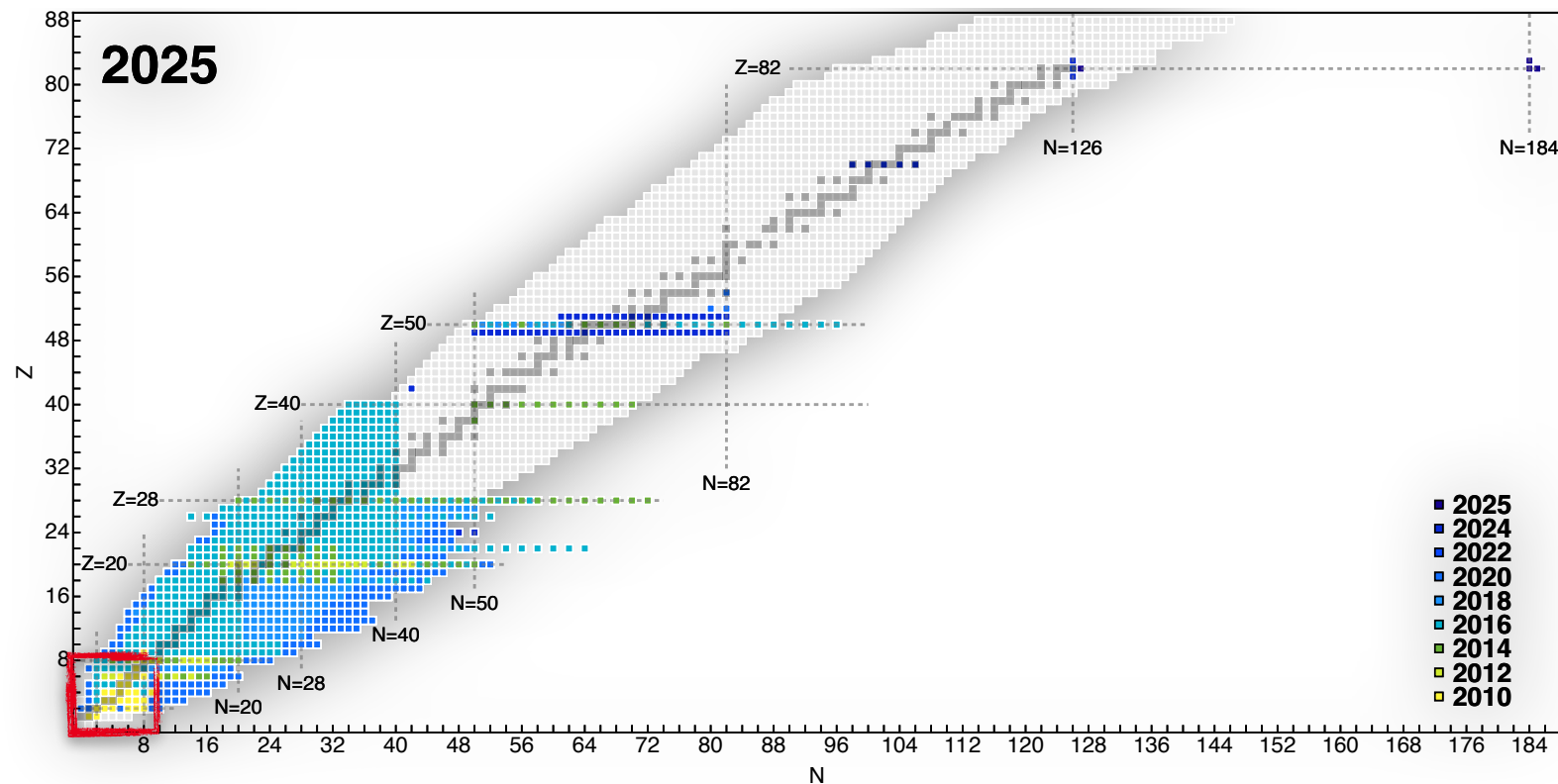
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- **Prohibitively complicated to extend to heavier systems**



Marcucci et al., Front. Phys. 8:69 (2020)



LIGHT NUCLEI ($A \lesssim 20$)

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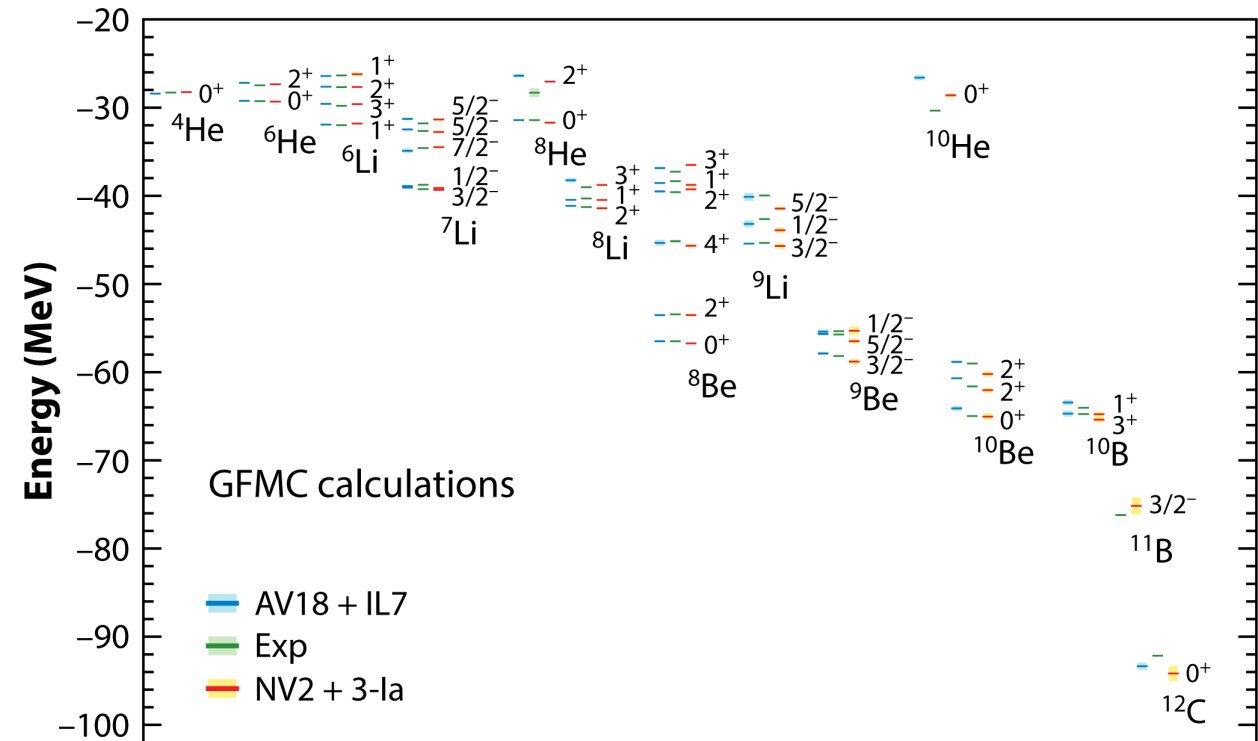
QUANTUM MONTE CARLO METHODS

Lynn, Tews, Gandolfi, Lovato, *Annu. Rev. Nucl. Part. Sci.* 69, 279-305 (2019)



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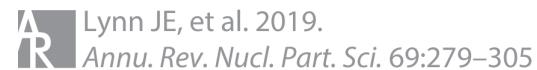
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Lynn JE, et al. 2019.
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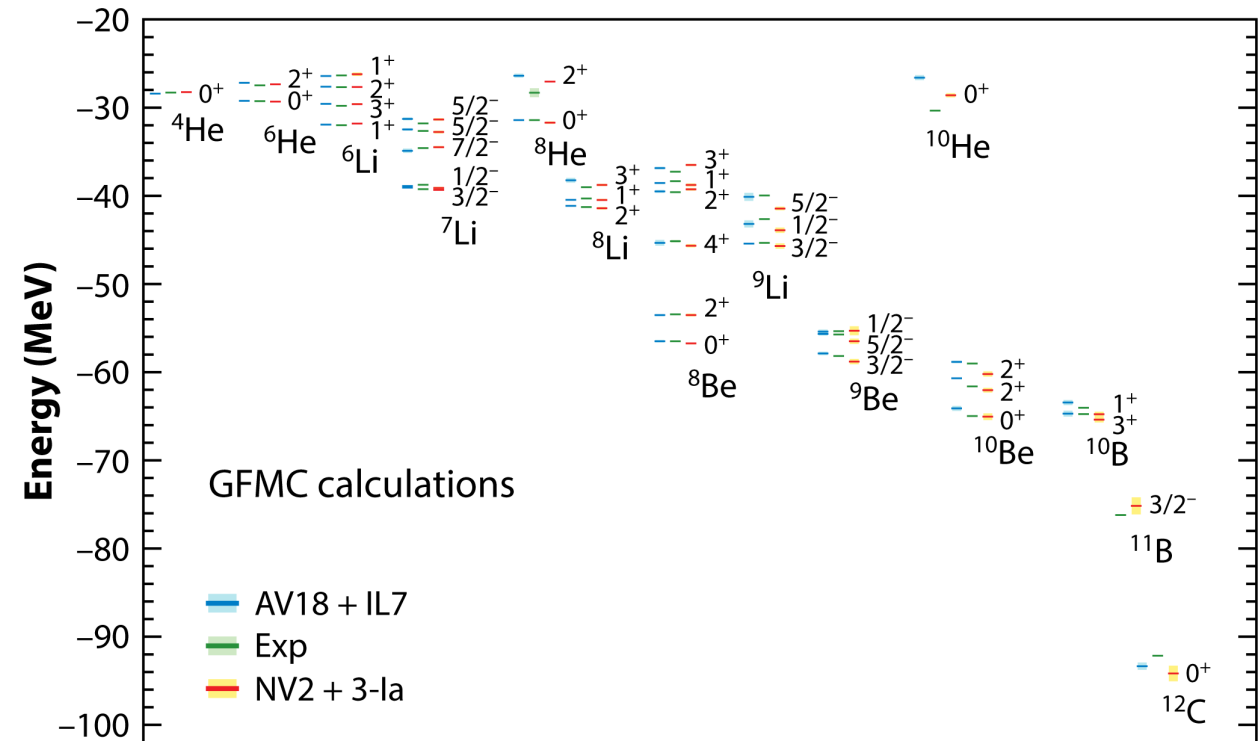
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- Different variants:

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- Approximate ground state energy

$$E_V = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle}$$



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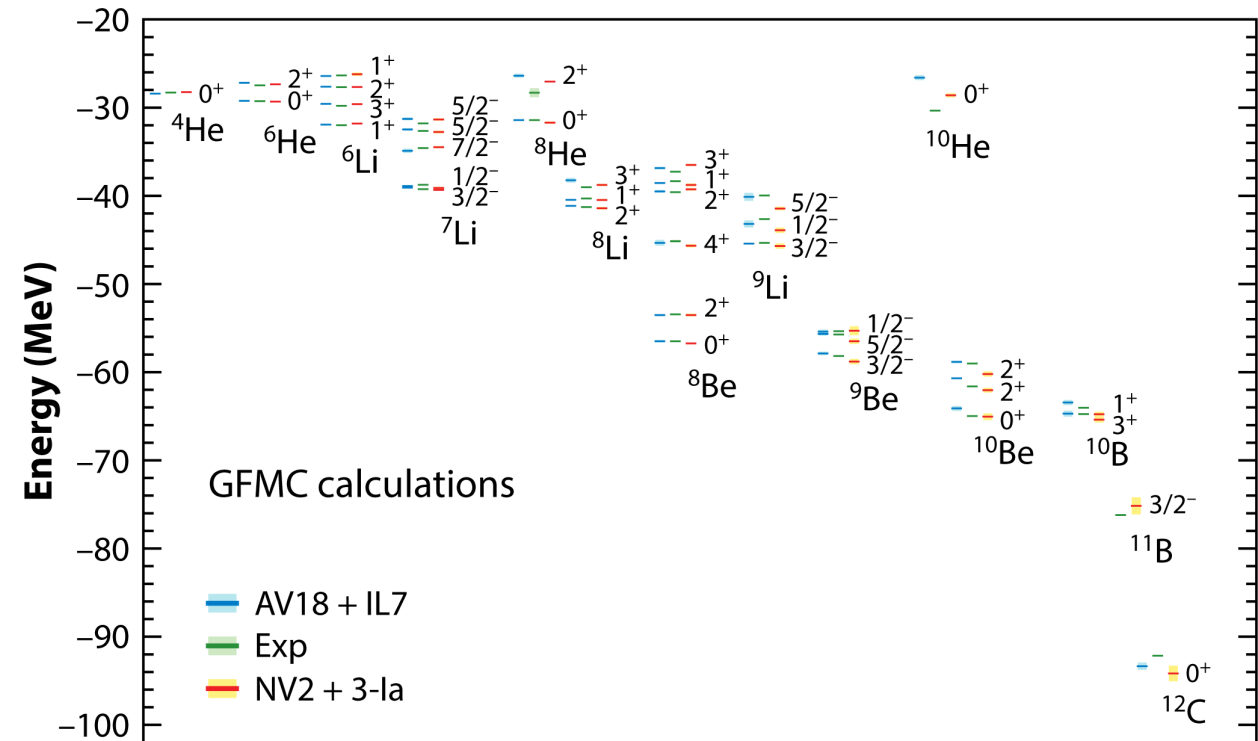
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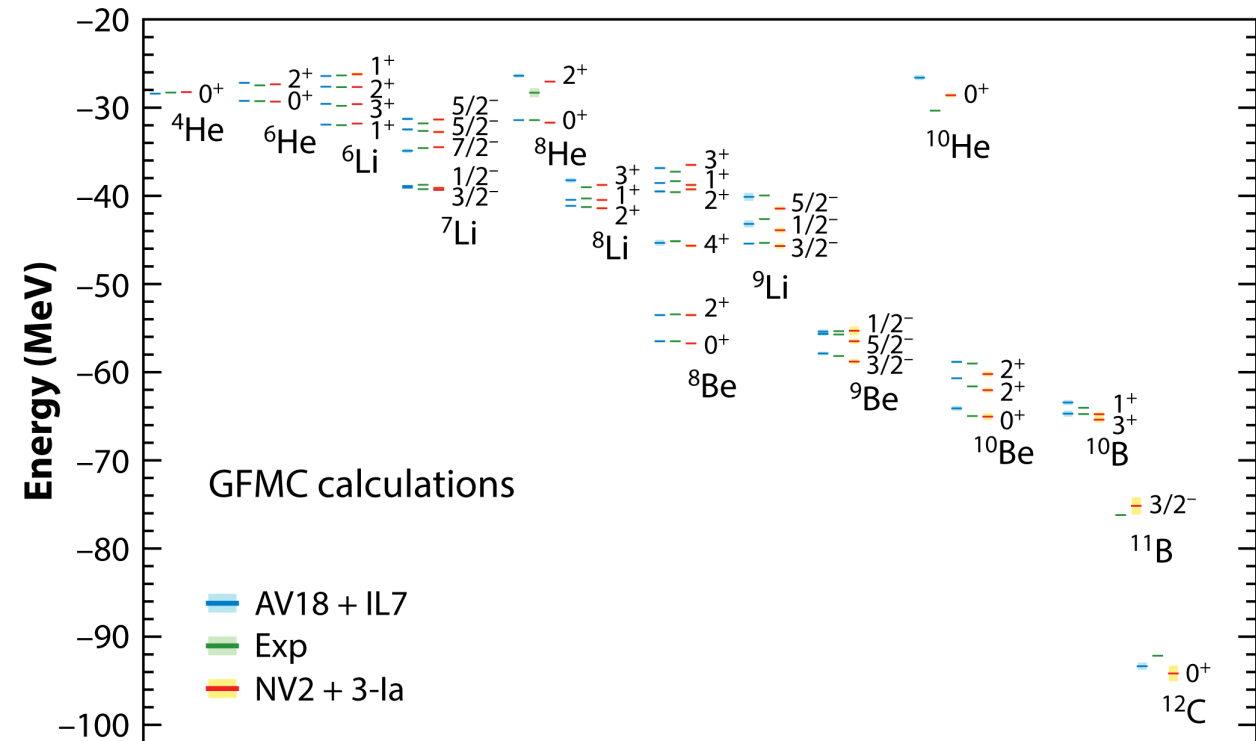
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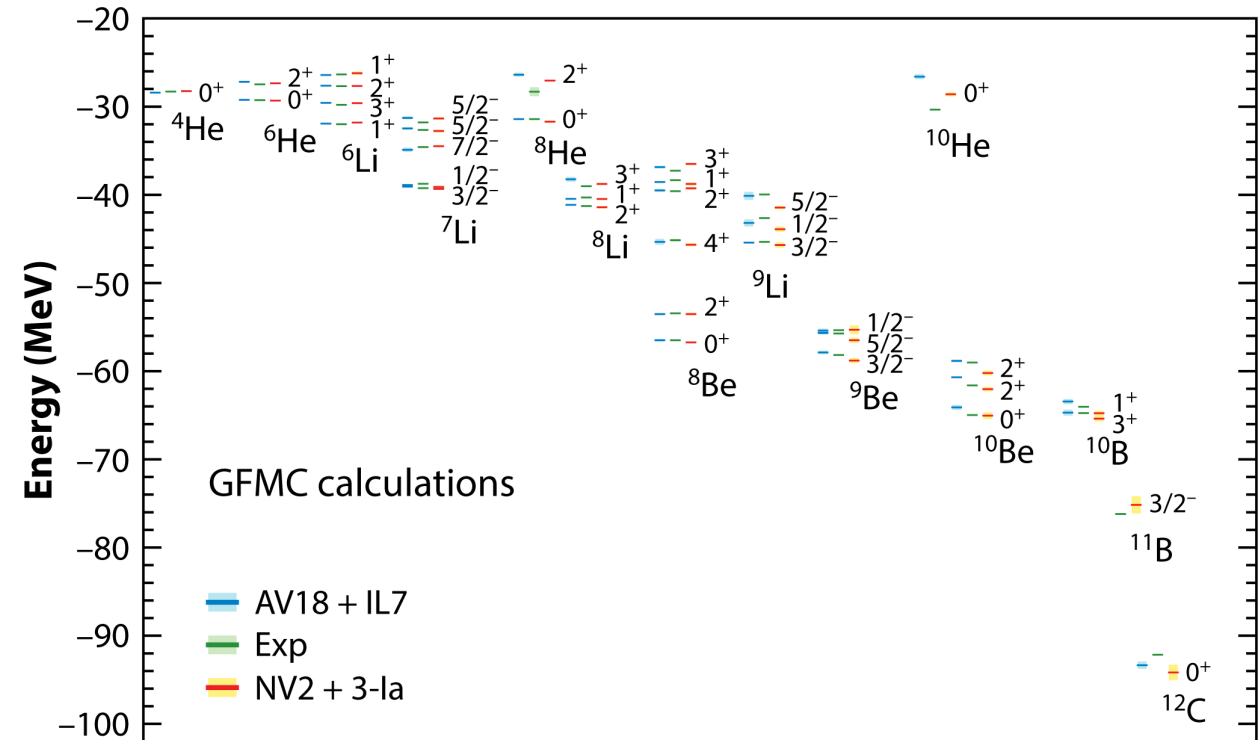
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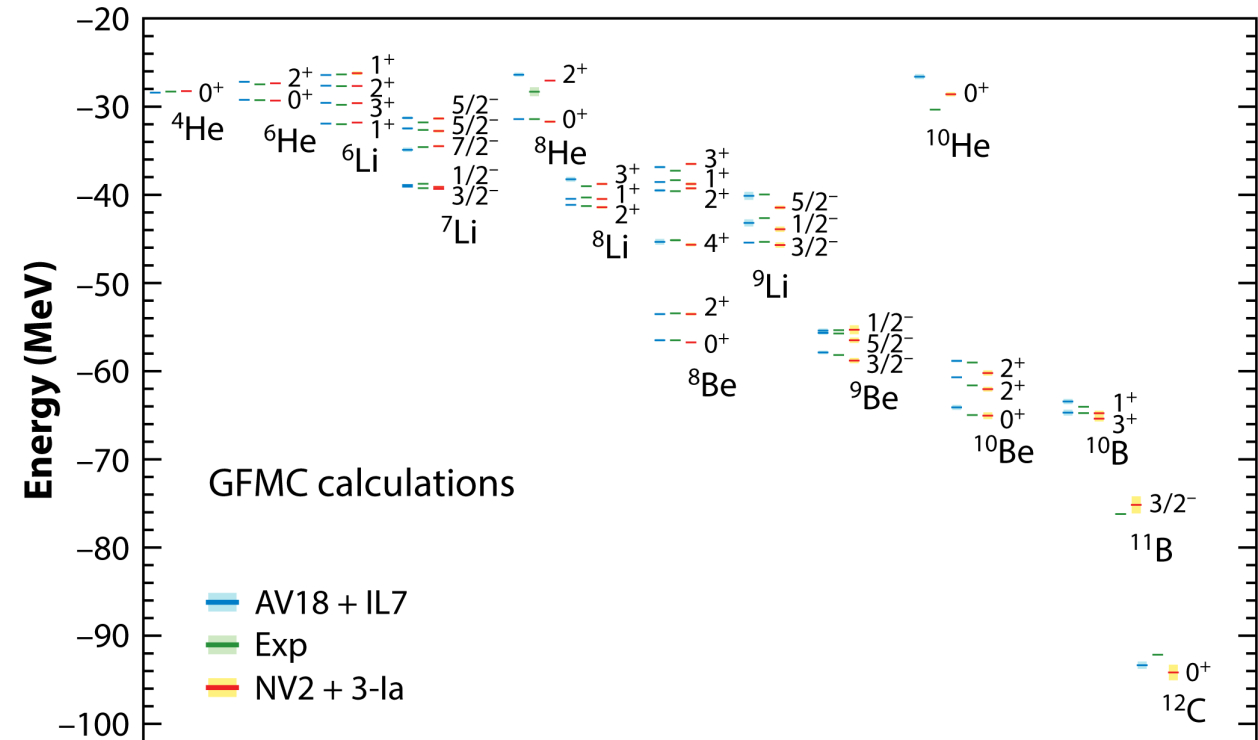
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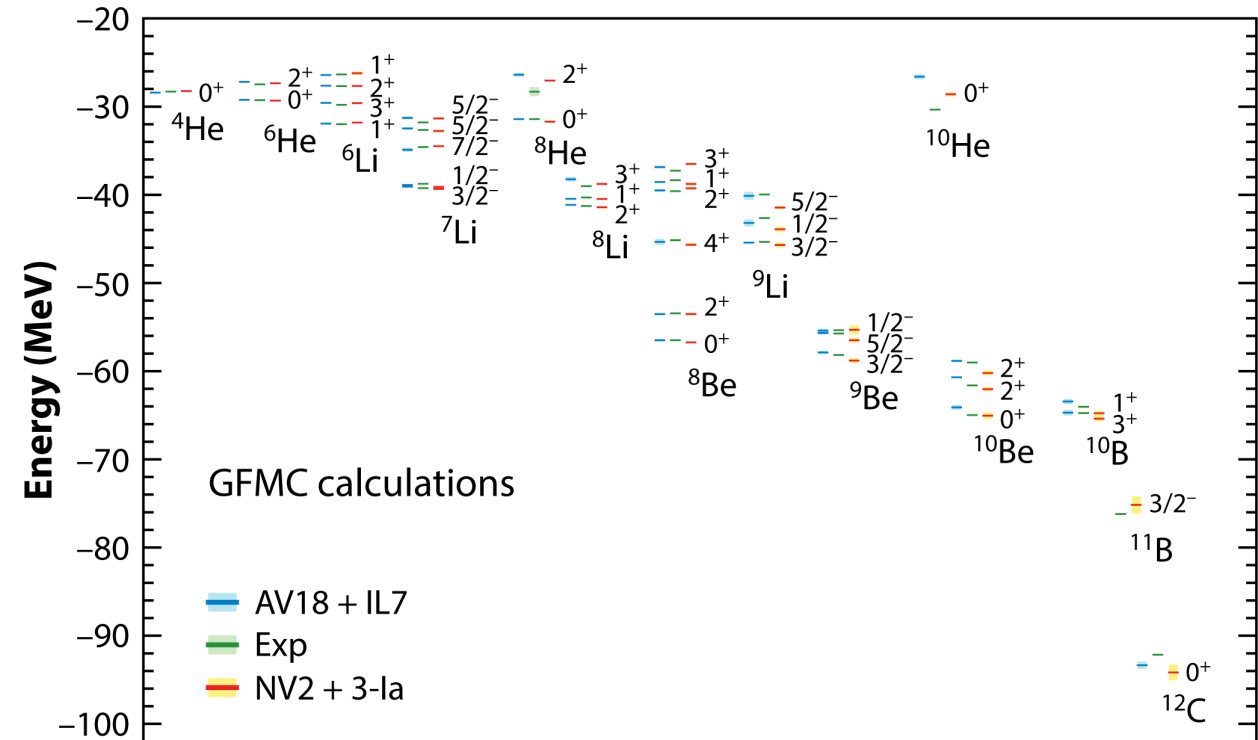
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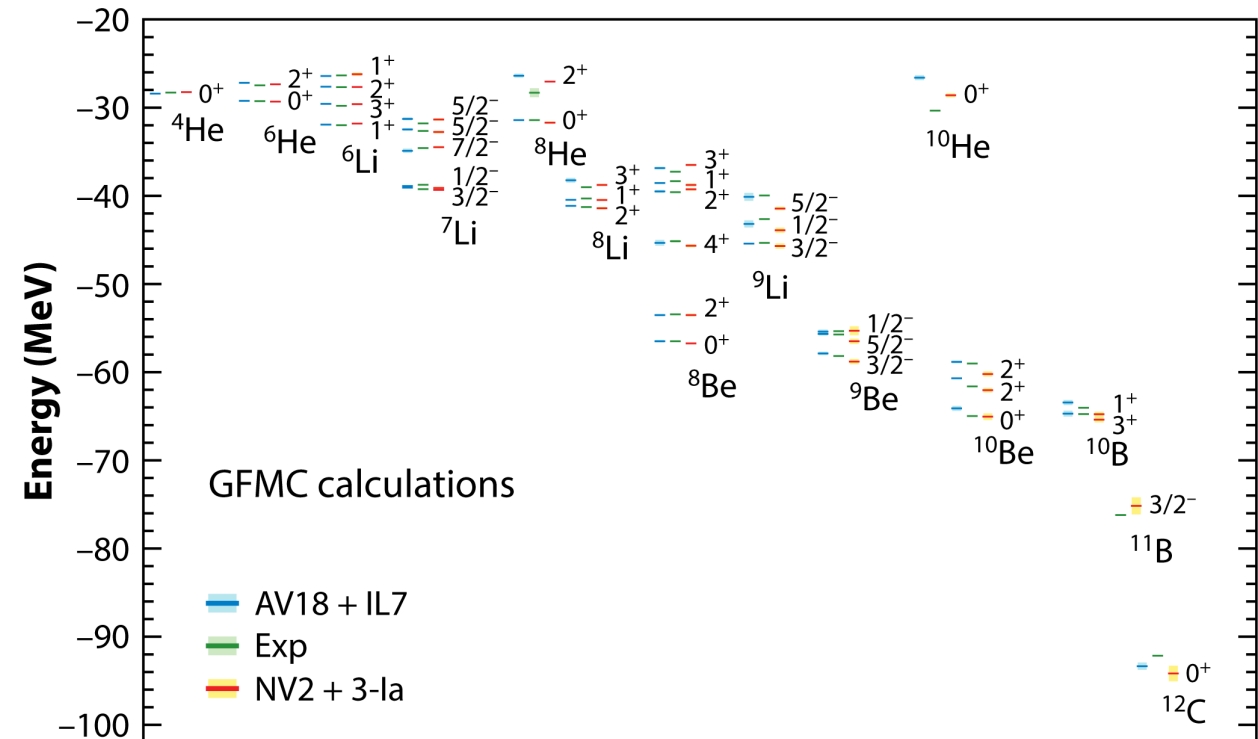
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- Sampling of spin/isospin states for better scaling with A

- Used for applications in light ($A \lesssim 16$) nuclei and for benchmarking other ab initio methods



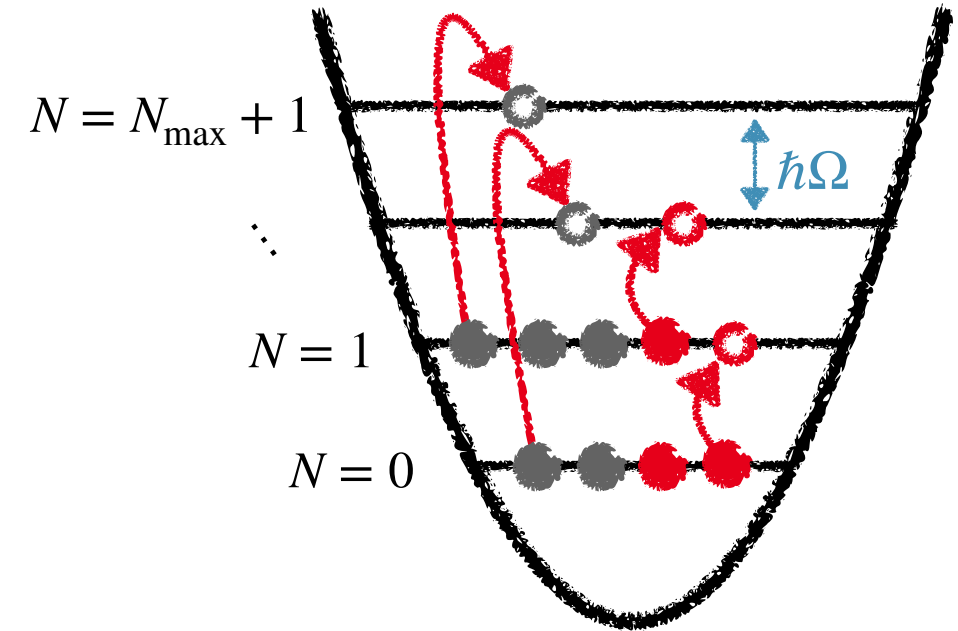
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NO-CORE SHELL MODEL (NCSM)

Barrett, Navrátil, Vary, Prog. Part. Nucl. Phys. 69, 131-181 (2013)



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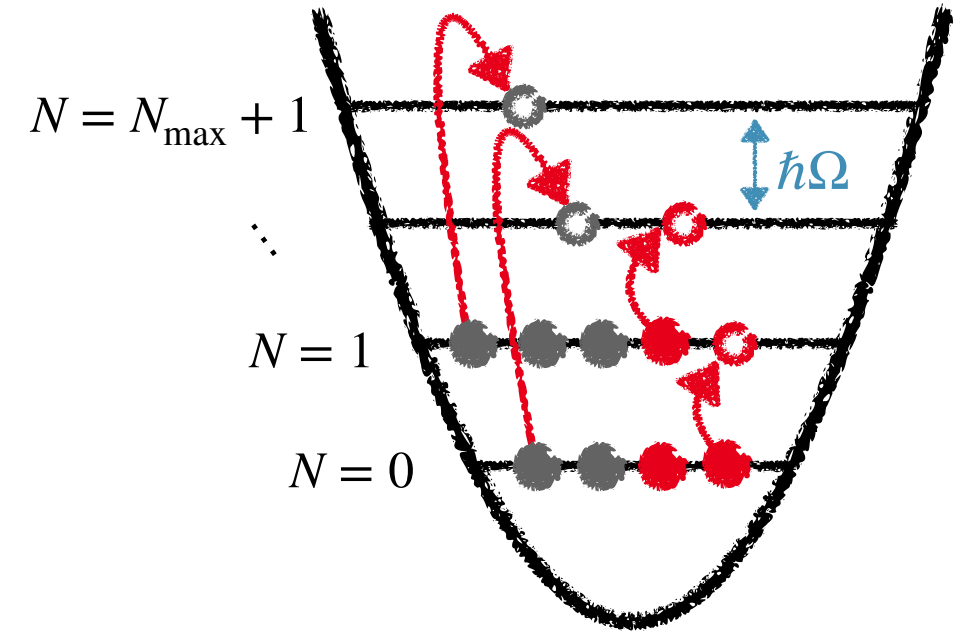


