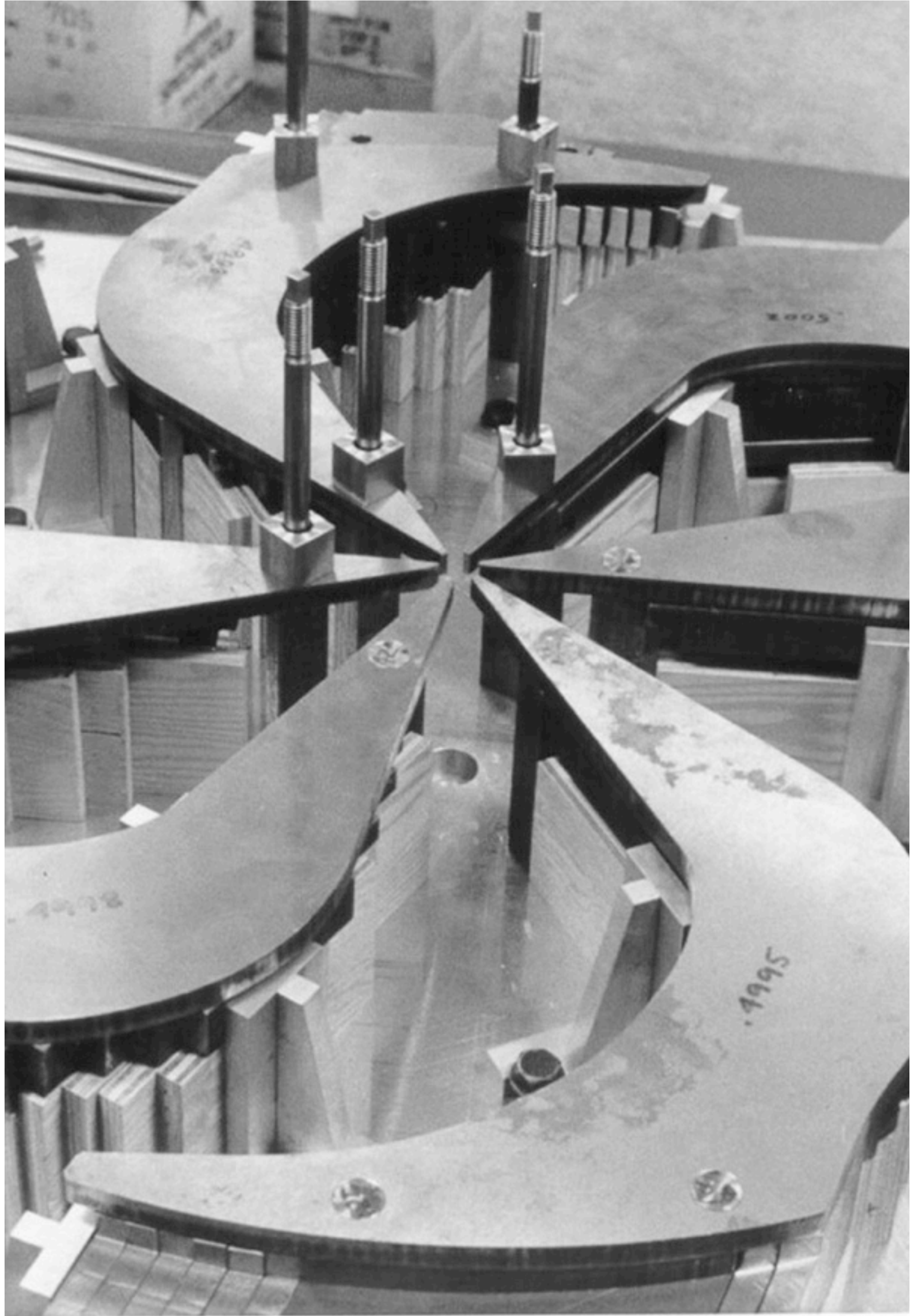
Ab initio nuclear correction to the Lamb shift

Extracting nuclear radii from precision muonic experiments



Collaborators: Petr Navratil, Michael Gennari

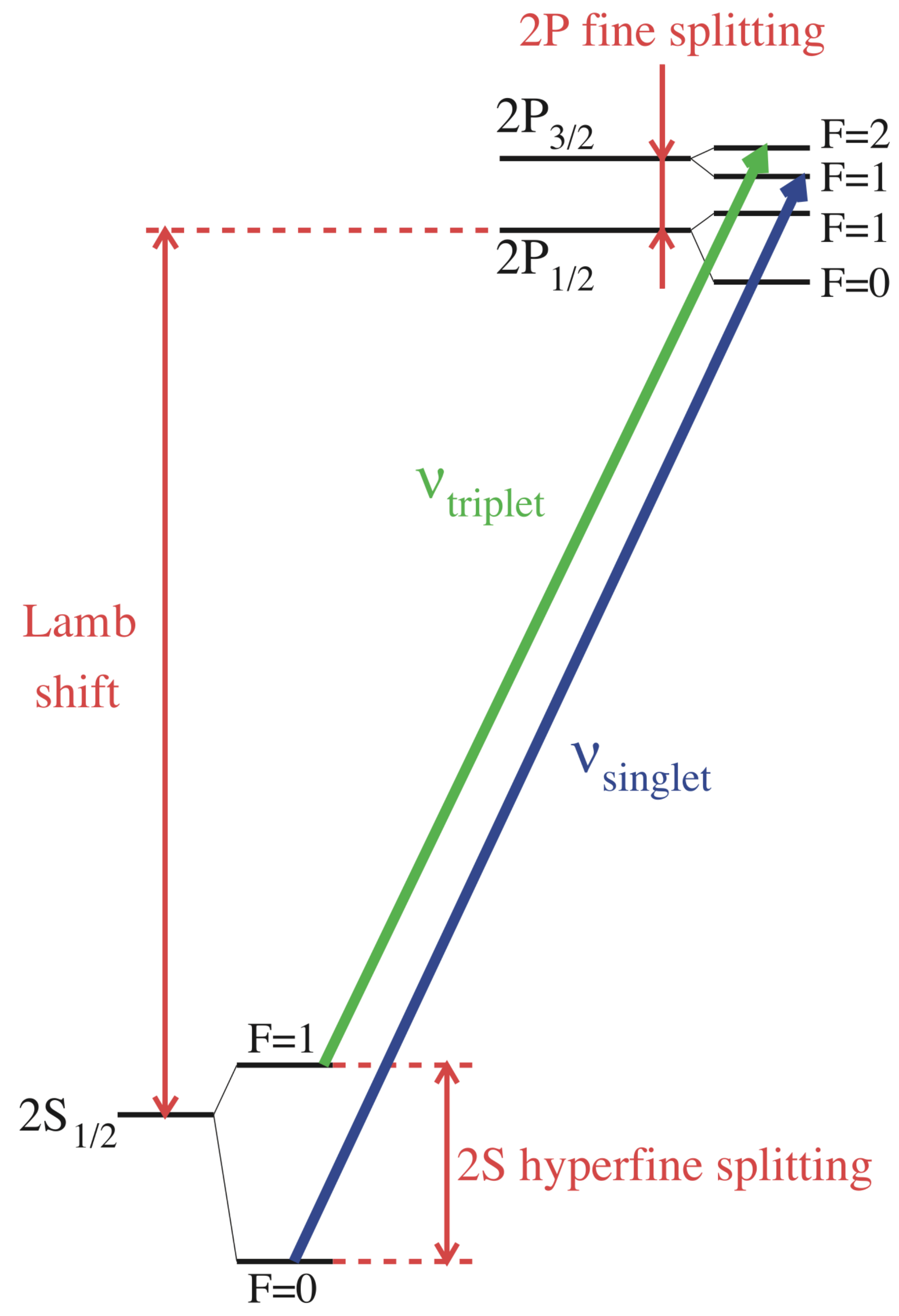
Mehdi Drissi
TRIUMF - Theory department

EPIC workshop

Sardinia Cagliari - 25th of September 2024

Discovery, accelerated

The muonic Lamb shift as a precision probe



[Antognini et al, Science (2013)]

The muonic Lamb shift as a precision probe

A key probe to develop the Standard Model…

~1900 **Observation of atomic spectra**

Discrete energy levels
Quantum theory

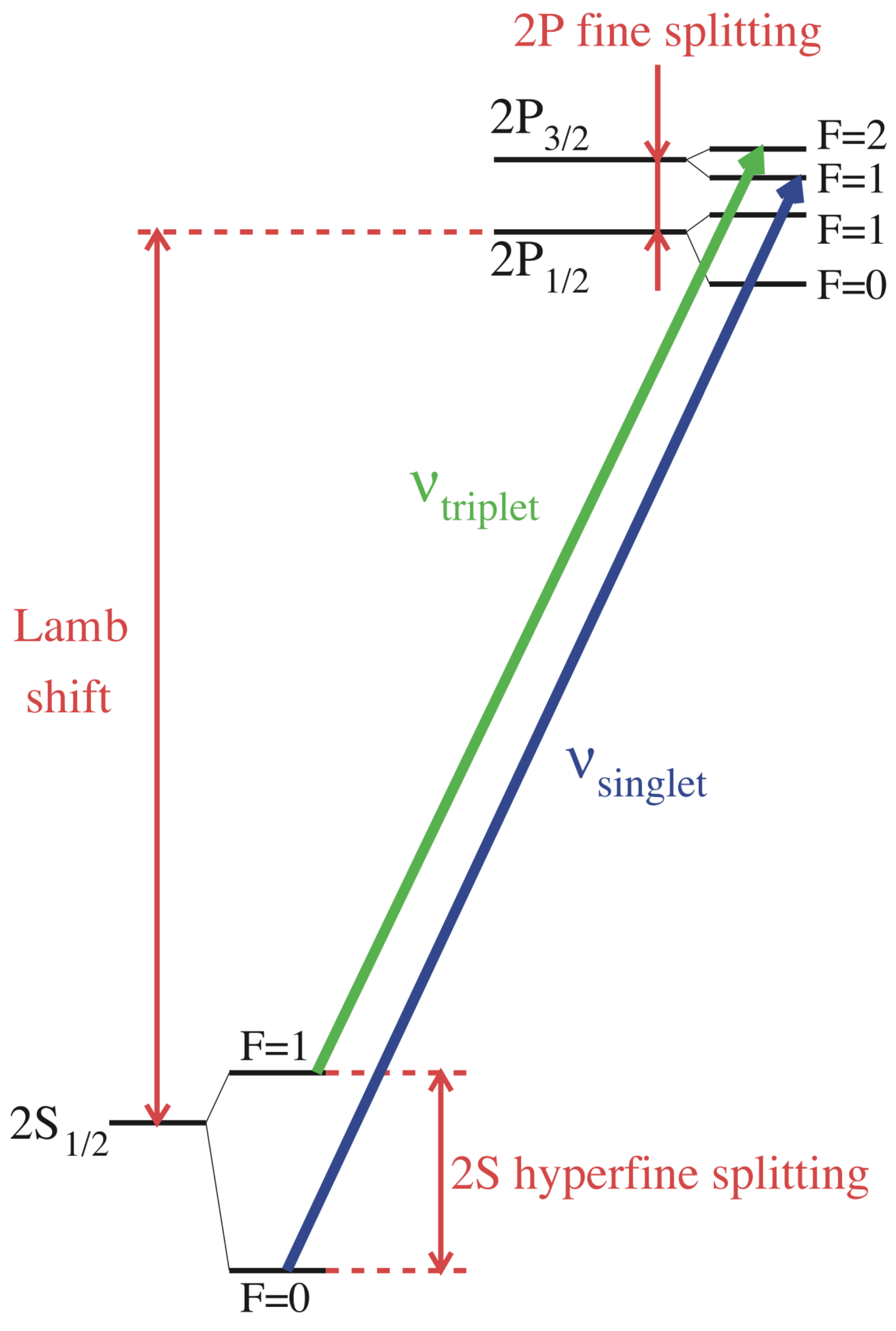
~1947 **Observation of Lamb shift between $2S_{1/2} - 2P_{1/2}$ states**

Vacuum polarization effect
Renormalization theory

~1965 **Quantum Electrodynamics**

Non-abelian generalization

~1970 **Standard Model of particle physics**



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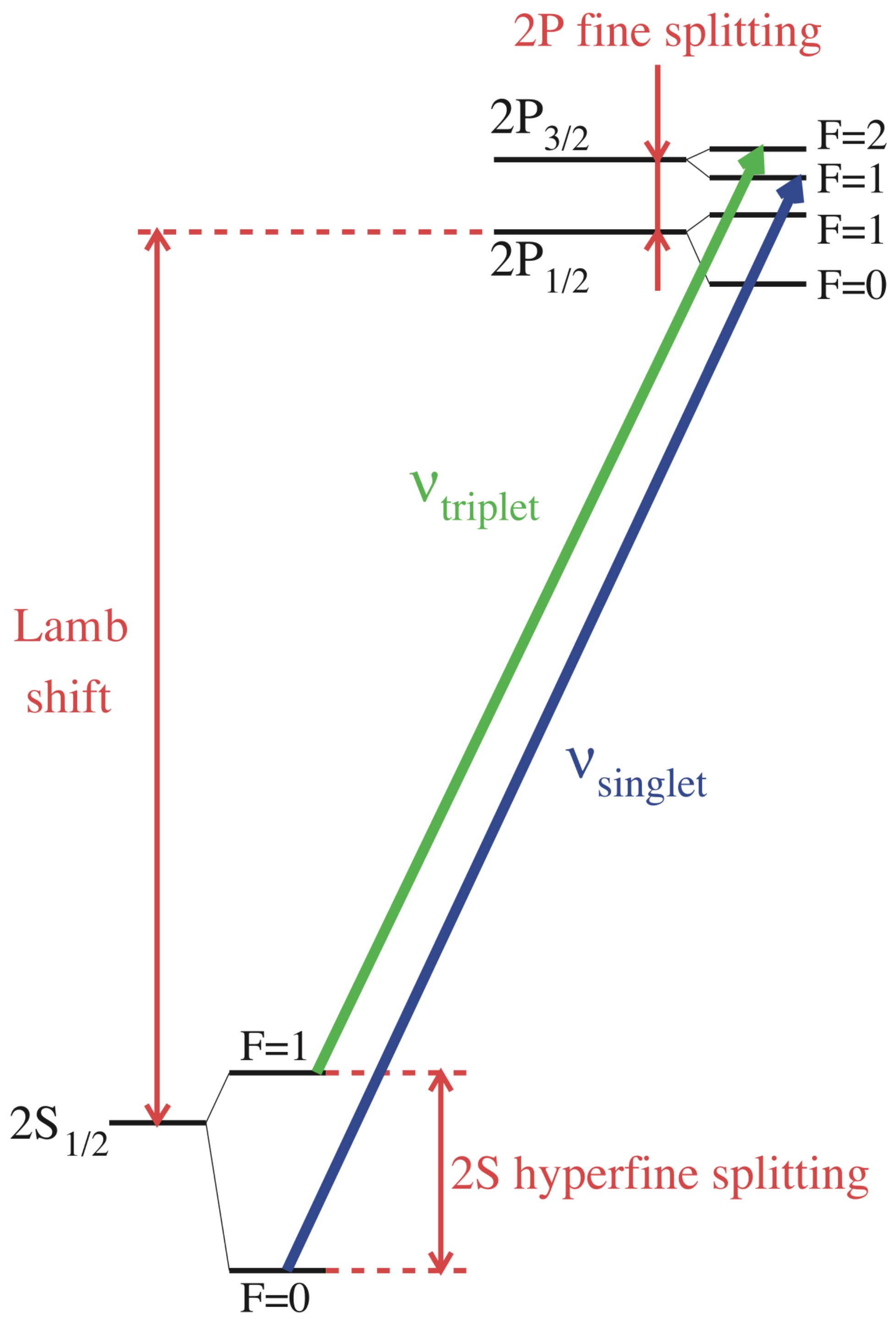

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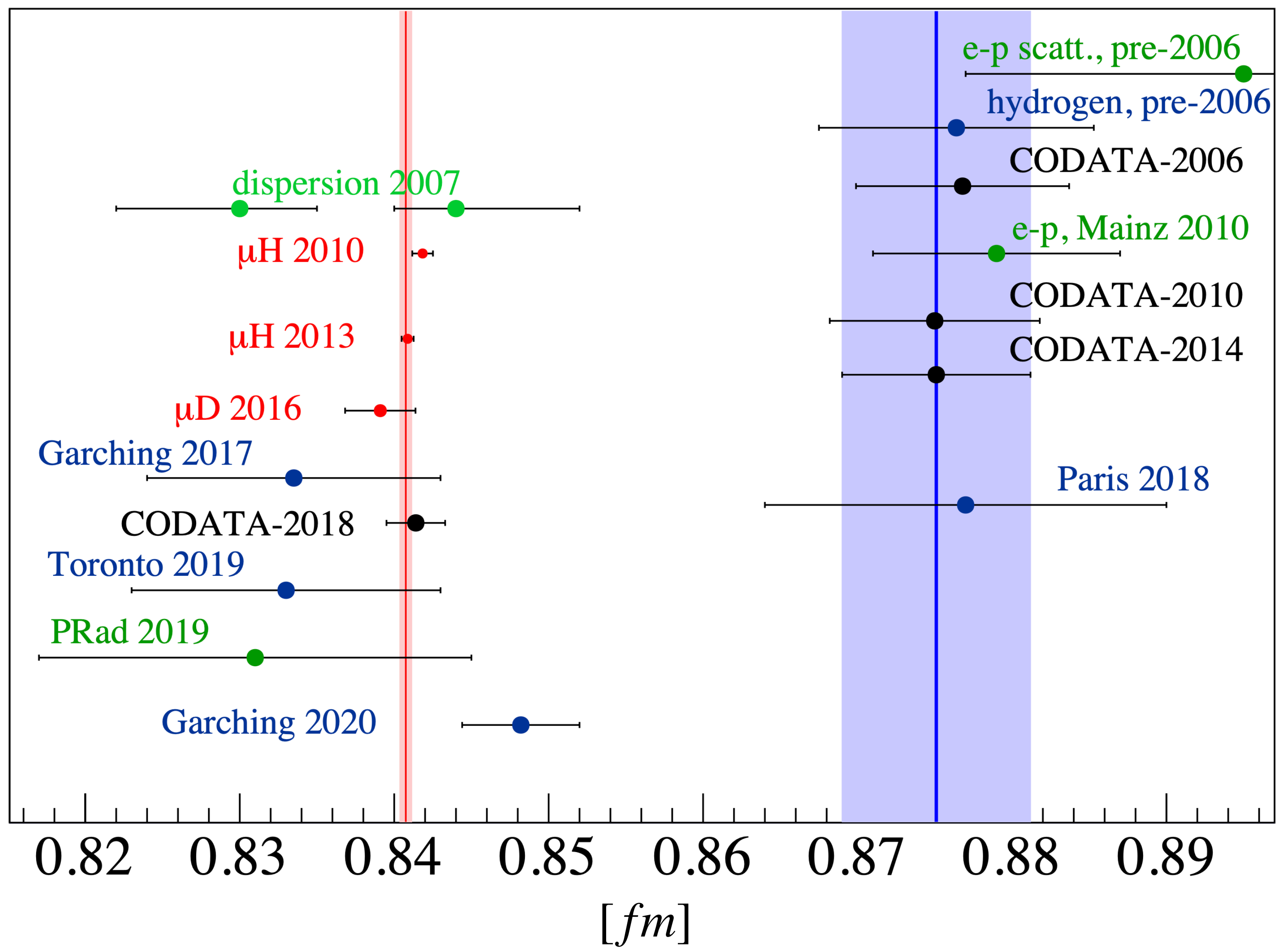

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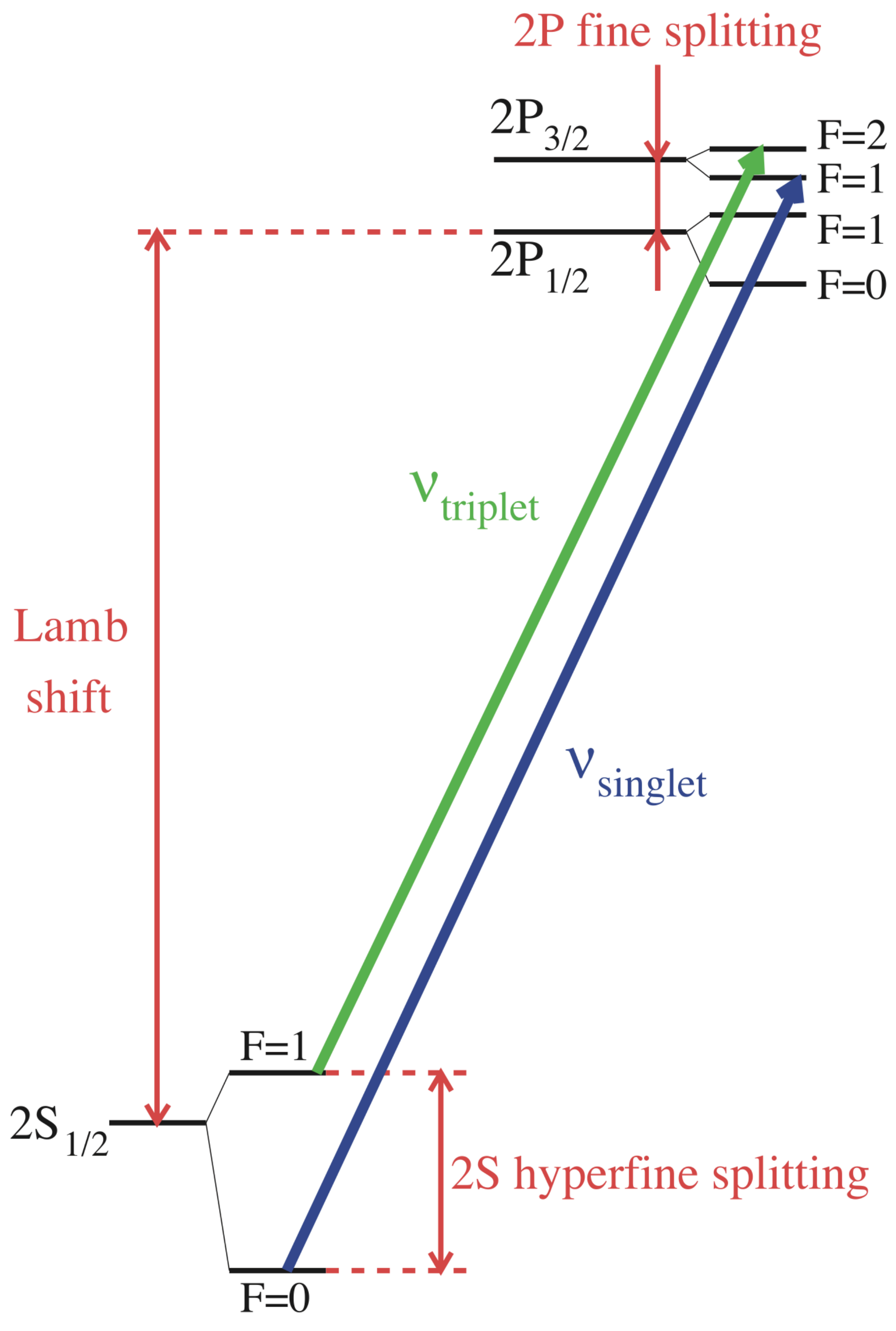

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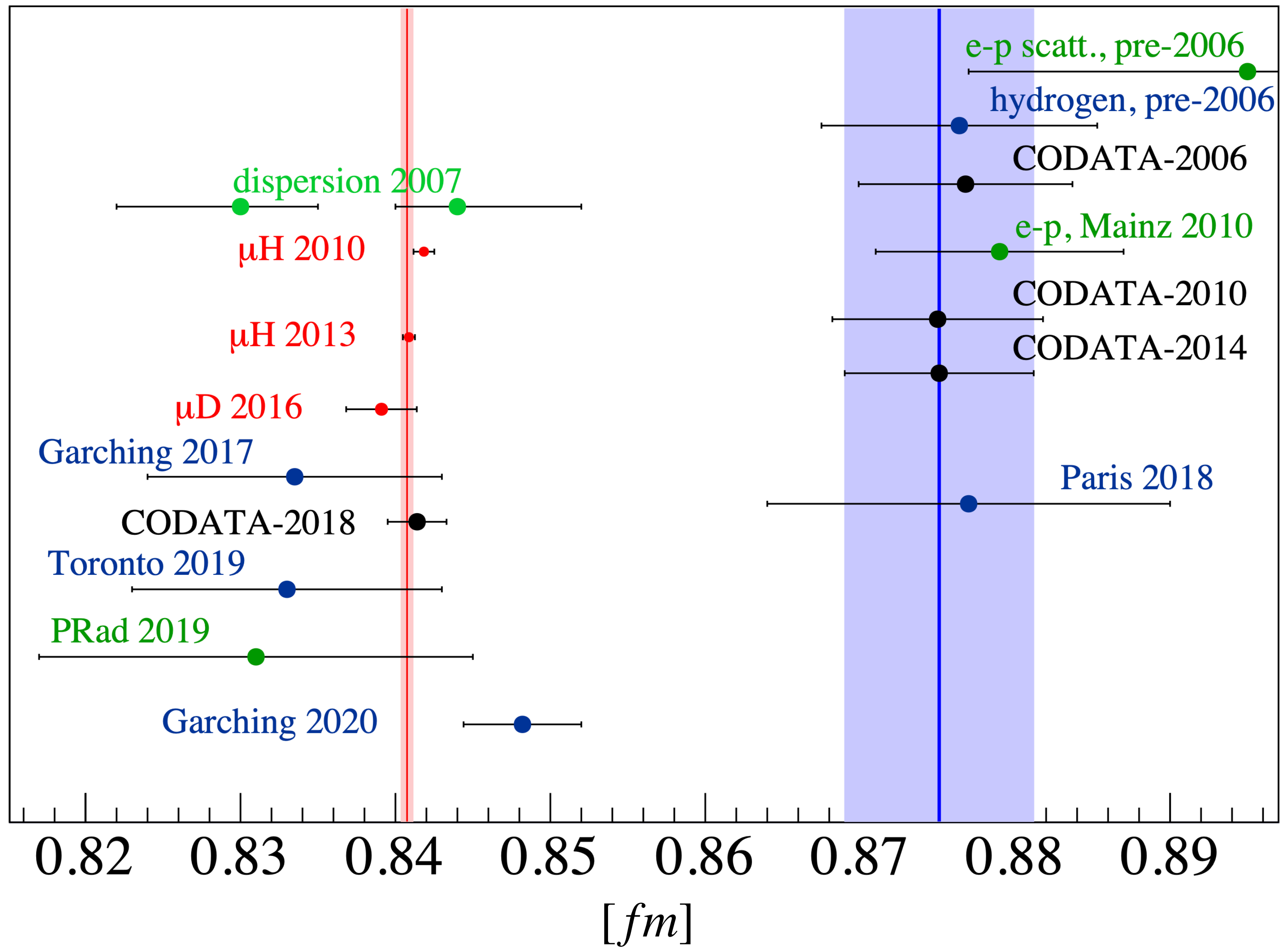
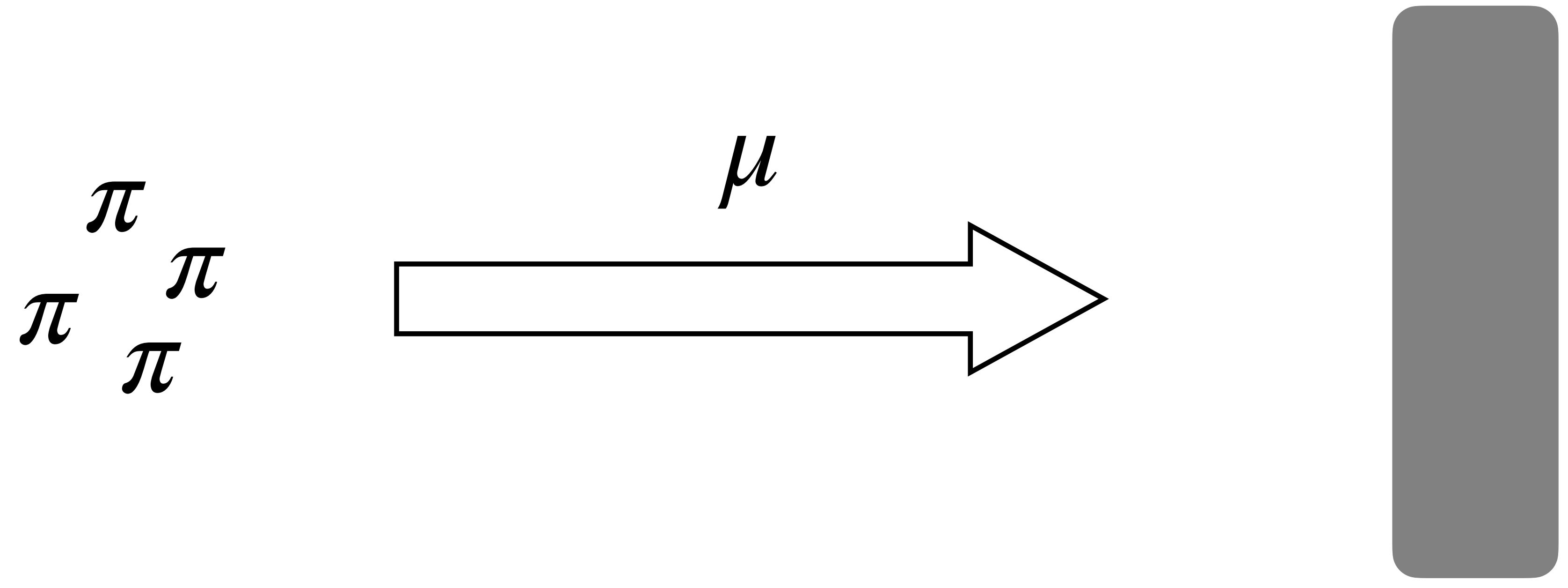


See Randolf Pohl's talk for more

Observing muonic atoms with X-rays

How to make muonic atom



(i) Pion decay: muon source

(ii) High intensity beam: momentum filtering, ...

(ii) Thick target: capture muons

Typically muons captured on orbitals with $n \sim \sqrt{\frac{m_\mu}{m_e}} \sim 14$

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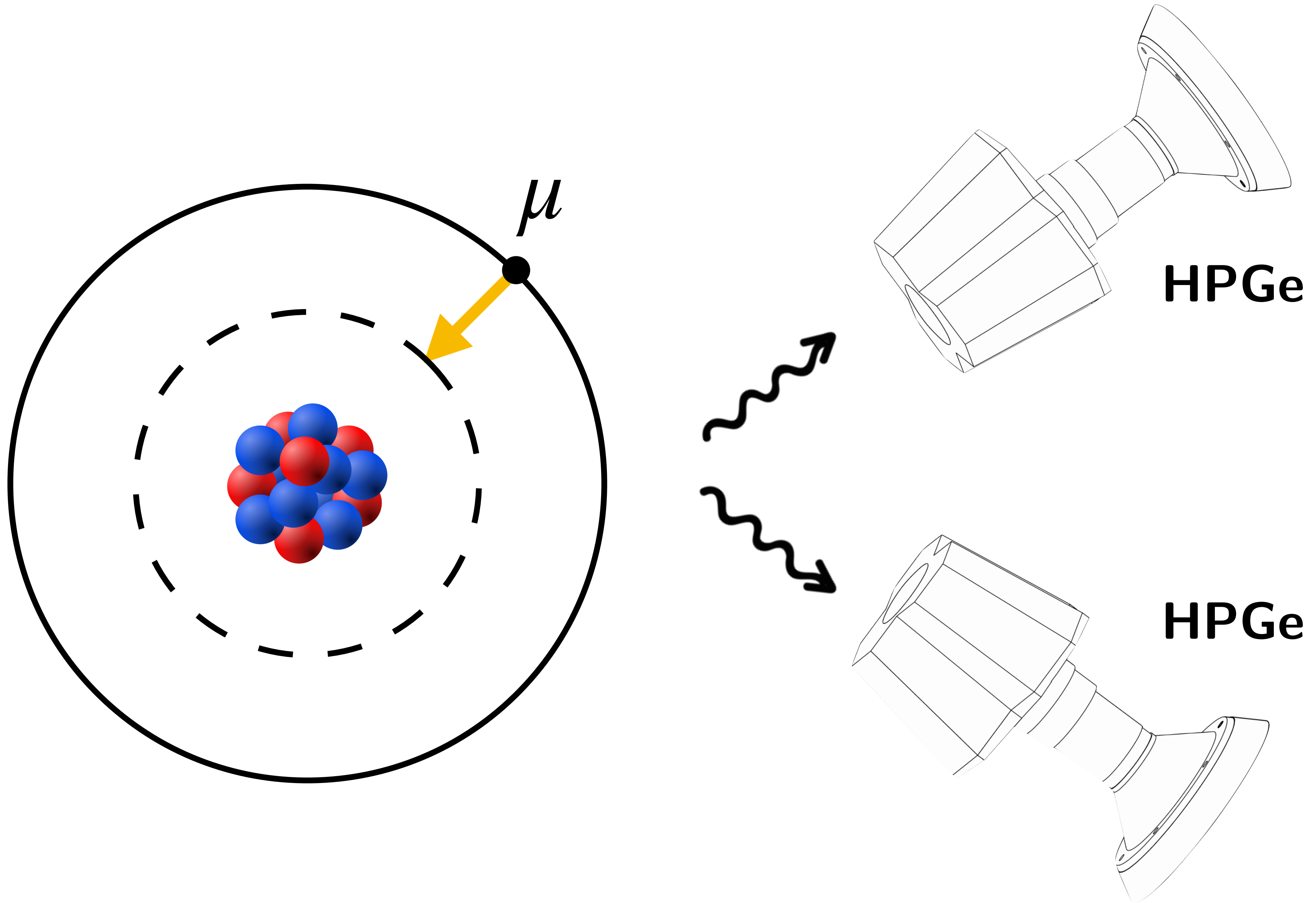

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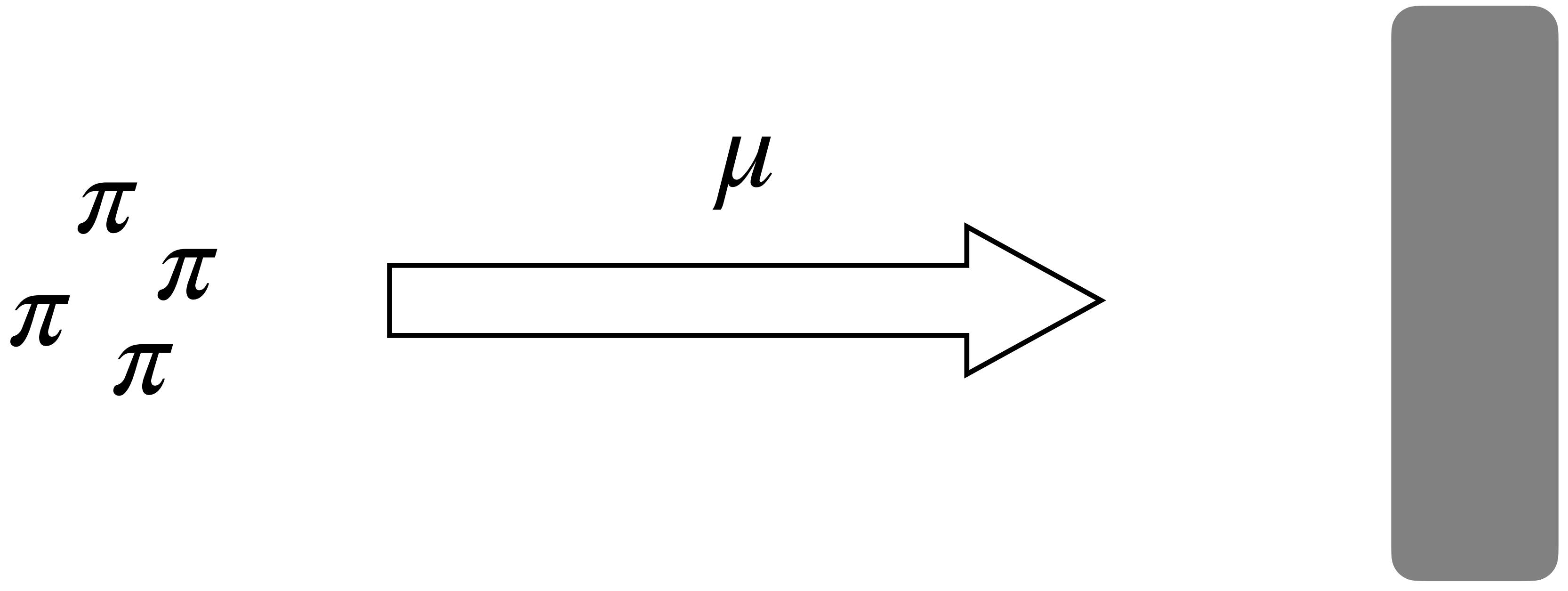

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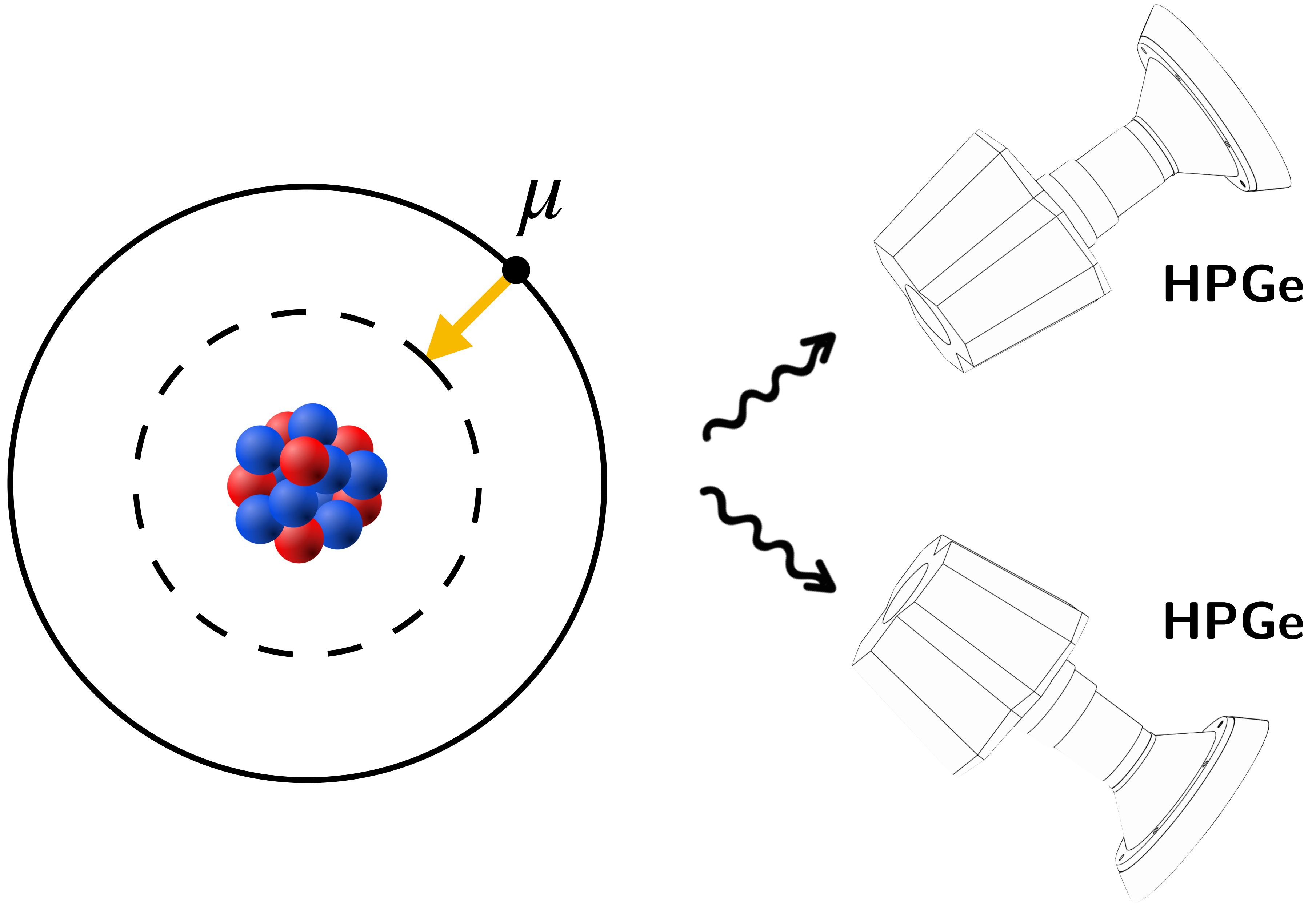

Muonic X-ray achievements

- Precise spectroscopy of almost all stable elements
- Specific transition targeted with low-latency lasers
- Absolute charge radii extracted $\Rightarrow$ **highest accuracy**

➡ **Higher sensitivity due to higher overlap** $\sim \left(\frac{m_\mu}{m_e}\right)^3 \sim 10^7$

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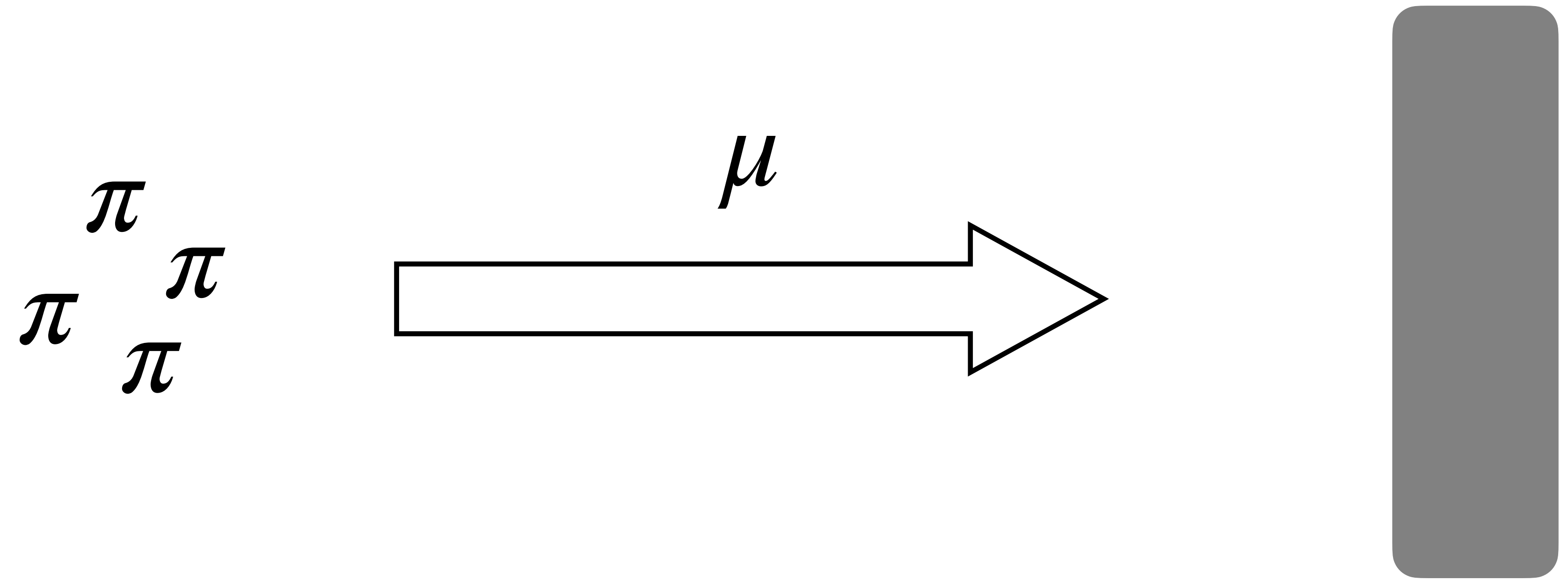

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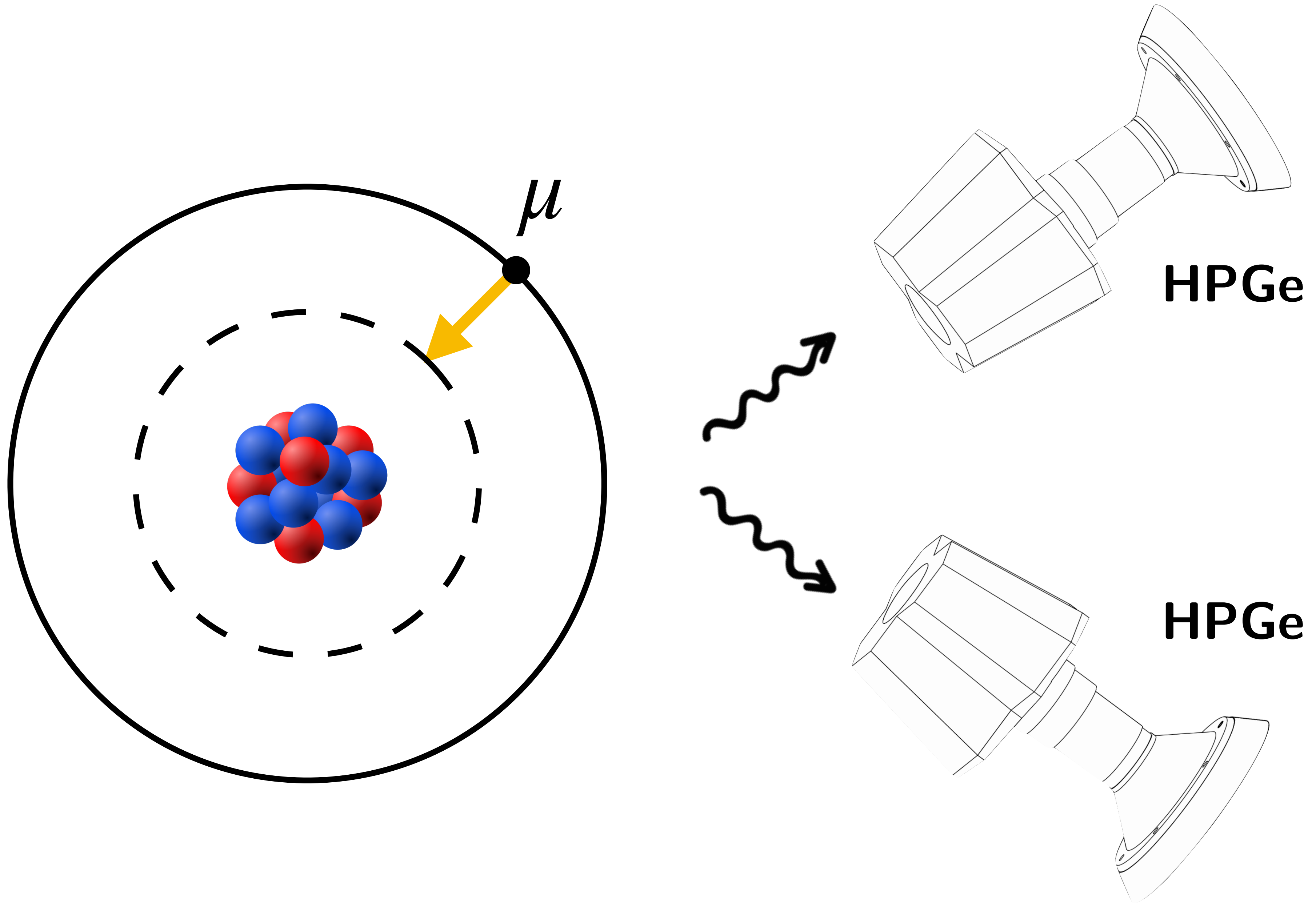