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- Solve the nuclear many-body problem

$$H^{(A)}\Psi^{(A)}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_A) = E^{(A)}\Psi^{(A)}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_A)$$



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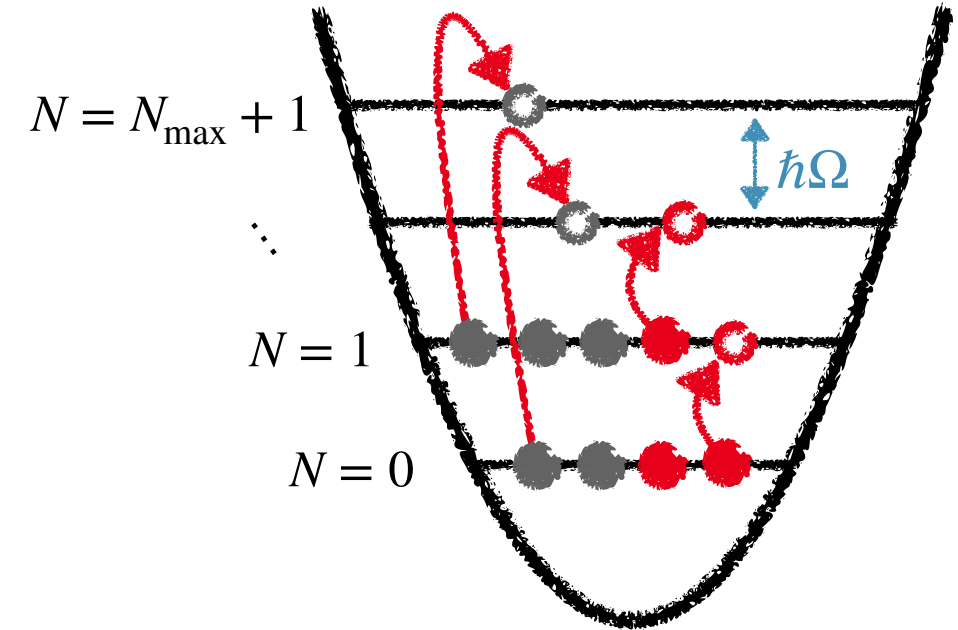
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- **Two- (NN)** and **three-body (3N)** forces from χ EFT:

$$H^{(A)} = \sum_{i=1}^A \frac{p_i^2}{2m} + \sum_{i<j=1}^A V_{ij}^{\text{NN}}(\mathbf{x}_i - \mathbf{x}_j) + \sum_{i<j<k=1}^A V_{ijk}^{\text{3N}}$$



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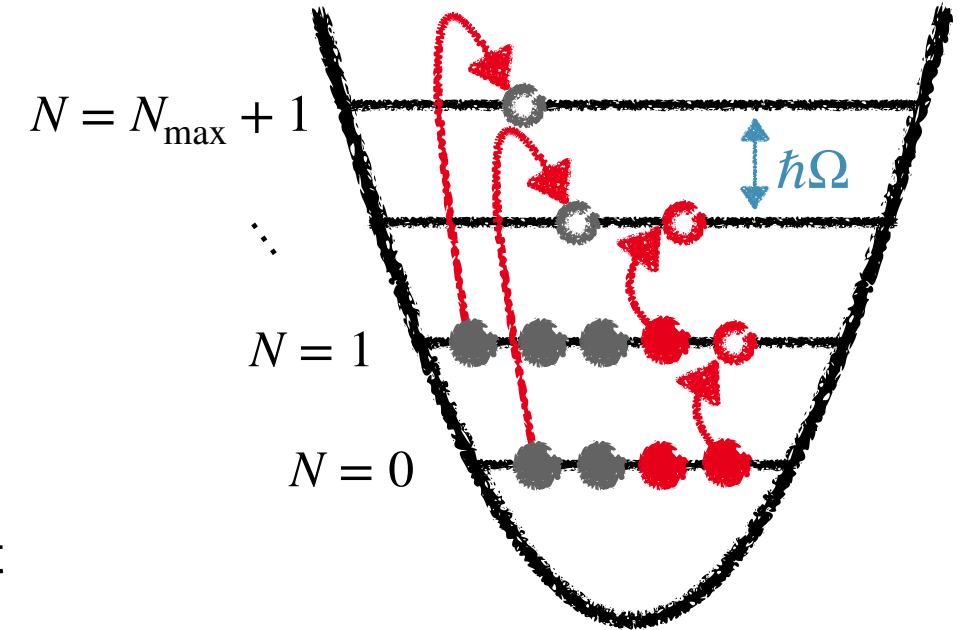
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- Expansion in Harmonic Oscillator (HO) Slater determinant (SD) basis:

$$\Psi_{\text{SD}}^{(A)} = \sum_{N=0}^{N_{\text{max}}} \sum_j c_{Nj}^{\text{SD}} \Phi_{\text{SD}Nj}^{\text{HO}}(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_A) = \psi^{(A)} \phi_{000}(\mathbf{R}_{\text{CM}})$$



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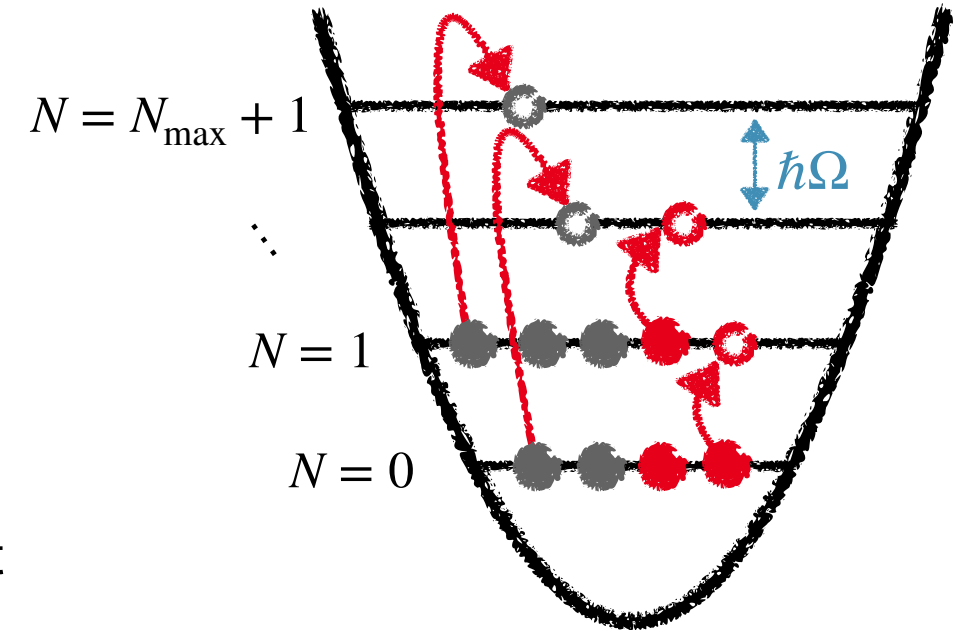
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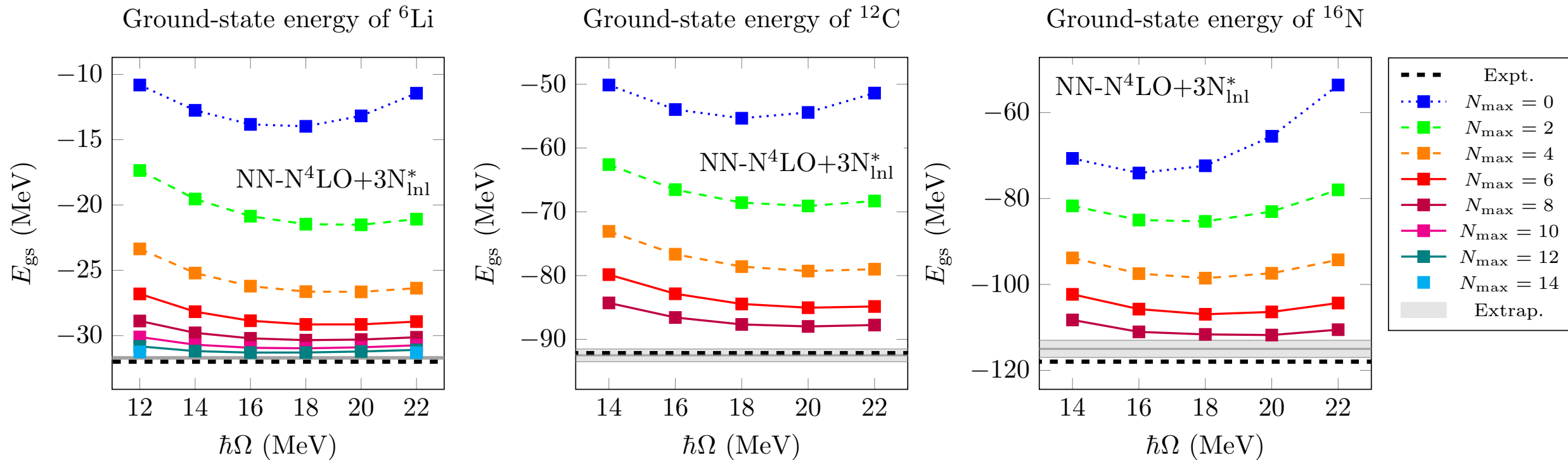
- Convergence to exact result with $N_{\text{max}} \rightarrow \infty$



CONVERGENCE OF NCSM CALCULATIONS



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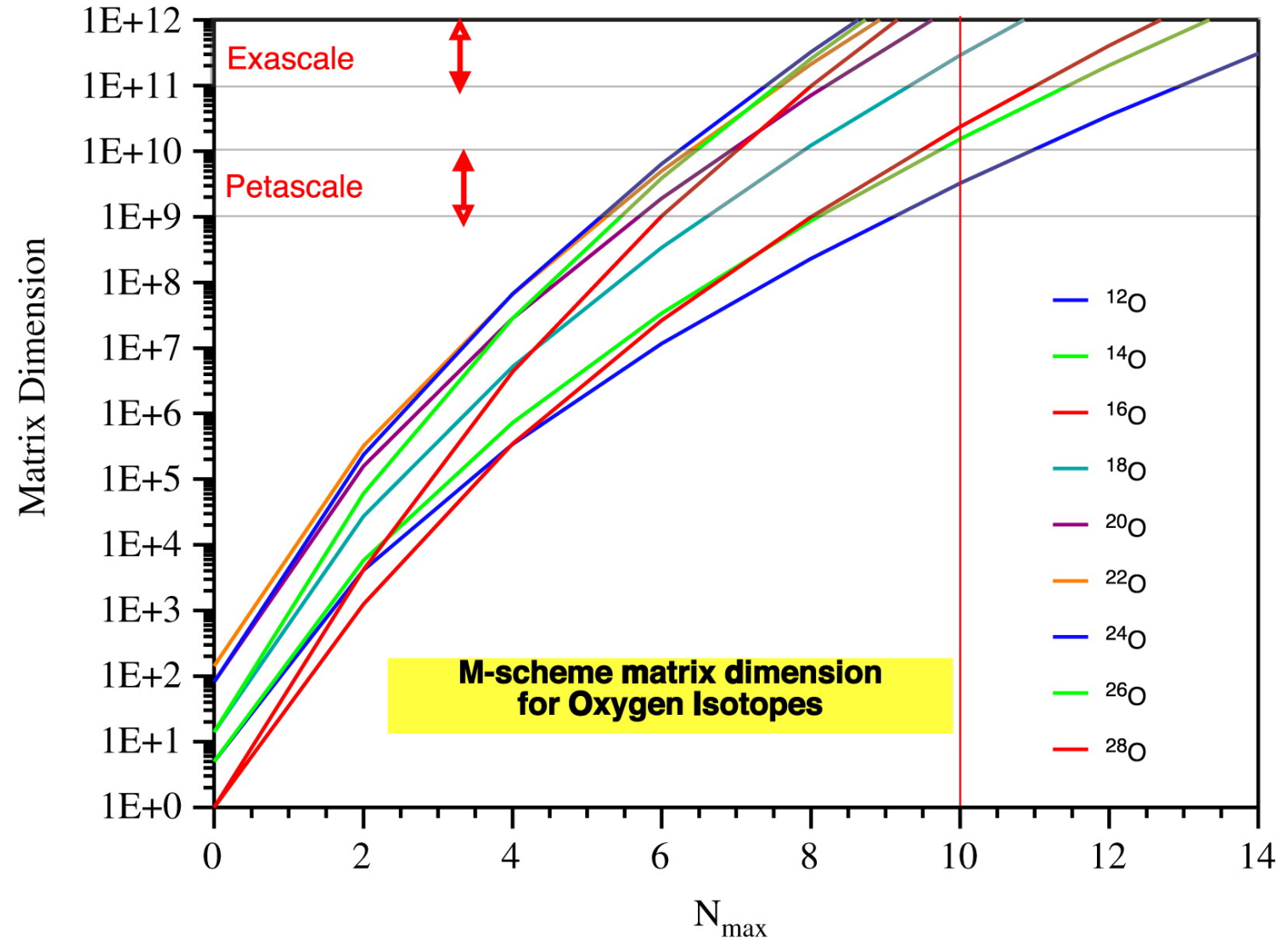
Jokiniemi, Navrátil, Kotila, Kravvaris, Phys. Rev. C 109, 065501 (2024)

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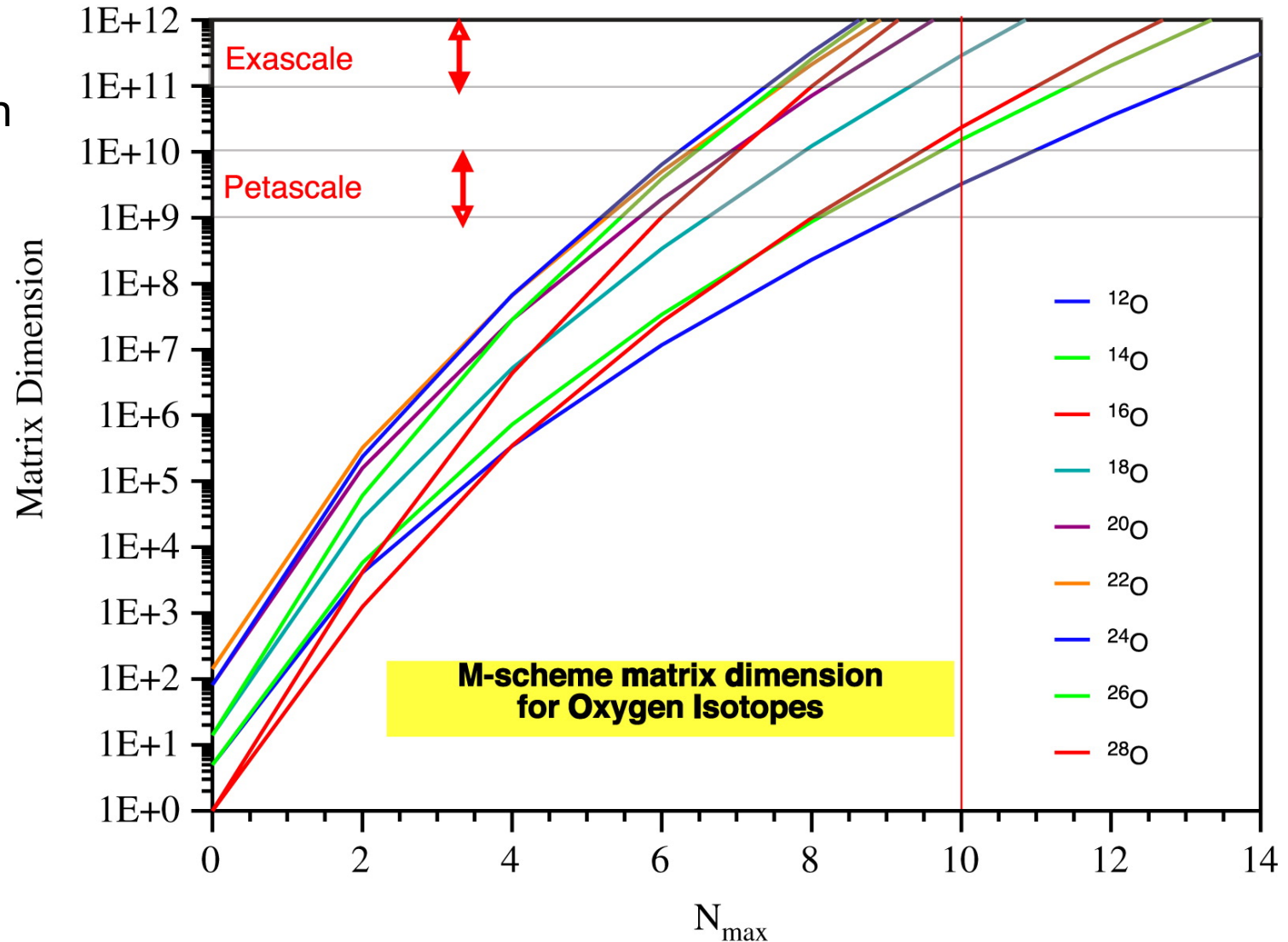
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- **Dimension of the Hamiltonian matrix grows combinatorially with $N_{\max}$ and A**



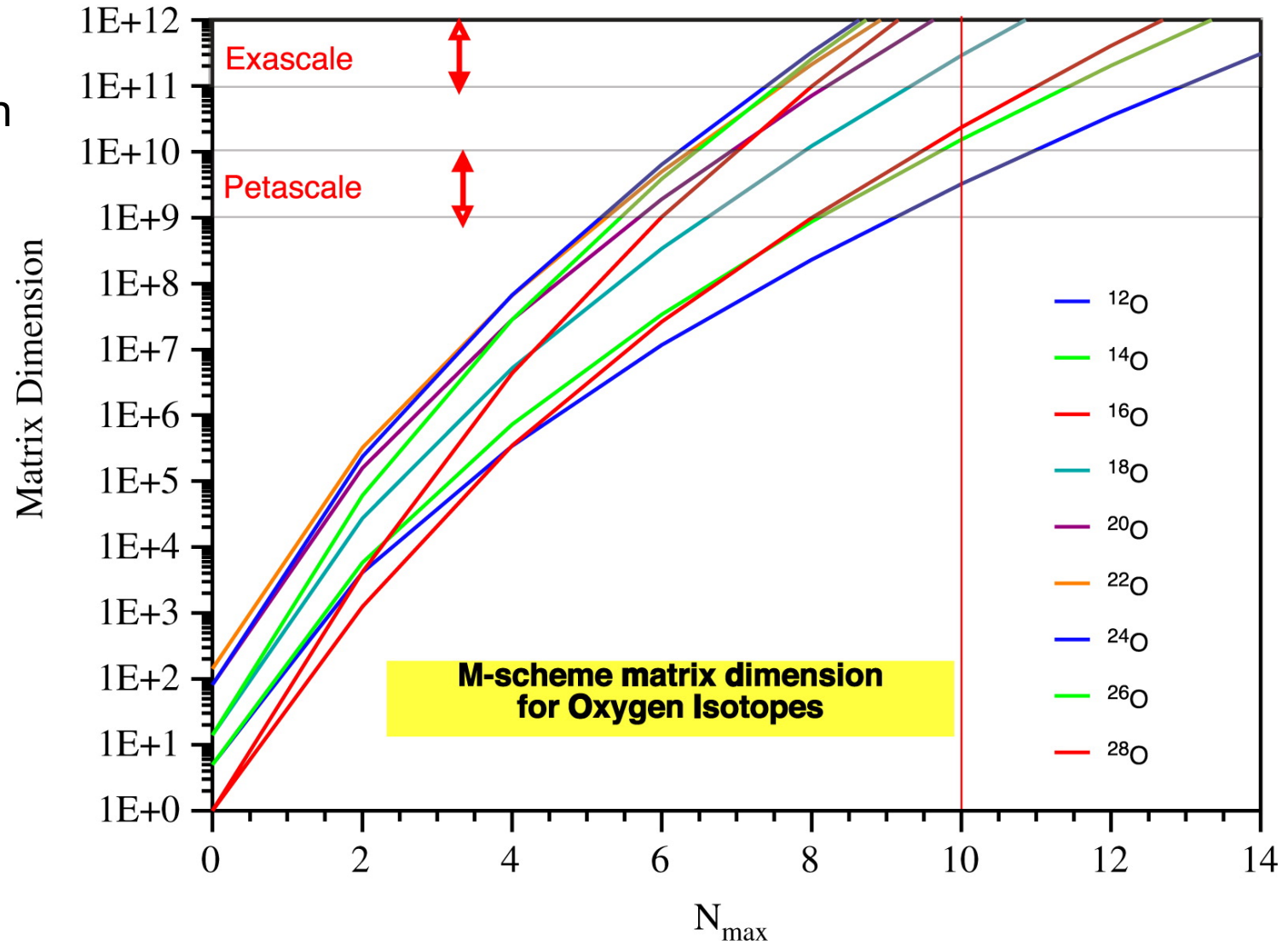
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- **Dimension of the Hamiltonian matrix grows combinatorially** with $N_{\max}$ and A
- Converged calculations with $NN + 3N$ forces possible for nuclei with $A \lesssim 20$



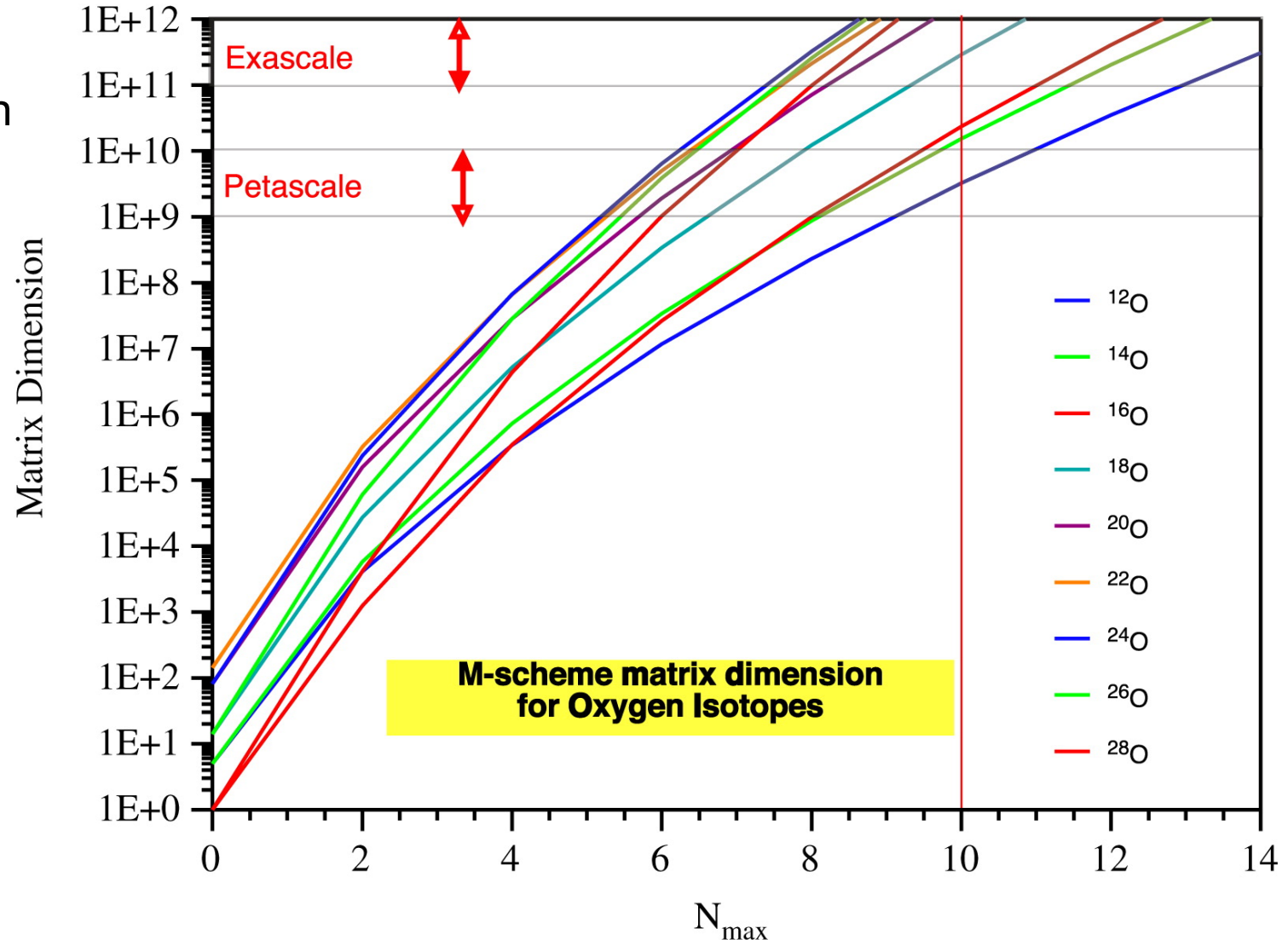
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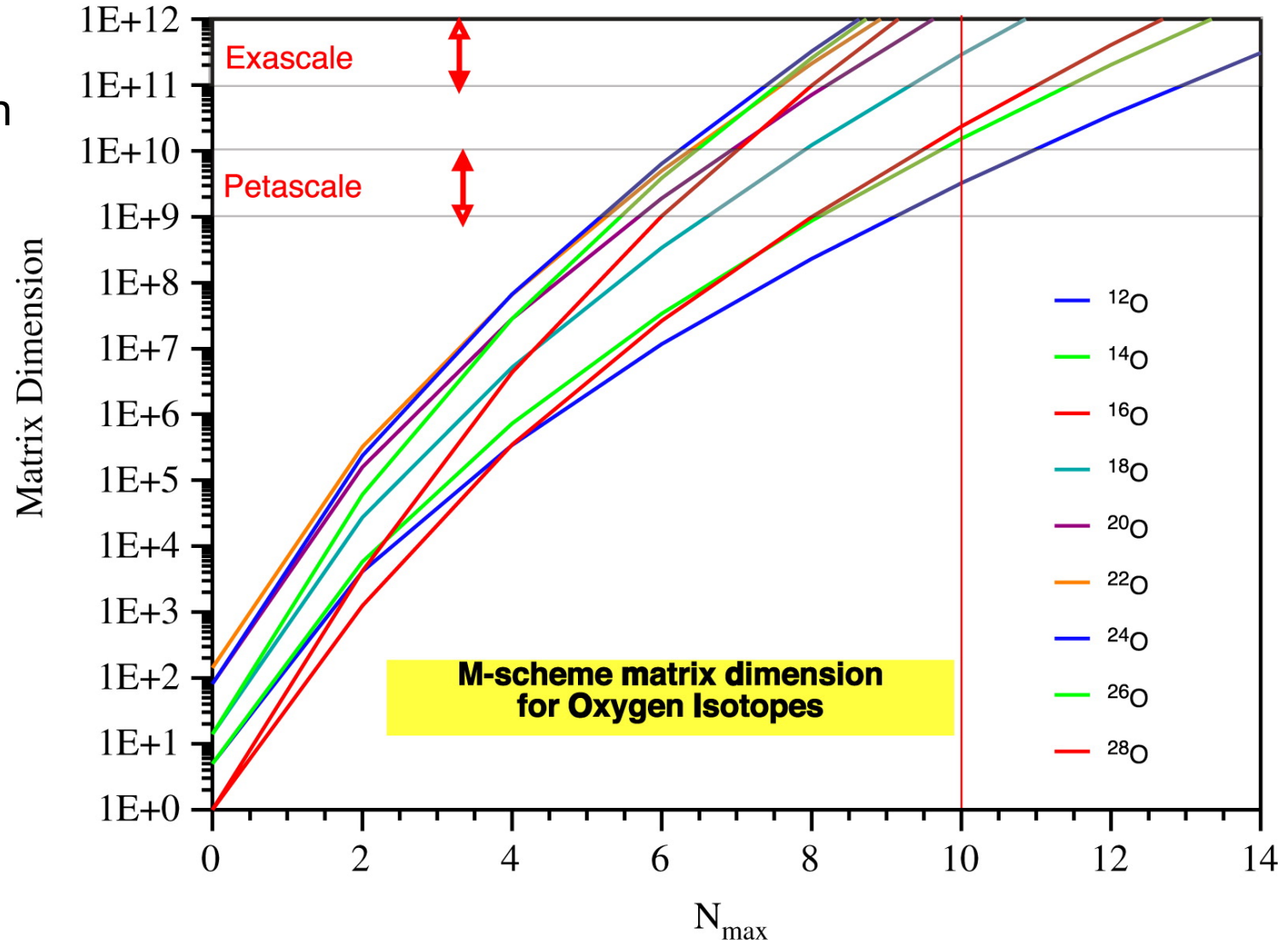
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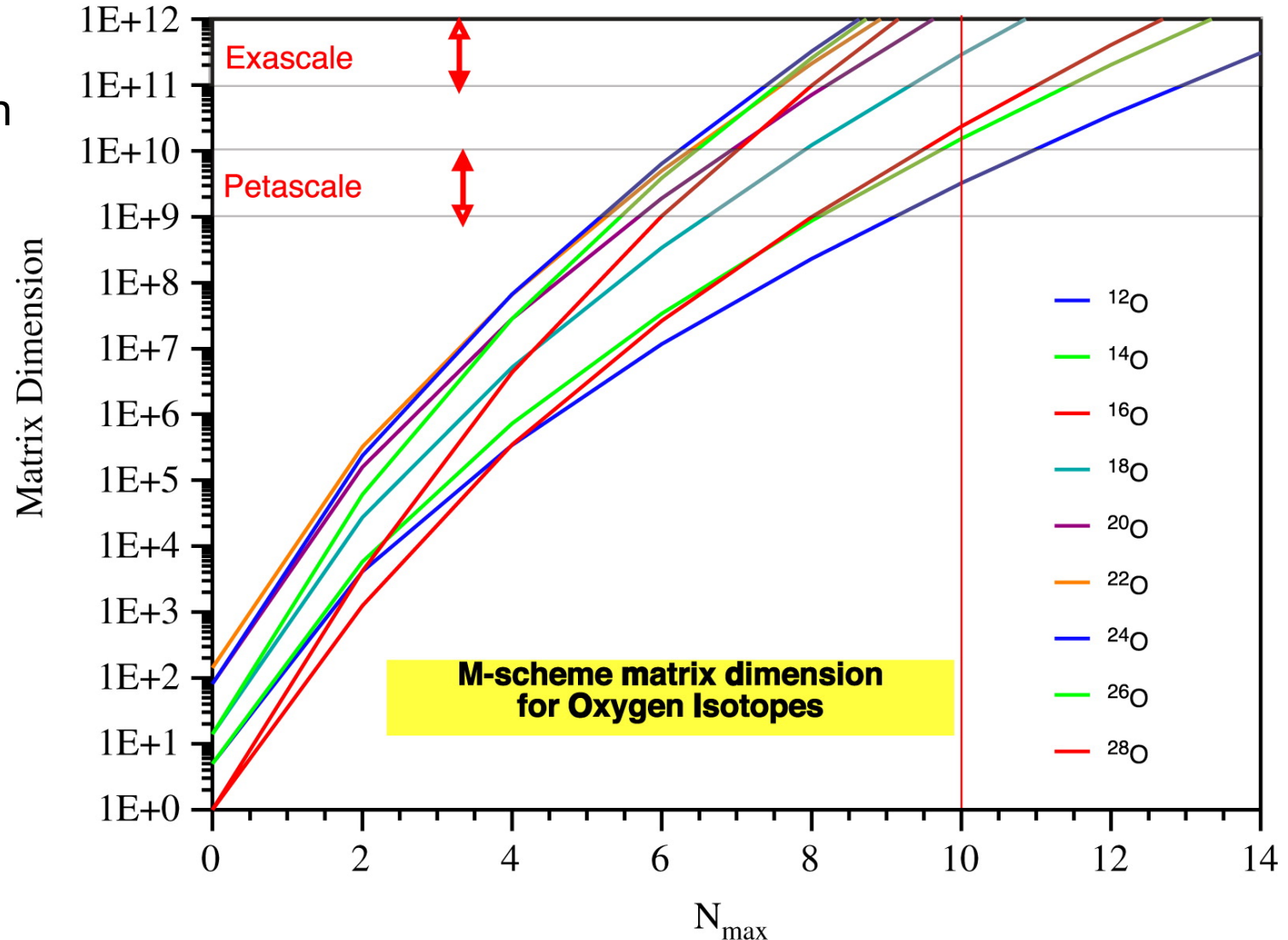
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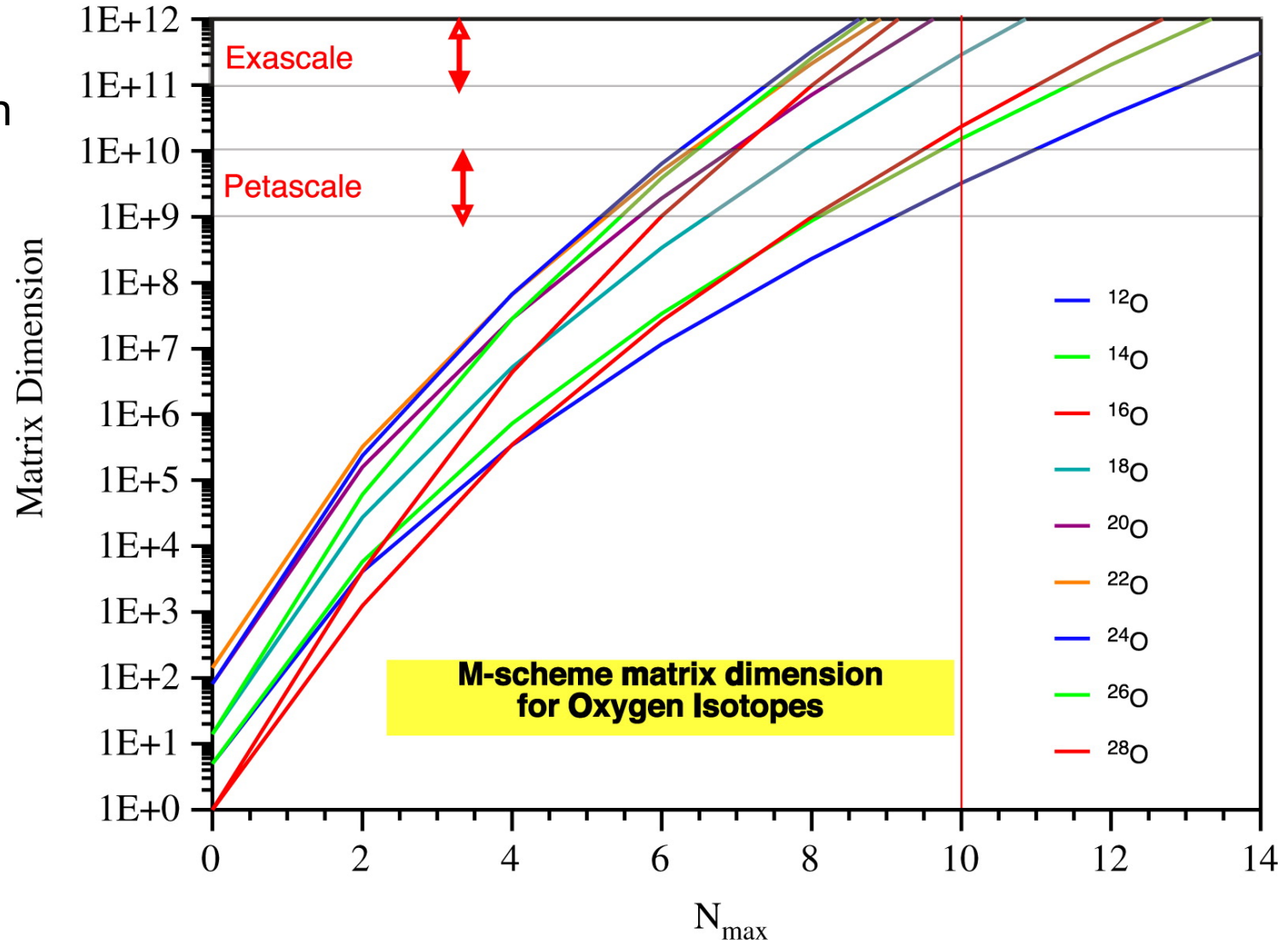
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Barrett, Navrátil, Vary, Prog. Part. Nucl. Phys. 69, 131-181 (2013)