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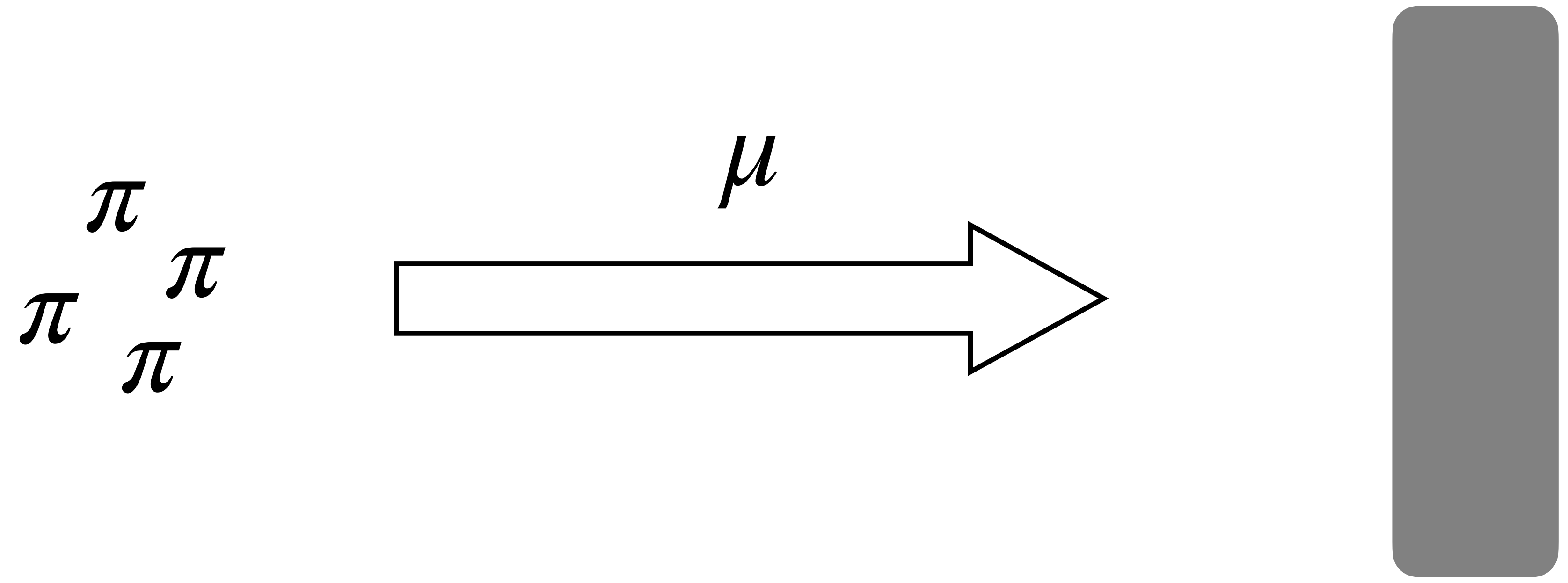

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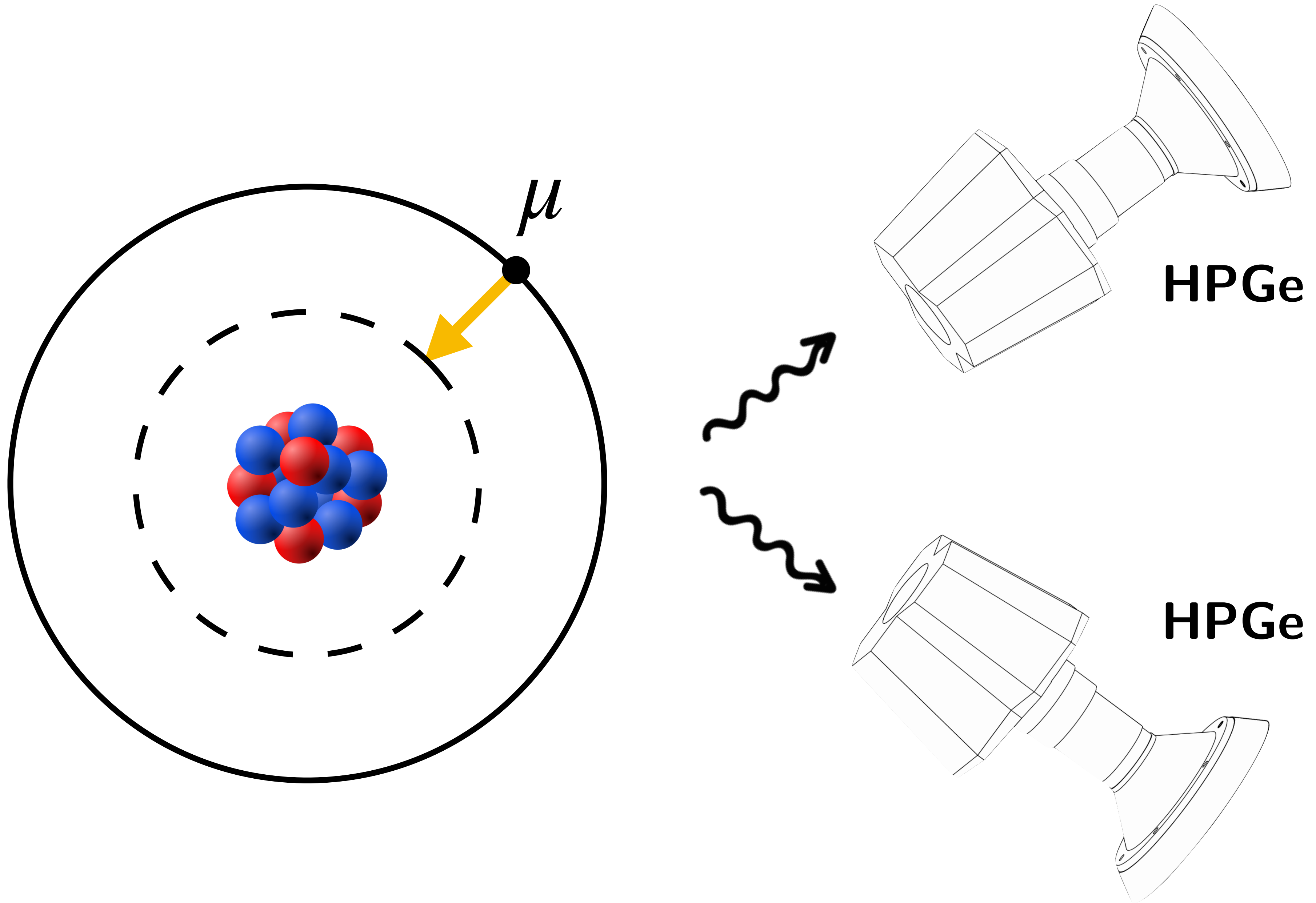

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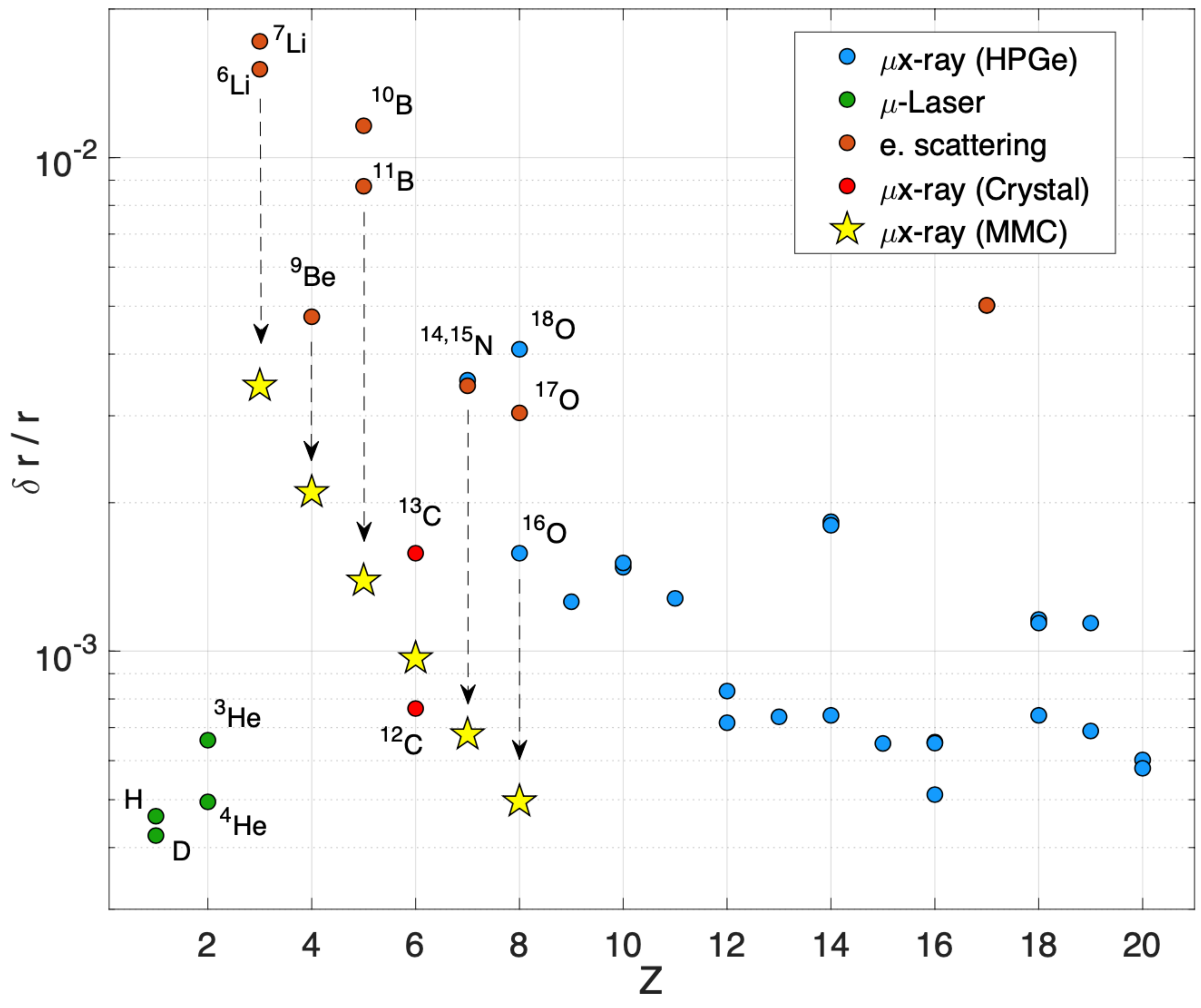
Reaching high resolution for light nuclei



[Antognini et al, arXiv:2210.16929]
NuPECC Long Range Plan 2024

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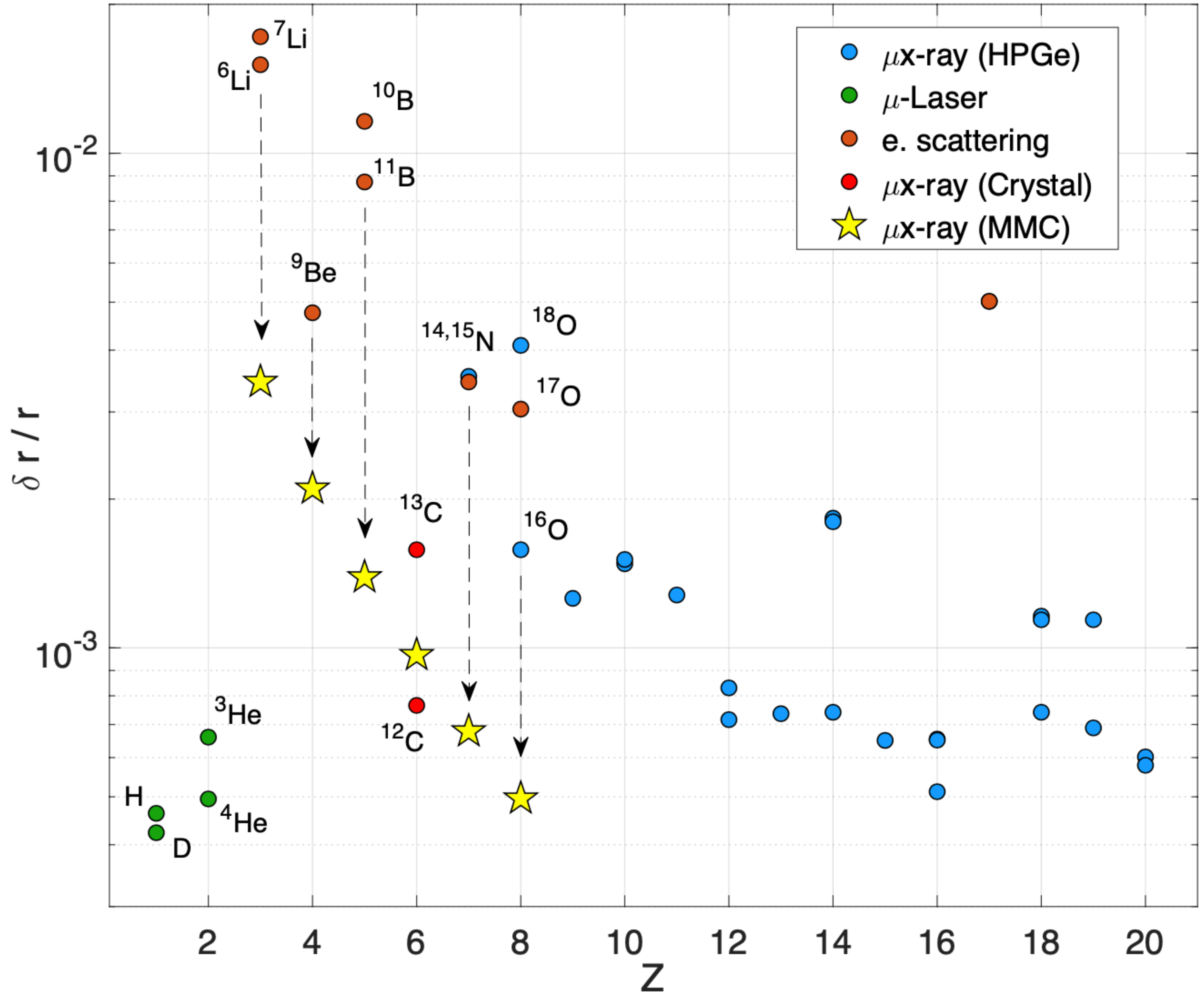

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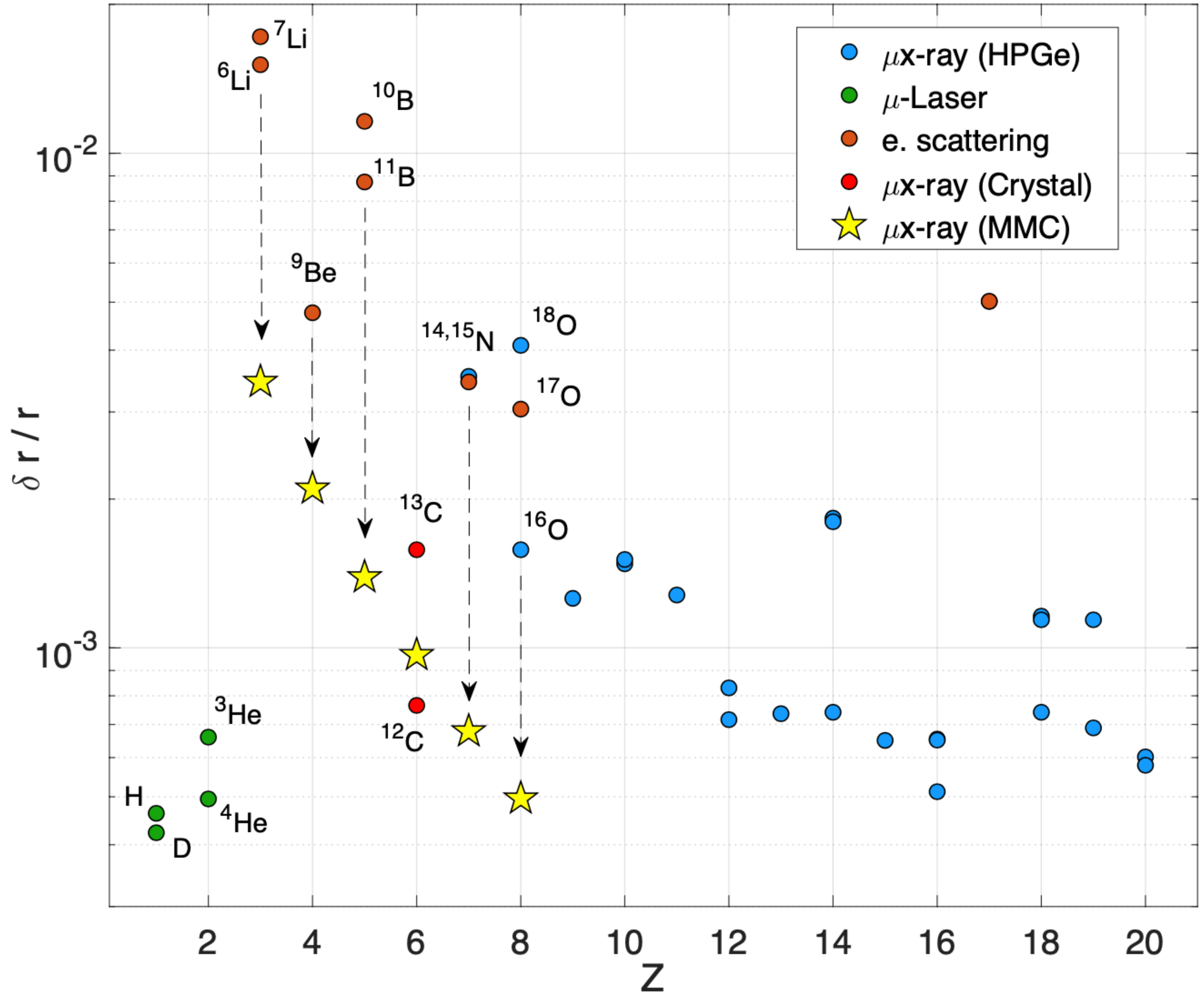

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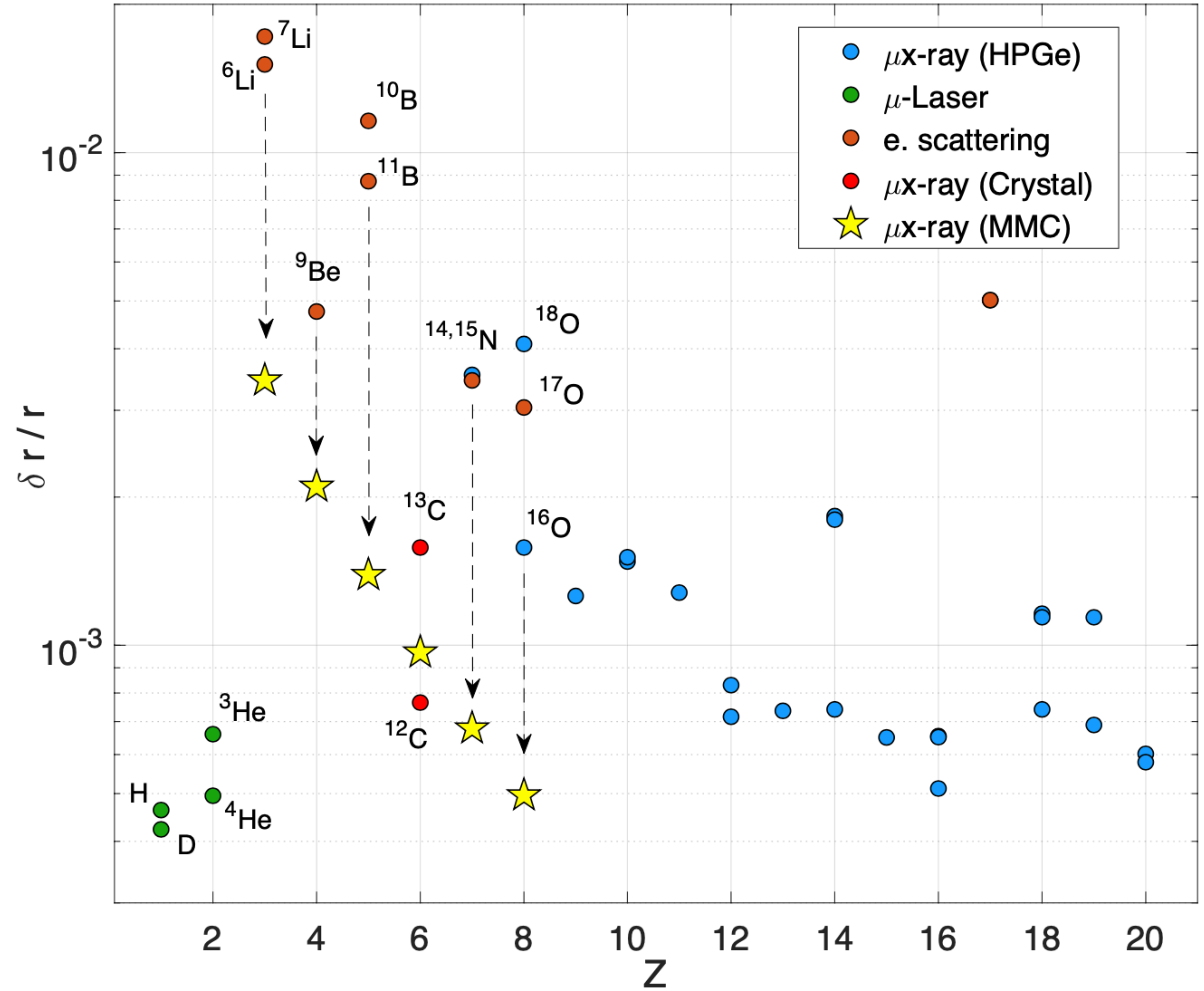