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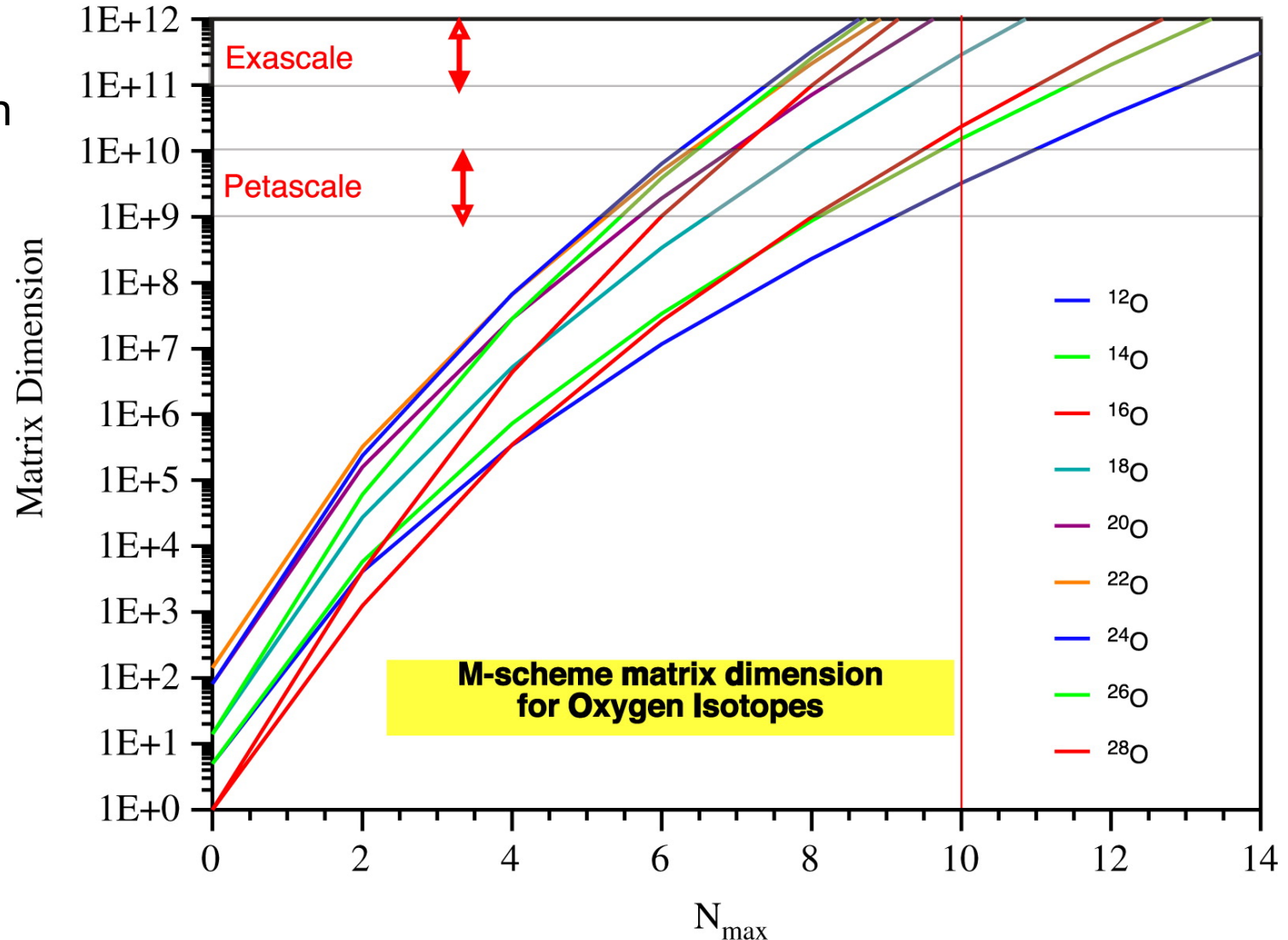
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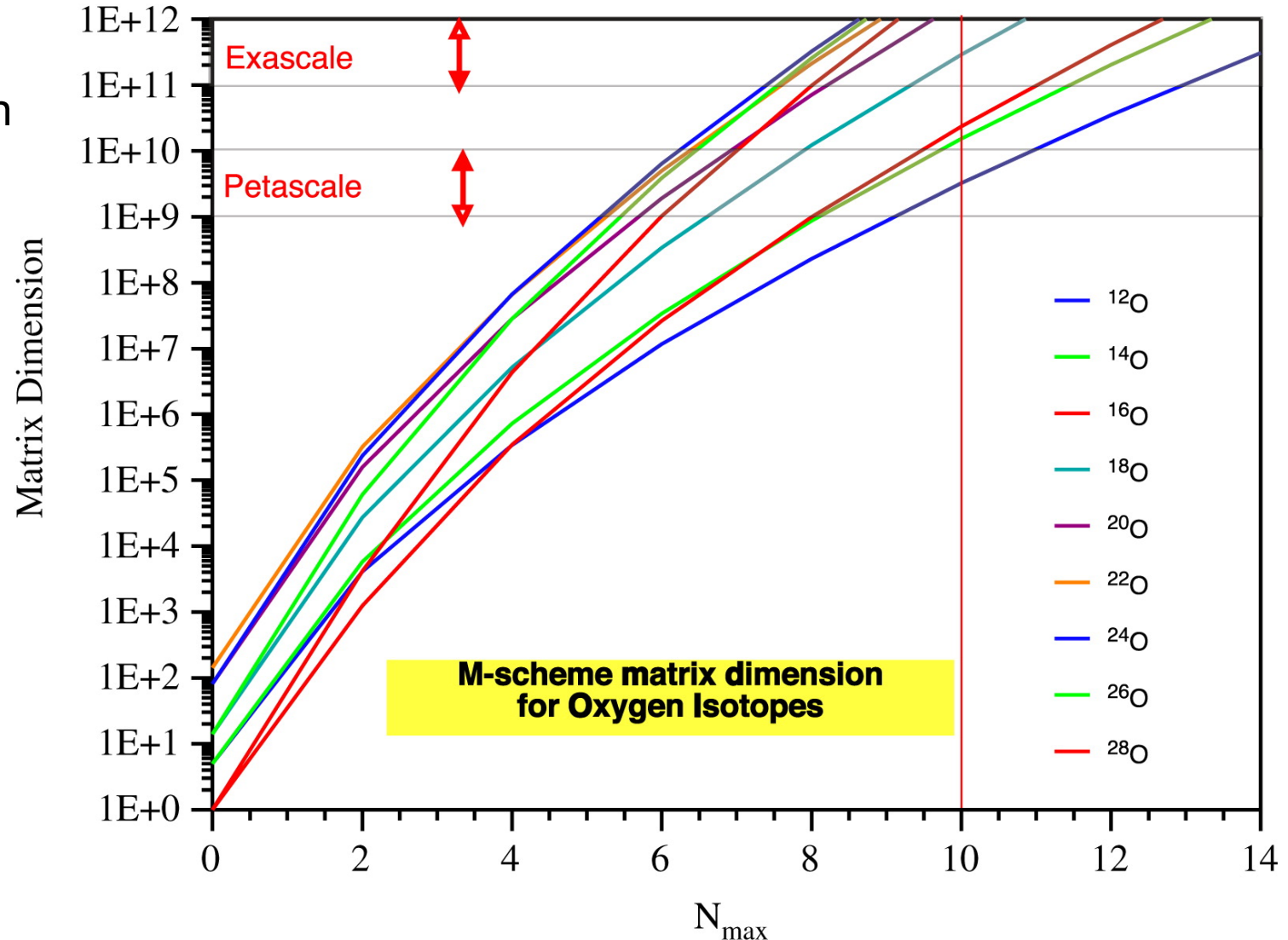
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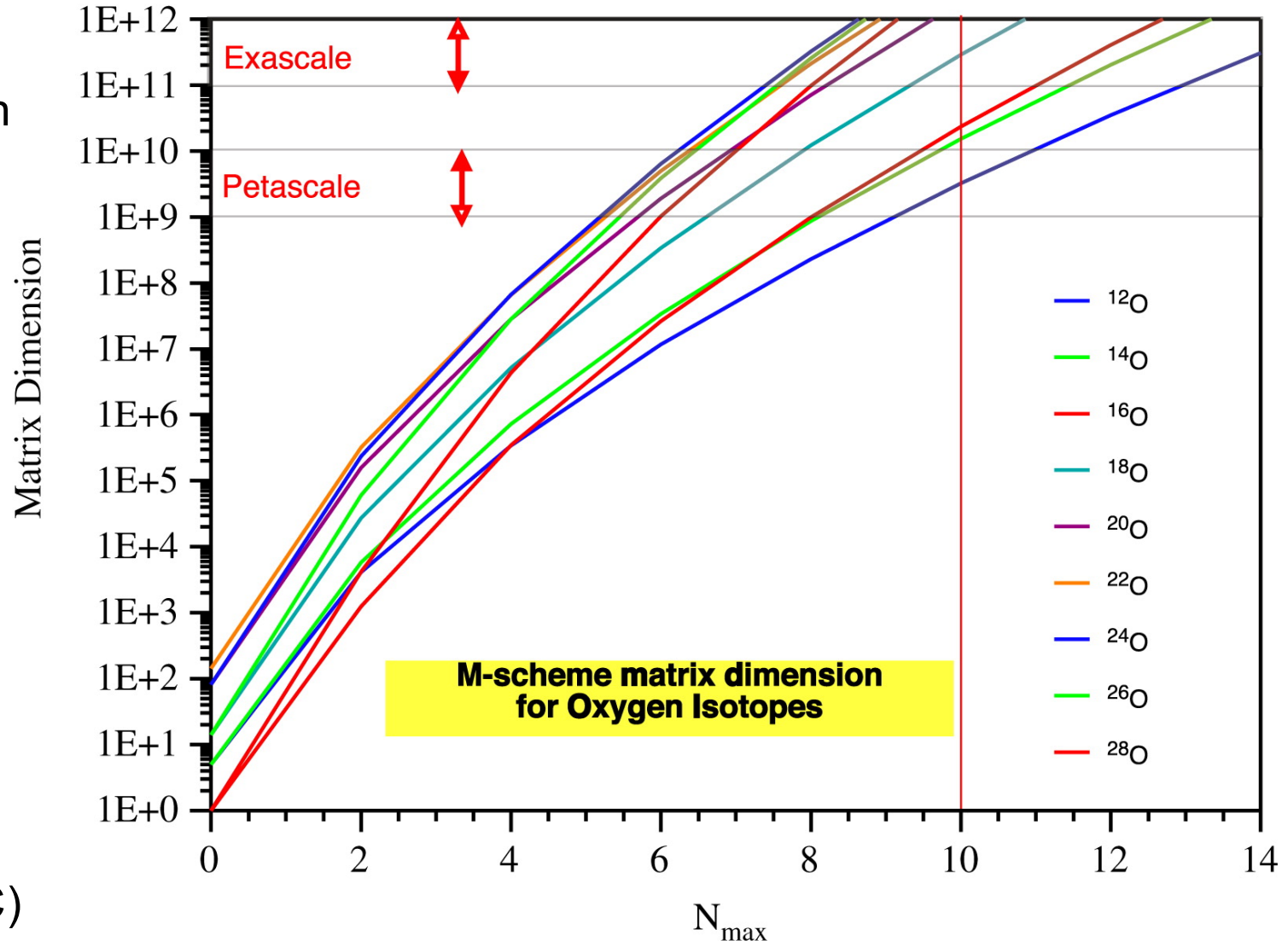
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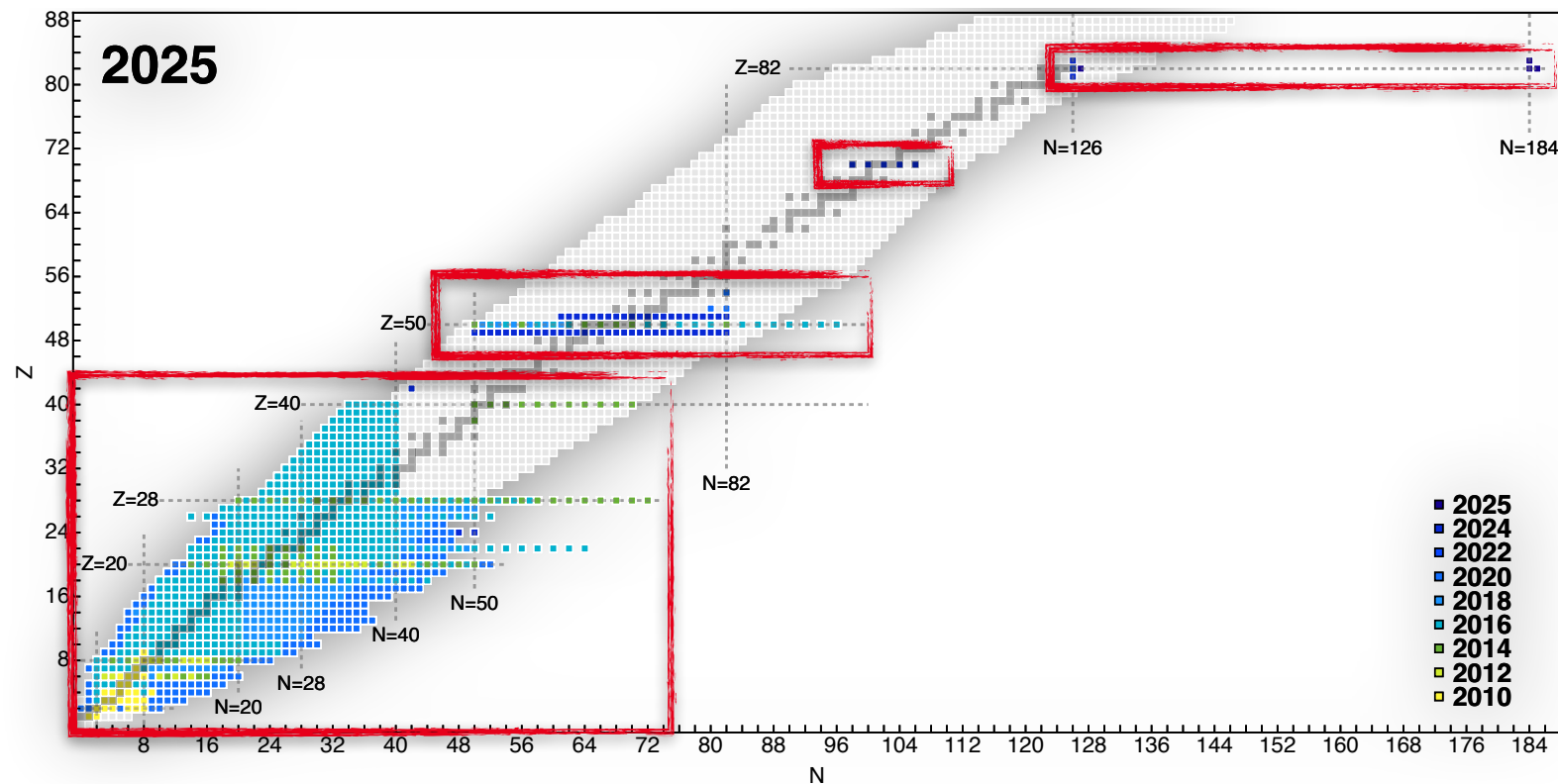
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MEDIUM-HEAVY TO HEAVY NUCLEI

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- **These methods often rely on Hamiltonian normal-ordered with respect to the reference state**

$$H = E_0 + \sum_{ij} f_{ij} \{a_i^\dagger a_j\} + \frac{1}{4} \sum_{ijkl} \Gamma_{ijkl} \{a_i^\dagger a_j^\dagger a_l a_k\} \left(+ \frac{1}{36} \sum_{ijklmn} W_{ijklmn} \{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\} \right)$$

HARTREE-FOCK THEORY

Suhonen, *"From Nucleons to Nucleus: concepts of microscopic nuclear theory"* (2007)

$$H = T + V = \sum_{\alpha\beta} t_{\alpha\beta} a_{\alpha}^{\dagger} a_{\beta} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma}$$



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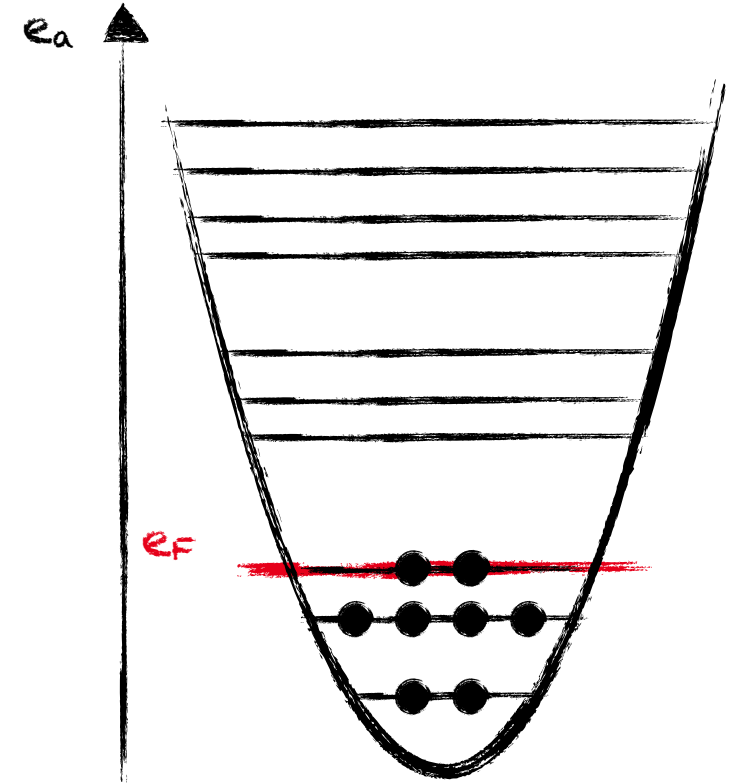
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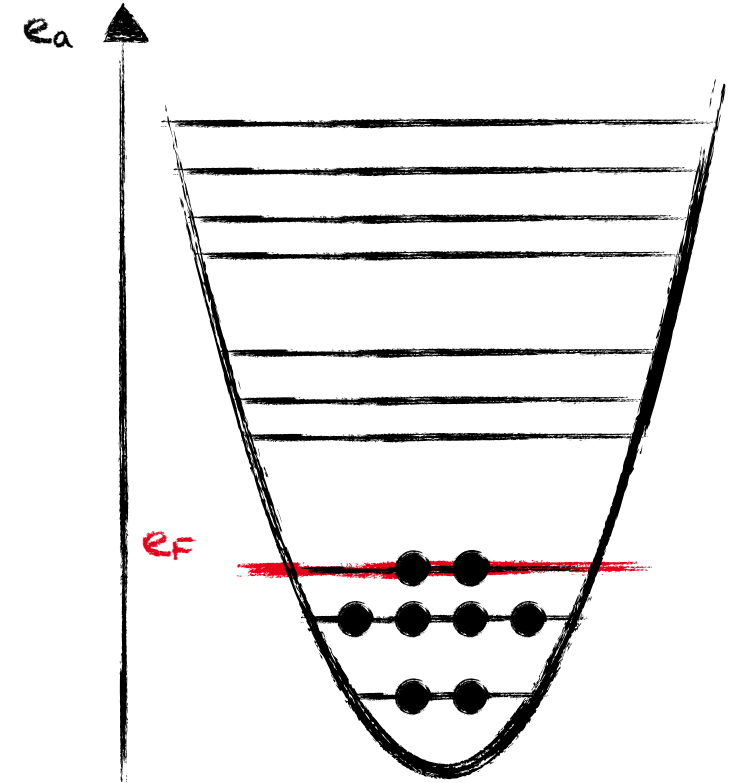


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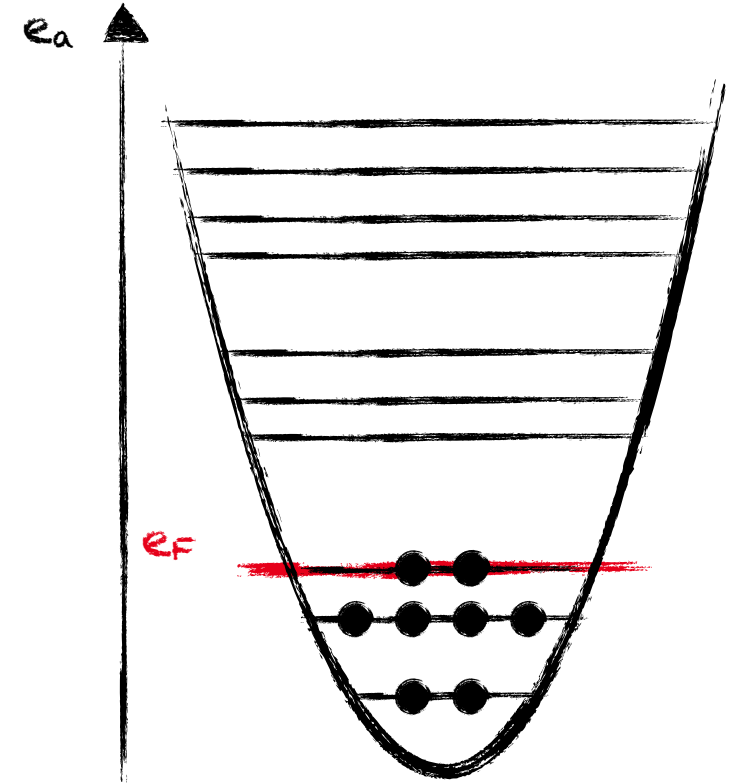
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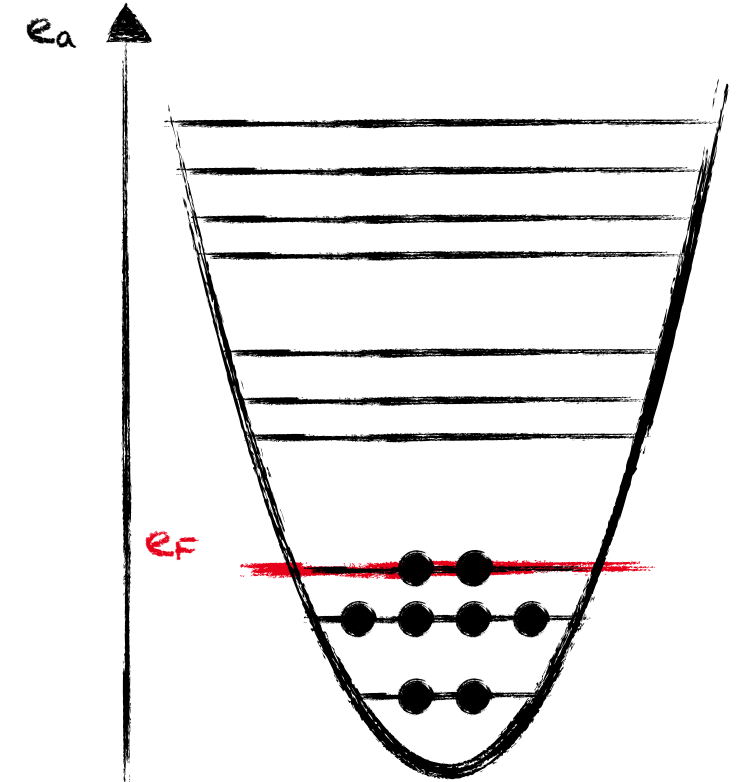
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Mean field



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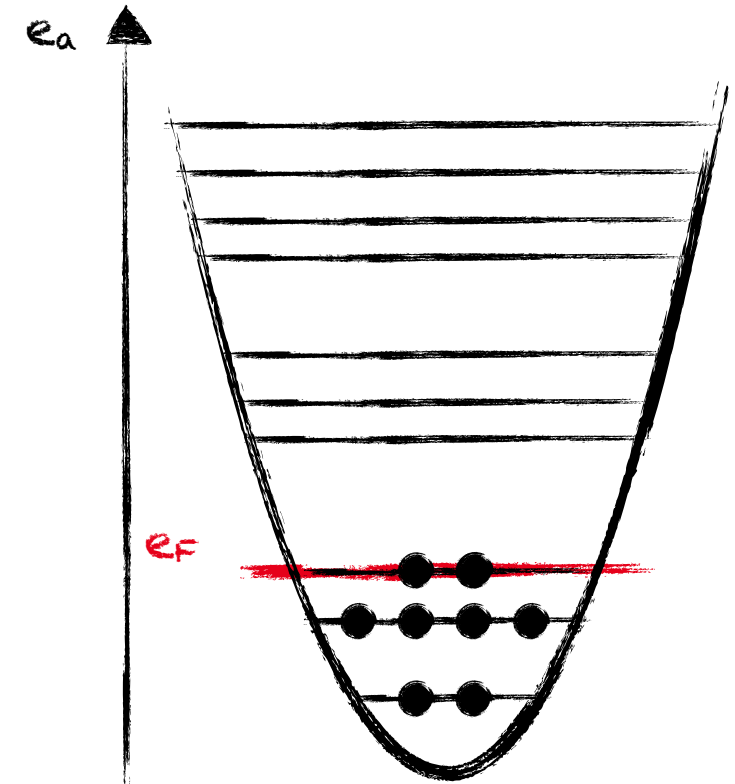
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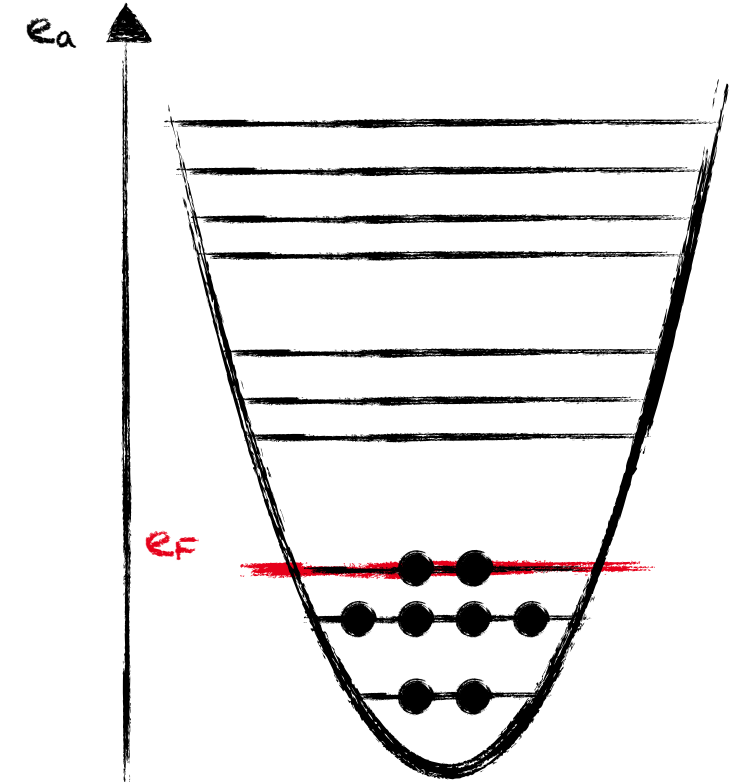
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**Residual
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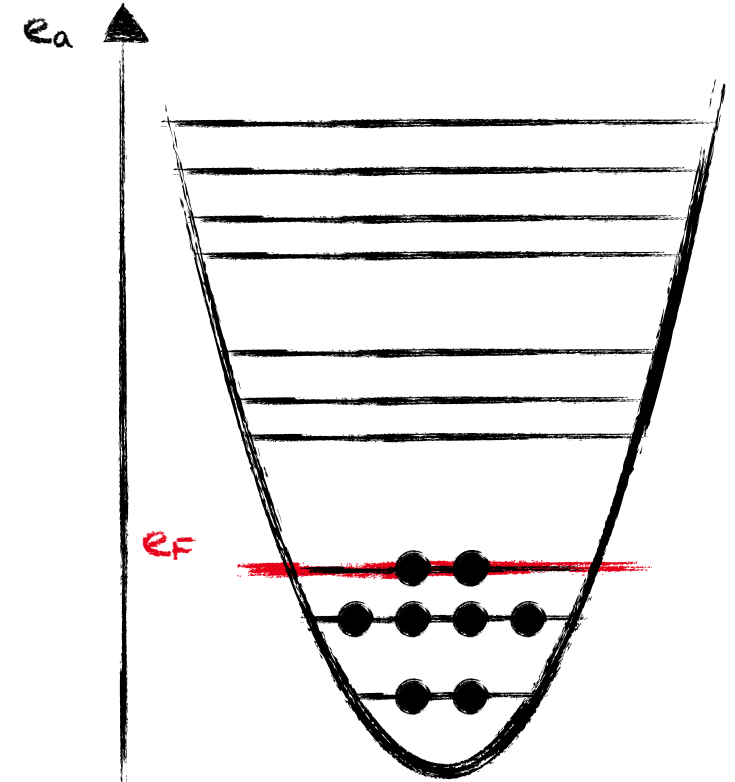
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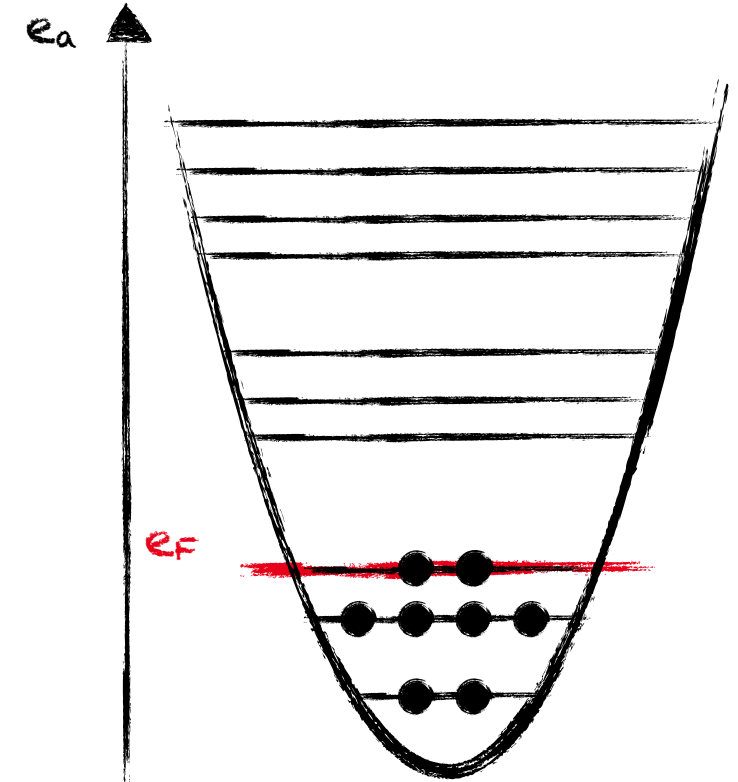
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MANY-BODY PERTURBATION THEORY