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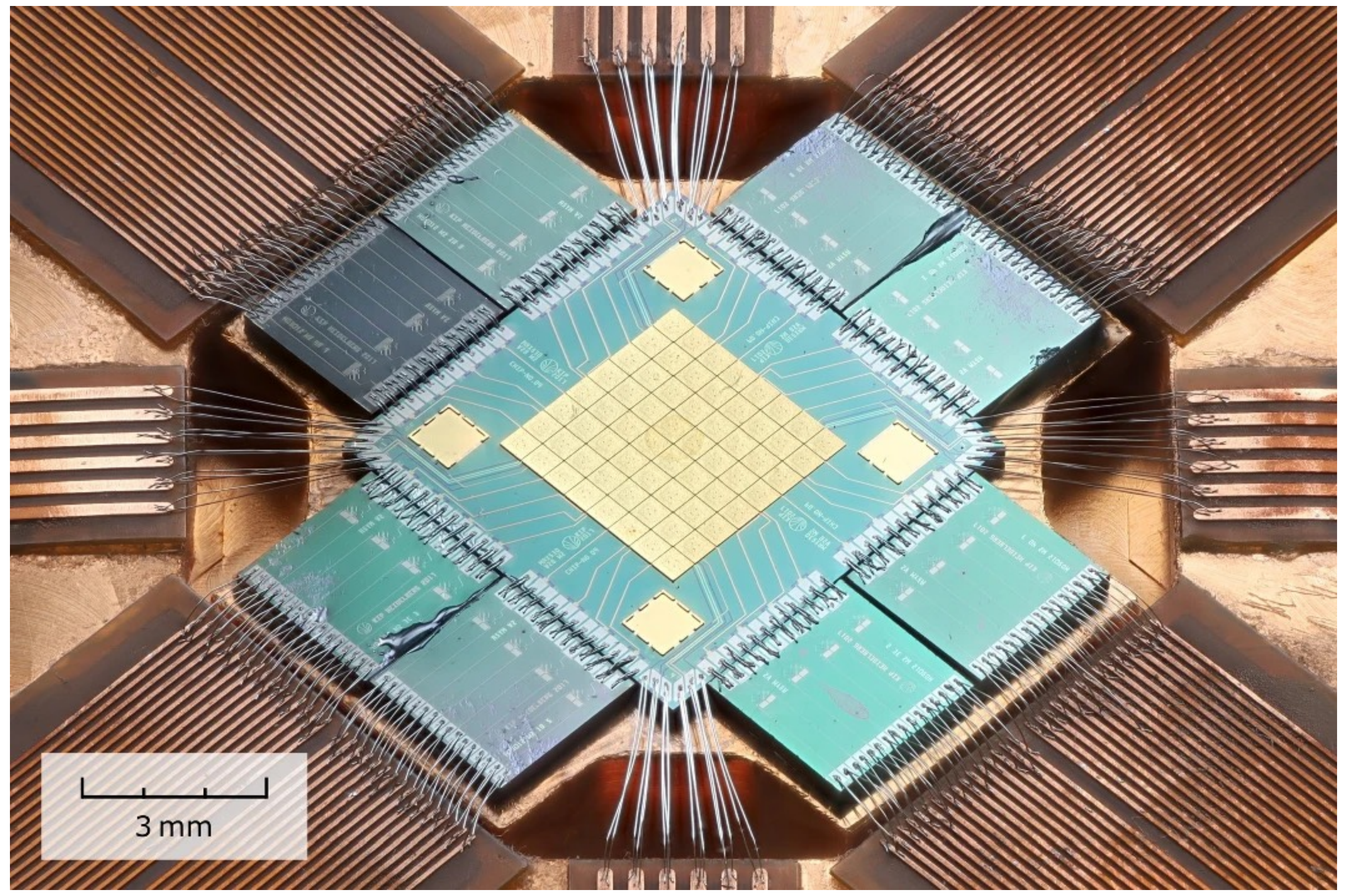

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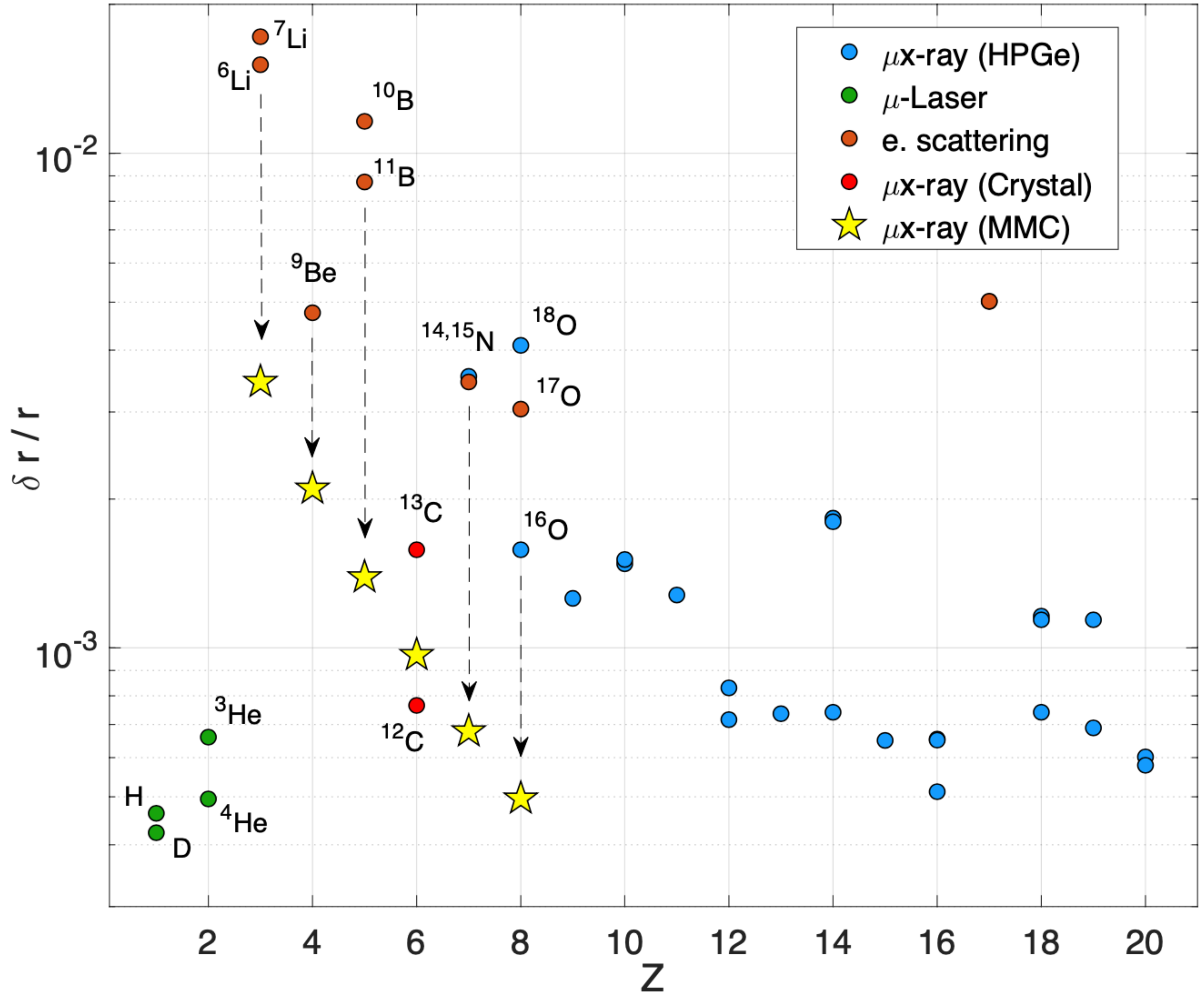

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Theoretical challenge: reach 10 meV uncertainty!

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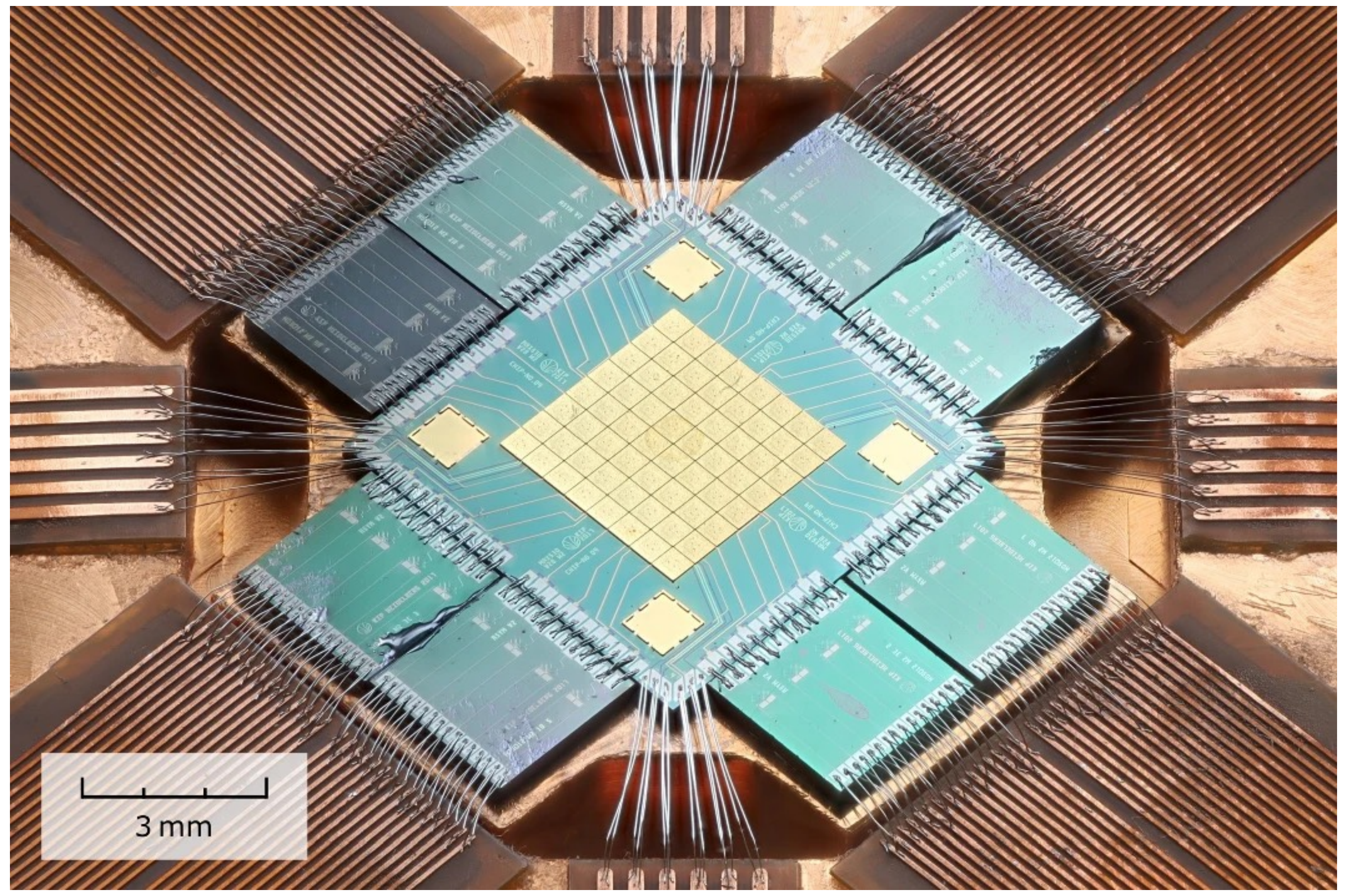

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Outline

- **Theoretical modeling**
  - Lamb-shift to atomic energy levels
  - Two-photon exchange corrections
- **Calculations for $^{7}\mathrm{Li}$**
  - No-Core Shell Model
  - Nuclear polarizability of $^{7}\mathrm{Li}$

From energy levels to nuclear structure

Converting experimental data

- What to do once precise value of energy levels is known ?
  - Can be used to **test fundamental constants** like R_∞, α, m_e
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  - Can be used to test validity of **many-body calculations**

- Example in practice: Lamb shift in meV $2S_{1/2} - 2P_{1/2}$ (r_x in fm)

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$$\Delta E(\mu\mathrm{H}) = 206.0336(15) - 5.2275(10) \times r_p^2 + 0.0332(20)$$
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  - ✓ In practice use **effective instantaneous potential**
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Bound states QED contributions

Bound muon within potential

- Zero-order: one-body Coulomb interaction
  - Solve exactly for $H_0 = \dfrac{\vec{p}^2}{2m_r} - \dfrac{Z\alpha}{r}$
  - $E_{nl} = -\dfrac{(Z\alpha)^2 m_r}{2n^2} \equiv E^{(0)}$
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  - Finite nuclear mass $\Rightarrow$ recoil and relativistic corrections
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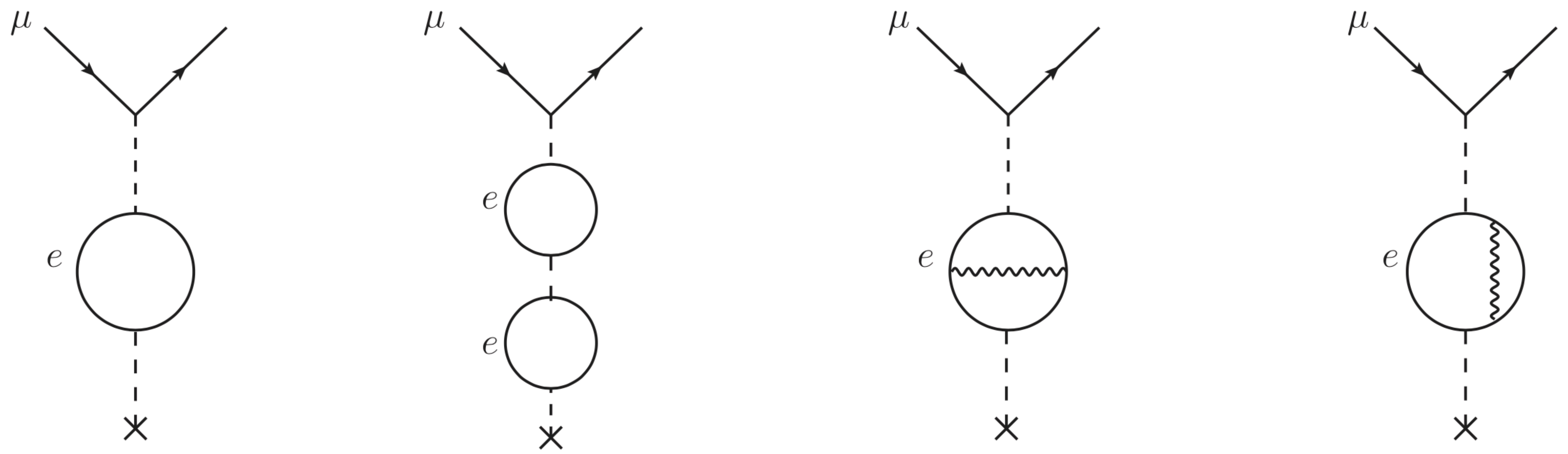

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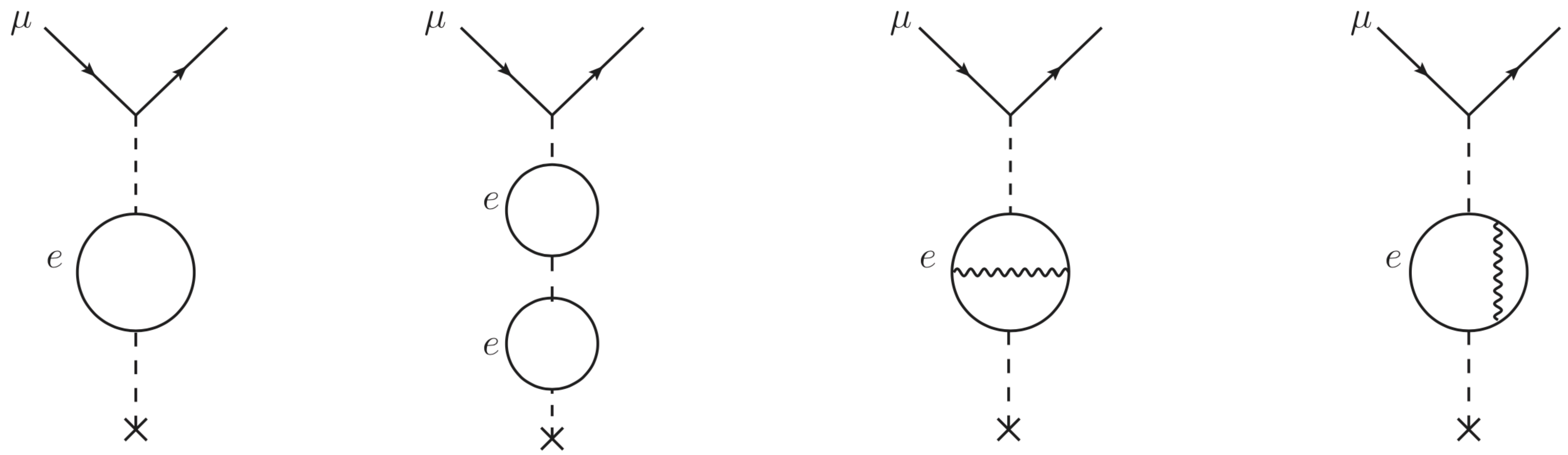

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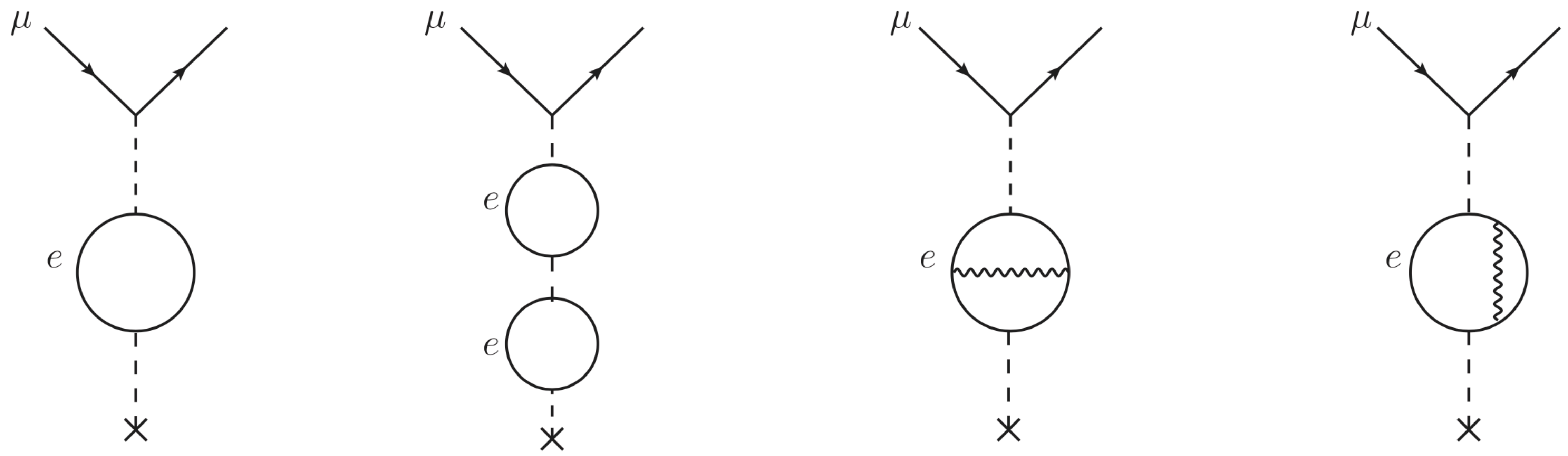
  - Electron vacuum polarization: $a_\mu \sim \lambda_e \Rightarrow$ **main one!**
  - Finite nuclear mass $\Rightarrow$ recoil and relativistic corrections
  - Muon self-energy terms

Example: electron vacuum polarization corrections



$$-\frac{g^{\mu\nu}}{q^2} \to \frac{g^{\mu\nu}}{q^2\left(1+\bar{\omega}\left(\frac{q^2}{m_e}\right)\right)}$$ where $\bar{\omega} \equiv$ 1PI expanded in powers of α

$$-\frac{g^{\mu\nu}}{q^2} \to \frac{g^{\mu\nu}}{q^2}\left(1+\rho^{(1)}+\rho^{(2)}+\dots\right)$$

$$\Rightarrow \quad \boxed{V^{(i)}(r) = -(Z\alpha)\int \frac{\mathrm{d}^3\vec{q}}{(2\pi)^3}\frac{4\pi}{\vec{q}^{\,2}}\;\rho^{(i)}(-\vec{q}^{\,2})\;e^{i\vec{q}.\vec{r}}}$$

$$\Rightarrow \quad E_{nl} = E^{(0)} + \langle V^{(1)}\rangle + \langle V^{(2)}\rangle + \langle V^{(1)}\frac{1}{(E_0-H_0)'}V^{(1)}\rangle + \dots$$

[Pachucki et al. Review of Modern Physics (2024)]

Bound states QED contributions

Section	Order	Correction	μH	μD	μ^3He$^+$	μ^4He$^+$
III.A	$\alpha(Z\alpha)^2$	eVP$^{(1)}$	205.007 38	227.634 70	1641.886 2	1665.773 1
III.A	$\alpha^2(Z\alpha)^2$	eVP$^{(2)}$	1.658 85	1.838 04	13.084 3	13.276 9
III.A	$\alpha^3(Z\alpha)^2$	eVP$^{(3)}$	0.007 52	0.008 42(7)	0.073 0(30)	0.074 0(30)
III.B	$(Z, Z^2, Z^3)\alpha^5$	Light-by-light eVP	−0.000 89(2)	−0.000 96(2)	−0.013 4(6)	−0.013 6(6)
III.C	$(Z\alpha)^4$	Recoil	0.057 47	0.067 22	0.126 5	0.295 2
III.D	$\alpha(Z\alpha)^4$	Relativistic with eVP$^{(1)}$	0.018 76	0.021 78	0.509 3	0.521 1
III.E	$\alpha^2(Z\alpha)^4$	Relativistic with eVP$^{(2)}$	0.000 17	0.000 20	0.005 6	0.005 7
III.F	$\alpha(Z\alpha)^4$	μSE$^{(1)}$ + μVP$^{(1)}$, LO	−0.663 45	−0.769 43	−10.652 5	−10.926 0
III.G	$\alpha(Z\alpha)^5$	μSE$^{(1)}$ + μVP$^{(1)}$, NLO	−0.004 43	−0.005 18	−0.174 9	−0.179 7
III.H	$\alpha^2(Z\alpha)^4$	μVP$^{(1)}$ with eVP$^{(1)}$	0.000 13	0.000 15	0.003 8	0.003 9
III.I	$\alpha^2(Z\alpha)^4$	μSE$^{(1)}$ with eVP$^{(1)}$	−0.002 54	−0.003 06	−0.062 7	−0.064 6
III.J	$(Z\alpha)^5$	Recoil	−0.044 97	−0.026 60	−0.558 1	−0.433 0
III.K	$\alpha(Z\alpha)^5$	Recoil with eVP$^{(1)}$	0.000 14(14)	0.000 09(9)	0.004 9(49)	0.003 9(39)
III.L	$Z^2\alpha(Z\alpha)^4$	nSE$^{(1)}$	−0.009 92	−0.003 10	−0.084 0	−0.050 5
III.M	$\alpha^2(Z\alpha)^4$	$\mu F_1^{(2)}$, $\mu F_2^{(2)}$, μVP$^{(2)}$	−0.001 58	−0.001 84	−0.031 1	−0.031 9
III.N	$(Z\alpha)^6$	Pure recoil	0.000 09	0.000 04	0.001 9	0.001 4
III.O	$\alpha(Z\alpha)^5$	Radiative recoil	0.000 22	0.000 13	0.002 9	0.002 3
III.P	$\alpha(Z\alpha)^4$	hVP	0.011 36(27)	0.013 28(32)	0.224 1(53)	0.230 3(54)
III.Q	$\alpha^2(Z\alpha)^4$	hVP with eVP$^{(1)}$	0.000 09	0.000 10	0.002 6(1)	0.002 7(1)