Tichai, Roth, Duguet, Front. Phys. 8:164 (2020); Hergert, Front. Phys. 8:379 (2020)



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MANY-BODY PERTURBATION THEORY



Tichai, Roth, Duguet, Front. Phys. 8:164 (2020); Hergert, Front. Phys. 8:379 (2020)

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MANY-BODY PERTURBATION THEORY



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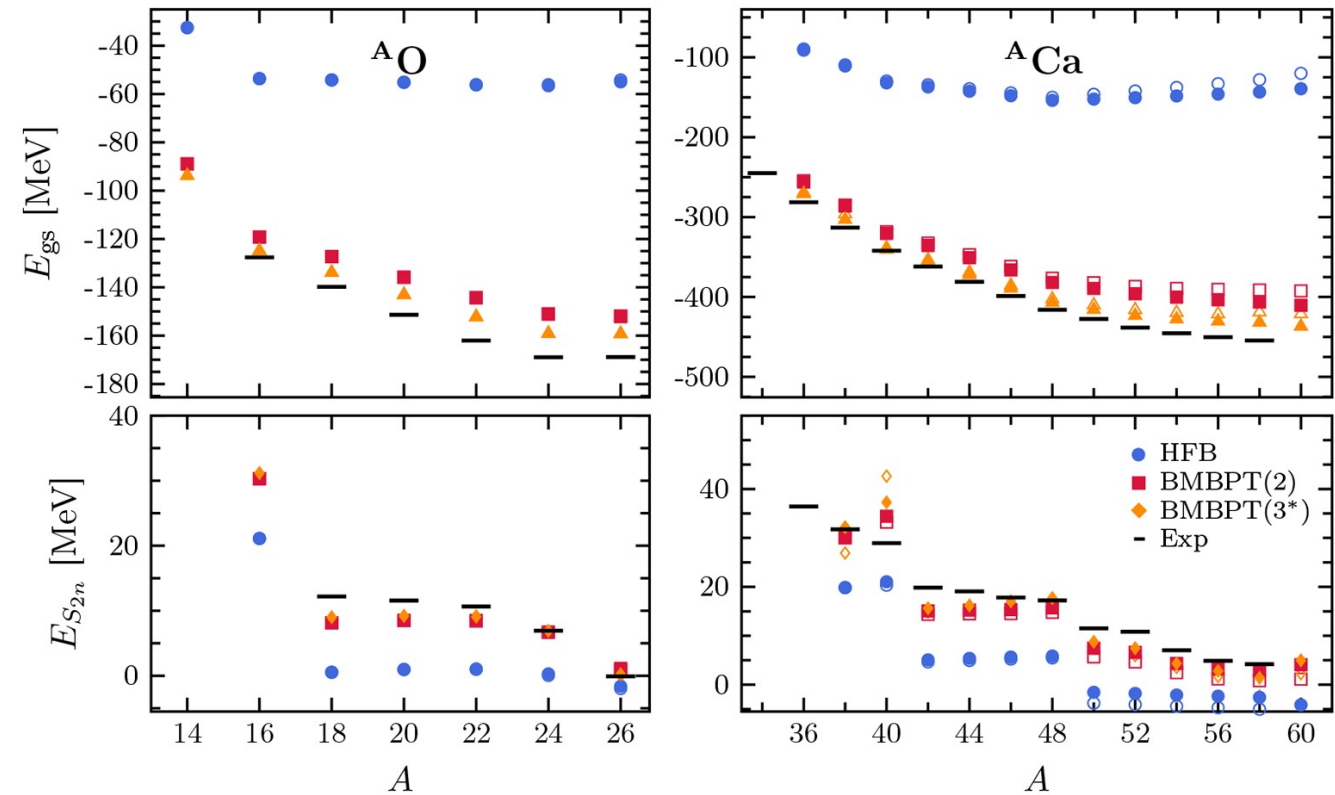
Hands-on session
by P. Arthuis on
Thursday afternoon

MANY-BODY PERTURBATION THEORY

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



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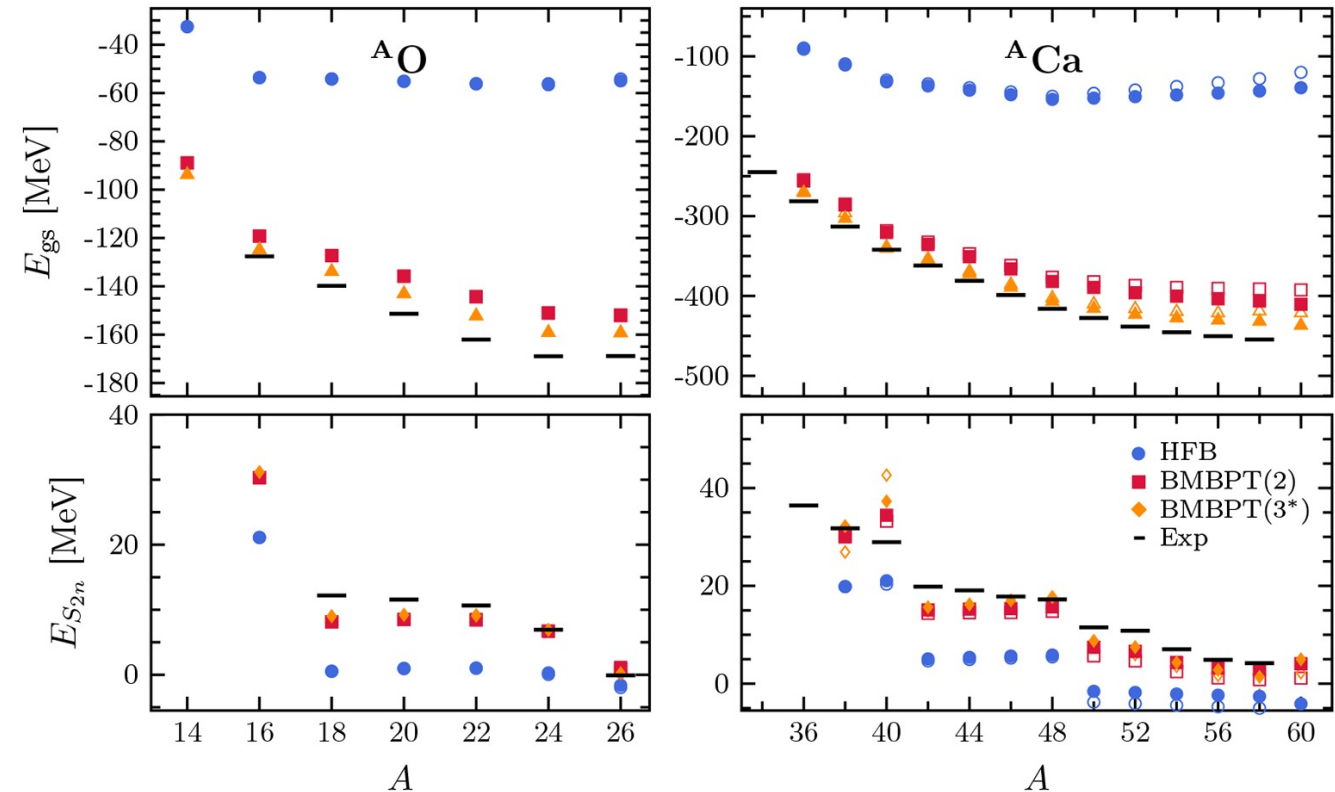
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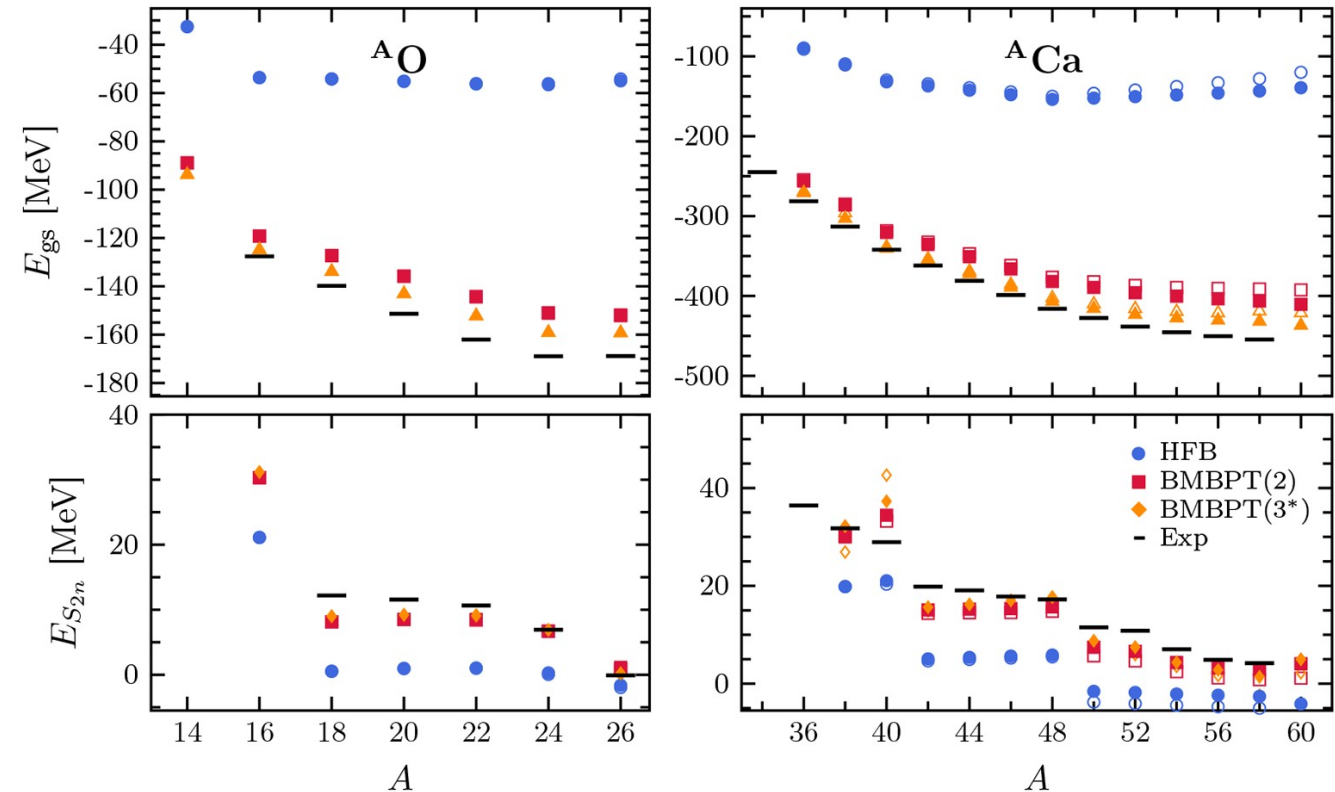
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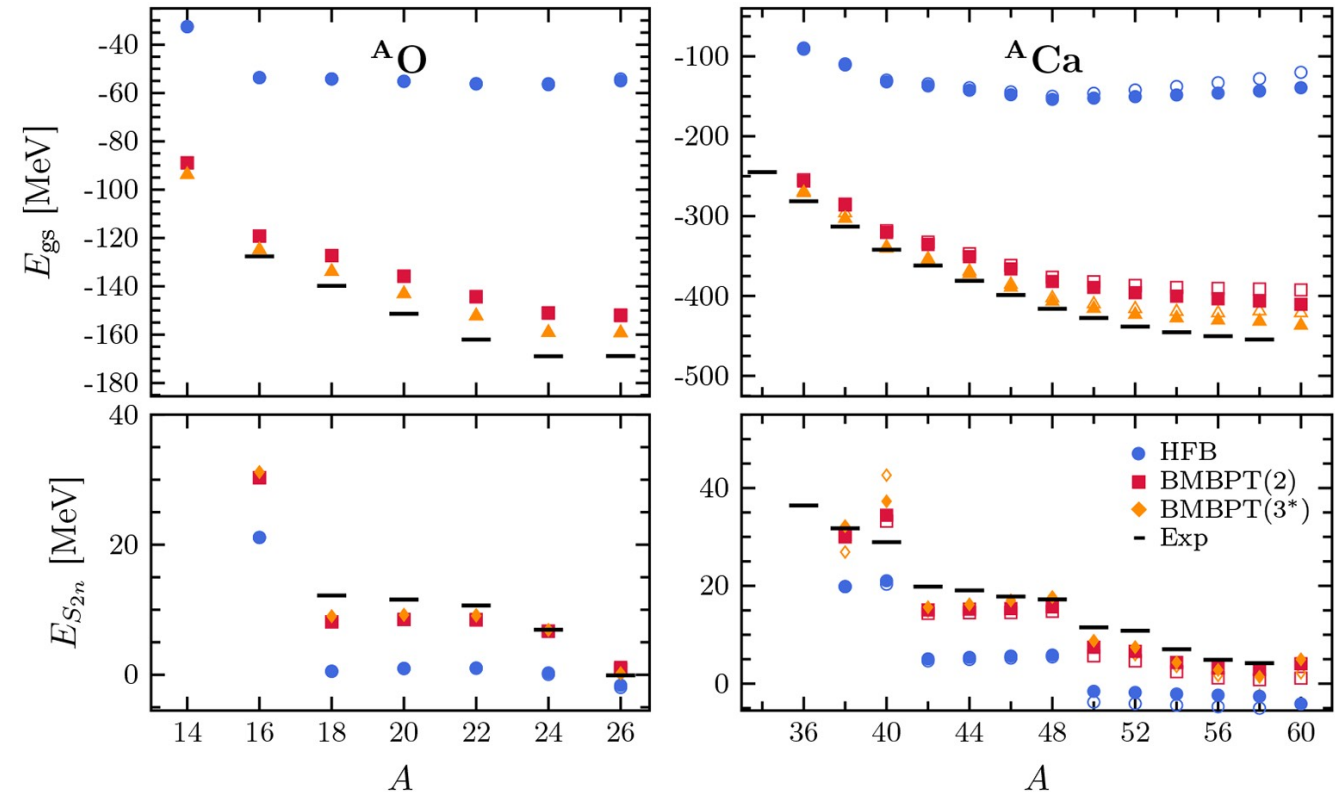
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MANY-BODY PERTURBATION THEORY

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- Very practical for uncertainty quantification
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- Extensions to open-shell nuclei:



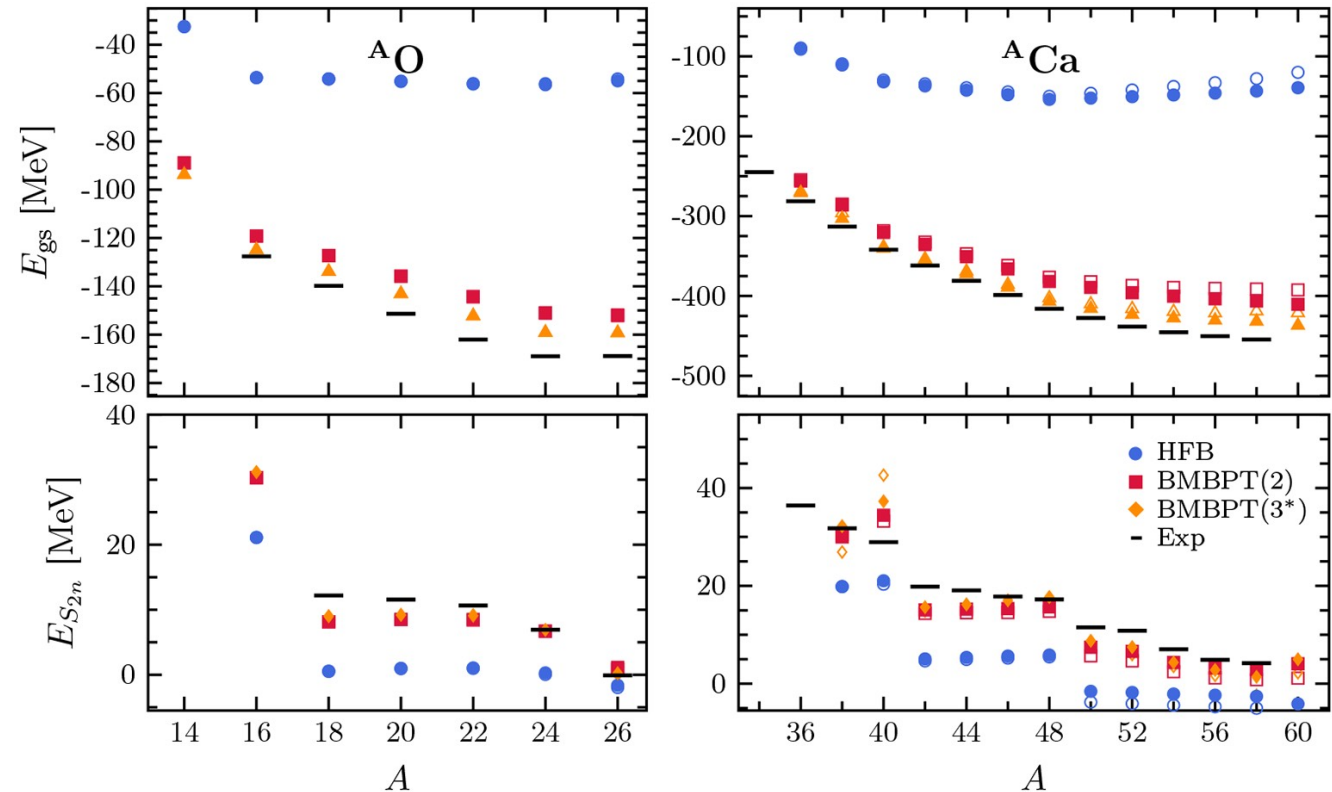
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- Extensions to open-shell nuclei:
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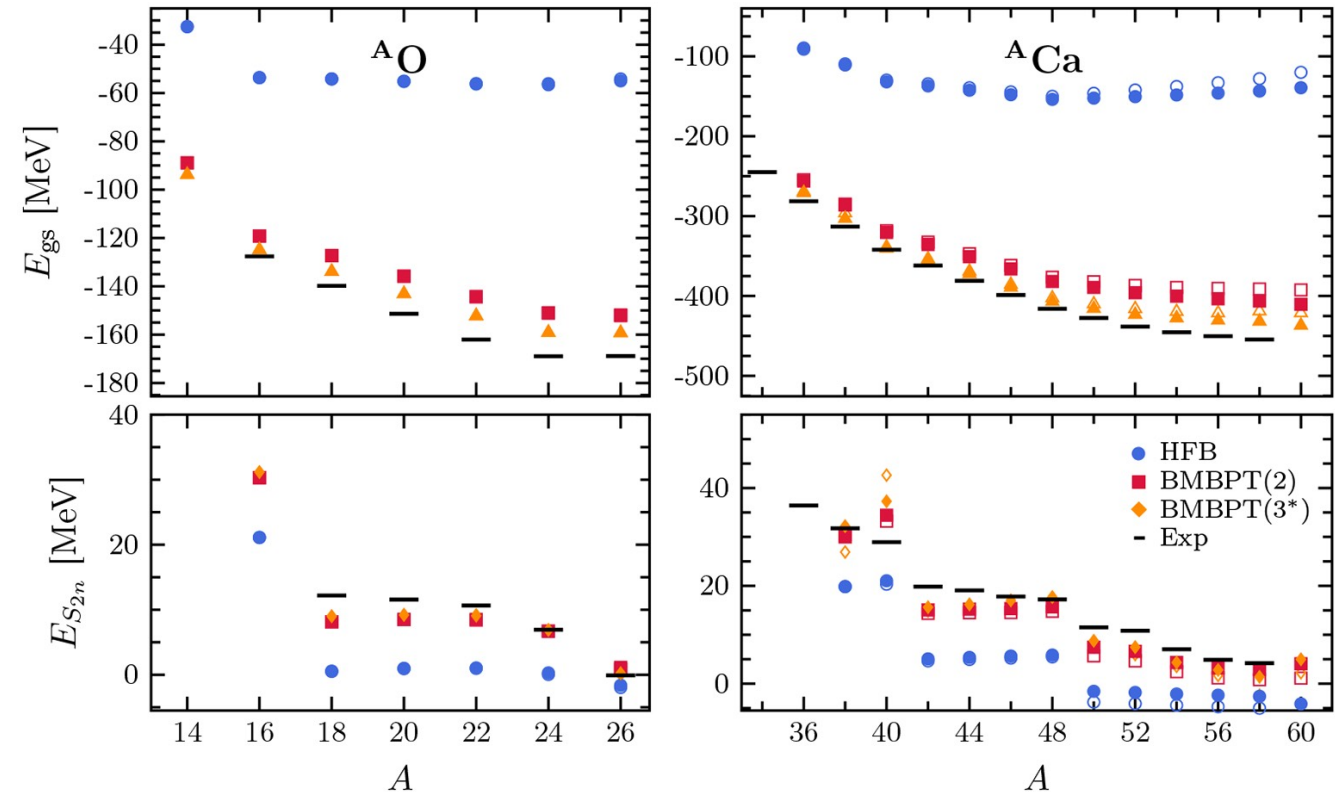
MANY-BODY PERTURBATION THEORY



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

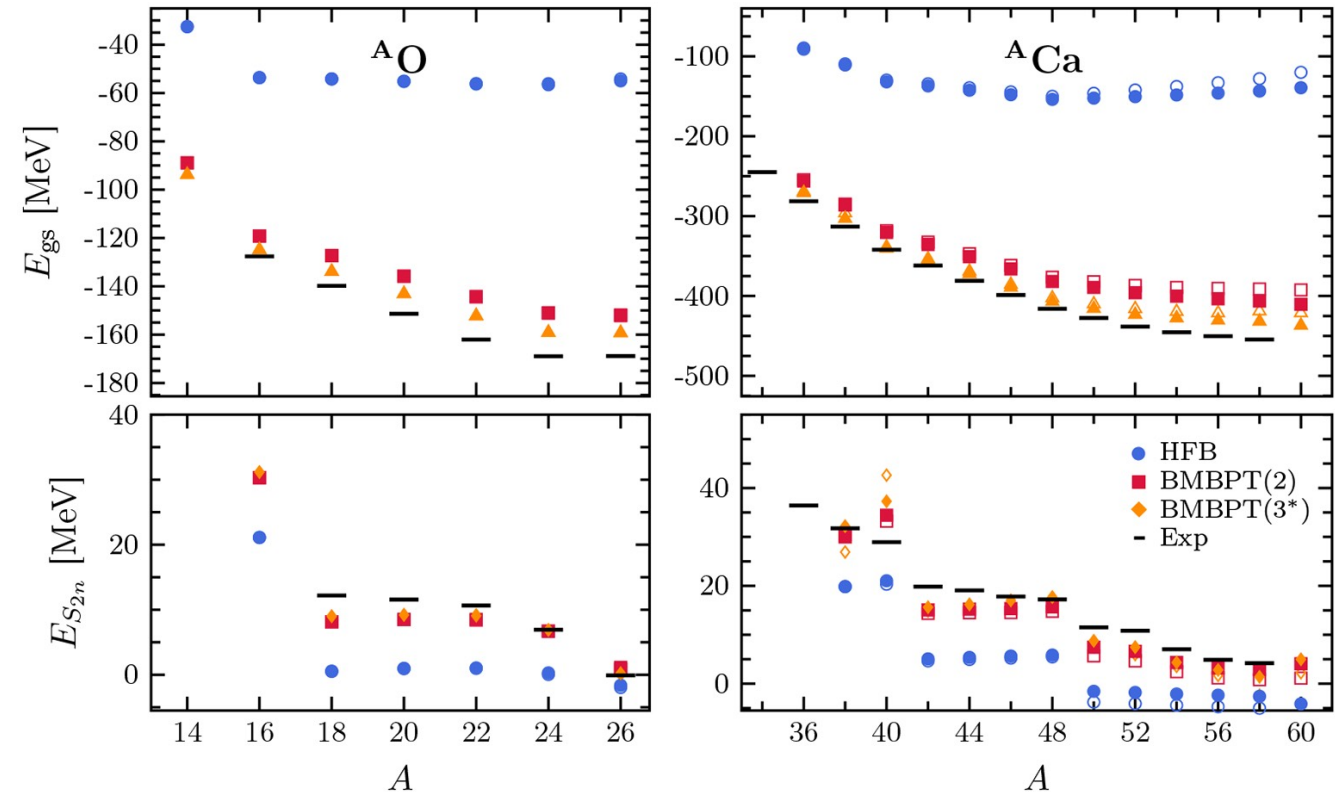
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SELF-CONSISTENT GREEN'S FUNCTIONS

Somá, Front. Phys. 8:340 (2020); Dickhoff, Barbieri, Progr. Part. Nucl. Phys. 52, 377-496 (2004)



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SELF-CONSISTENT GREEN'S FUNCTIONS



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Somá, Front. Phys. 8:340 (2020); Dickhoff, Barbieri, Progr. Part. Nucl. Phys. 52, 377-496 (2004)

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Initial guess (e.g. Hartree-fock)

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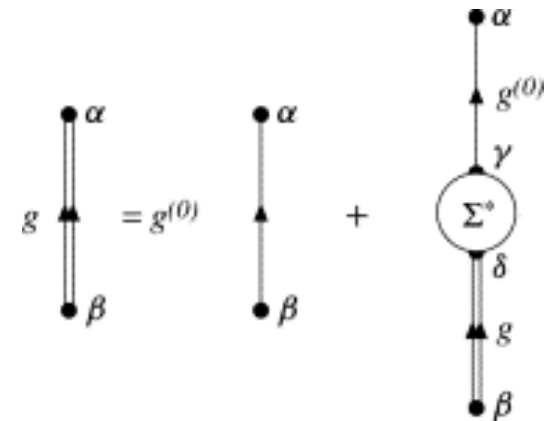
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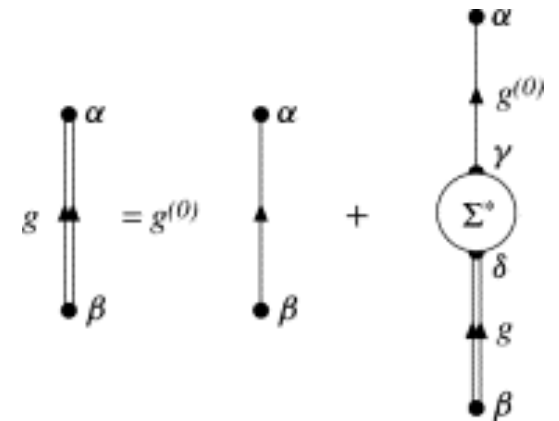
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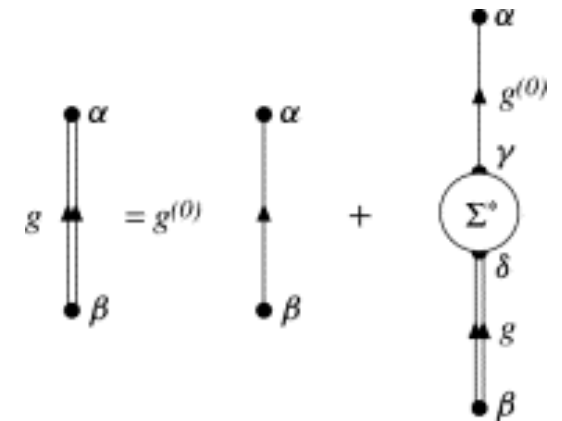
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- One-body observables, spectroscopy of $A \pm 1$ systems

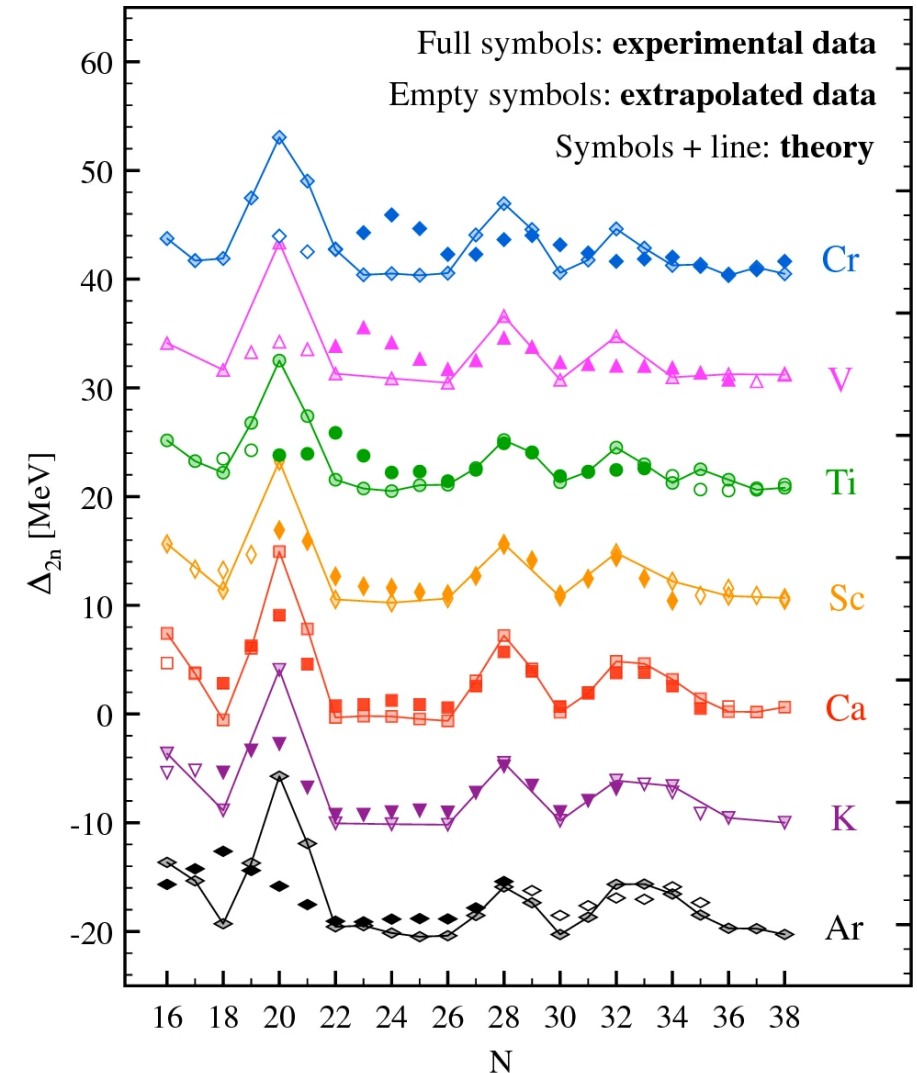


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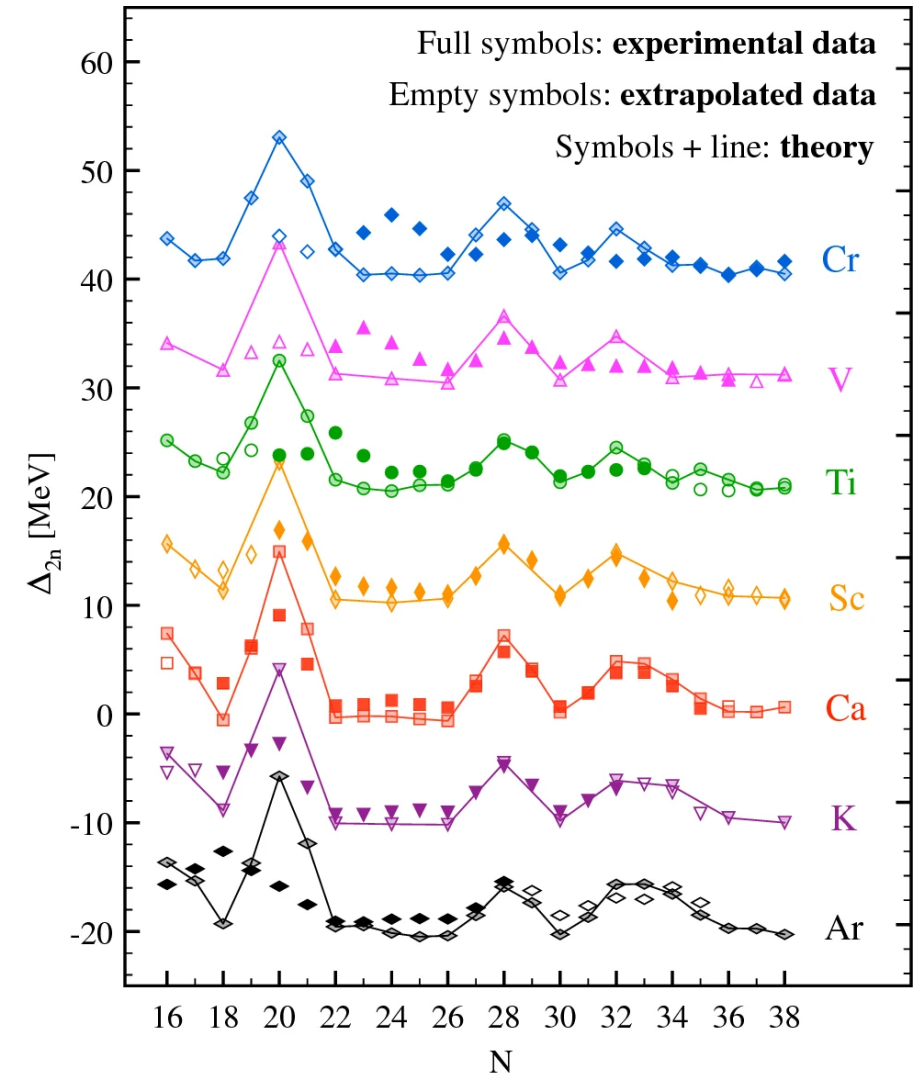
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- Implemented through **Algebraic Diagrammatic Construction** at order n [ADC(n)]



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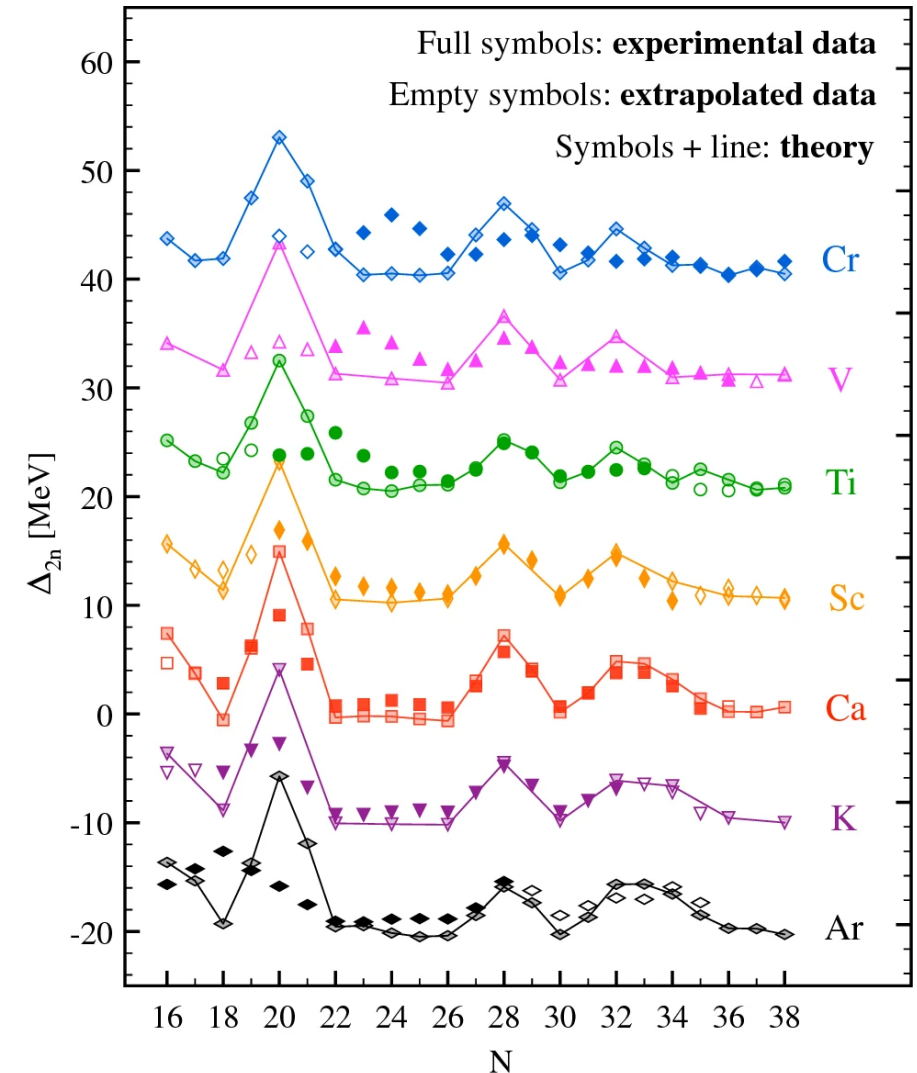
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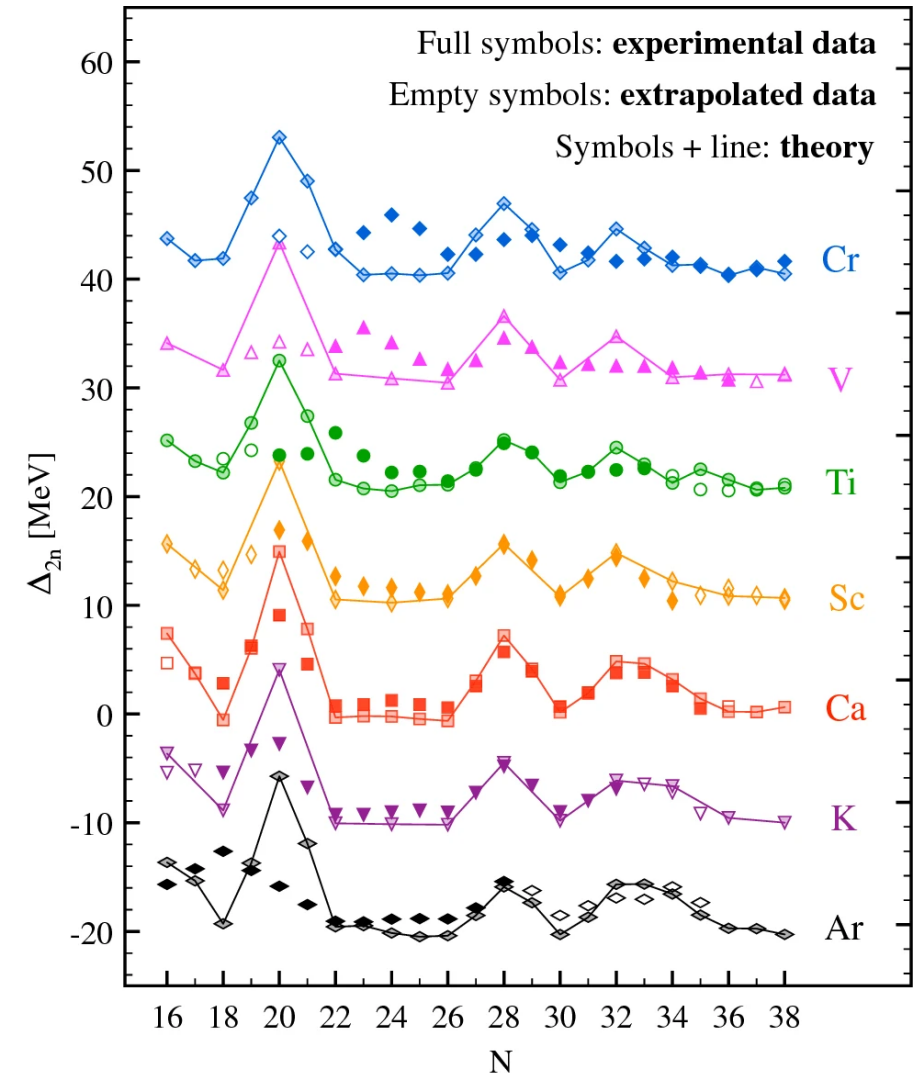
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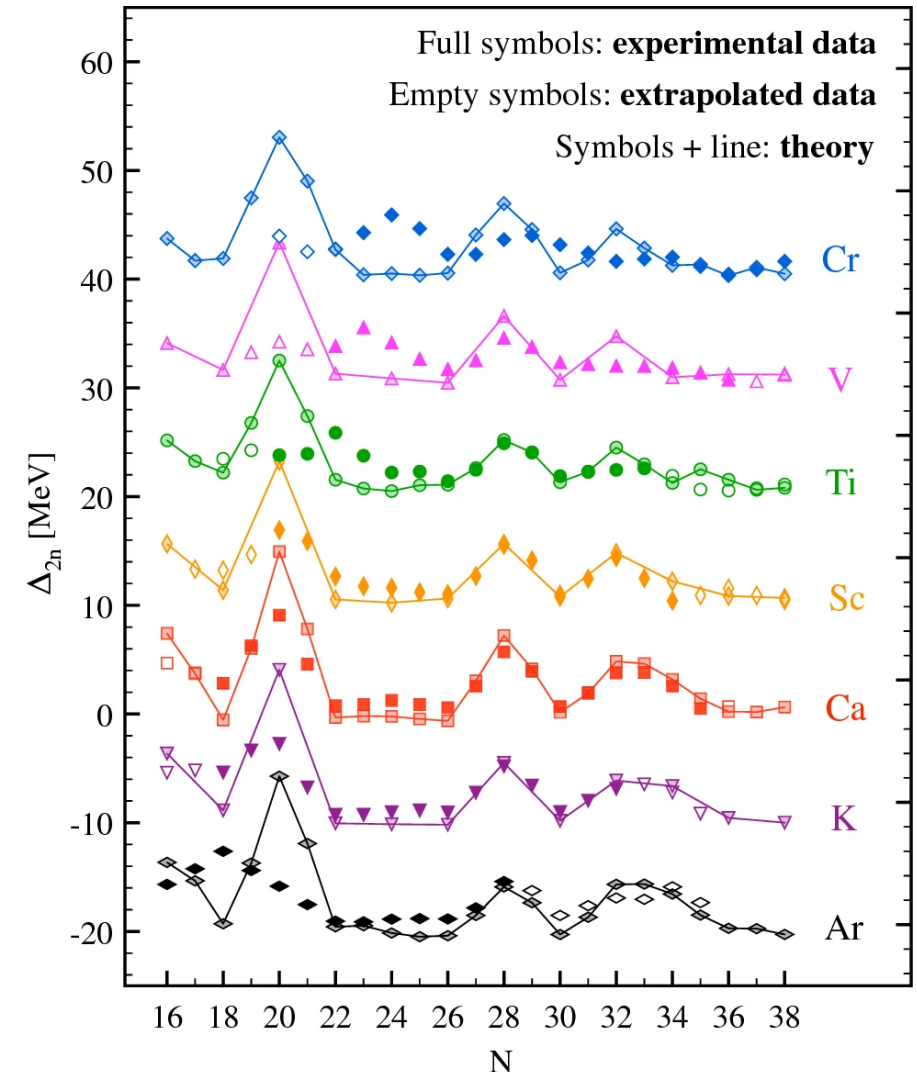
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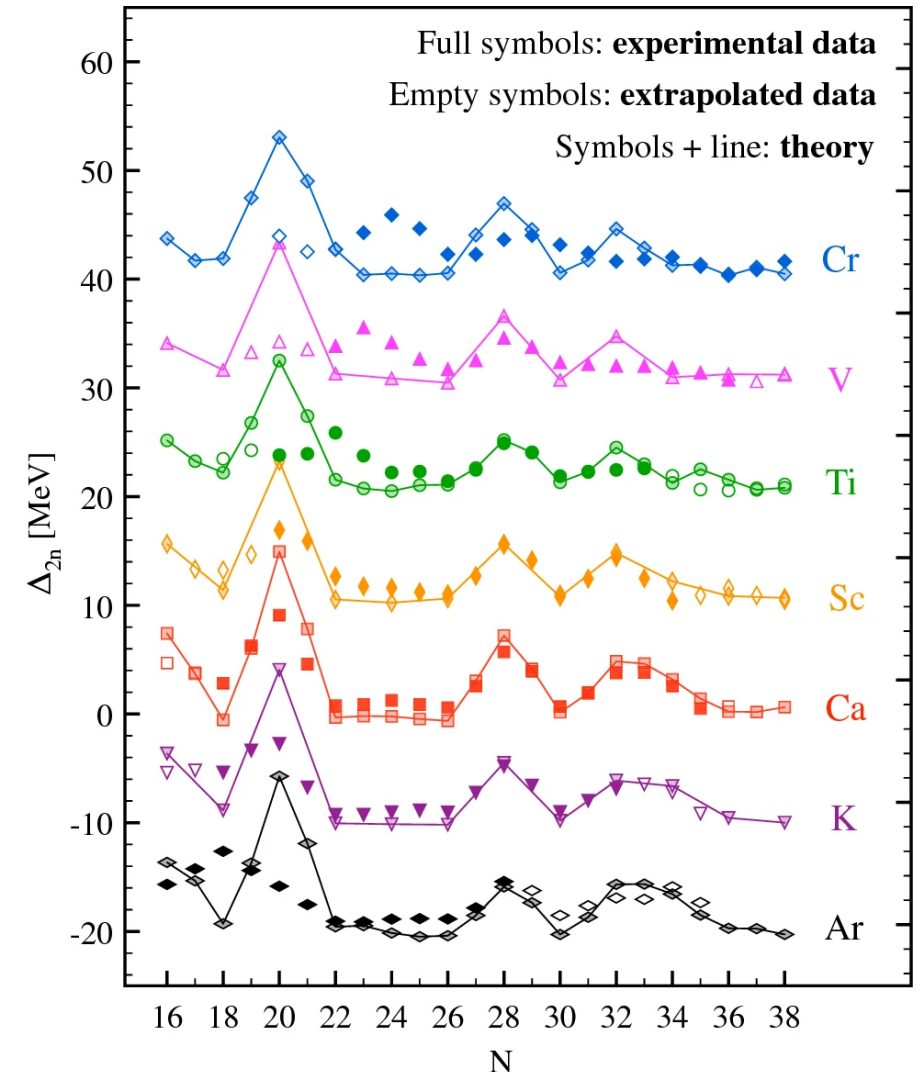
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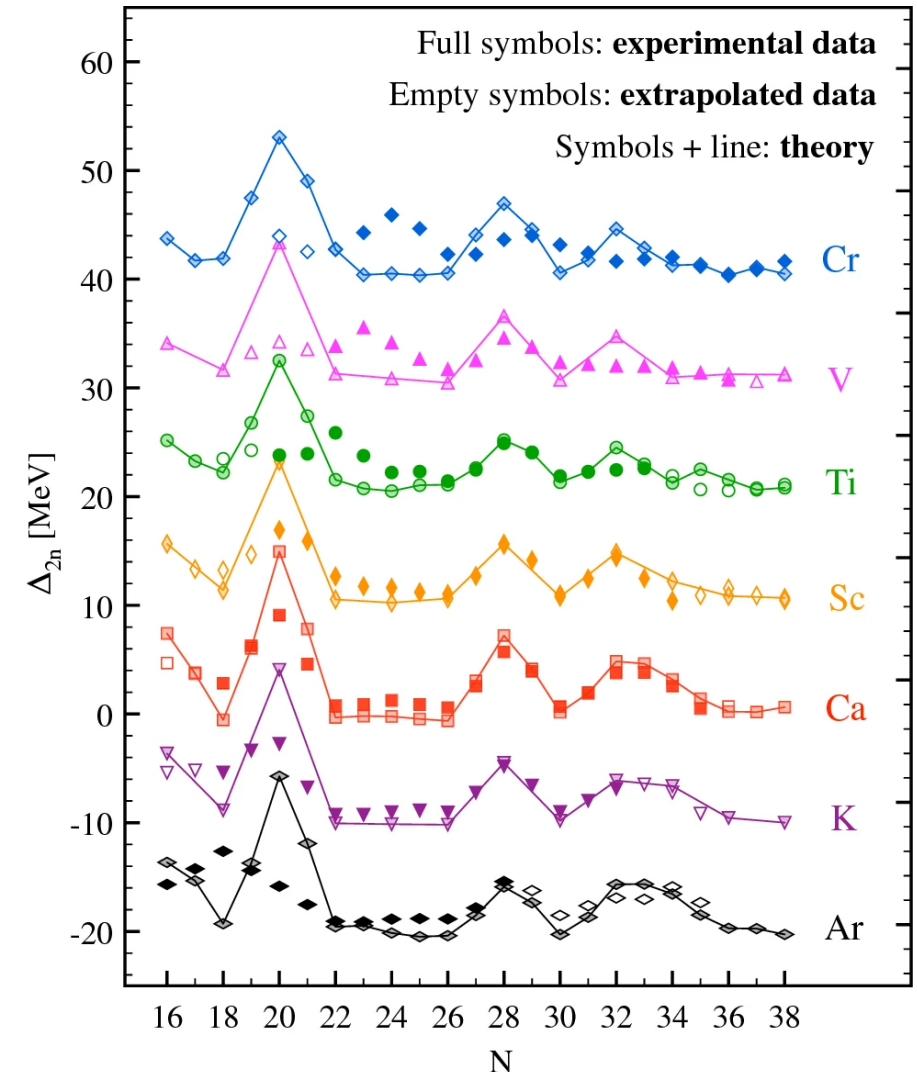
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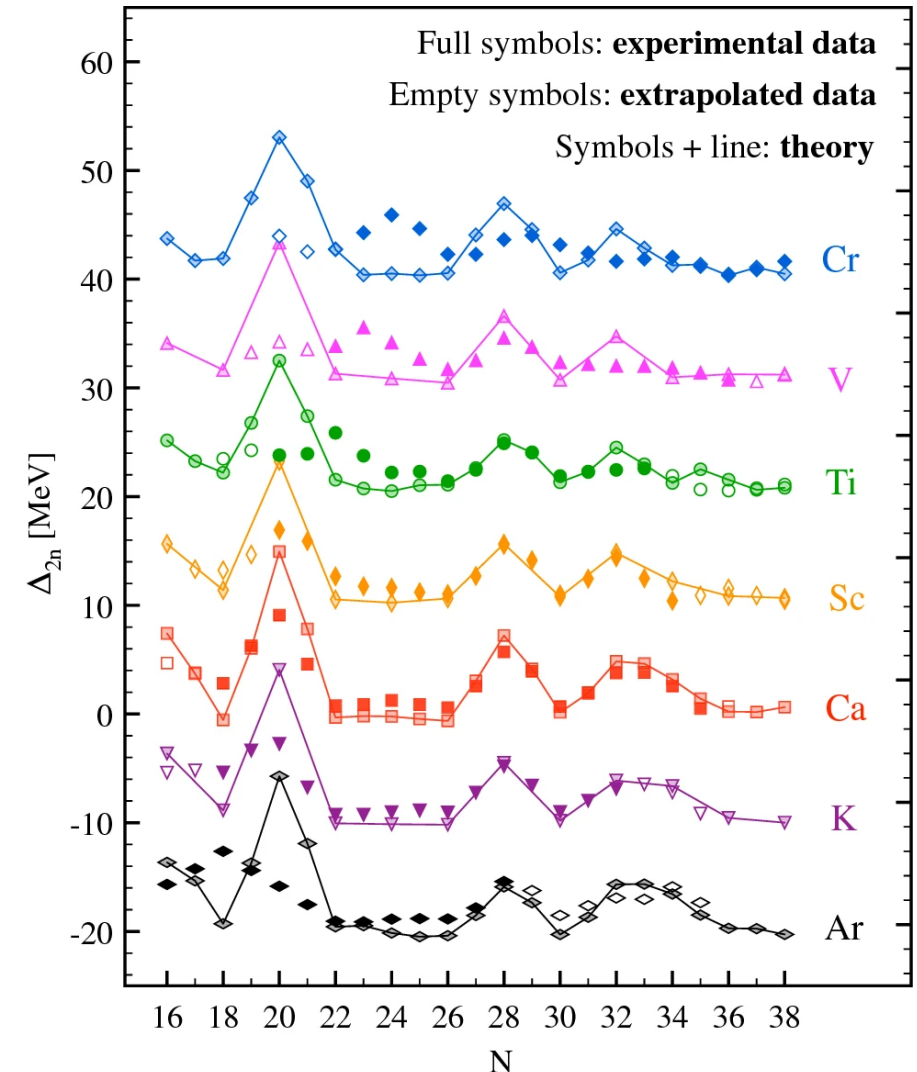
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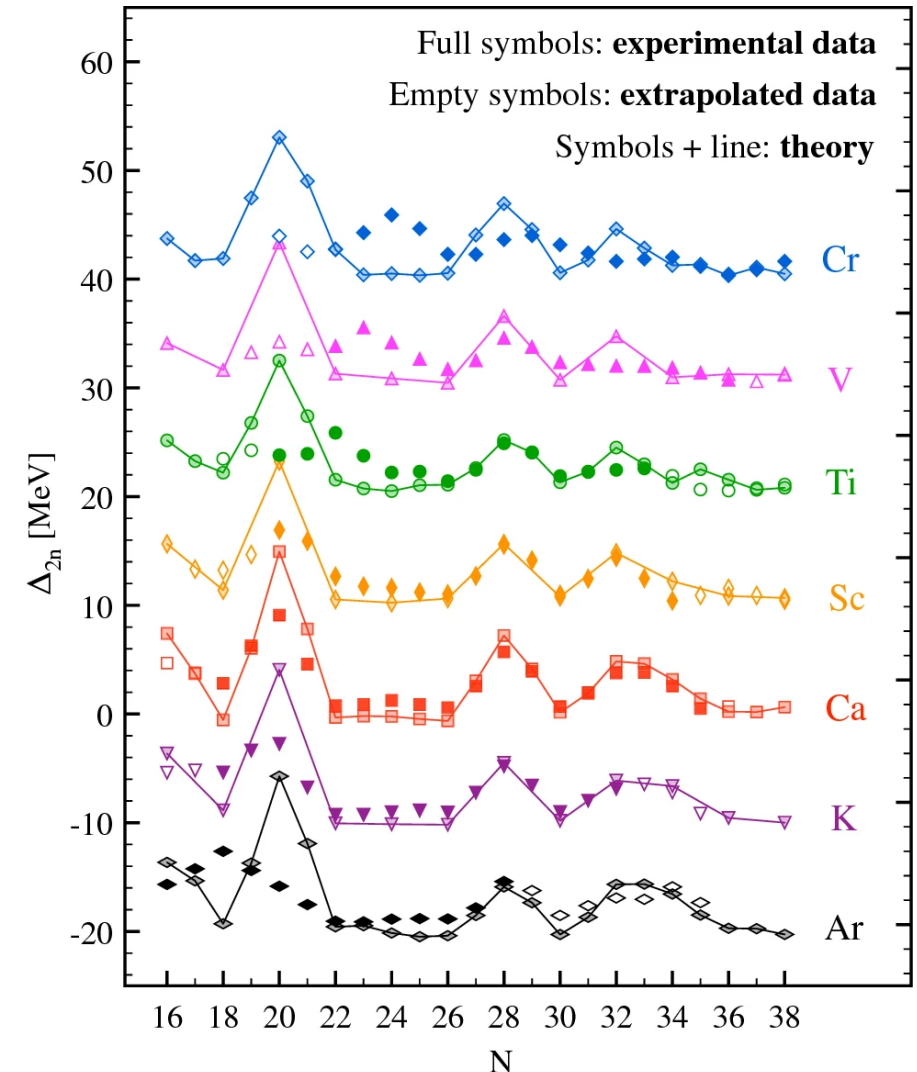
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Somá, Barbieri, Duguet, Navrátil, EPJA 57, 135 (2021)

COUPLED-CLUSTER METHOD

Hagen, Papenbrock, Hjorth-Jensen, Dean, Rep. Prog. Phys. 77, 096302 (2014)



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COUPLED-CLUSTER METHOD

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- **Exponential Ansatz** for the wave function

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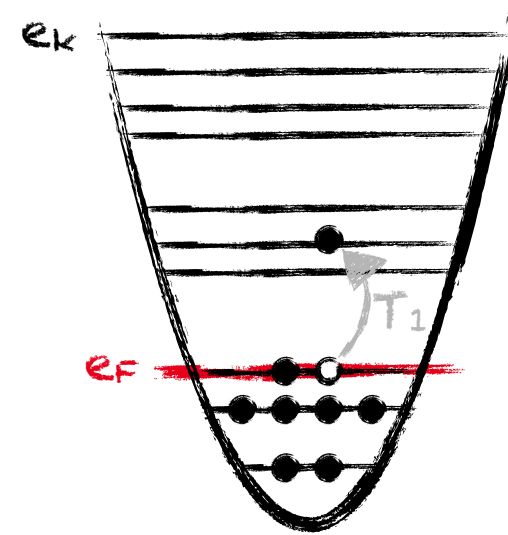
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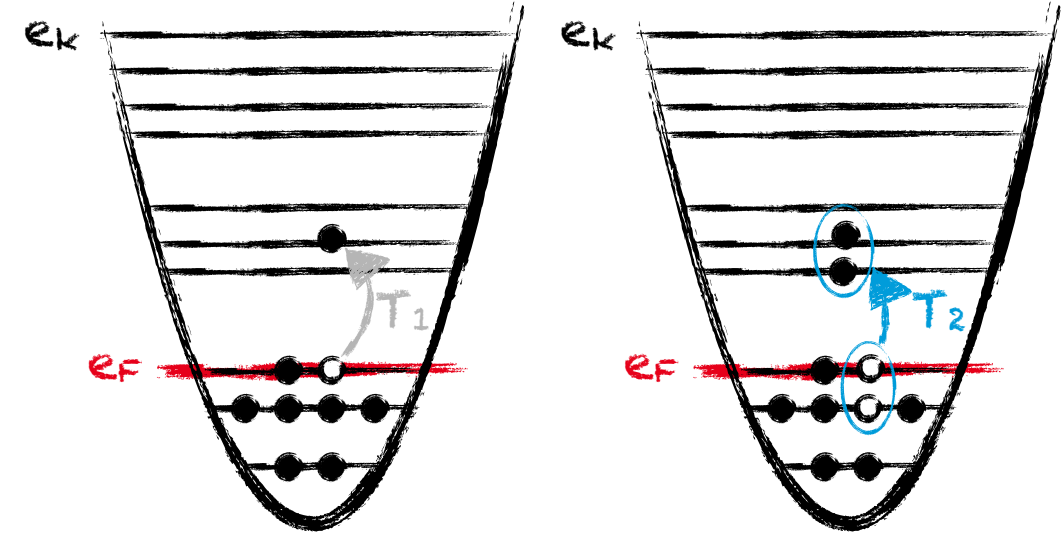
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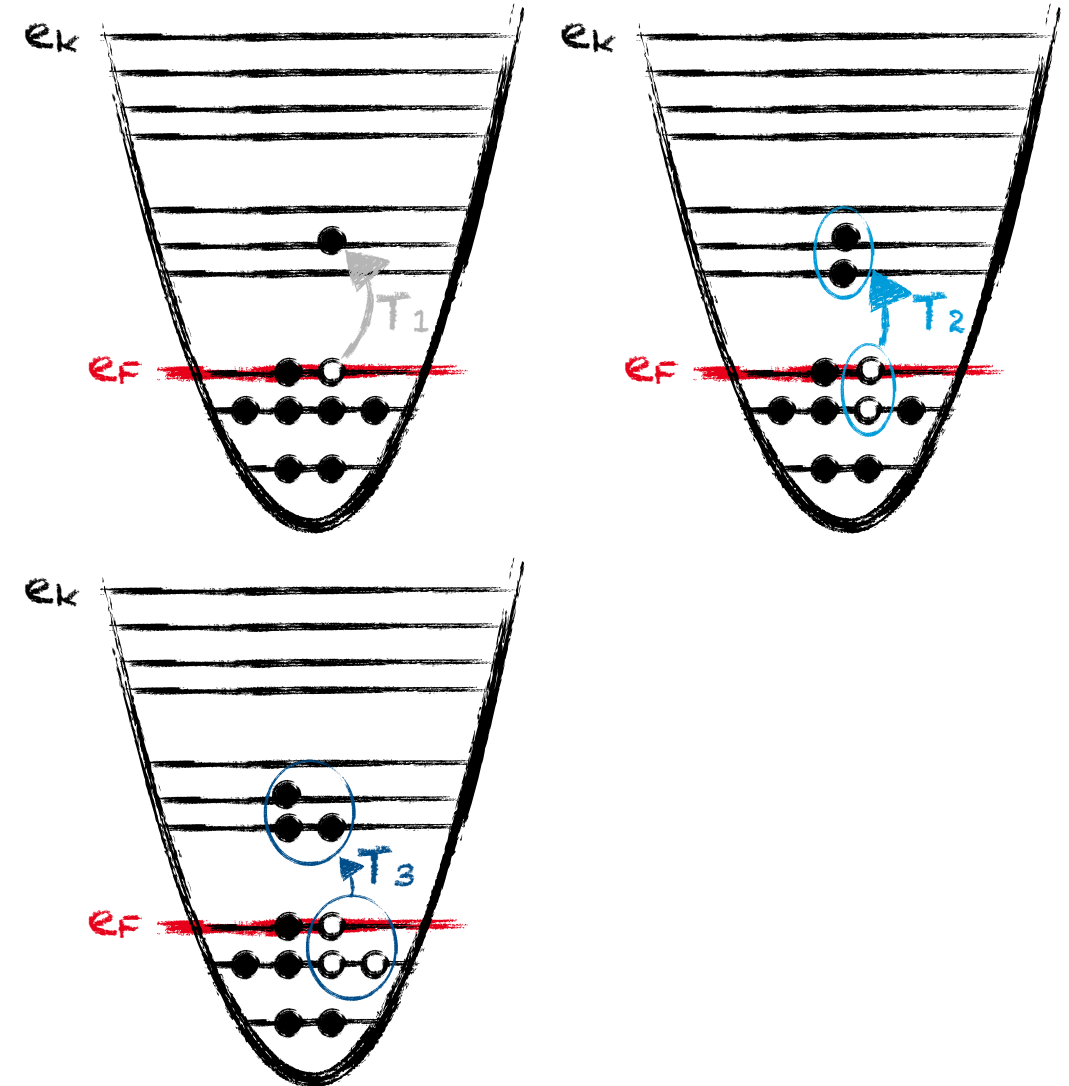
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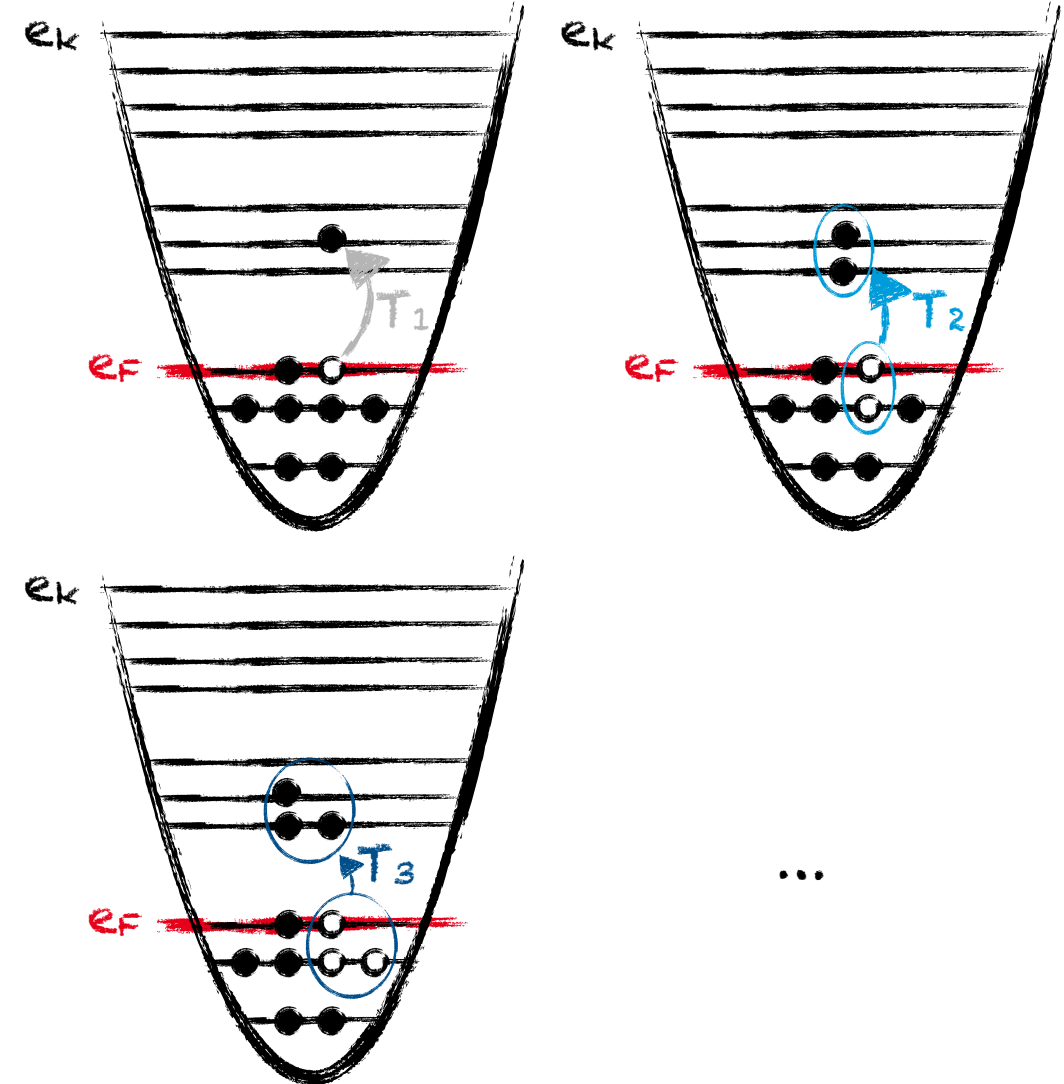
CCSD