[Pachucki et al. Review of Modern Physics (2024)]

Finite size nuclear contributions

Finite nuclear size contribution

- Correction to account for non-point like nucleus
  - Similar approach as pure QED contributions
  - Multipole expansion of charge distribution
  - ➡ Main contributions $\propto r_c^2$

- Beyond charge radius contributions
  - In principle higher order terms leads to multipoles of ρ
  - Experiments not precise enough for now
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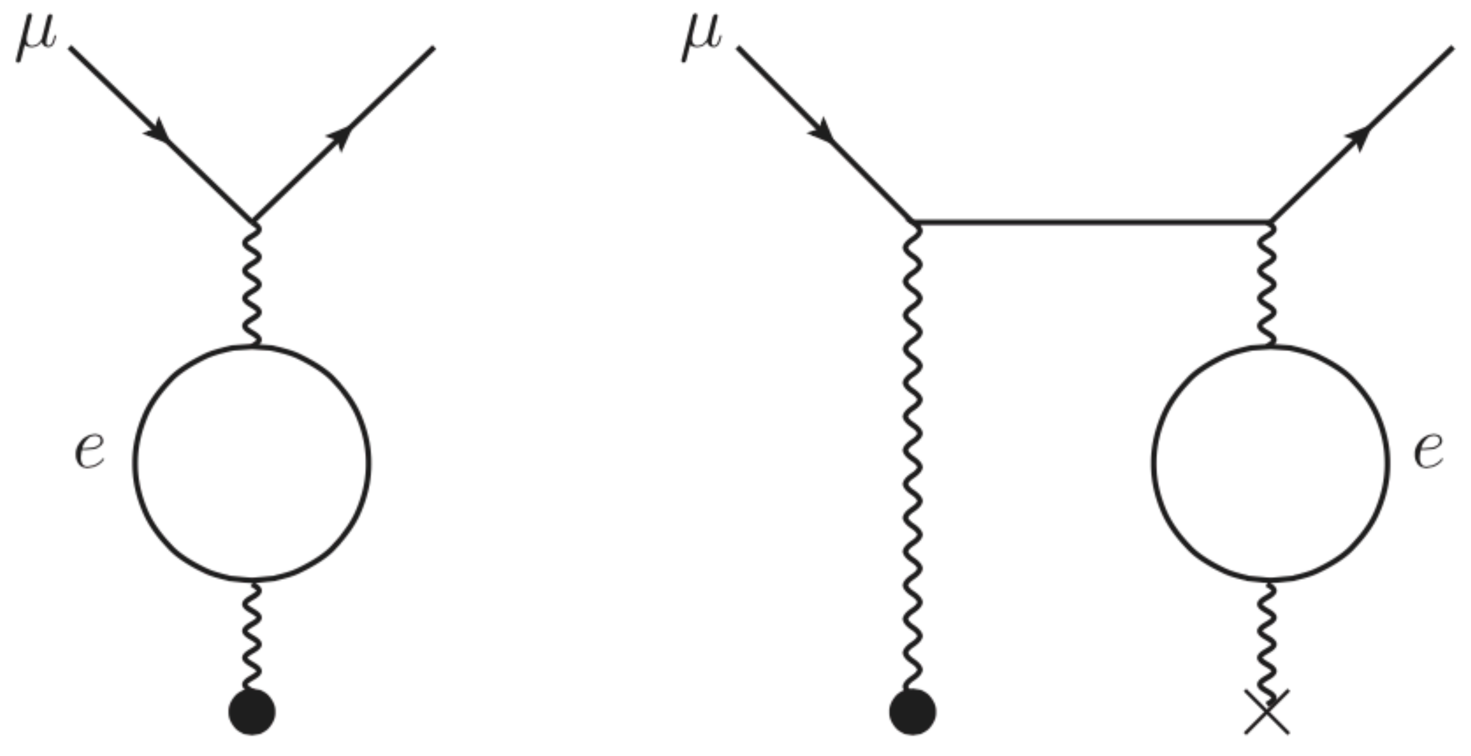

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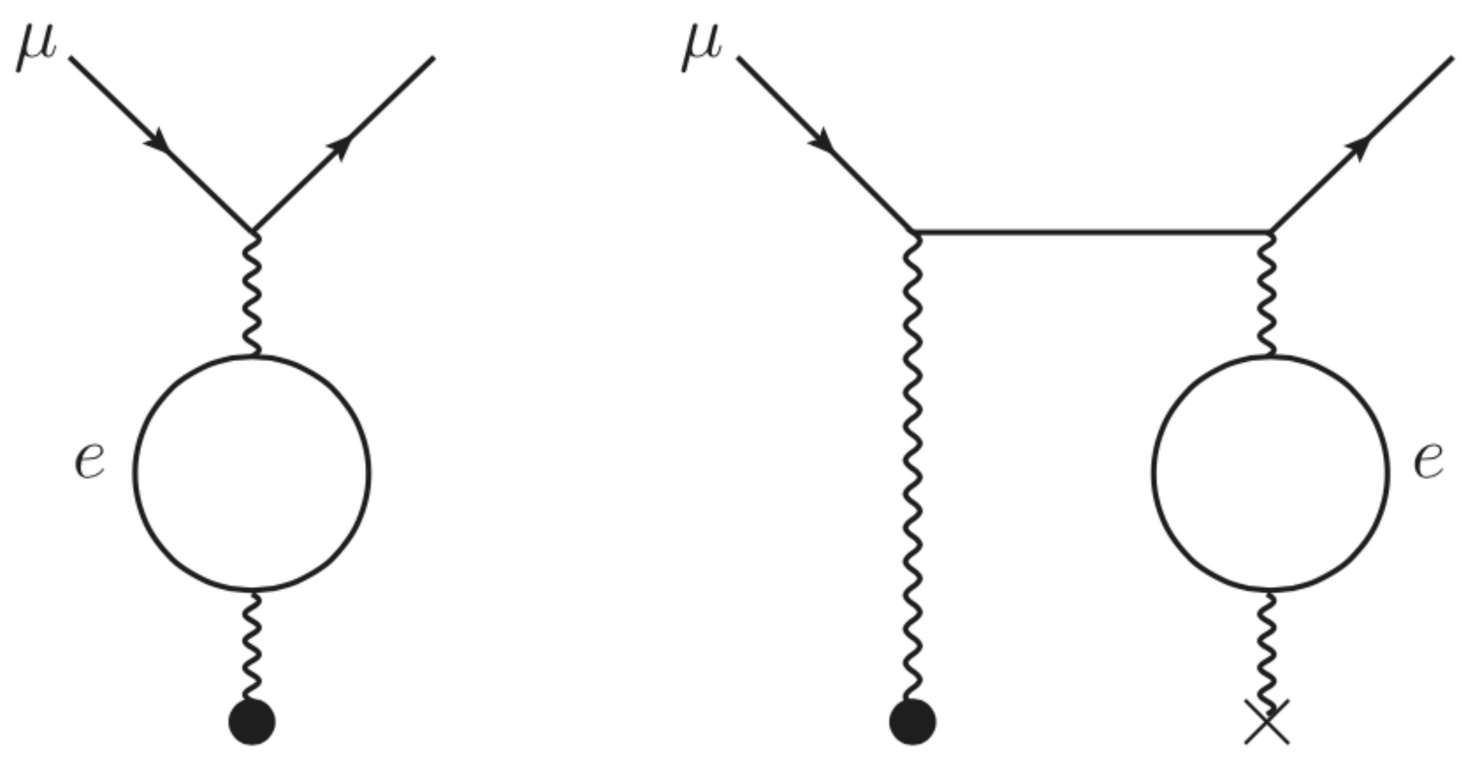

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Section	Order	Correction	μH	μD	μ^3He$^+$	μ^4He$^+$
IV.A	$(Z\alpha)^4$	r_C^2	$-5.197\,5r_p^2$	$-6.073\,2r_d^2$	$-102.523r_h^2$	$-105.322r_\alpha^2$
IV.B	$\alpha(Z\alpha)^4$	eVP$^{(1)}$ with r_C^2	$-0.028\,2r_p^2$	$-0.034\,0r_d^2$	$-0.851r_h^2$	$-0.878r_\alpha^2$
IV.C	$\alpha^2(Z\alpha)^4$	eVP$^{(2)}$ with r_C^2	$-0.000\,2r_p^2$	$-0.000\,2r_d^2$	$-0.009(1)r_h^2$	$-0.009(1)r_\alpha^2$

Nuclear structure dependent corrections

Nuclear structure effects

- Corrections accounting for non static effects
  - Nucleus is no longer treated as an external potential
  - Main contribution from **two-photon exchange** δ_{TPE}
  - **Nuclear excited states** become necessary

➡ δ_{TPE} contributes at $(Z\alpha)^5$

- Beyond TPE
  - Further corrections three-, four-, ... photon exchange
  - Combinations with vacuum polarization, etc

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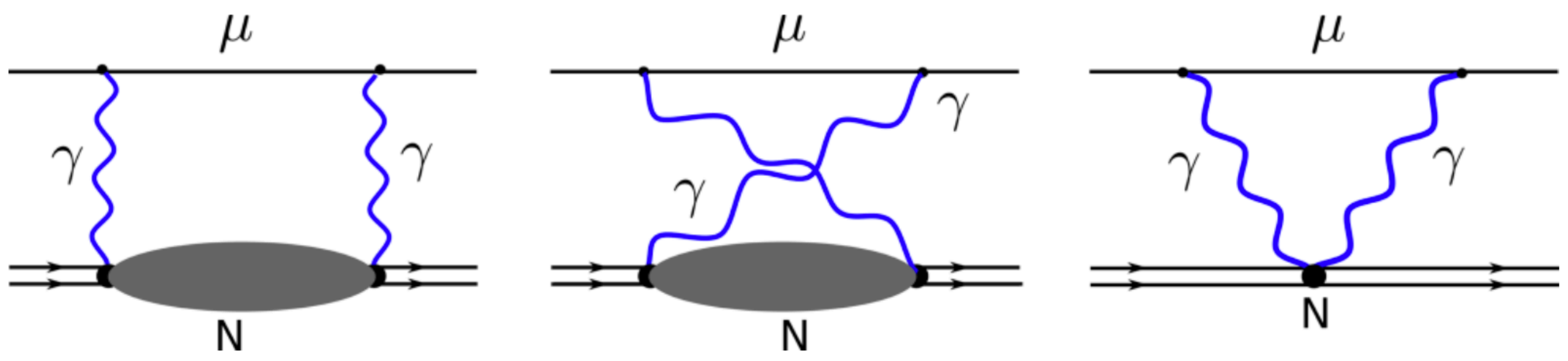
Two photon exchanges contributions



$$\boxed{\Delta E_{nl} = -\frac{(4\pi Z\alpha)}{m_r}\,|\,\phi_{nl}(0)\,|^2\,\mathrm{Im}\int \frac{\mathrm{d}^4 q}{(2\pi)^4} D^{\mu\rho}(q) D^{\nu\tau}(-q)\; t_{\mu\nu}(q,k)\; T_{\rho\tau}(q,-q)}$$

with:

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- $t_{\mu\nu} \equiv$ the lepton tensor
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- $k \equiv (m_r, 0)$

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See Vadim Lensky's talk for more details

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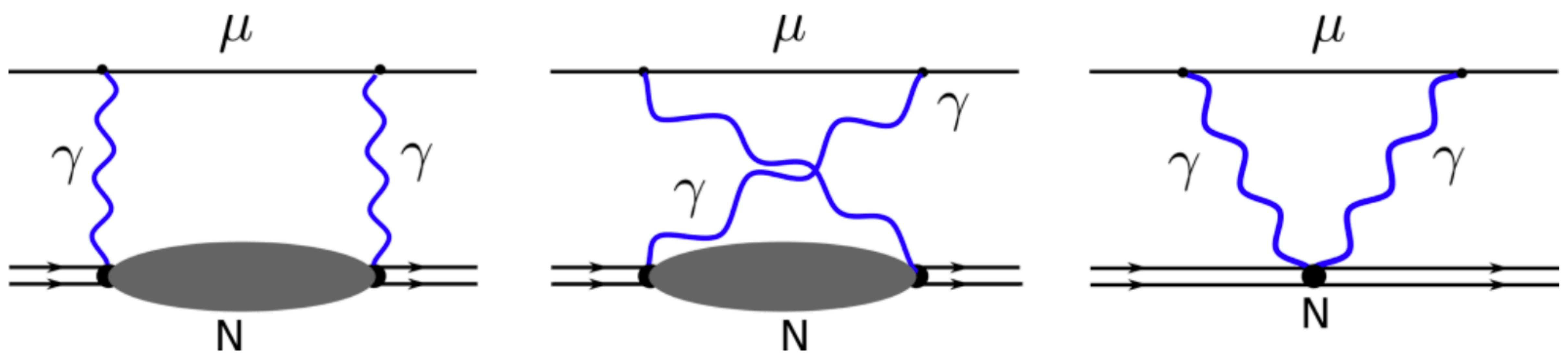

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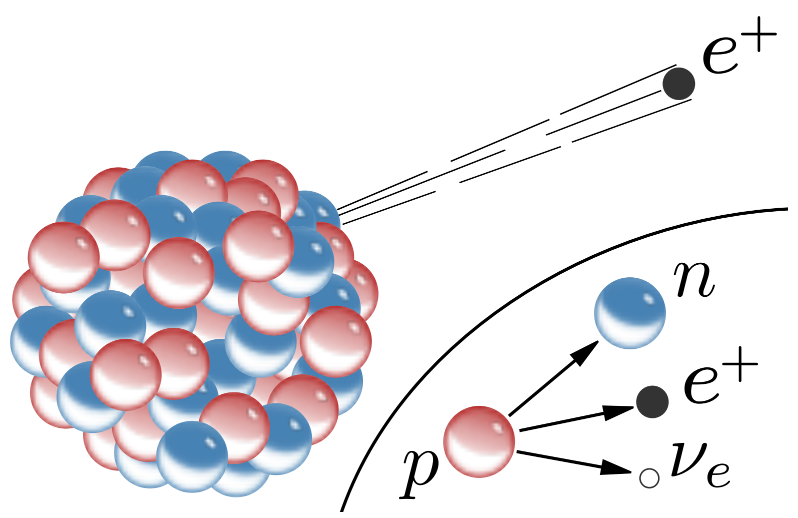
Intermezzo: successful application to β-decay

Superallowed β-decay



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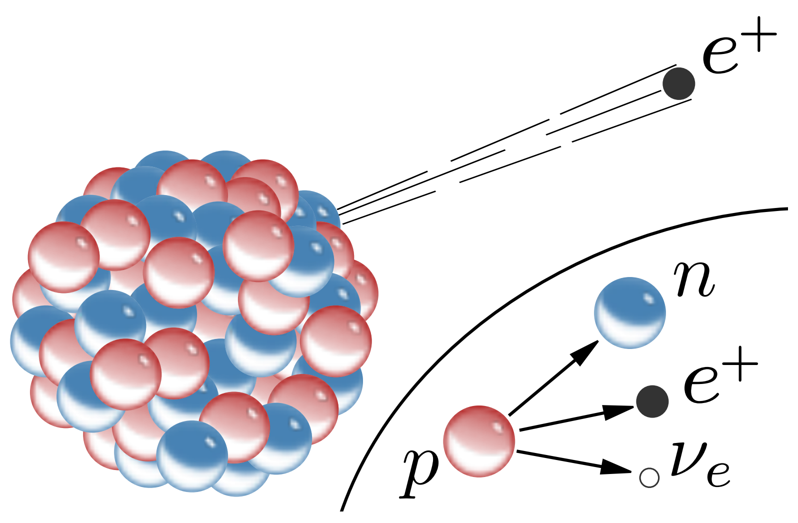

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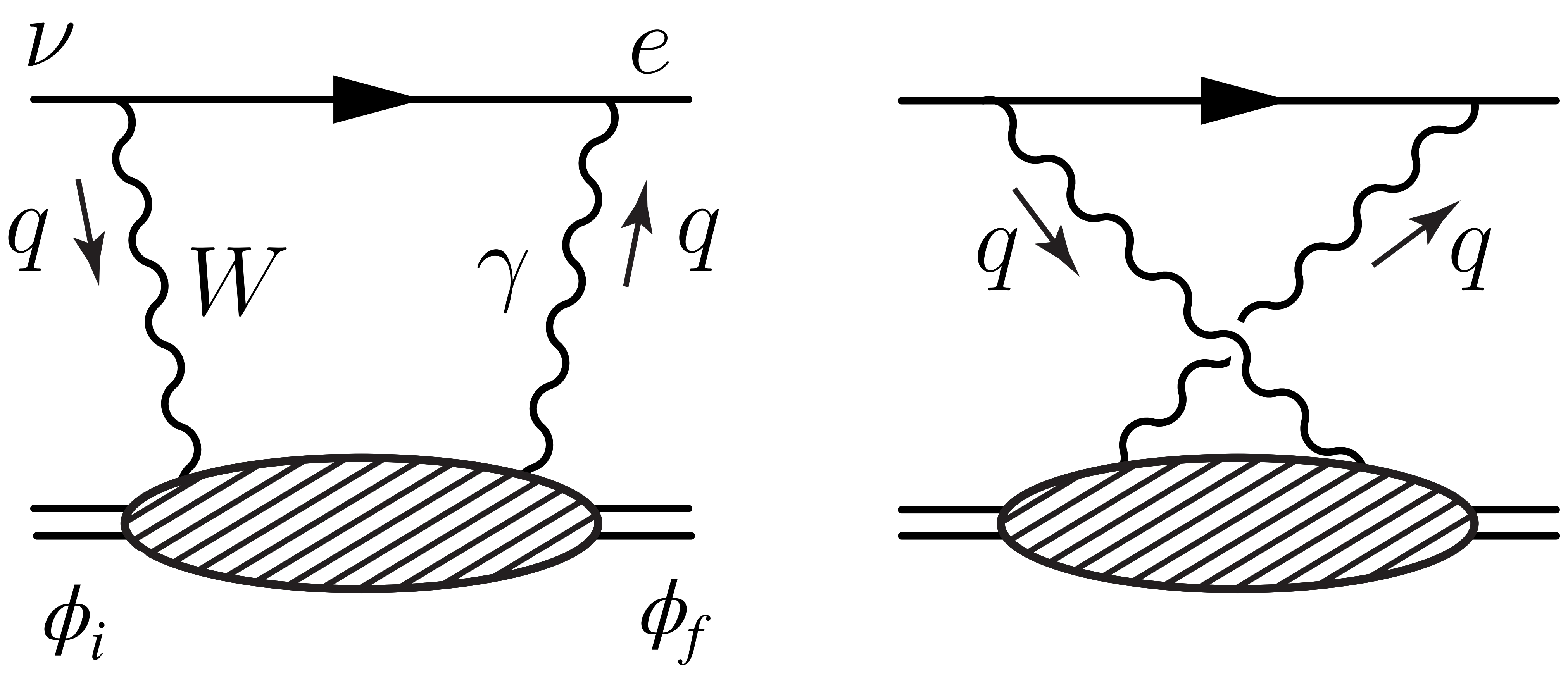

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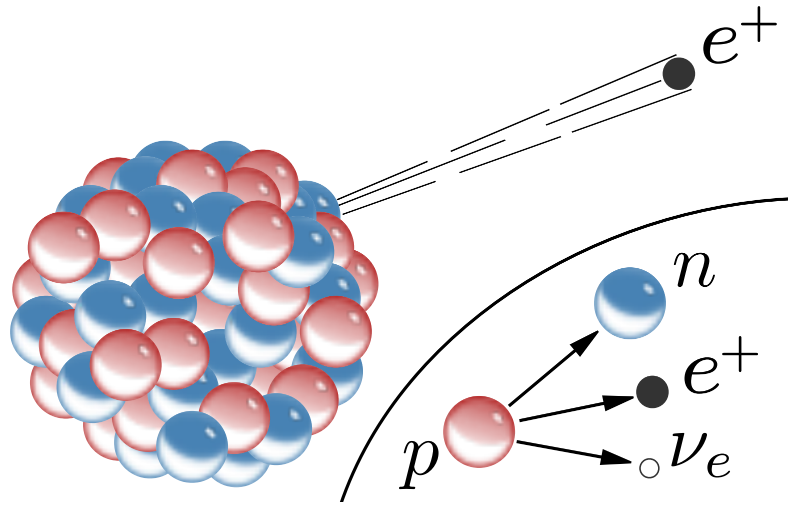

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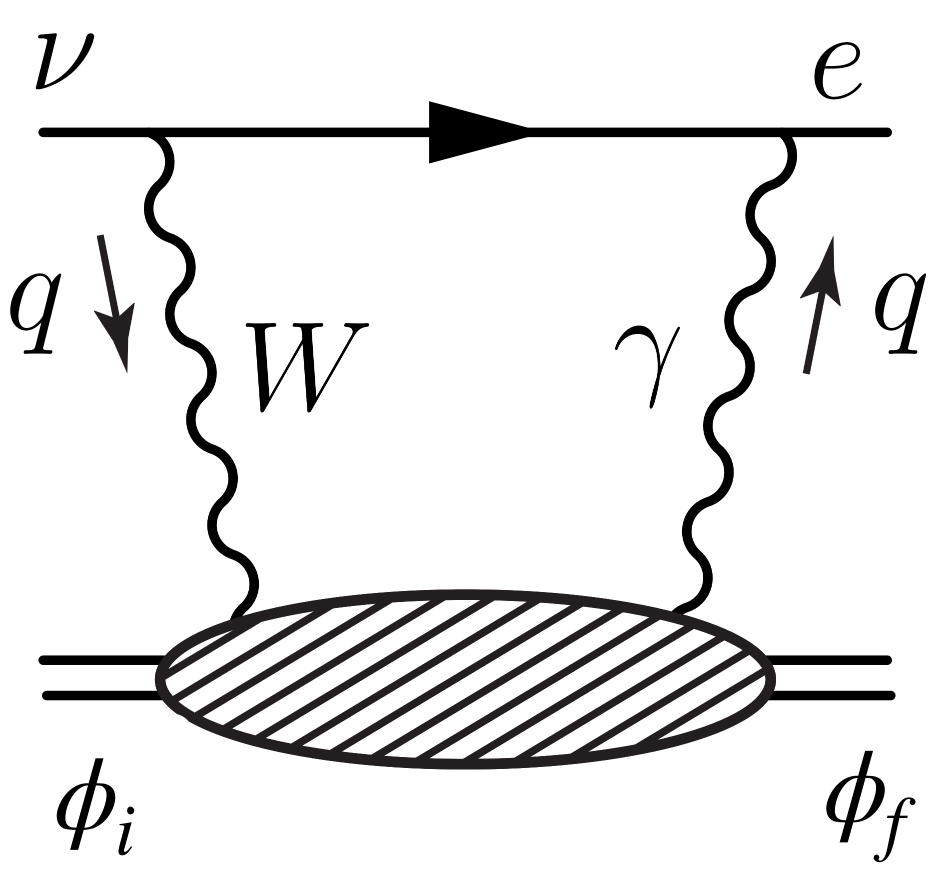

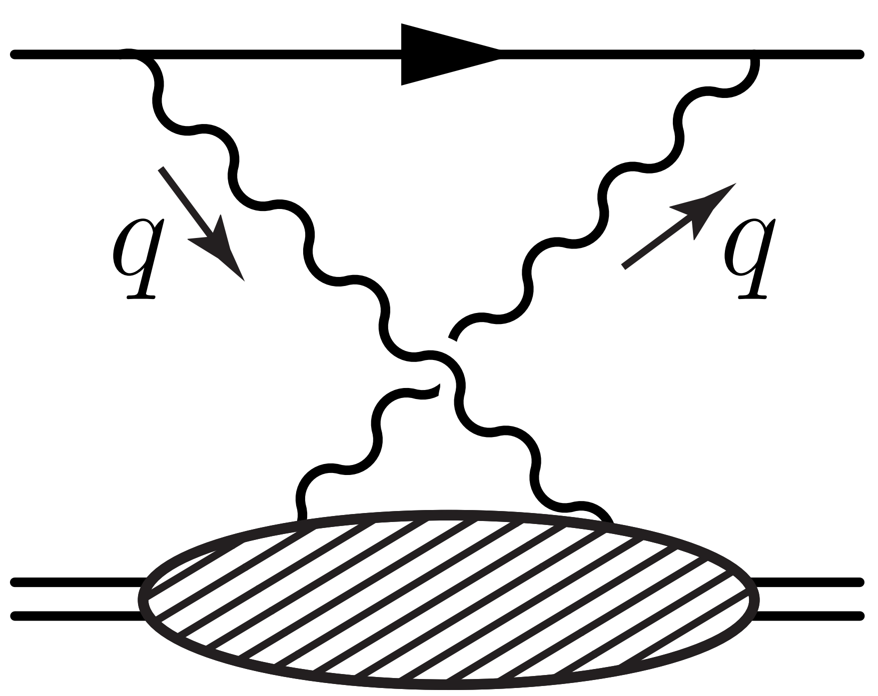

Box diagram expression

$$\Box^{\mathrm{nucl}}_{\gamma W}(E_e) = \frac{e^2}{M_F}\mathfrak{Re}\int \frac{d^4q}{(2\pi)^4}\frac{M_W^2}{M_W^2 - q^2}\frac{\left(Q^2 + M\nu\frac{p_e\cdot q}{p\cdot p_e}\right)T_3^{\mathrm{nucl}}(\nu,|\vec{q}\,|)}{[(p_e-q)^2 - m_e^2 + i\varepsilon](q^2+i\varepsilon)M\nu}$$

- M_F = Fermi matrix element ($=\sqrt{2}$ in the isospin limit)
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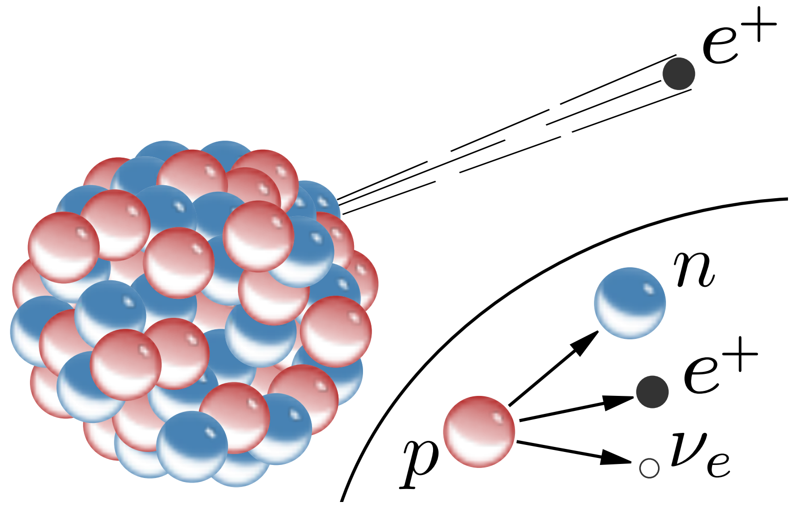

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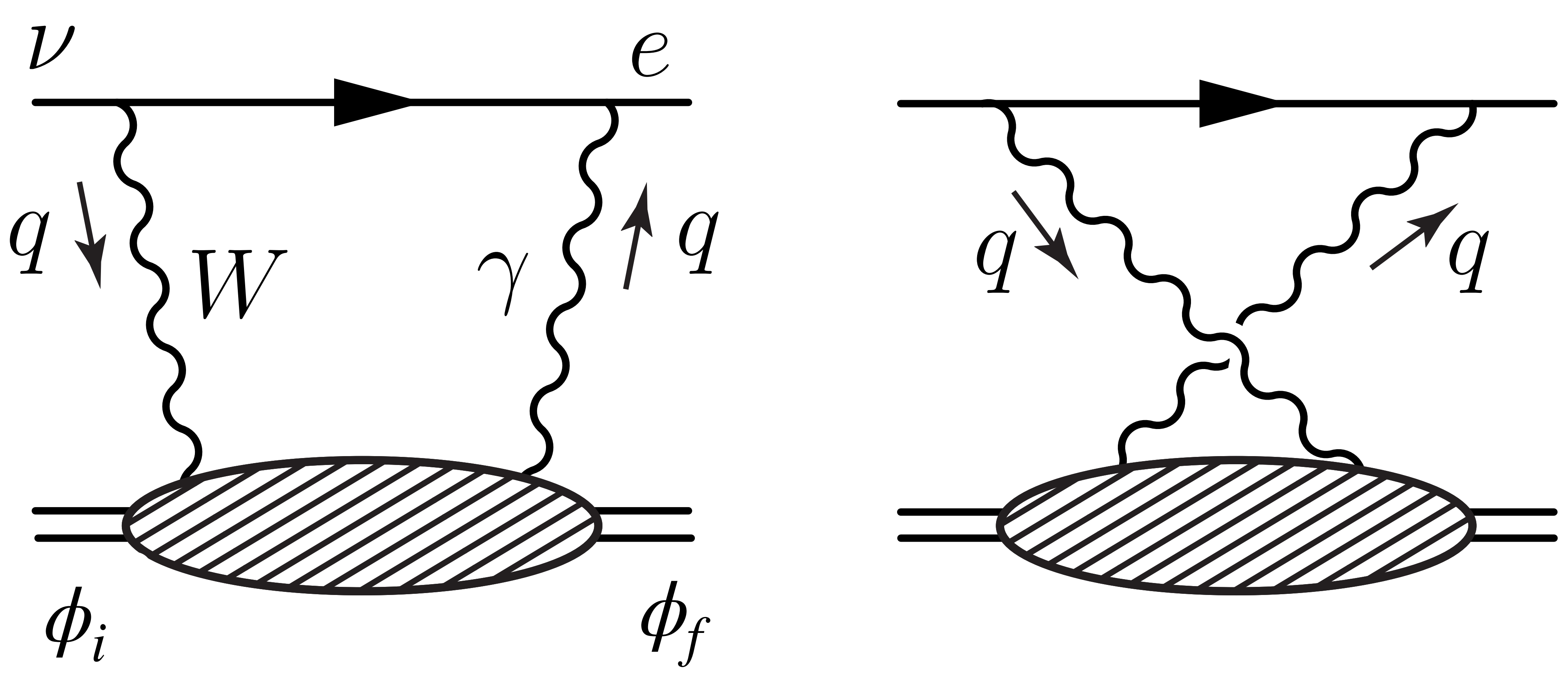

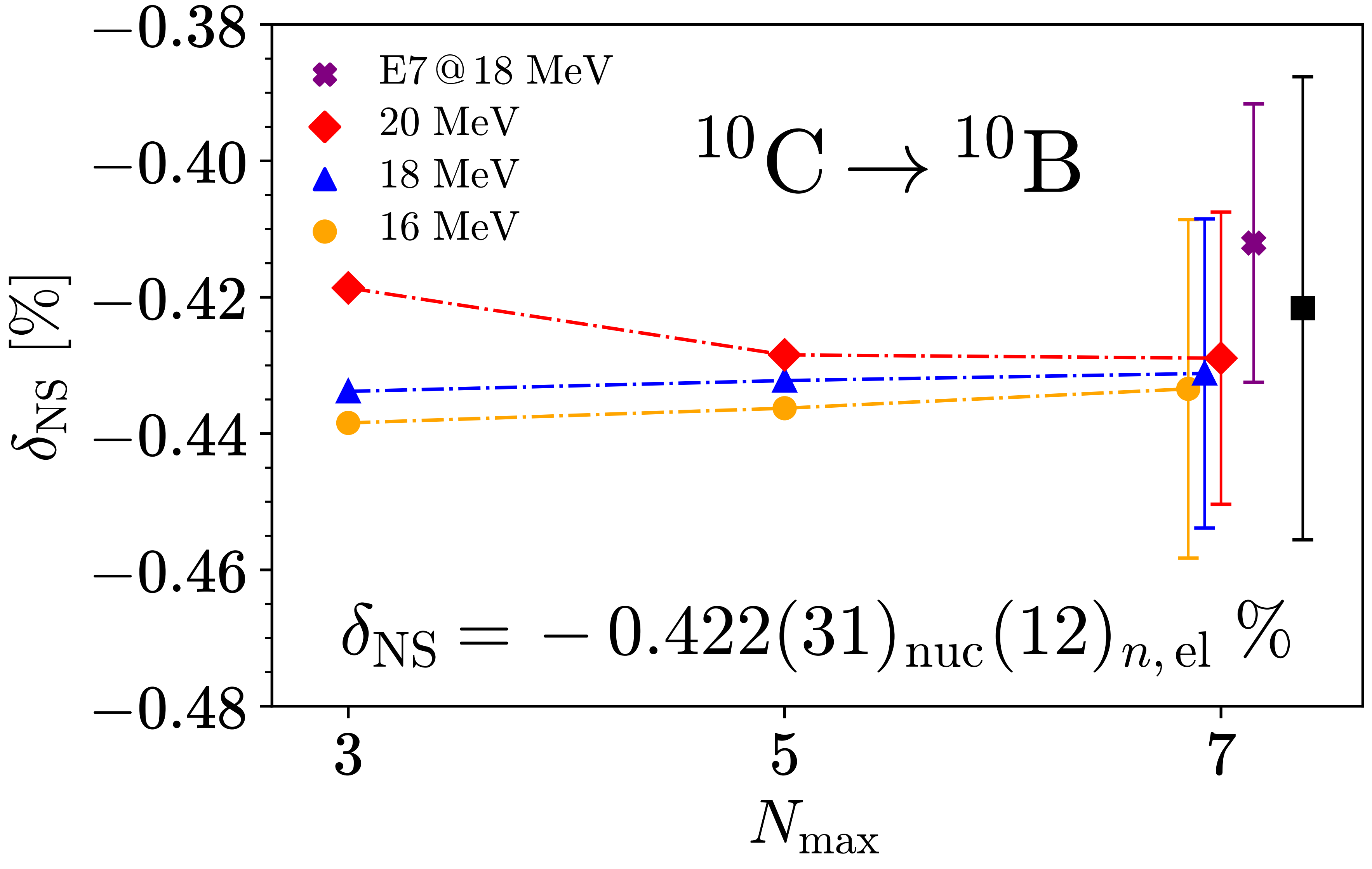

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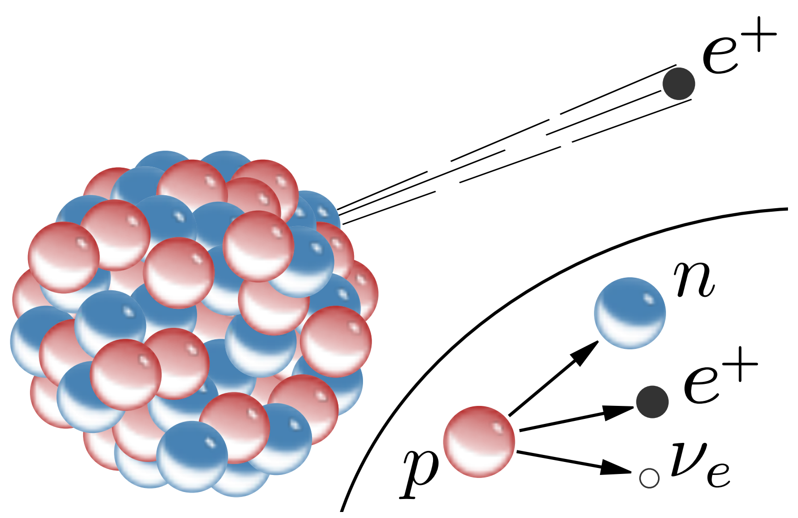

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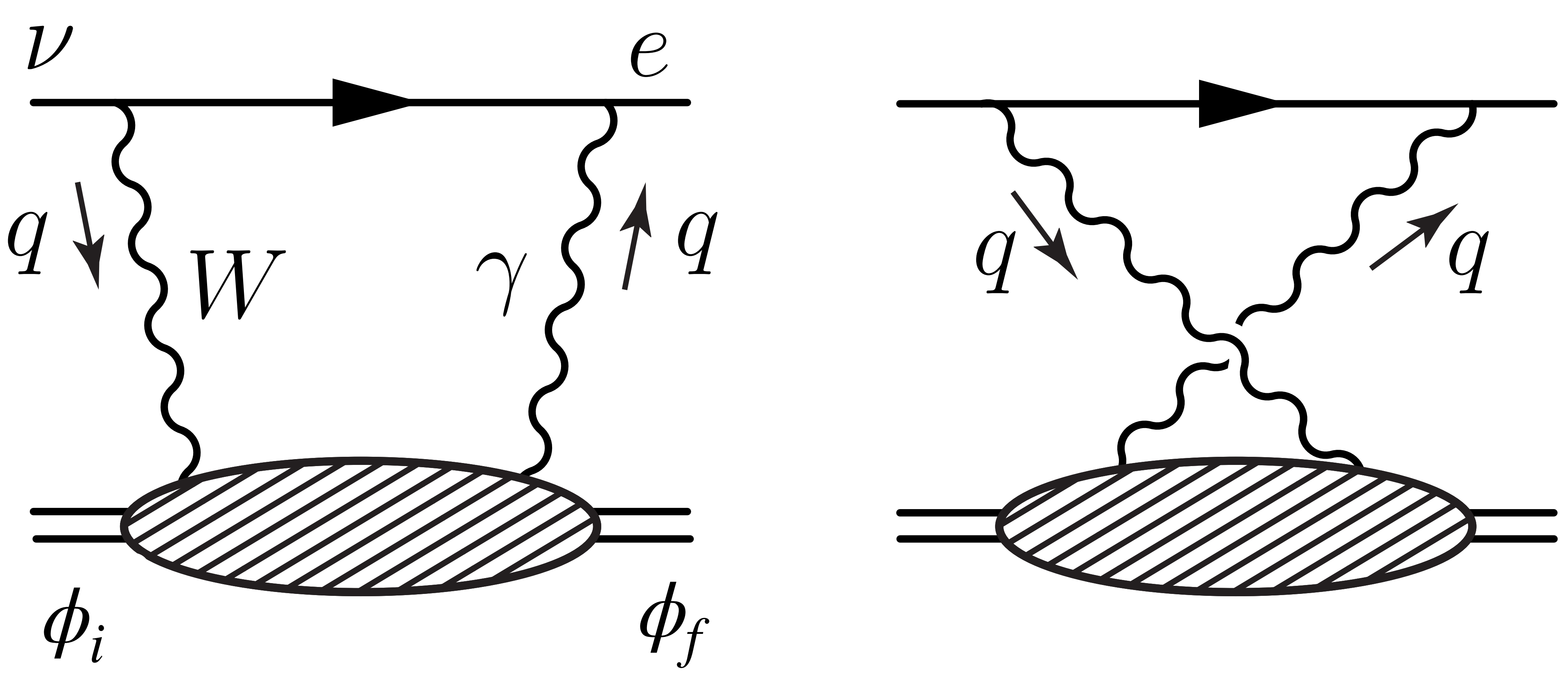

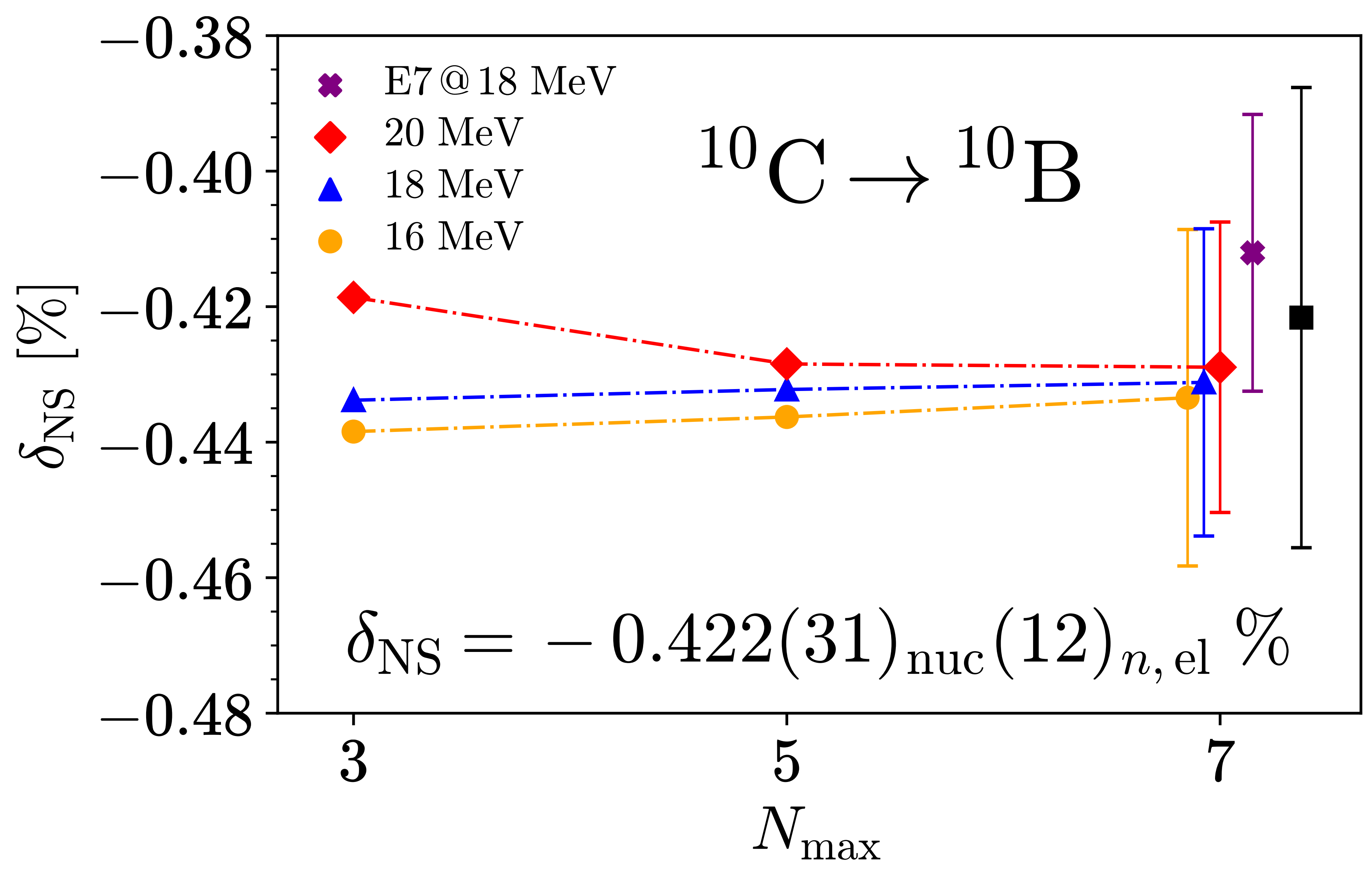

See Michael Gennari's poster for more details !

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Outline

- **Theoretical modeling**
  - Lamb-shift to atomic energy levels
  - Two-photon exchange corrections
- **Calculations for $^7\mathrm{Li}$**
  - No-Core Shell Model
  - Nuclear polarizability of $^7\mathrm{Li}$

Nuclear Compton Tensor

Pure electromagnetic part

- Leptonic tensor:
  - Wave-function approx: free muon propagator + $\phi_{1s}(0)$
  - ➡ **Decouple leptonic from nuclear part**

$$t_{\mu\nu}(q,k) = \frac{\frac{1}{4}\mathrm{Tr}\left[\gamma_\mu(\not{k} - \not{q} + m_r)\gamma_\nu(\not{k} + m_r)\right]}{(k-q)^2 - m_r^2 + i\epsilon}$$

- Photon propagator:
  - Use Coulomb gauge
  - ➡ **Decouple charge and transverse contributions**

$$D^{\mu\nu}(q) = \begin{pmatrix} \frac{1}{\vec{q}^{\,2}} & 0 \\ 0 & \frac{1}{q^2}\left(\delta_{ij} - \frac{q_i q_j}{\vec{q}^{\,2}}\right) \end{pmatrix}$$

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[Bernabeu et al, Nuclear Physics A (1974)]

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Decomposition of two-photon exchange

- Nucleon/Nucleus decomposition: (in the end use DR)

$$\boxed{\delta_{TPE} = (\delta^N_{el} + \delta^N_{pol}) + (\delta^A_{el} + \delta^A_{pol})}$$

Nuclear modeling

Model used of nuclear currents

- Multipole decomposition of nuclear currents
  [Donnelly, Haxton, Atomic and Nuclear Data Tables (1979)]
  - $M_{JM_J;TM_T}(q) \equiv \int d^3x\ \mathbf{M}_J^{M_J}(qx) J_0(x)_{TM_T}$
  - $T^E_{JM_J;TM_T}(q) \equiv \int d^3x \left[\frac{1}{q}\nabla \times \vec{\mathbf{M}}^{M_J}_{JJ}(qx)\right] . \vec{J}(x)_{TM_T}$
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➡ **Truncation at $J = 3$**

Nuclear modeling

Model used of nuclear currents

- Multipole decomposition of nuclear currents

  [Donnelly, Haxton, Atomic and Nuclear Data Tables (1979)]

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- Electromagnetic current modeling
  - Decomposed within the seven operator basis
  - Form factors given by the isovector dipole model
  - $f_{SN}(q) = \left(1 + \frac{q^2}{M_V^2}\right)^{-2}$, $F^{(T)}_{1,2}(q) = F^{(T)}_{1,2}(0)\, f_{SN}(q)$

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Model used of nuclear many-body state

- Ab initio nuclear interaction [Entem et al. (2017)] [Somà et al. (2020)]
  - Two chiral interactions considered
  - N4LO-E7 and N3LO

  ➡ **Estimate interaction uncertainty**

- Model space
  - Harmonic oscillator Slater determinant
  - Vary $\hbar\Omega$ and $N_{\max}$

  ➡ **Estimate model space uncertainty**

- Many-body approximation
  - No-Core Shell Model
  - More details in next section

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Need expression of δ^A_{pol} in terms of multipole currents !