CCSDT

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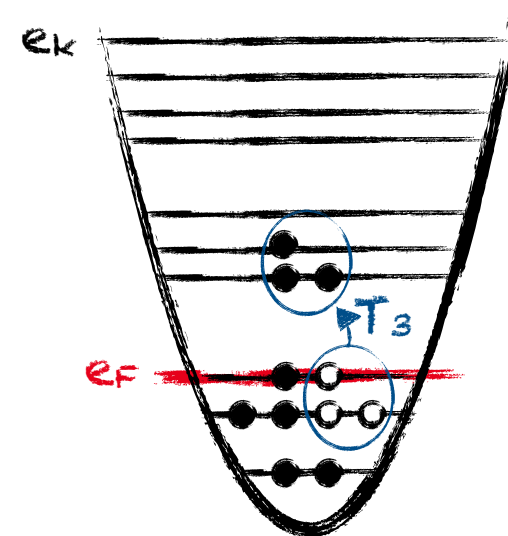
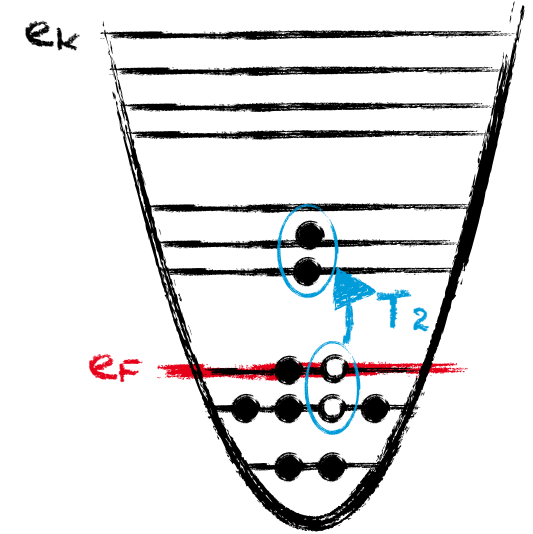
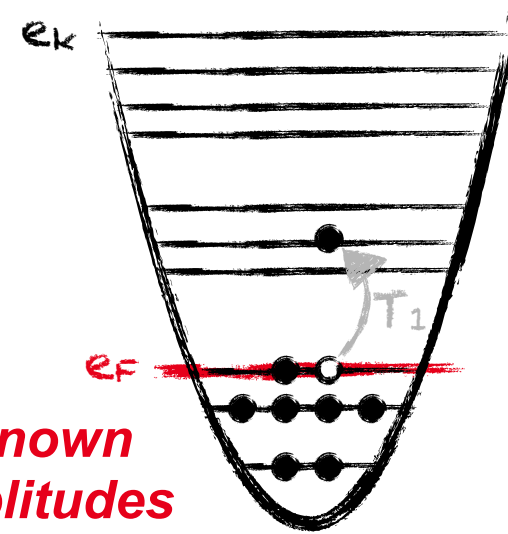
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CCSDT

Unknown
amplitudes



...

COUPLED CLUSTER EQUATIONS

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COUPLED CLUSTER EQUATIONS



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- Solve the unknown cluster amplitudes $t_{ijk\dots}^{abc\dots}$ from
$$\langle \Phi_i^a | e^{-\hat{T}} H_N e^{\hat{T}} | \Phi \rangle = 0 ,$$
$$\langle \Phi_{ij}^{ab} | e^{-\hat{T}} H_N e^{\hat{T}} | \Phi \rangle = 0 ,$$
$$\dots$$
where $|\Phi_{ijk\dots}^{abc\dots}\rangle \equiv \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_c^\dagger \dots \hat{a}_k \hat{a}_j \hat{a}_i | \Phi \rangle$

COUPLED CLUSTER EQUATIONS



Hagen, Papenbrock, Hjorth-Jensen, Dean, *Rep. Prog. Phys.* **77**, 096302 (2014)

- Select a reference state $|\Phi\rangle = \prod_{i=1}^A a_i^\dagger |0\rangle$ (e.g. a Hartree-Fock Slater determinant)
- Compute energy $E_{CC} = \langle \Phi | e^{-\hat{T}} \hat{H}_N e^{\hat{T}} | \Phi \rangle$, where $\hat{H}_N = \hat{H} - \langle \Phi | \hat{H} | \Phi \rangle$
- Solve the unknown cluster amplitudes $t_{ijk\dots}^{abc\dots}$ from

$$\langle \Phi_i^a | e^{-\hat{T}} H_N e^{\hat{T}} | \Phi \rangle = 0 ,$$

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Computational cost (CCSD): $A^2 n^4$

...

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Hagen, Papenbrock, Hjorth-Jensen, Dean, *Rep. Prog. Phys.* **77**, 096302 (2014)

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- Note: $e^{\hat{T}}$ non-unitary $\rightarrow$ transformed Hamiltonian $\bar{H} = e^{-\hat{T}} \hat{H}_N e^{\hat{T}}$ non-Hermitian

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Non-variational method

Computational cost (CCSD): $A^2 n^4$

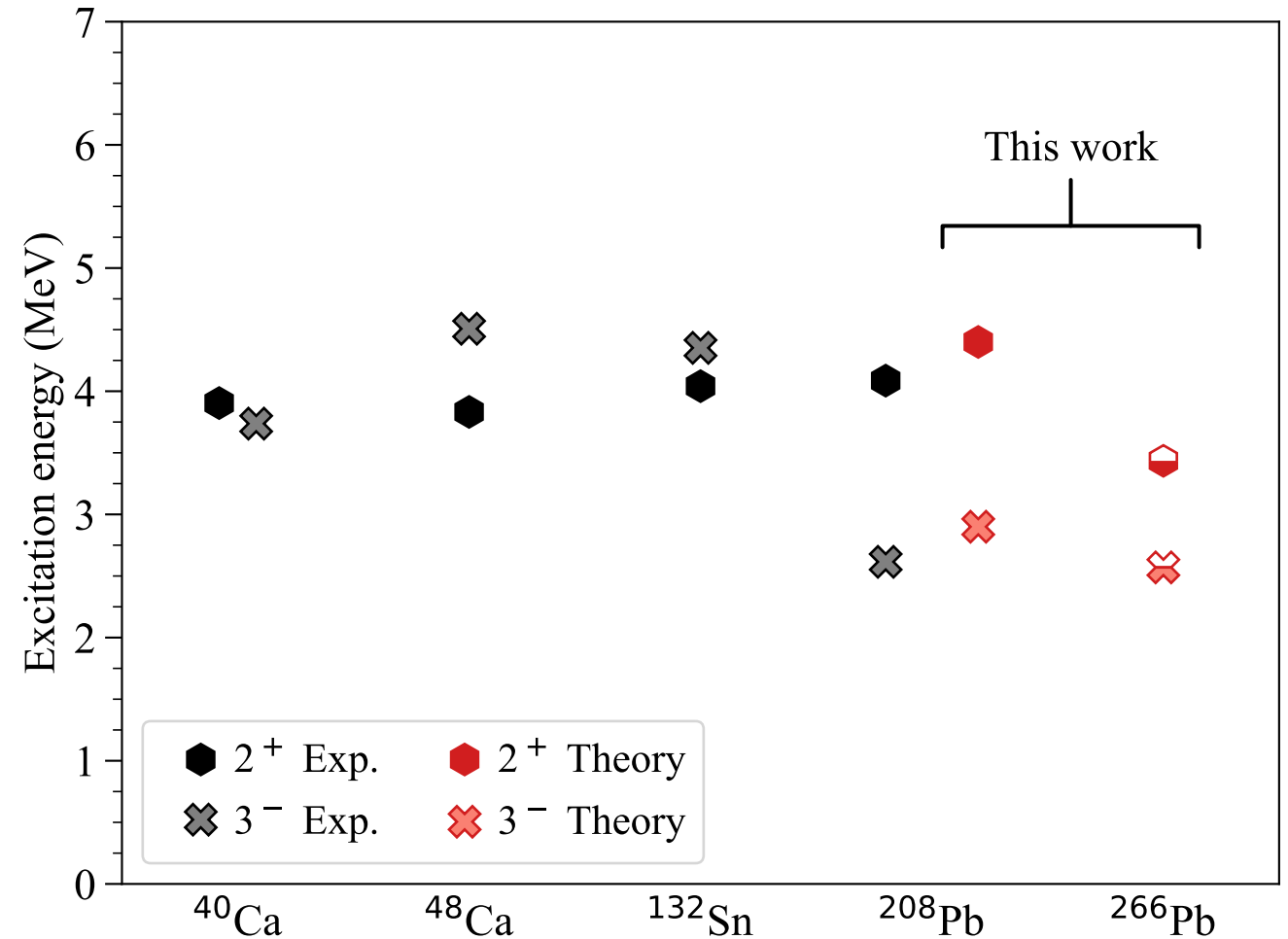
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COUPLED CLUSTER METHOD

Hagen, Papenbrock, Hjorth-Jensen, Dean, *Rep. Prog. Phys.* **77**, 096302 (2014)



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Bonaiti, Hagen, Papenbrock, *arXiv:2508.14217* (2025)

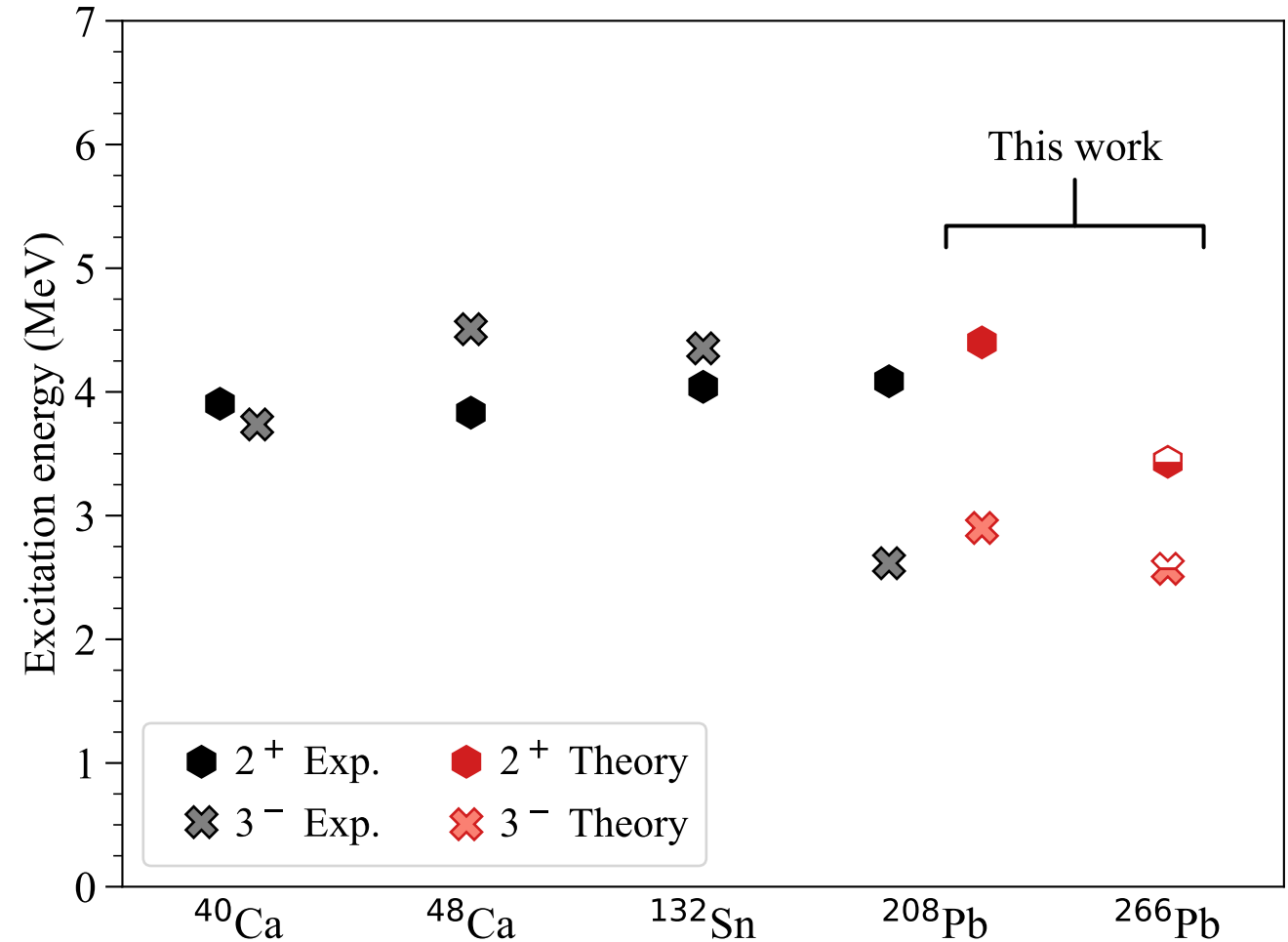
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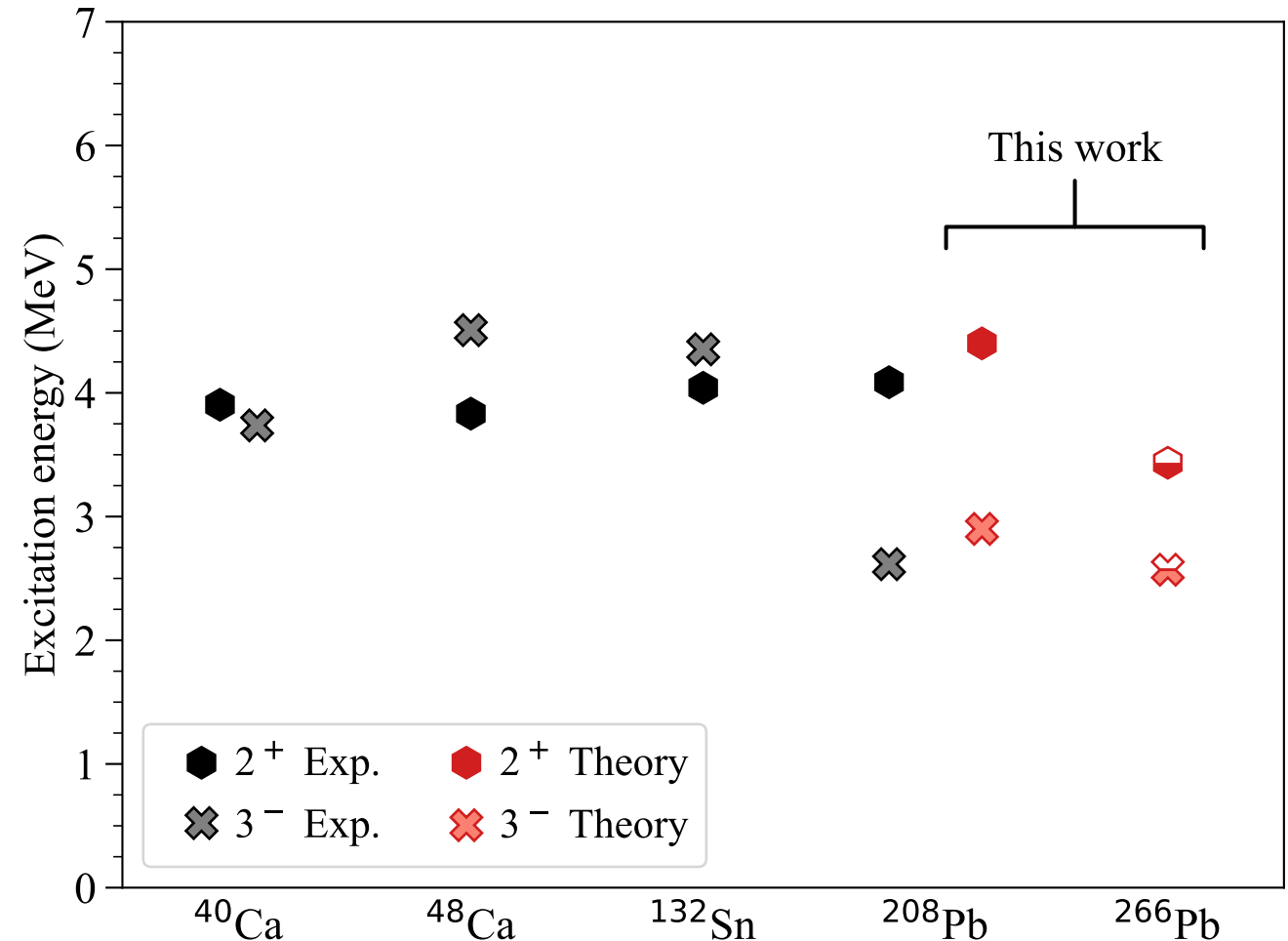
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Bonaiti, Hagen, Papenbrock, *arXiv:2508.14217* (2025)

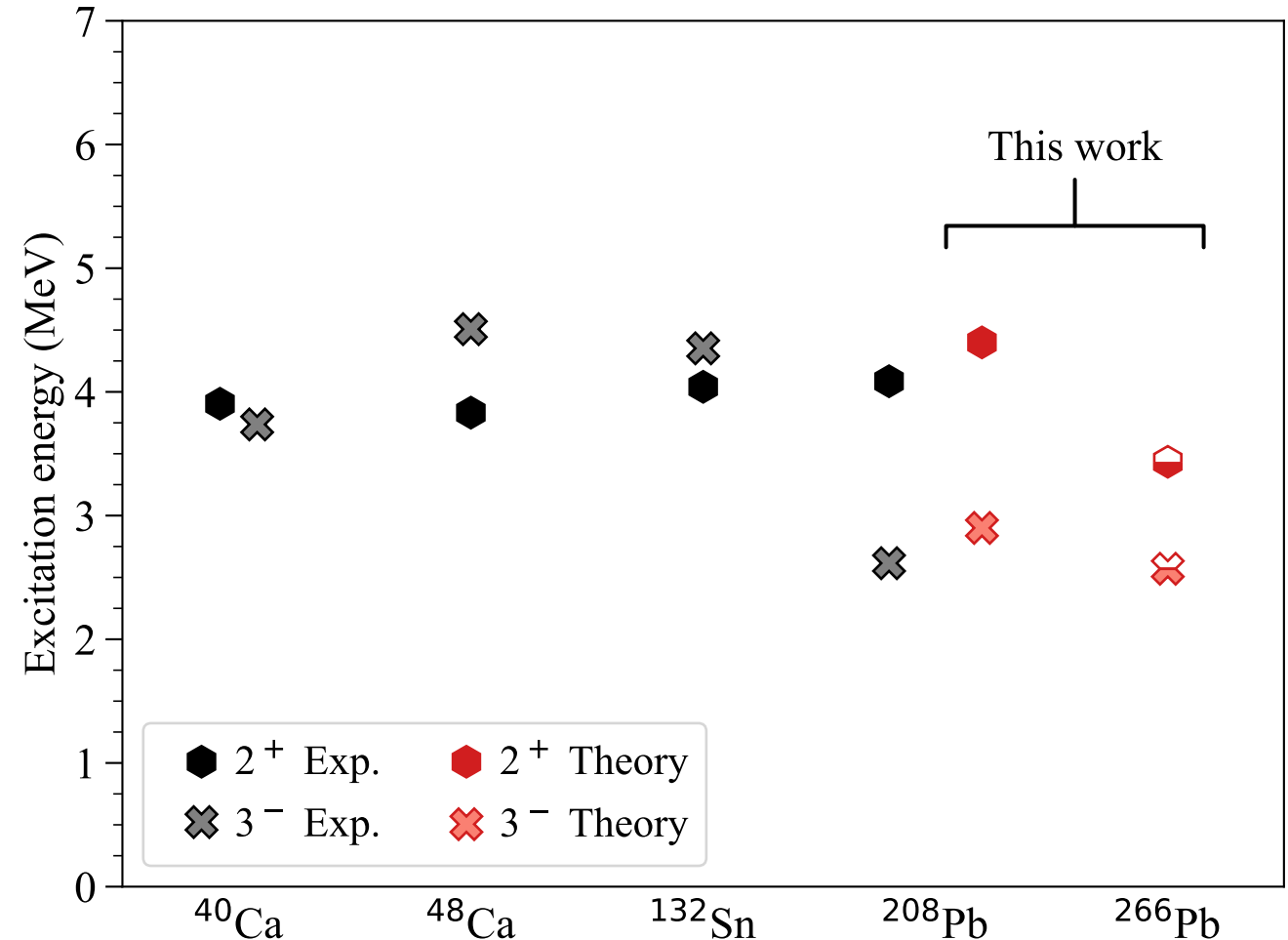
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Bonaiti, Hagen, Papenbrock, *arXiv:2508.14217* (2025)

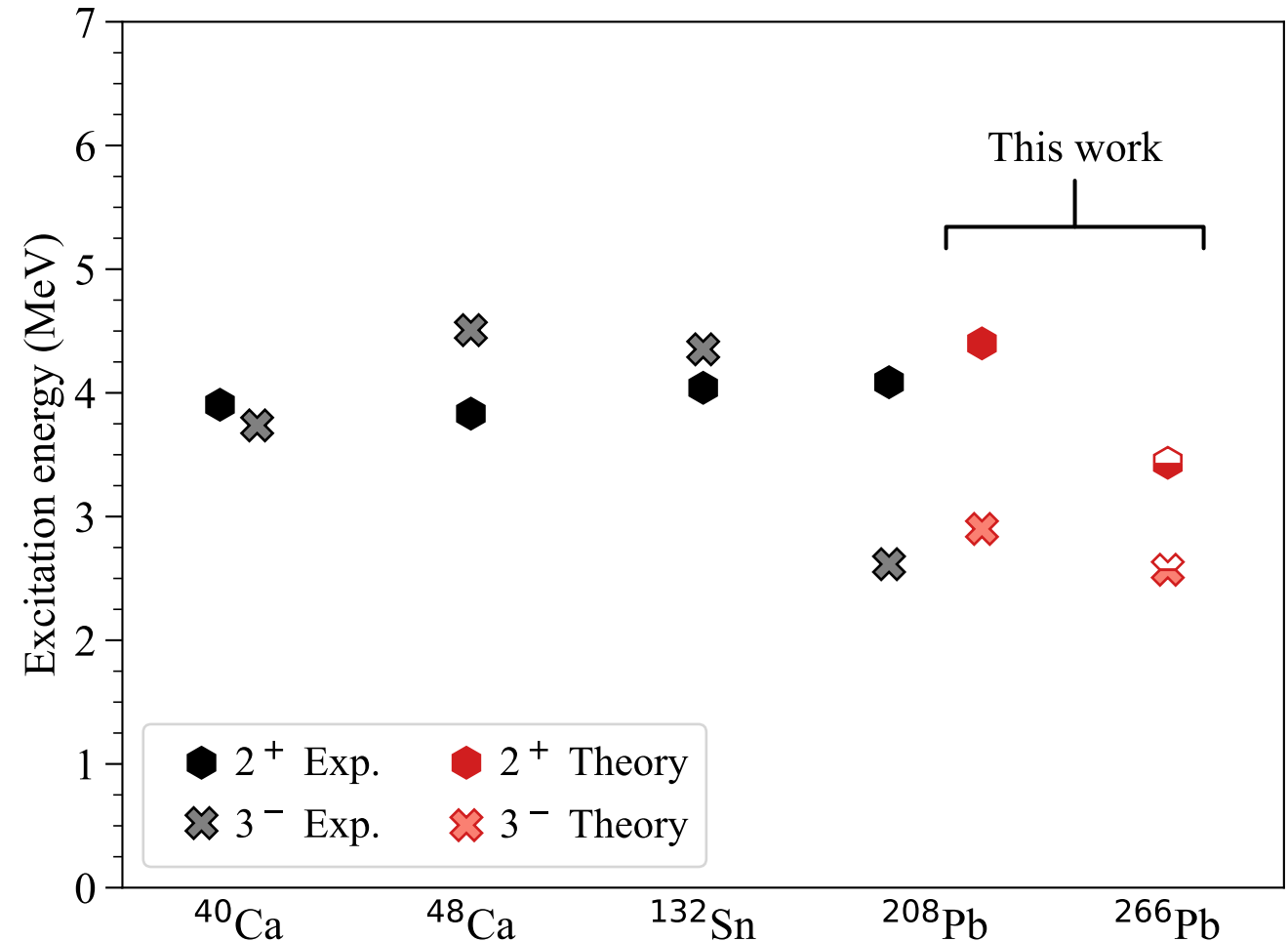
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Bonaiti, Hagen, Papenbrock, *arXiv:2508.14217* (2025)