Master formula

Inputs to evaluate nuclear polarizability

- Charge spectral function

$$S_{C,J}(\omega, q) \equiv \sum_{N \neq 0} |\langle N | M_{J0}(q) | \Psi \rangle|^2 \delta(E_N - E_0 - \omega)$$

- Transverse electric spectral function

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[Rosenfelder Nuclear Physics A (1983)]

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$$K_C(\omega,q) = \frac{1}{E_q}\left[\frac{1}{(E_q - m_r)(\omega + E_q - m_r)} - \frac{1}{(E_q + m_r)(\omega + E_q + m_r)}\right]$$

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Non-relativistic reduction

- Limit: $q \ll m_r$

➡ Only **charge** kernel remains ⇒ simpler + consistency check

$$K_C(\omega,q) \to K_{NR}(\omega,q) = \frac{1}{q^2\left(\frac{q^2}{2m_r}+\omega\right)}$$

$$K_L(\omega,q) \to 0$$

$$K_S(\omega,q) \to 0$$

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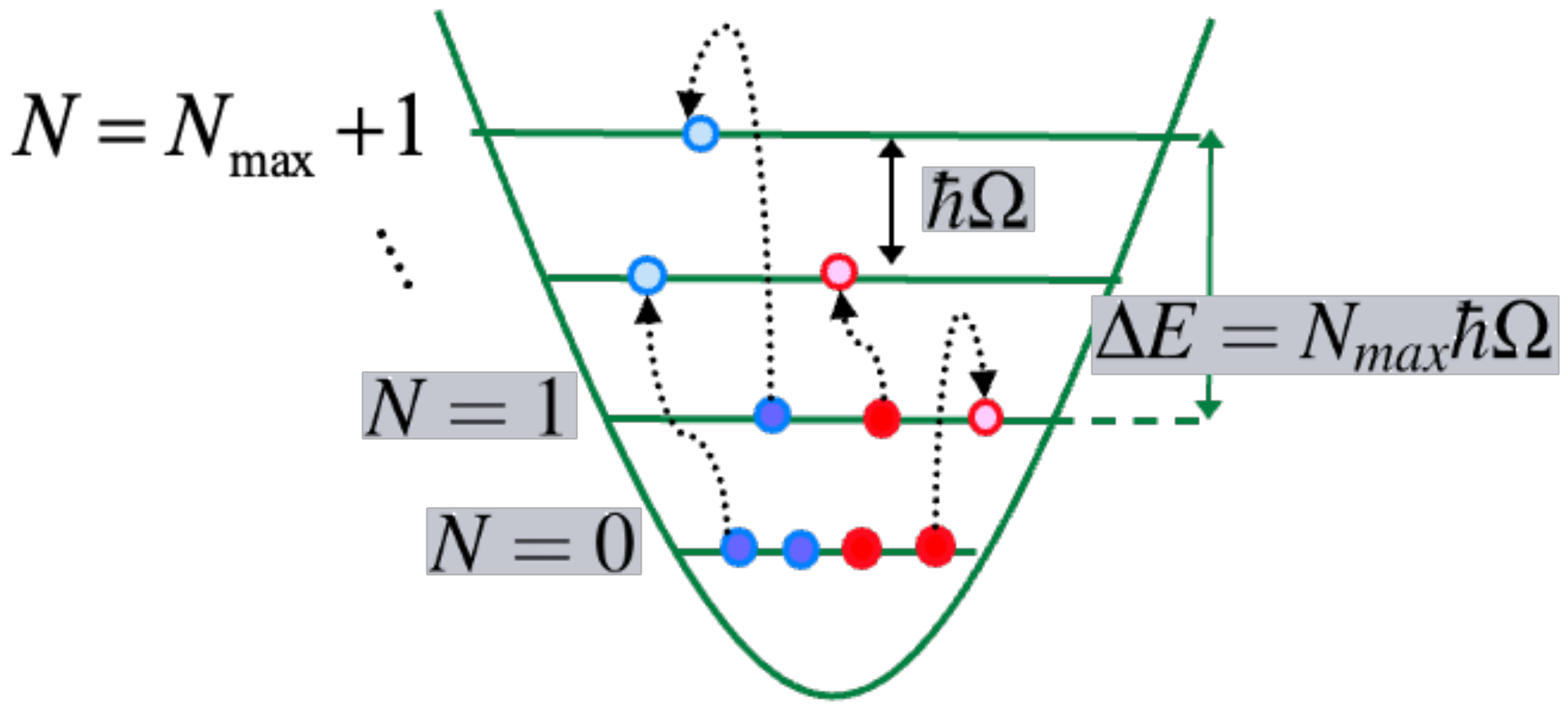
Outline

- **Theoretical modeling**
  - Lamb-shift to atomic energy levels
  - Two-photon exchange corrections
- **Calculations for $^{7}\mathrm{Li}$**
  - No-Core Shell Model
  - Nuclear polarizability of $^{7}\mathrm{Li}$

The No-Core Shell Model

Anti-symmetrized products of
many-body HO states



The No-Core Shell Model

Lanczos tridiagonalization algorithm [Lanczos (1950)]

- Initialization: normalized pivot $|\phi_1\rangle$
- Recursion: α_i, β_i and $|\phi_i\rangle$
  - $\beta_{i+1}|\phi_{i+1}\rangle = H|\phi_i\rangle - \alpha_i|\phi_i\rangle - \beta_i|\phi_{i-1}\rangle$
  - $\alpha_i = \langle\phi_i|H|\phi_i\rangle$ and β_{i+1} st $\langle\phi_{i+1}|\phi_{i+1}\rangle = 1$

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- Output:
  - Lanczos basis and coefficients $\{|\phi_i\rangle, \alpha_i, \beta_i\}$ → H **in Lanczos basis**
  - Lanczos basis ≡ orthonormal basis in Krylov space $\left\{|\phi_1\rangle, H|\phi_1\rangle, \ldots, H^{N_L}|\phi_1\rangle\right\}$

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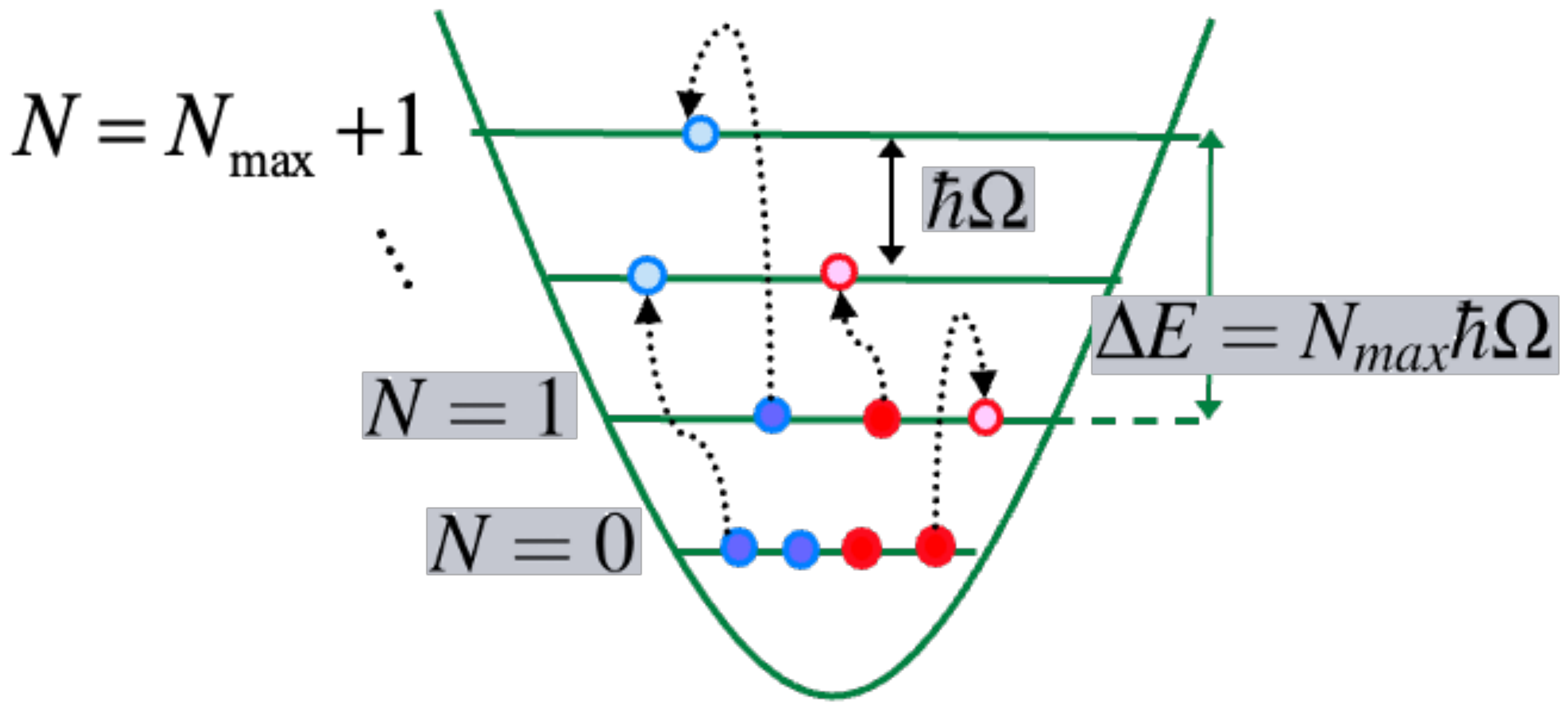

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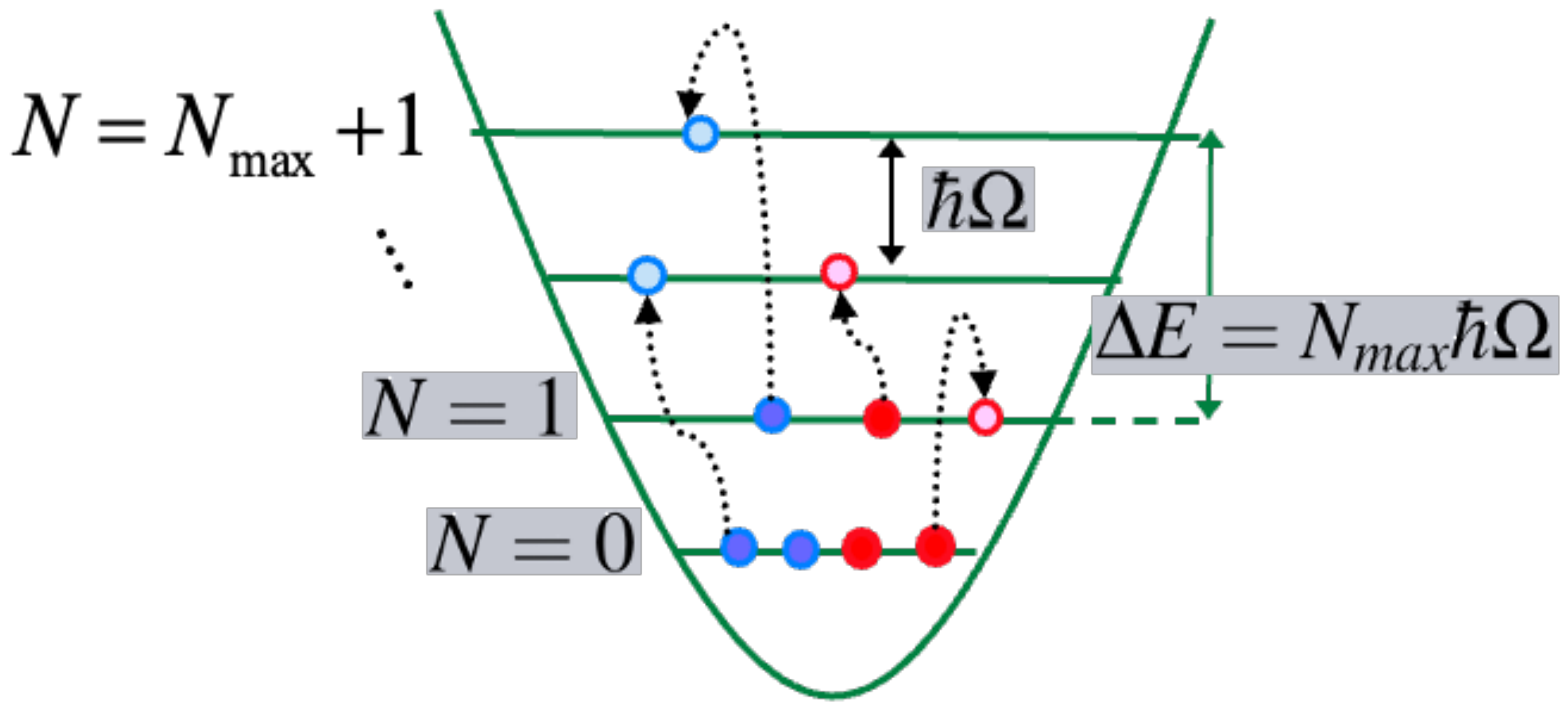

Application to nuclear structure

- Efficient calculation of spectra
  - Selection rules sparsity ⇒ **Fast matrix-vector multiplication**
  - In practice: $N_L \sim 100 - 200$ is sufficient to converge low-lying states
  - Cost of diagonalization of the tridiagonal matrix is negligible

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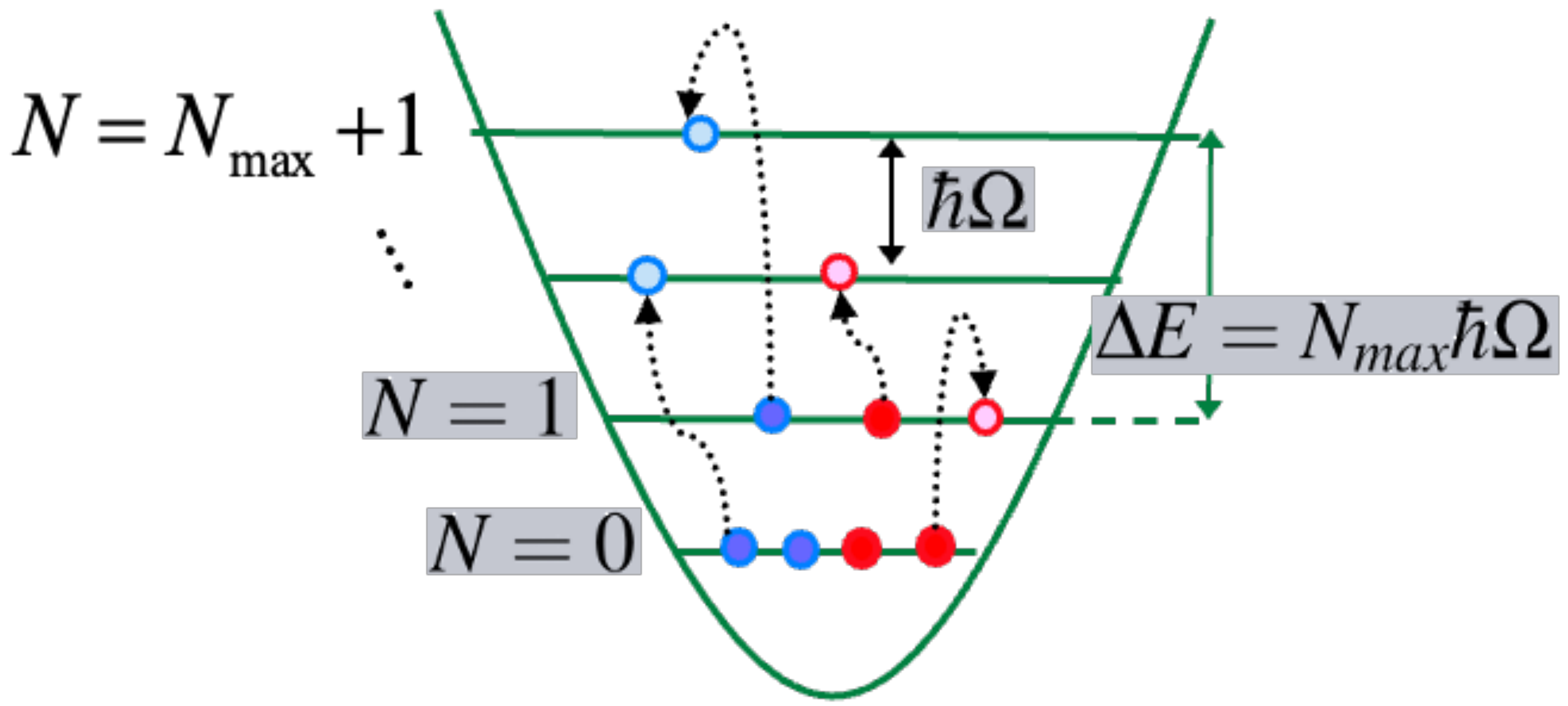

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Application to $^7\mathrm{Li}$

- Parameters of many-body calculation
  - $N_L = 200$ for $N_{max} = 1$ to 9
- Results
  - Ground-state of $^7\mathrm{Li}$ $|\Psi\rangle$ ⇒ **Starting point for δ^A_{pol}**

The Lanczos strength algorithm

Strength functions

- We need to compute
  - Eigenvalues: $E_N \Rightarrow$ obtained already with Lanczos
  - Overlaps: $|\langle N|O|\Psi\rangle|^2$ for each eigenstate and operator $\Rightarrow$ **expansive**
- Lanczos strength algorithm
  - Variant of Lanczos: extract only **relevant information**

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- For each operator O
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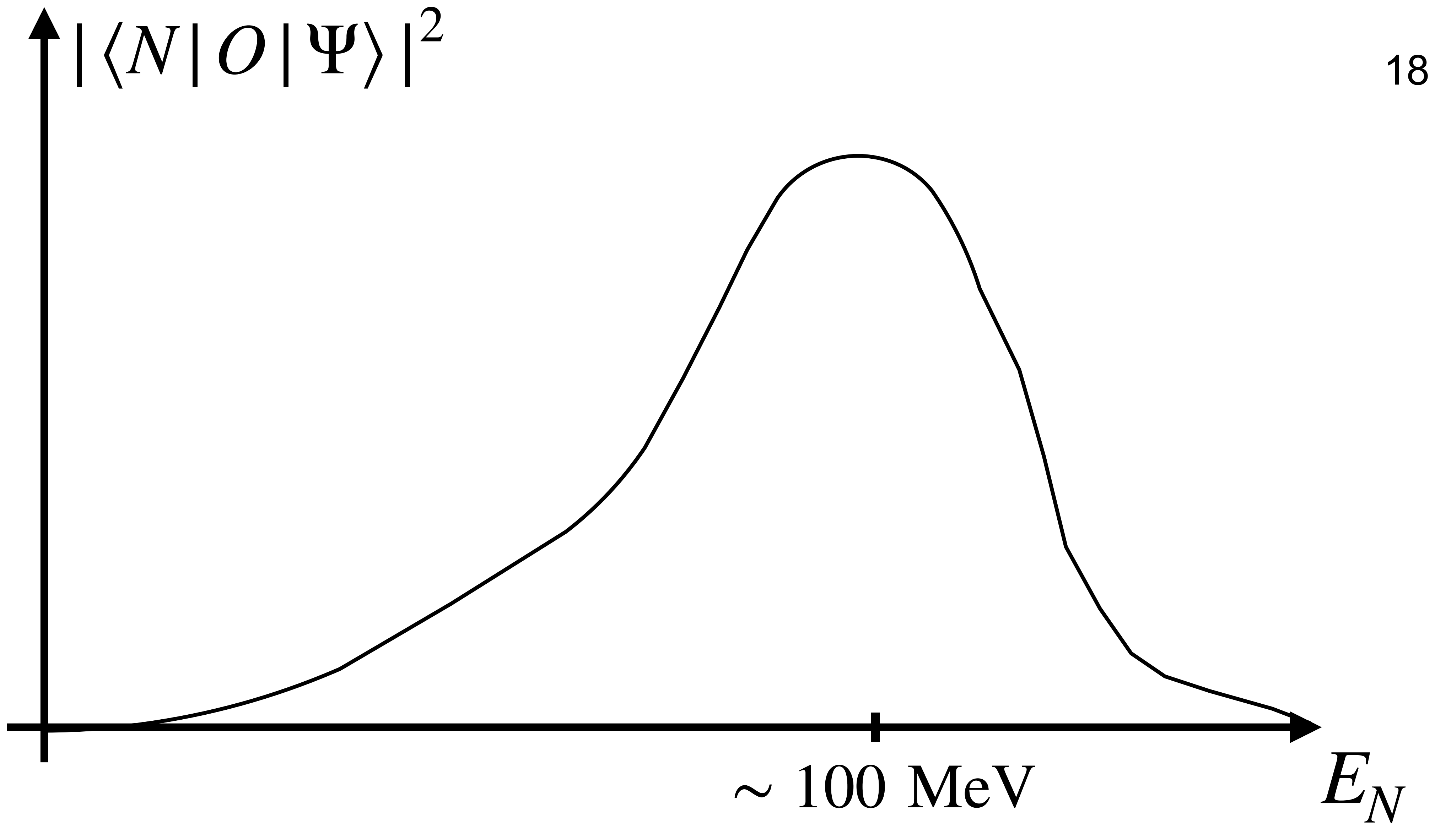