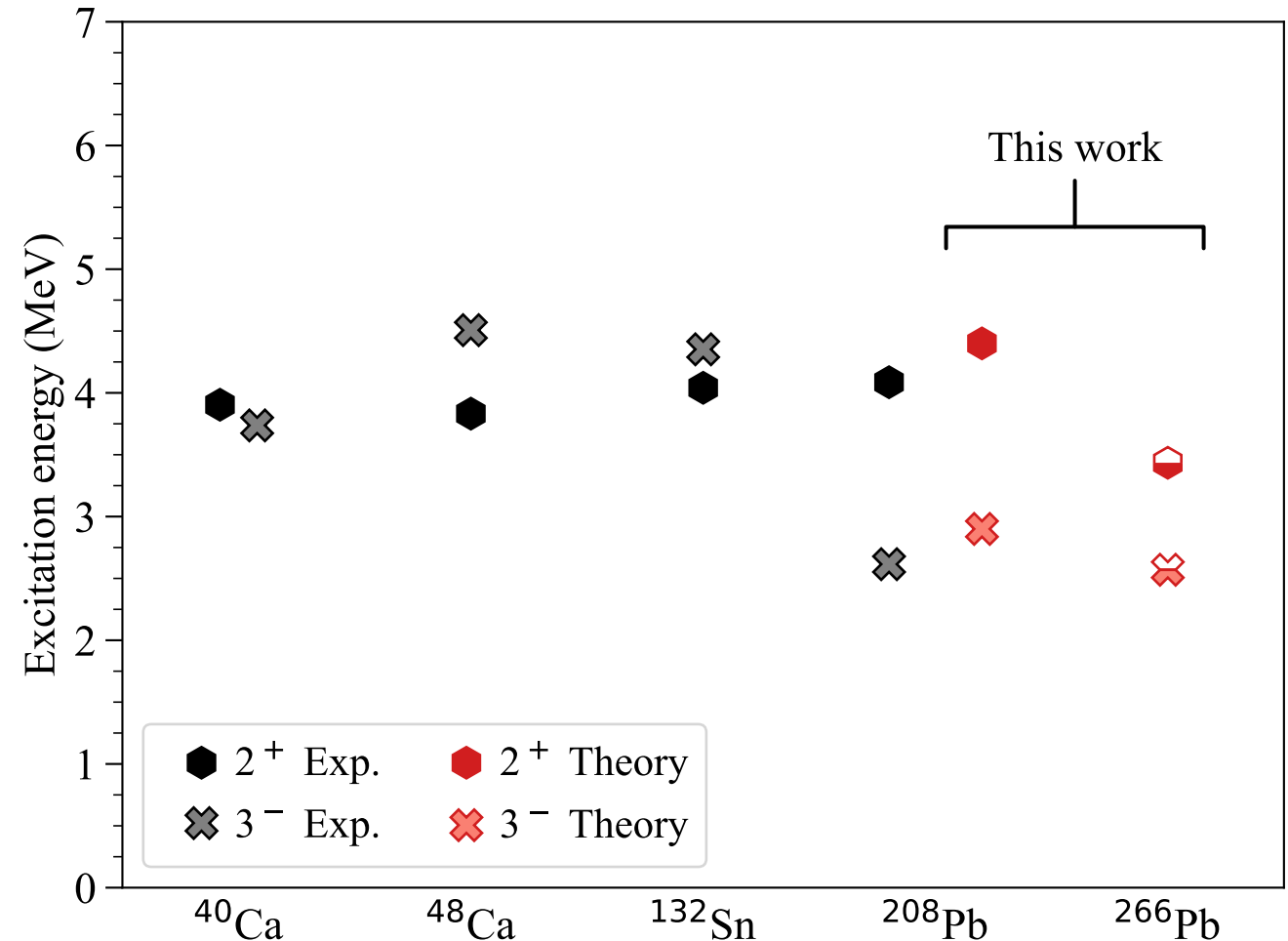
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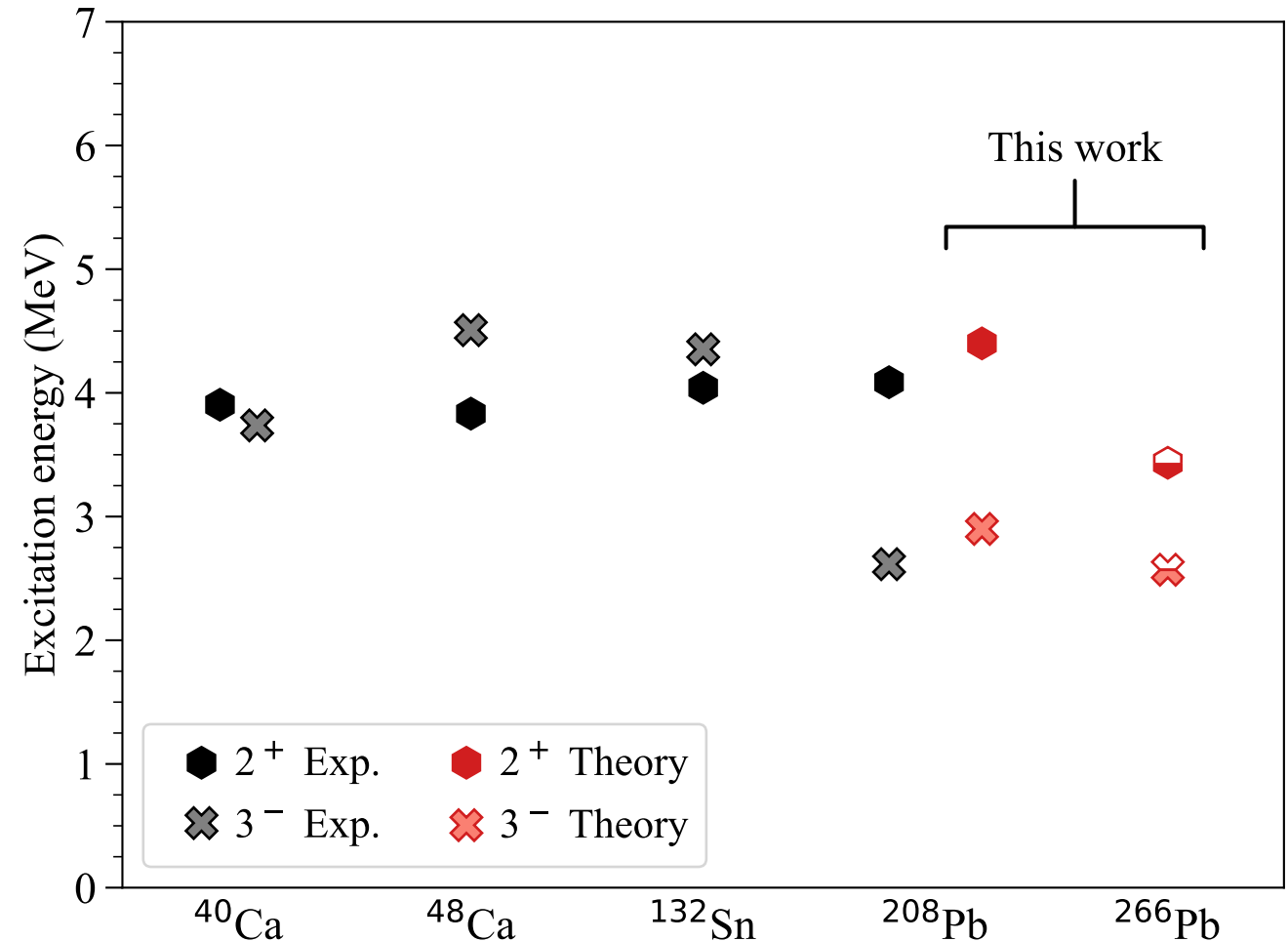
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Bonaiti, Hagen, Papenbrock, arXiv:2508.14217 (2025)

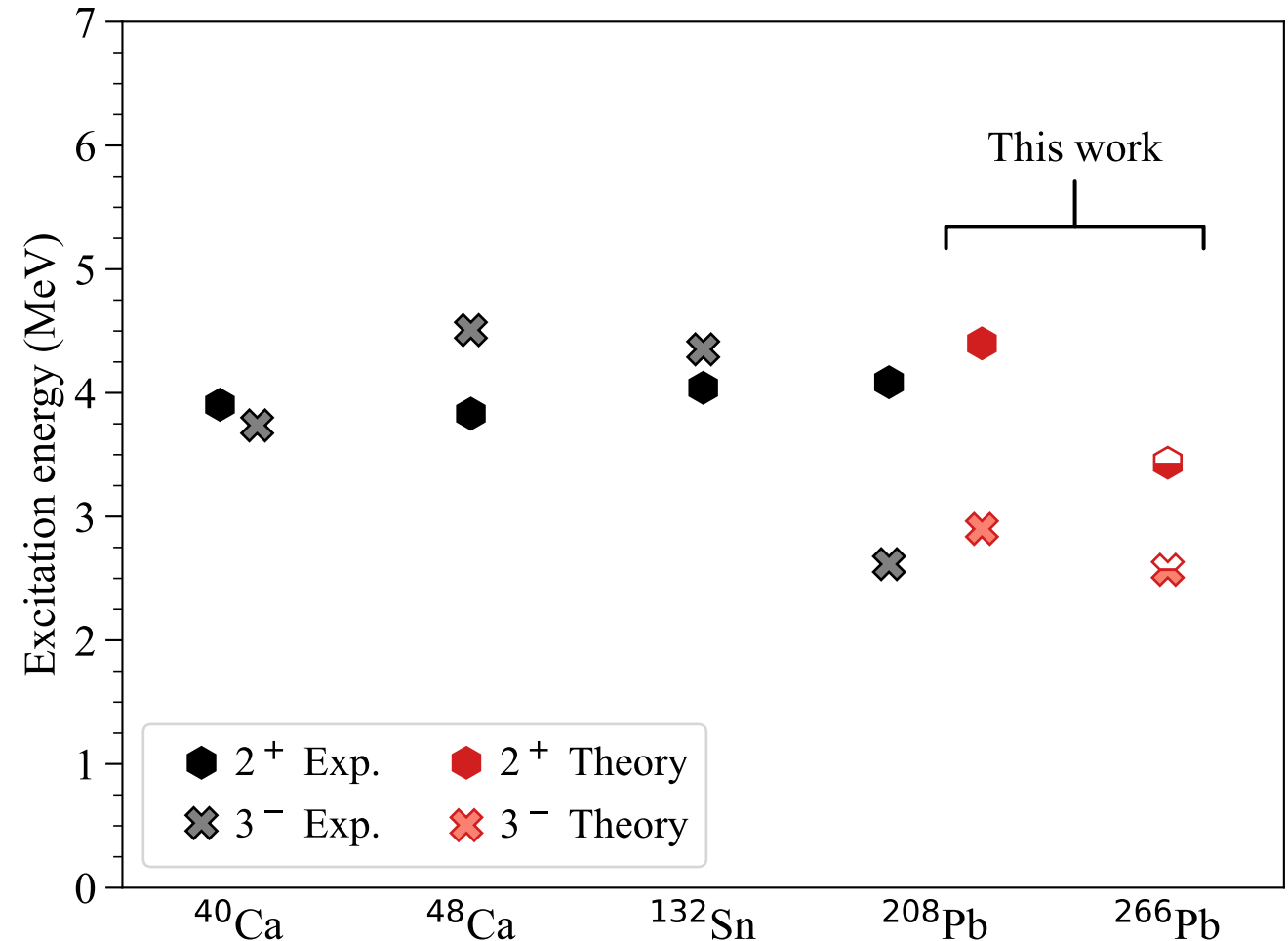
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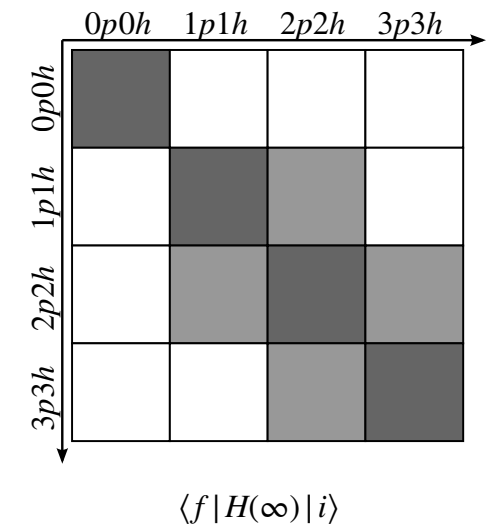
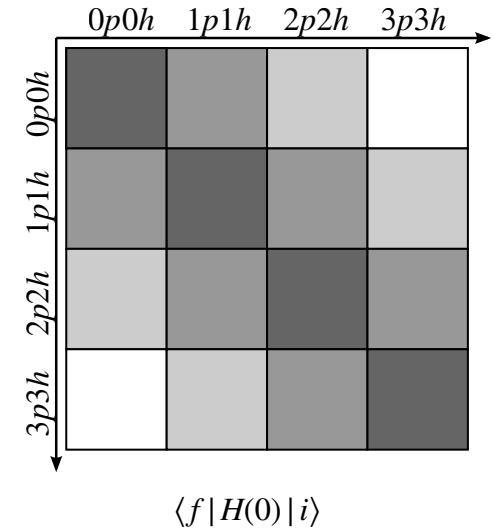
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IN-MEDIUM SIMILARITY RENORMALIZATION GROUP

Hergert, Bogner, Morris, Schwenk, Tsukiyama, Phys. Rep. 621, 165-222 (2016)



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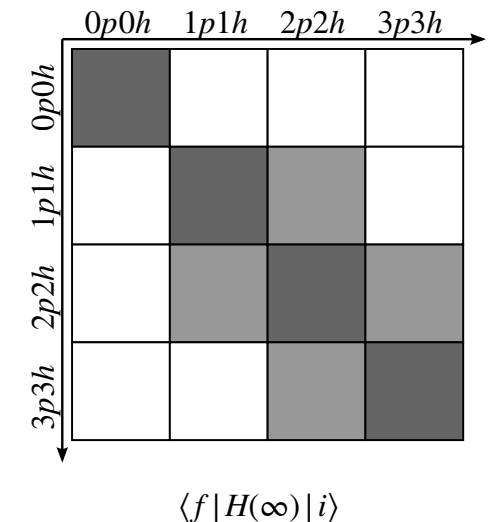
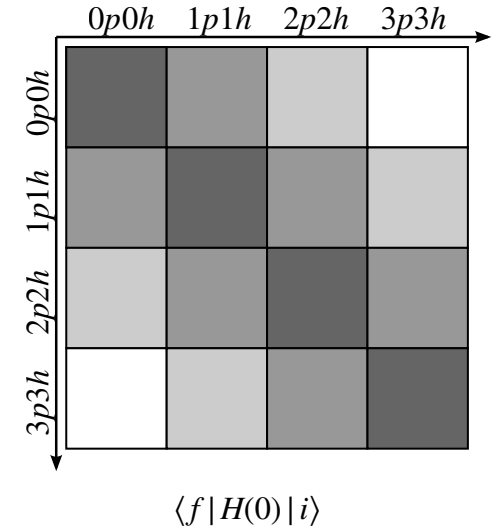
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Hergert, Bogner, Morris, Schwenk, Tsukiyama, Phys. Rep. 621, 165-222 (2016)

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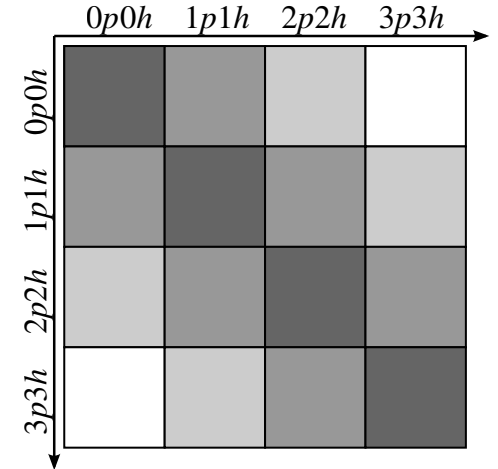
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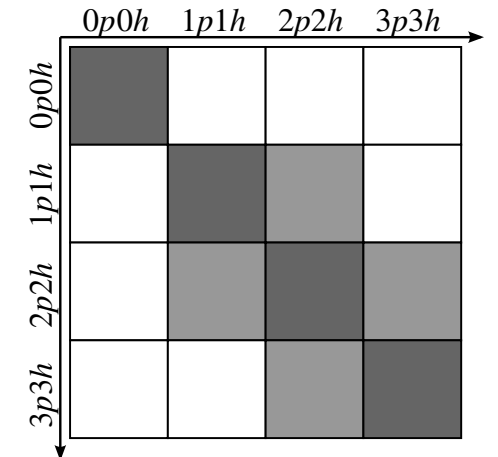
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$\langle f | H(0) | i \rangle$



$\langle f | H(\infty) | i \rangle$

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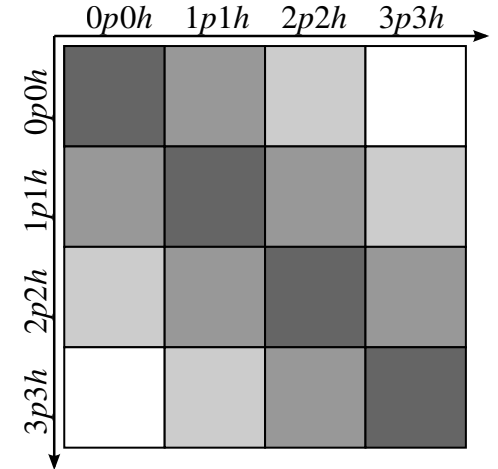
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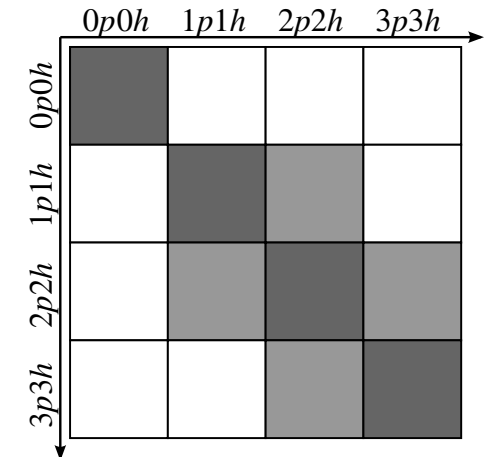
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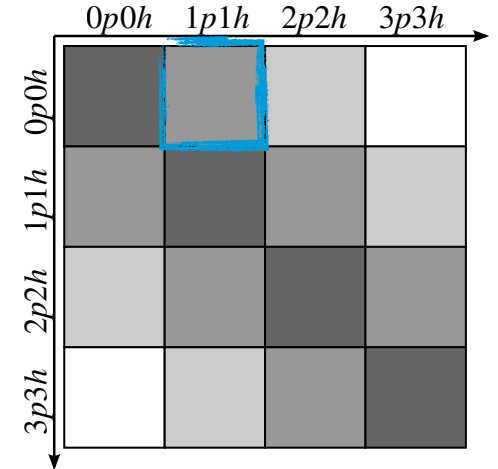
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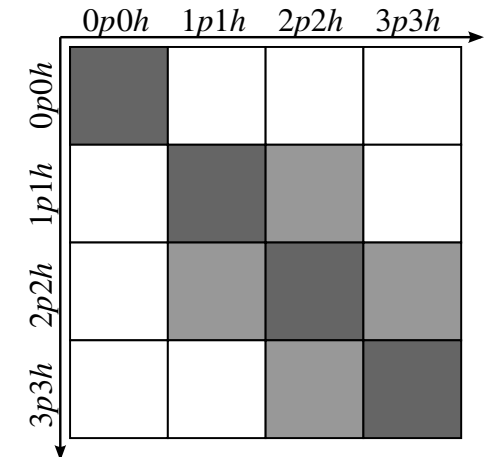
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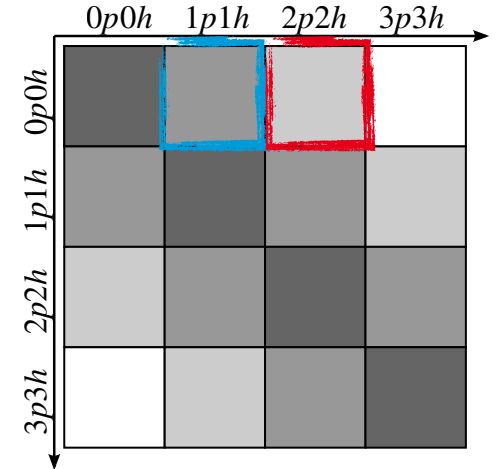
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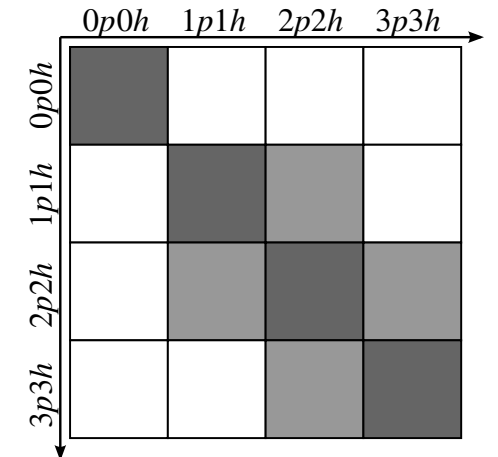
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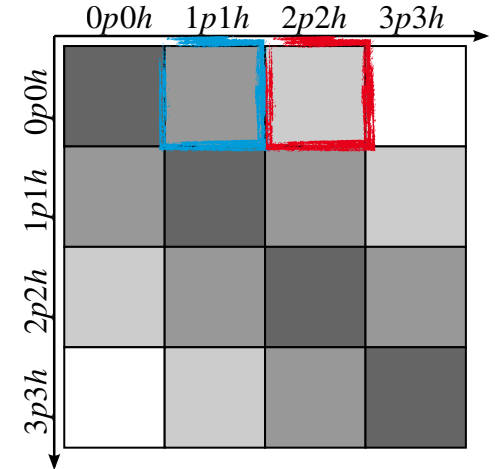
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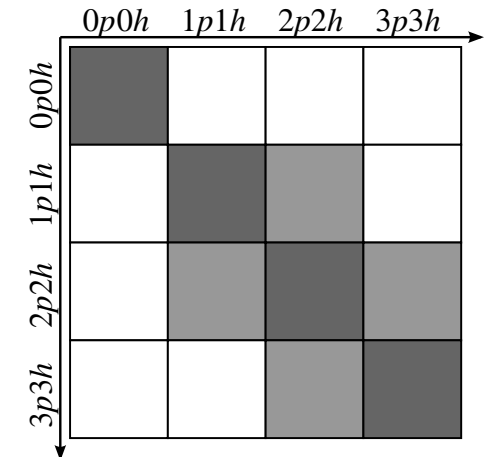
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$U(s) H U^\dagger(s)$ with different generator choices



$\langle f | H(0) | i \rangle$



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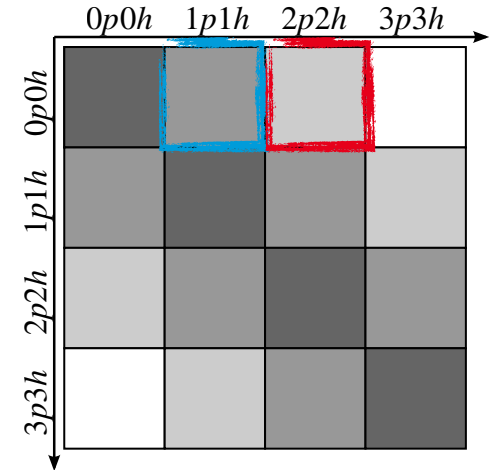
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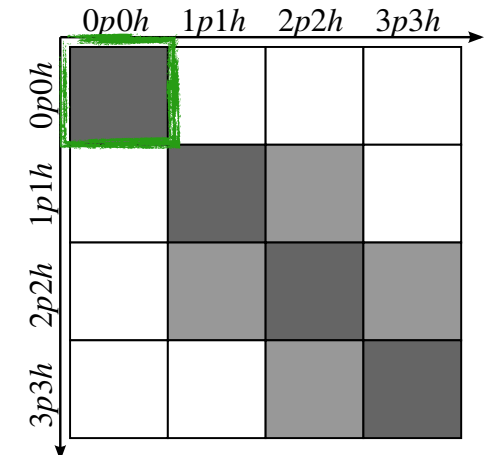
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- Ground-state properties** can then be easily obtained

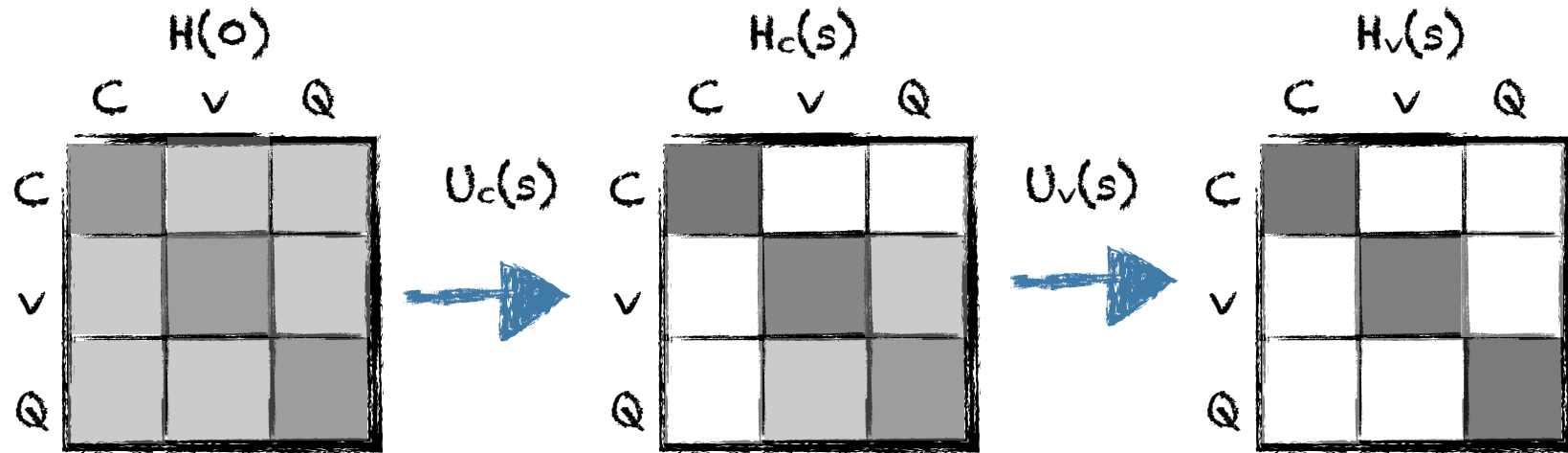
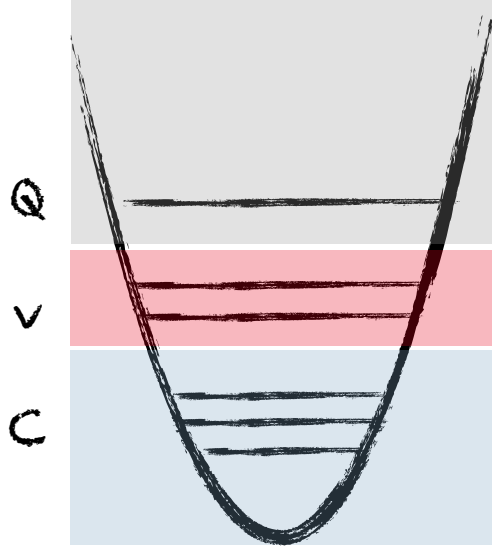


$\langle f | H(0) | i \rangle$



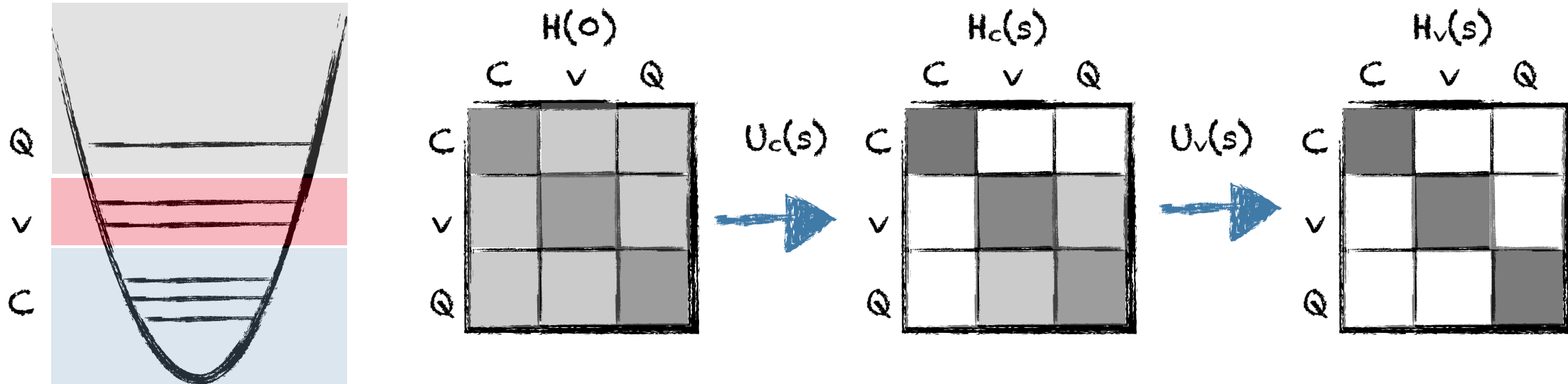
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VALENCE-SPACE IN-MEDIUM SIMILARITY RENORMALIZATION GROUP VS-IMSRG



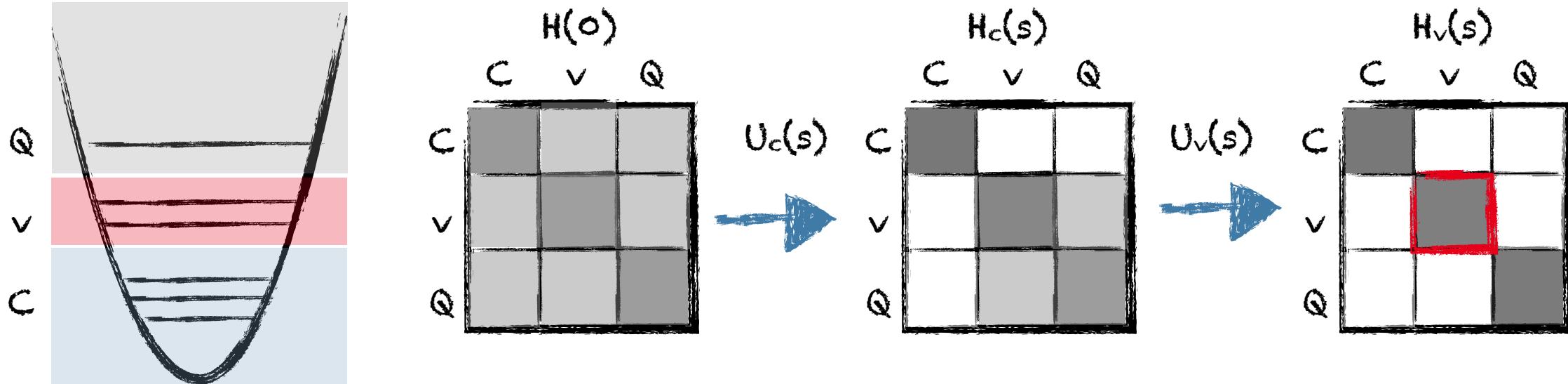
Stroberg et al., Phys. Rev. Lett. 118, 032502 (2017)

VALENCE-SPACE IN-MEDIUM SIMILARITY RENORMALIZATION GROUP VS-IMSRG



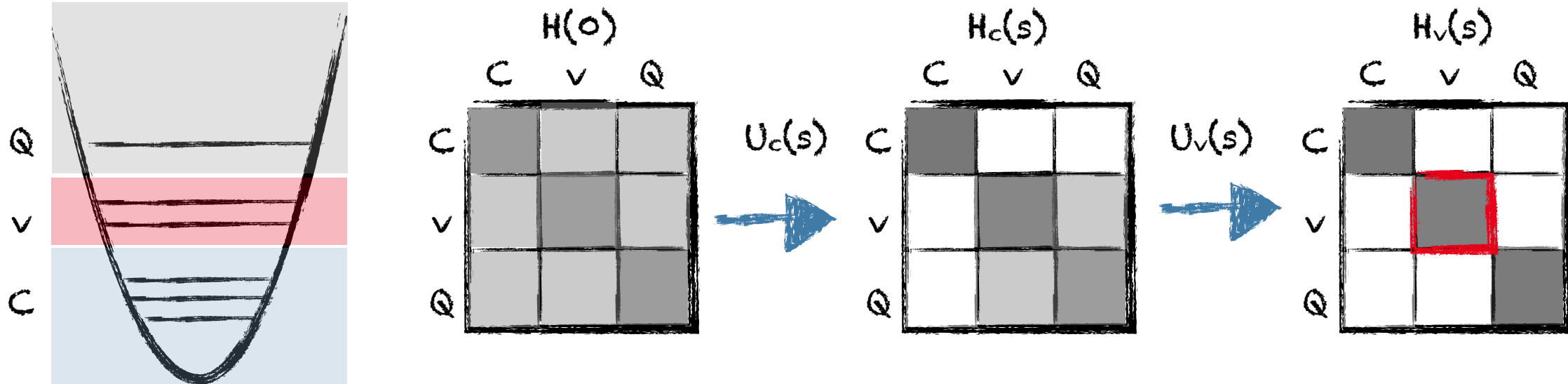
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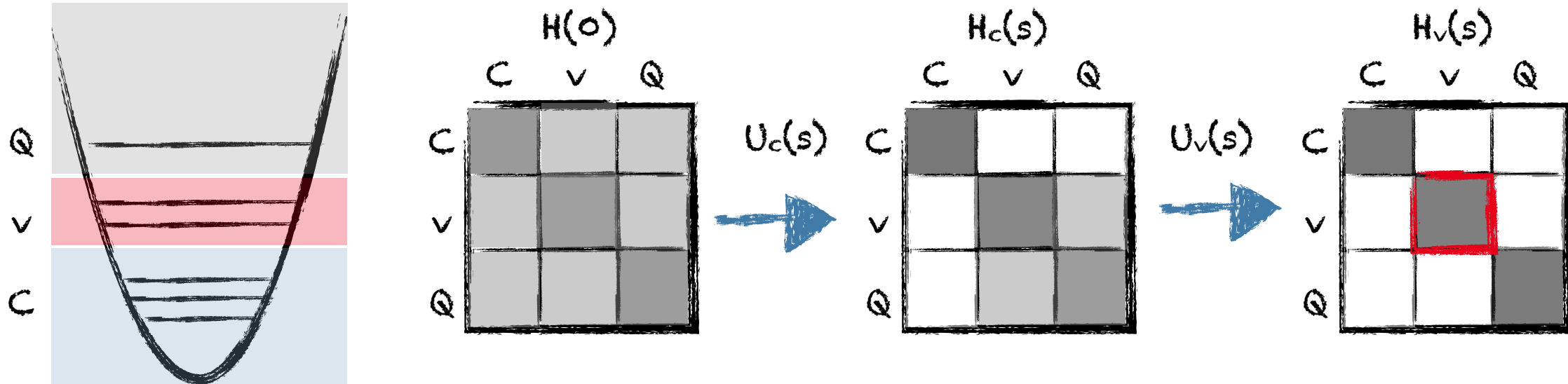
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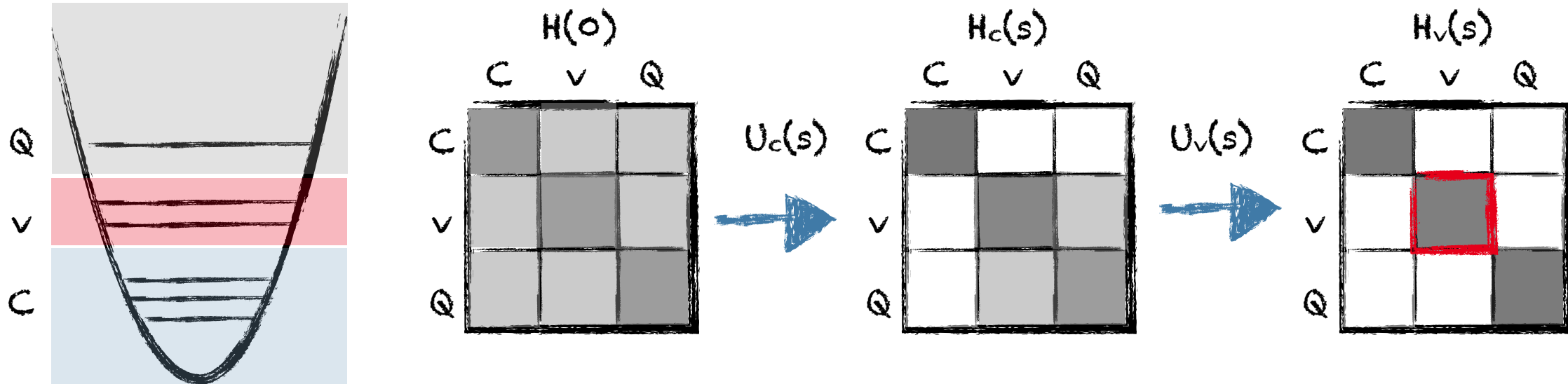
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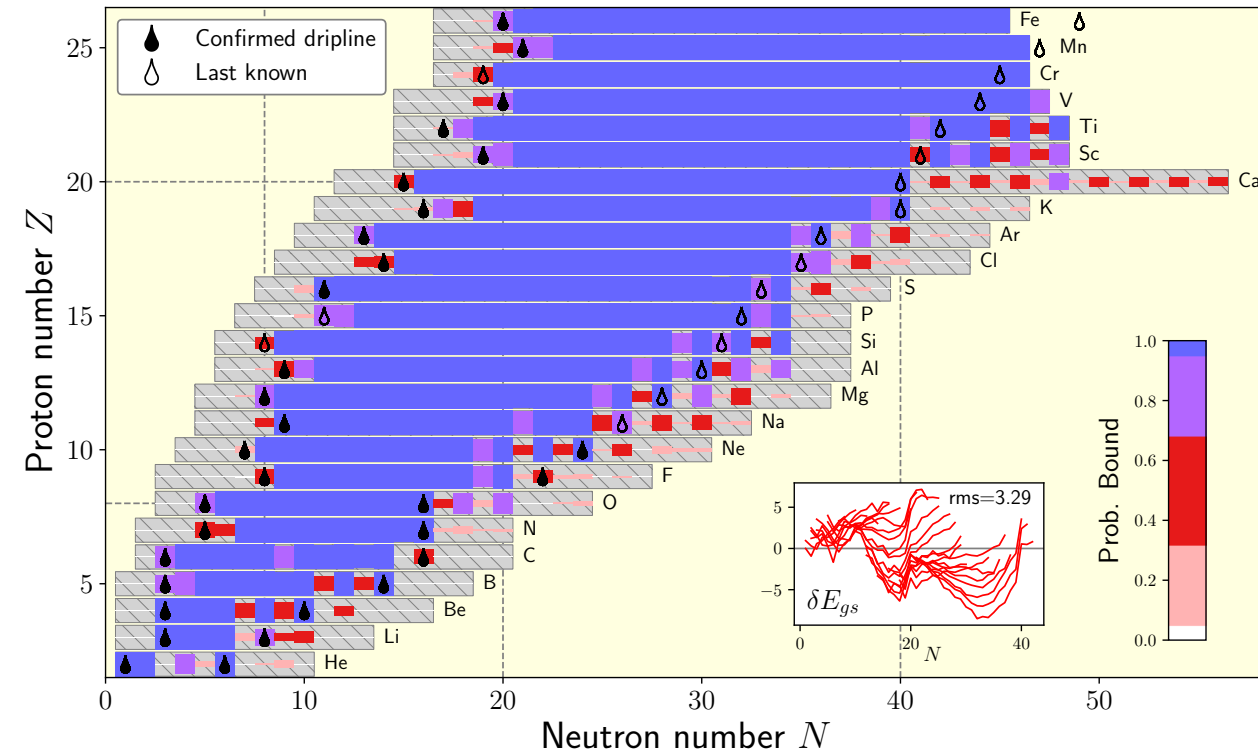
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VARIANTS OF IMSRG

Hergert, Front. Phys. 8:379 (2020)



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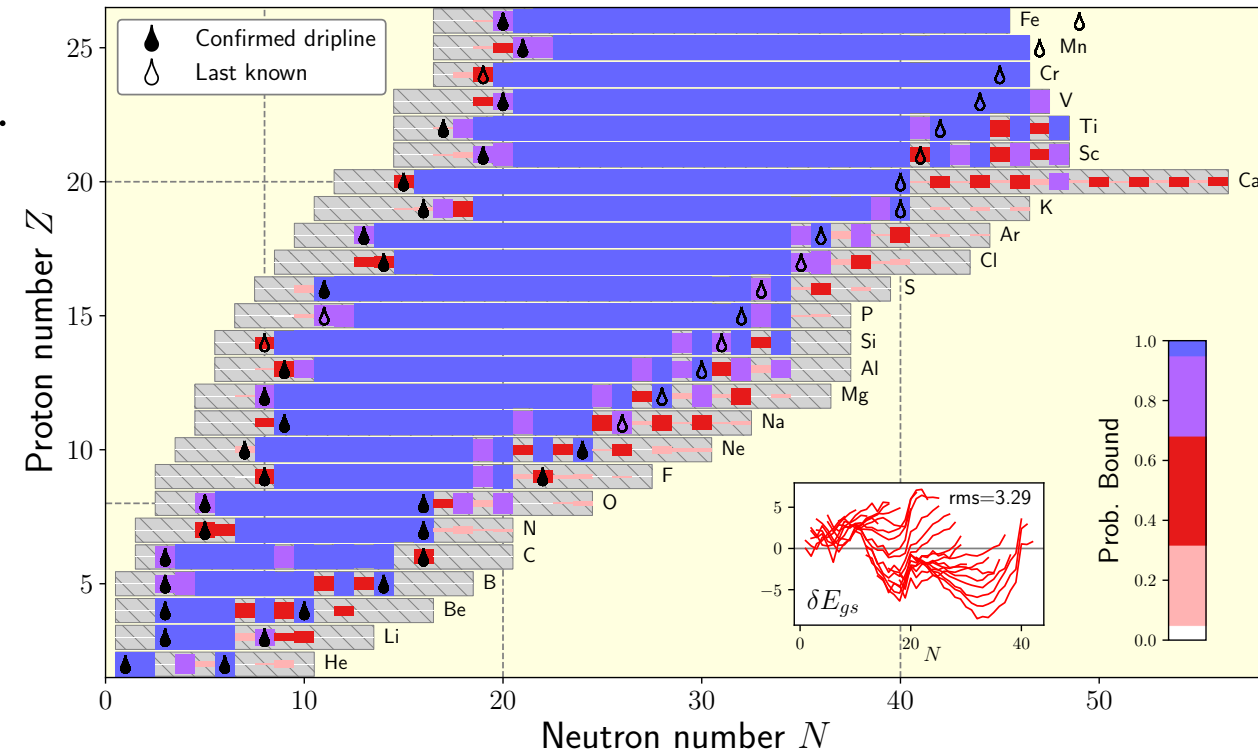
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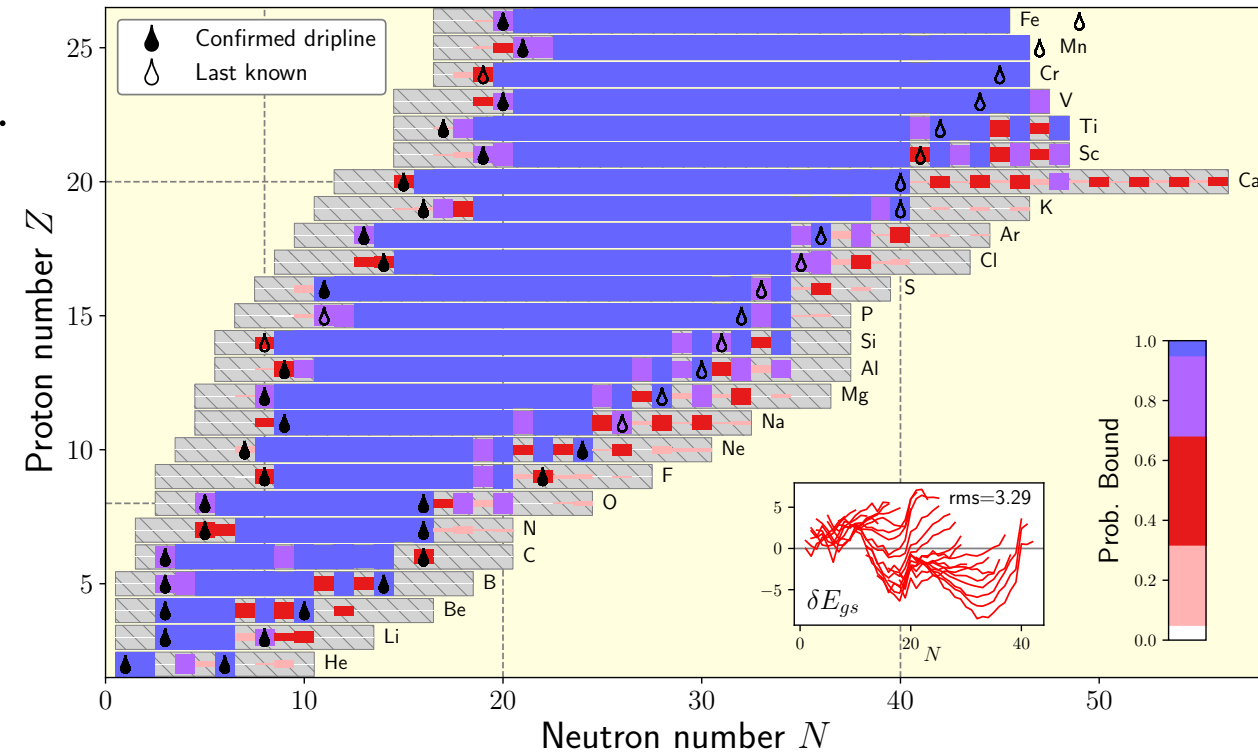
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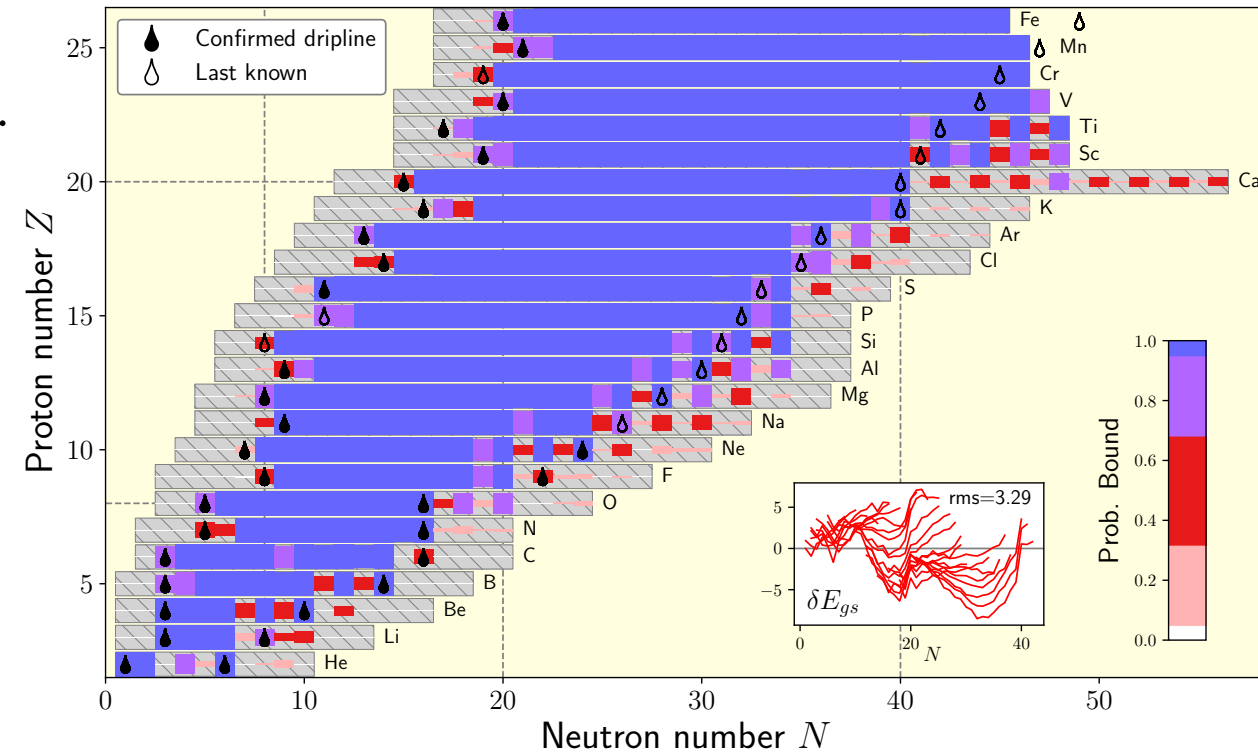
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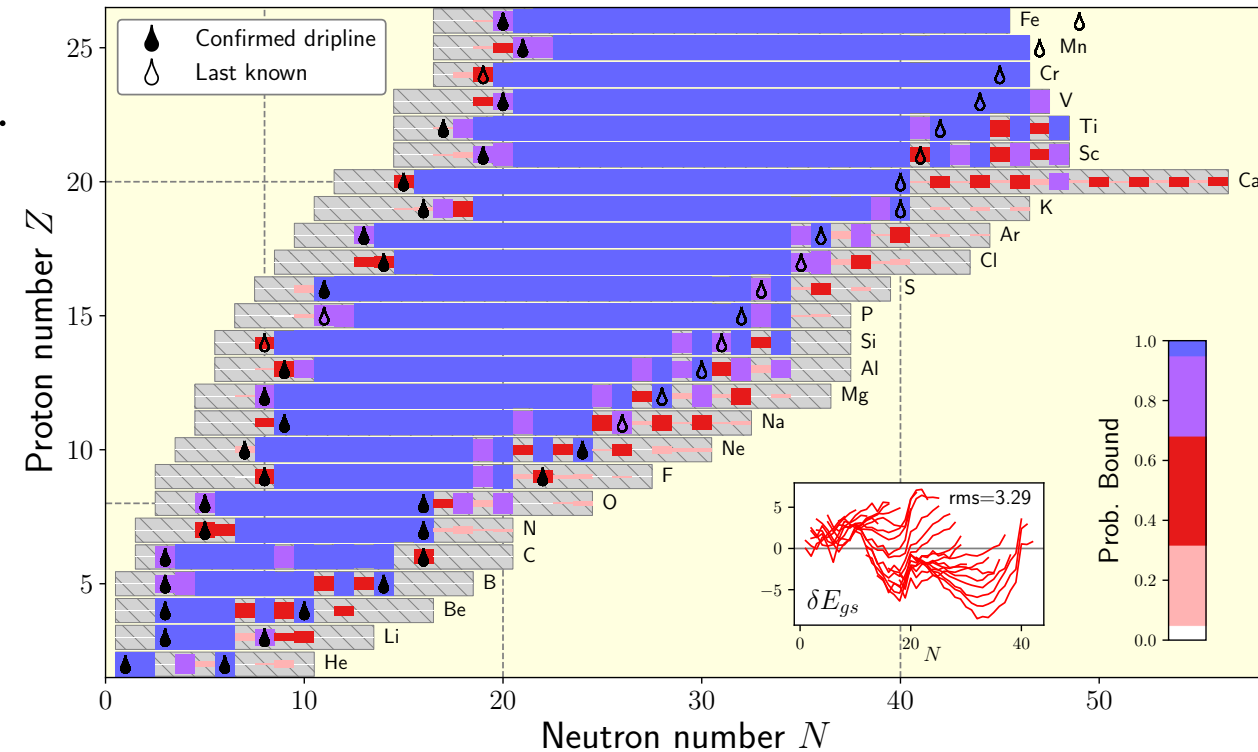
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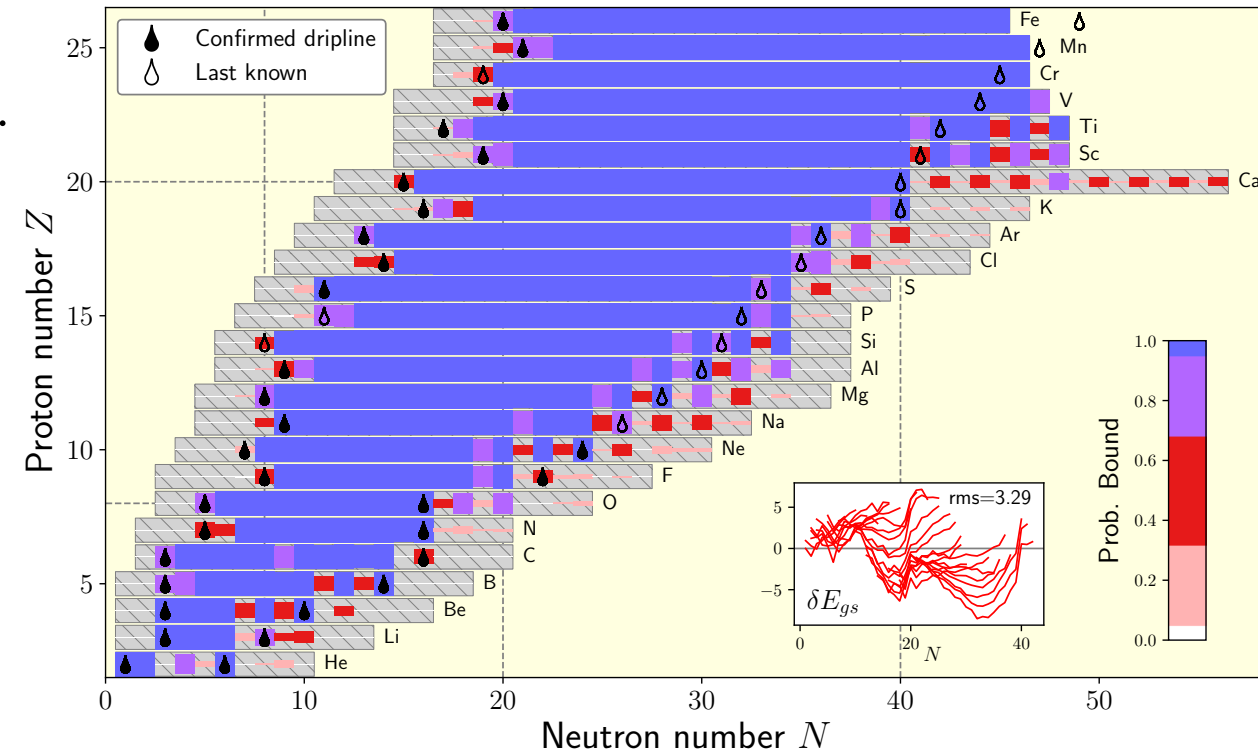


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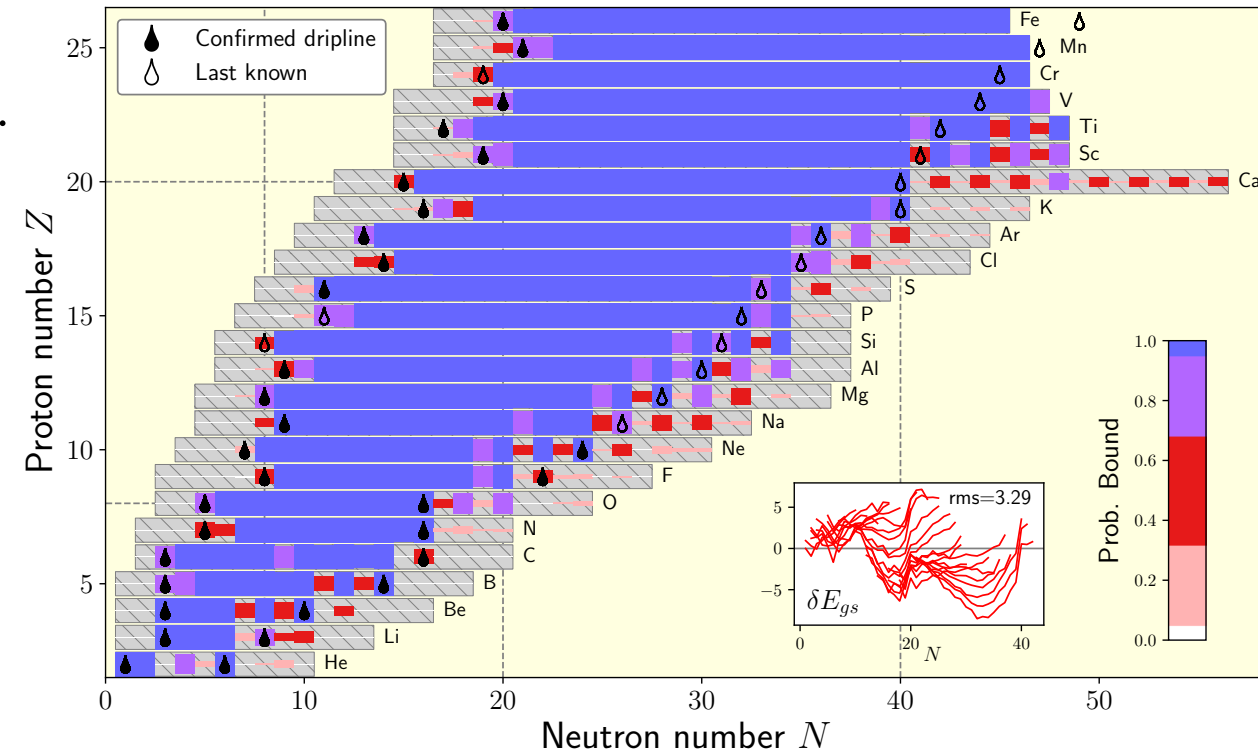


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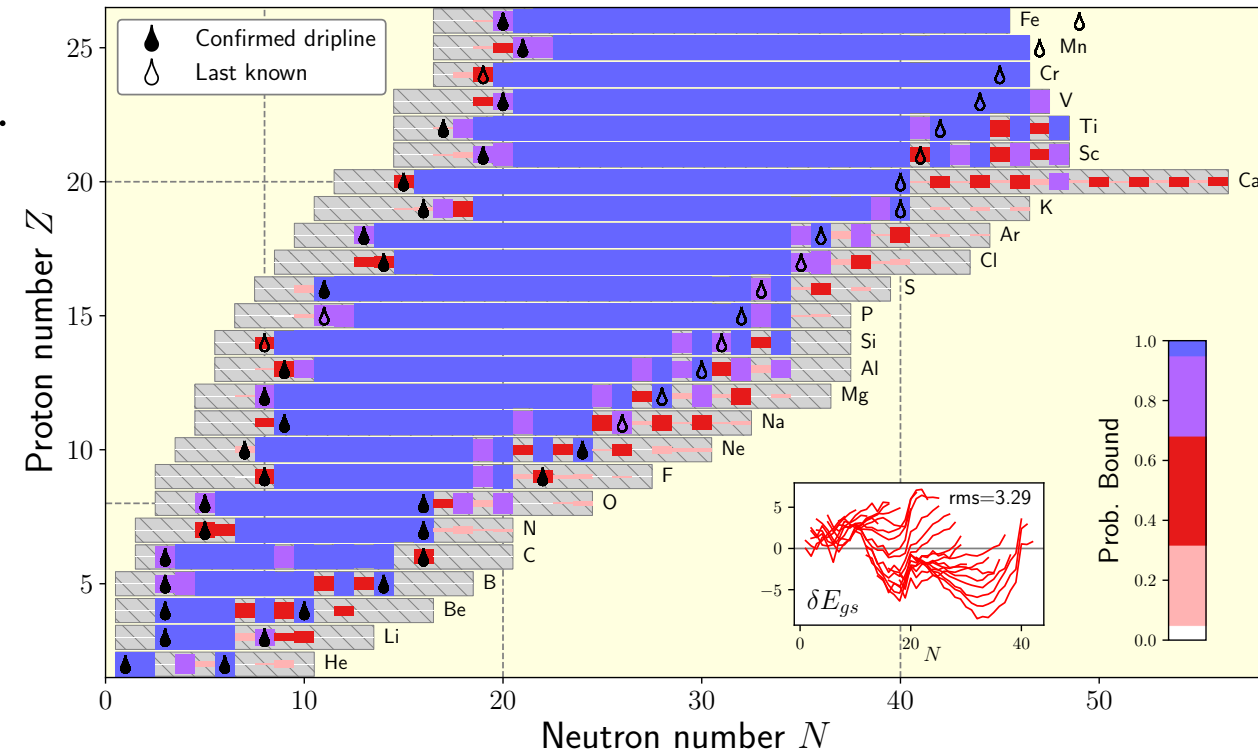


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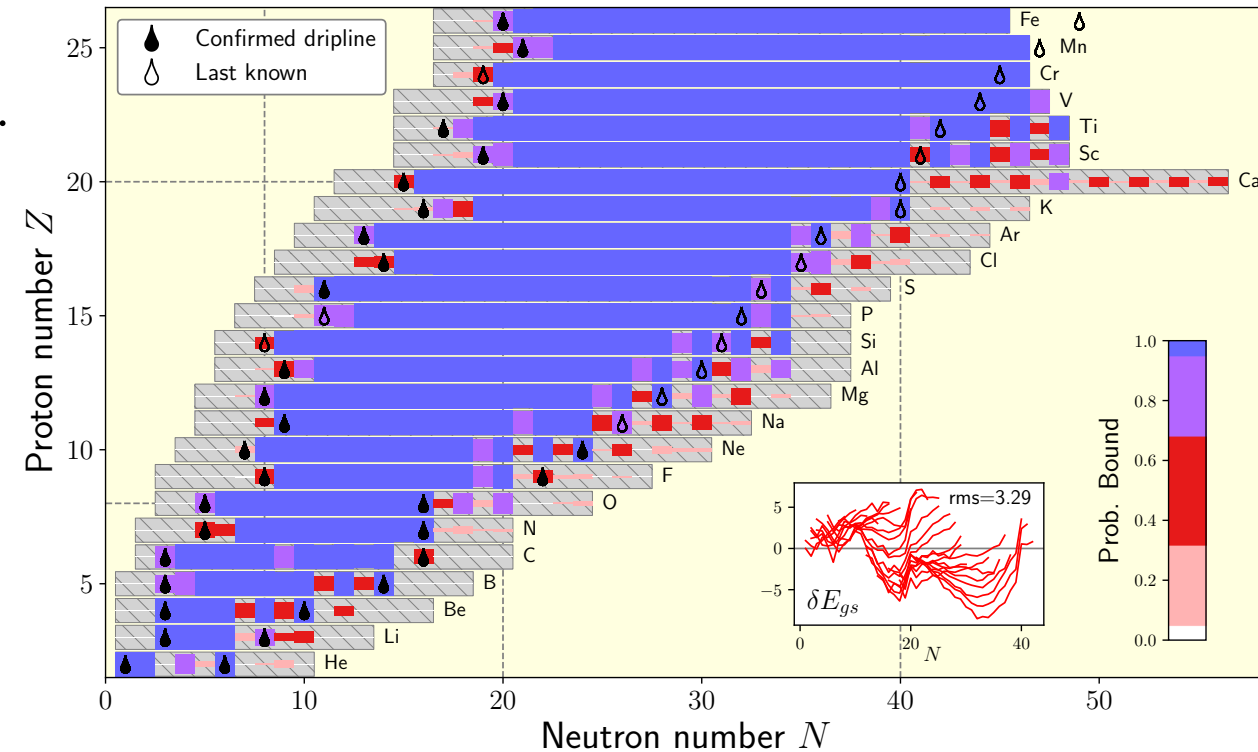
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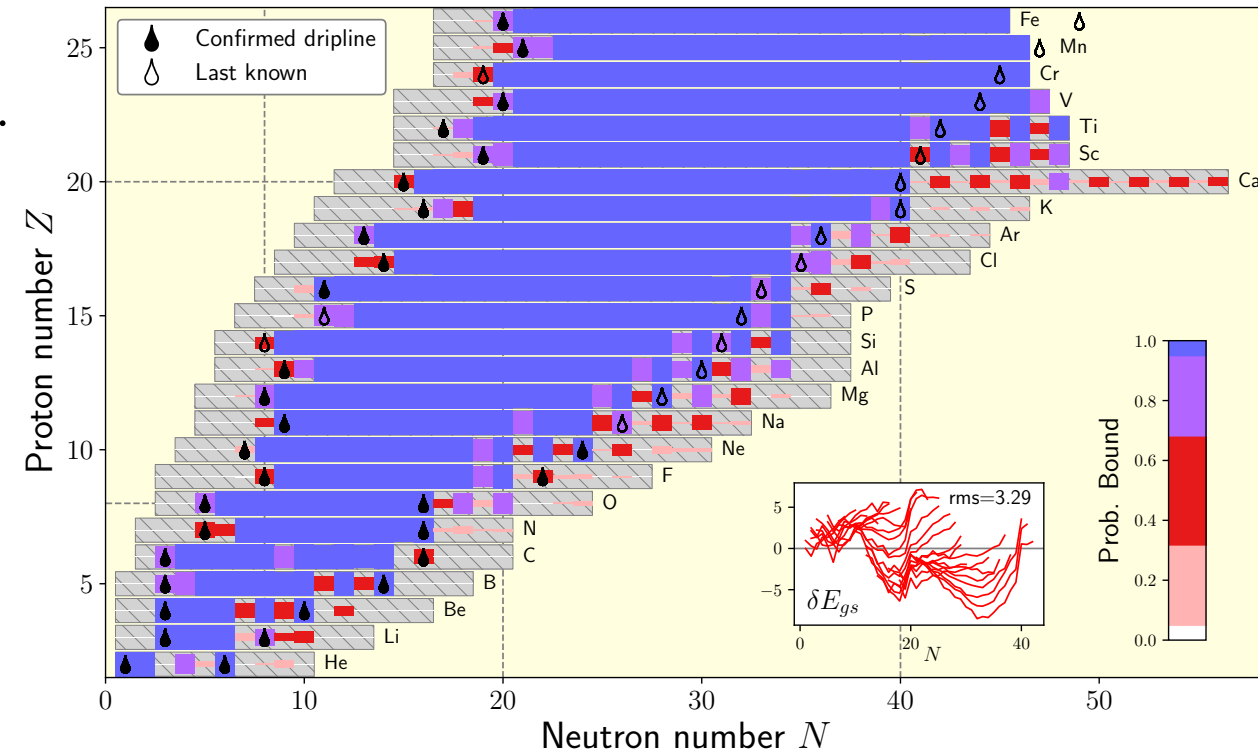


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TAKE-HOME MESSAGES

- **Exact solution of the nuclear many-body problem scales combinatorially** with mass number and basis size
- **“Virtually exact” methods** for $A \leq 5$ nuclei
 - Faddeev-Yakubovsky, Hyperspherical Harmonics
- **“Quasi exact” methods** for $A \leq 20$ nuclei
 - Quantum Monte Carlo, No-Core Shell Model
- **Expansion methods** for heavier nuclei
 - Many-Body Perturbation theory, Coupled Cluster, In-Medium Similarity Renormalization Group, Self-Consistent Green’s Functions
- ***Ab initio* nuclear theory is a fast growing field**

UP NEXT

Lecture 3 *From weak interactions to nuclear observables*