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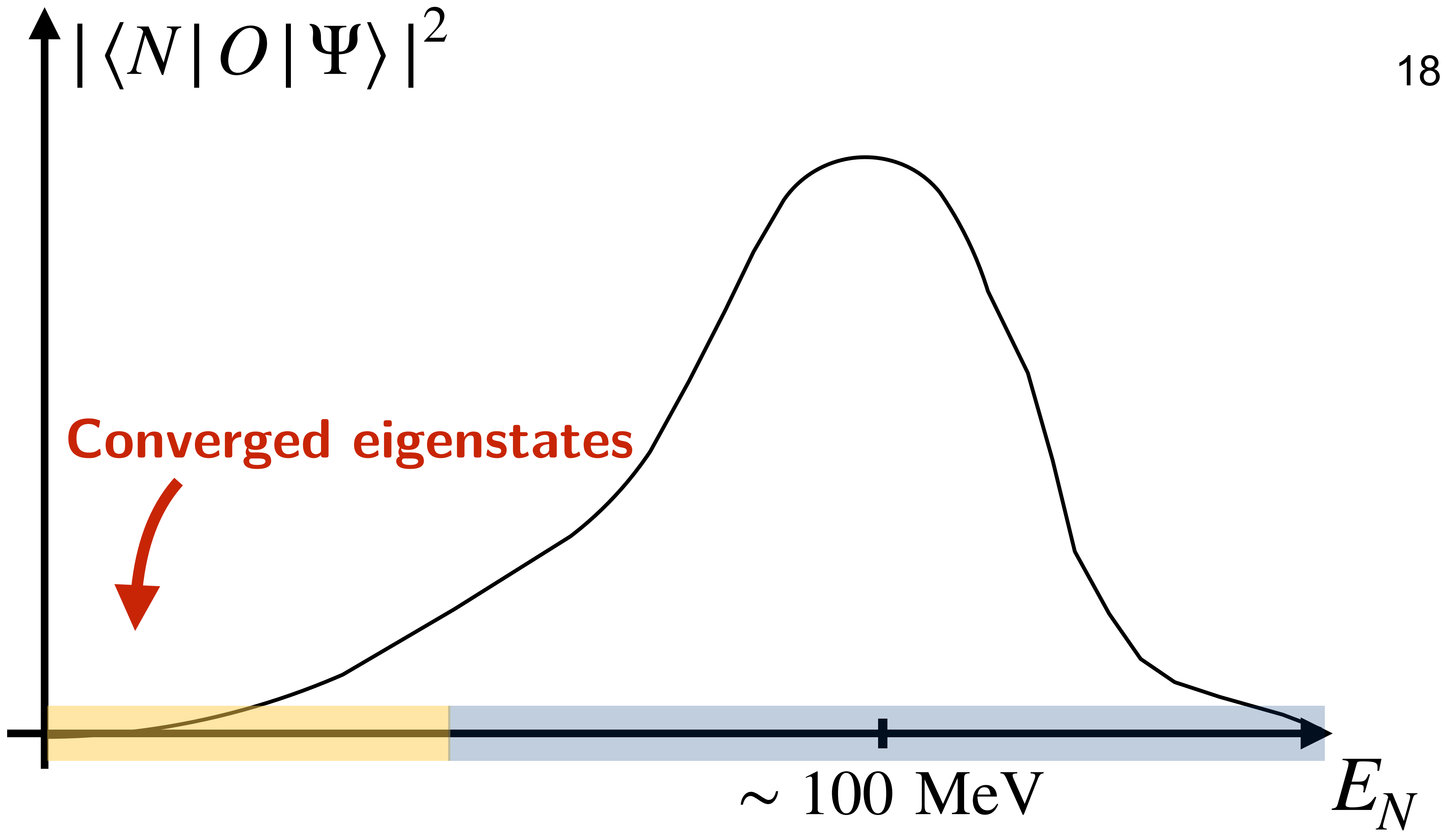

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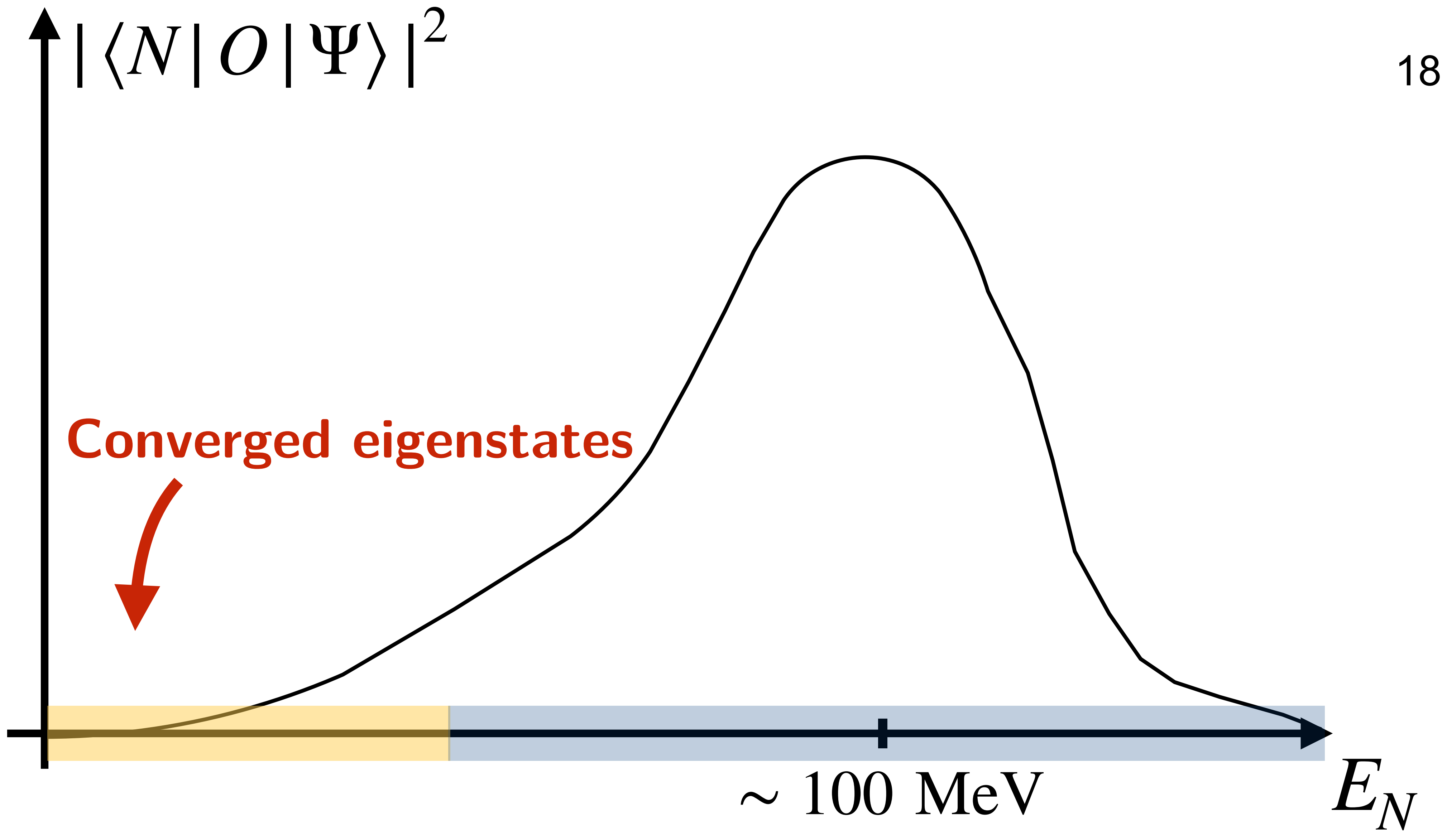

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  - Often the **strength is fragmented**
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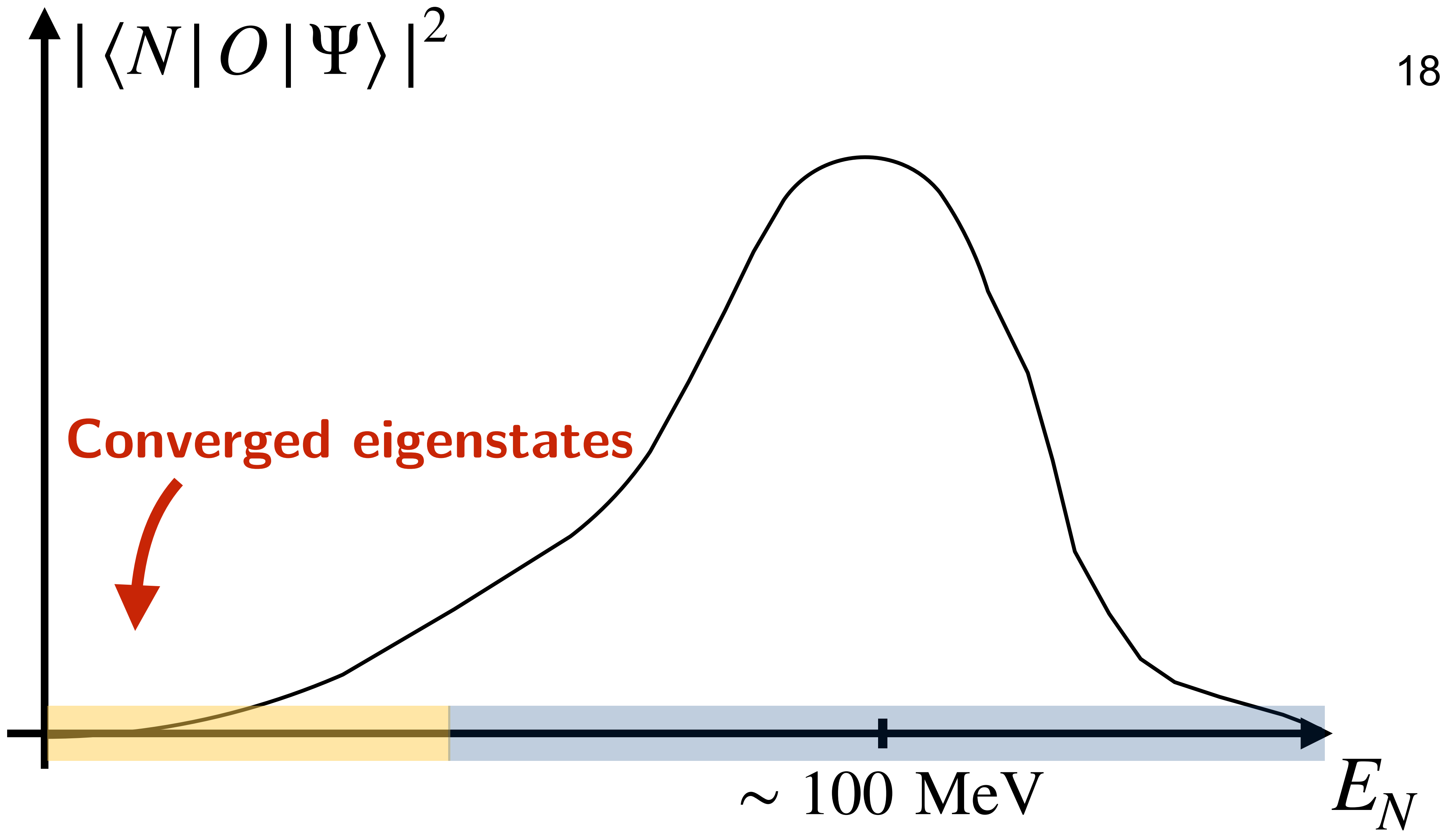

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Sum rules convergence

- Convergence problem
  - Often the **strength is fragmented**
  - Only low-lying states converged in general
- Lanczos strength algorithm
  - Recover exactly $\int \mathrm{d}\omega\ S_O(\omega)\ \omega^n$ for any $n \leq 2N_L$

➡ **Fast convergence of** $\int \mathrm{d}\omega\ f(\omega) S_O(\omega)$ (if f $\sim P_{100}(\omega)$)

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  - Nuclear polarizability of $^7\mathrm{Li}$

Testing convergence of sum rules for δ^A_{pol}

First tests of sum rule convergence

- Before running expansive $q-$dependent
  - Test convergence of strength integrals
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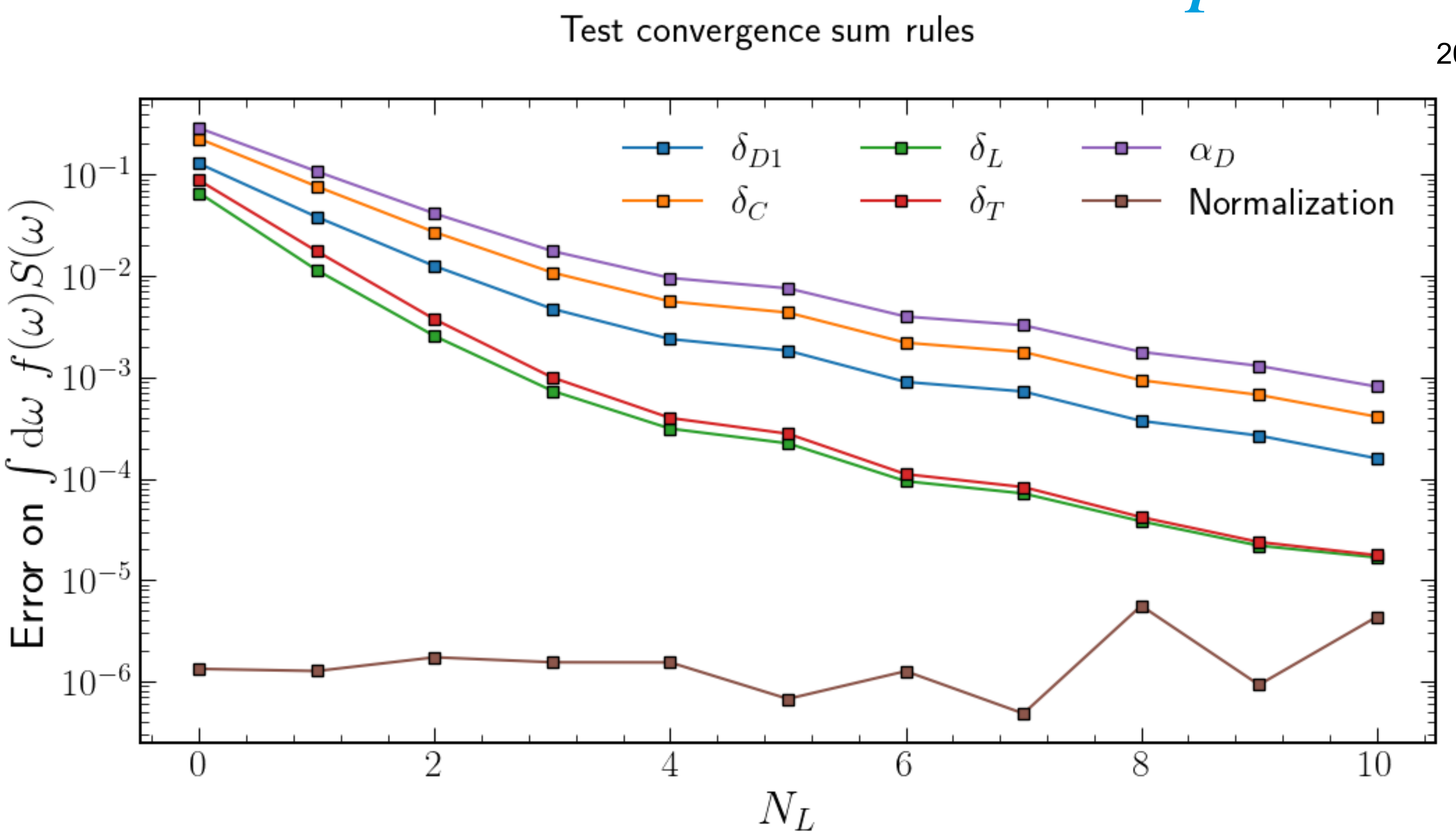

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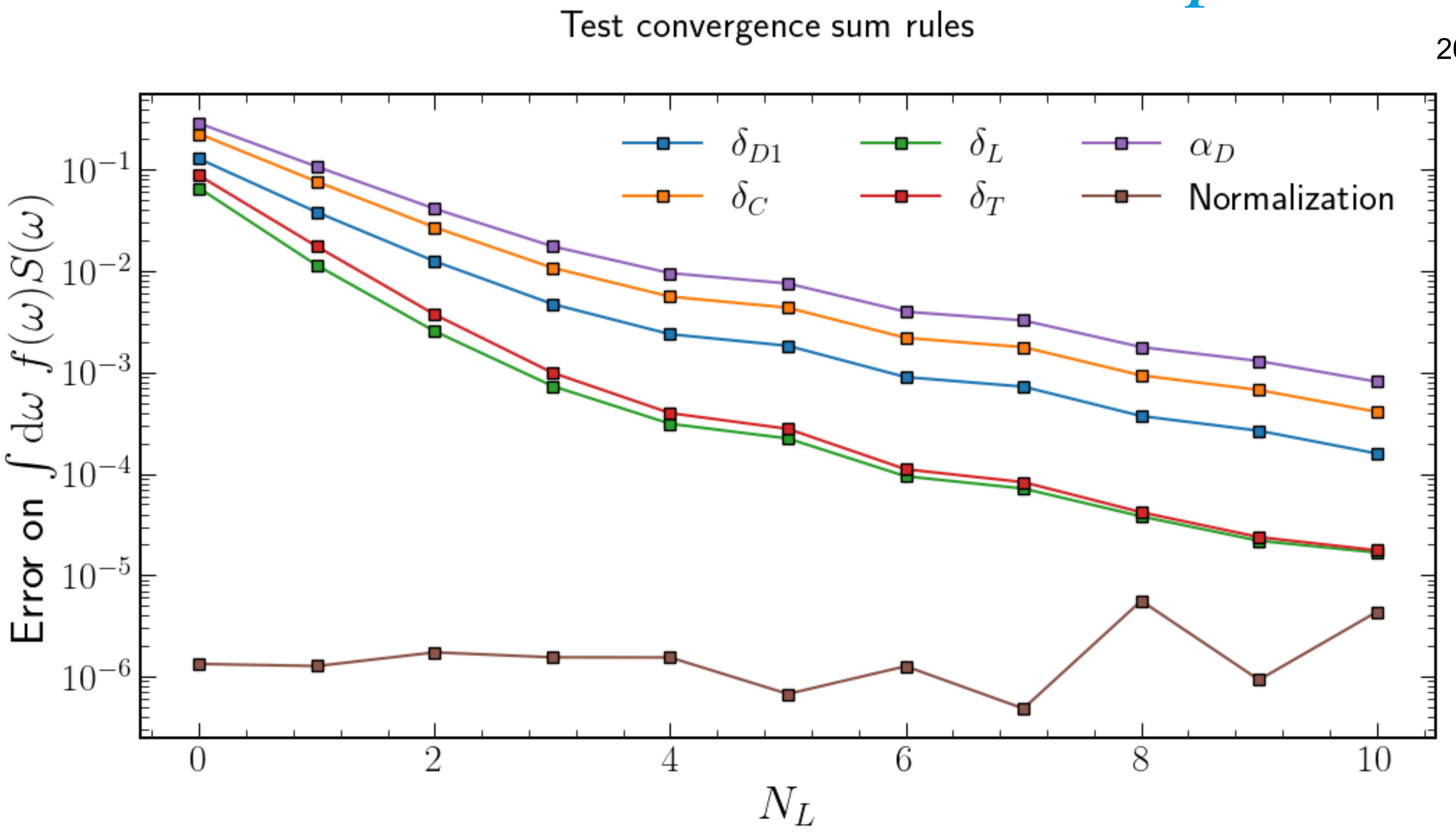
- Observations
  - Sum rules converge quickly $\Rightarrow N_L = 50$ is sufficient
  - Reaches plateau around $\sim 10^{-5}$ relative error



Testing convergence of sum rules for δ_{pol}^{A}

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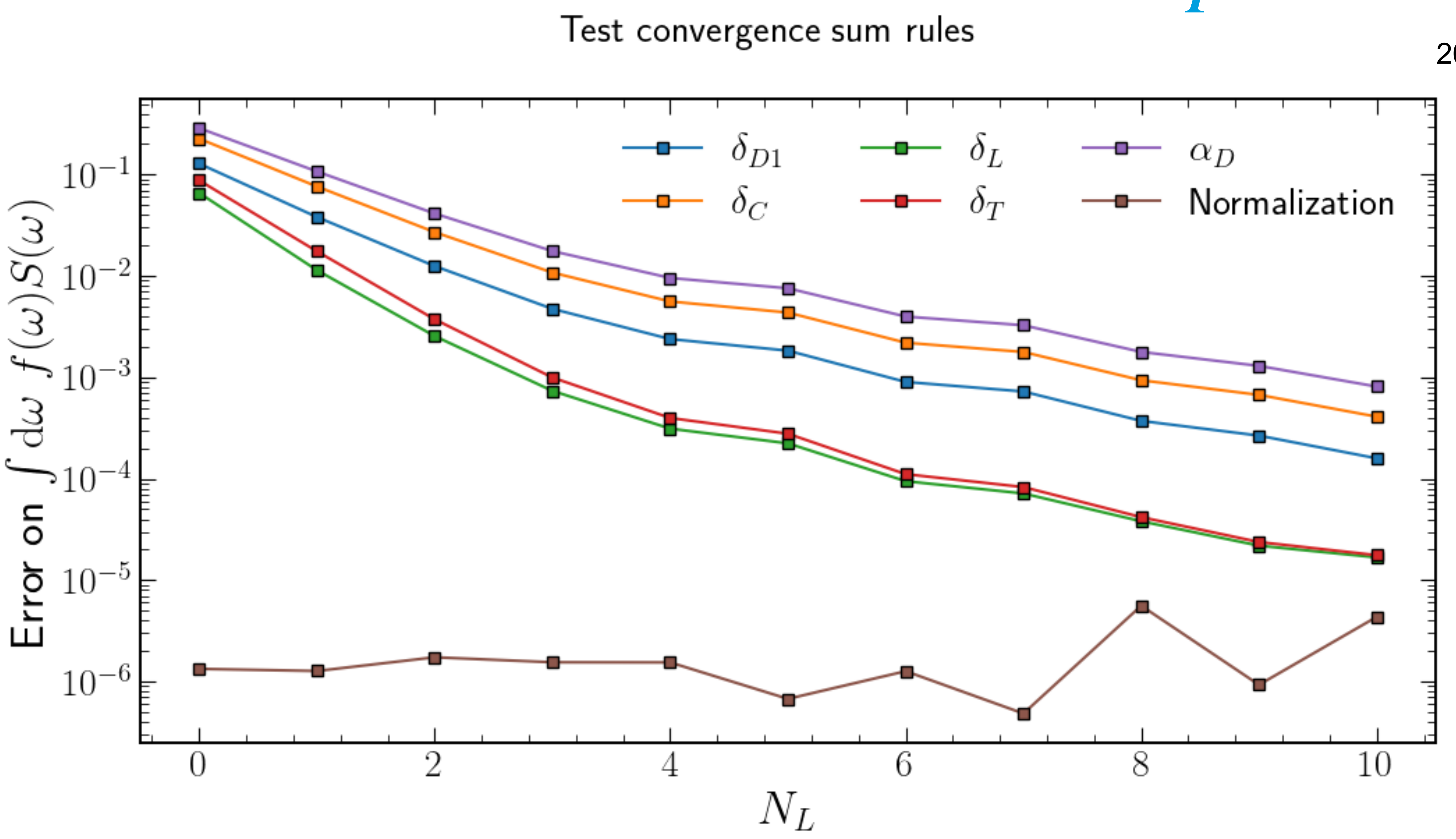

First conclusion: numerical noise from Lanczos algo is negligible

Next step: q-dependent calculations of δ_{pol}^{A} !

A first test case for N4LO-E7 and $N_{\max} = 7$

Numerical calculations

- $q_{\max} = 700$ MeV and $\Delta q = 10$ MeV
- 10 different operators for $J_{\max} = 3$

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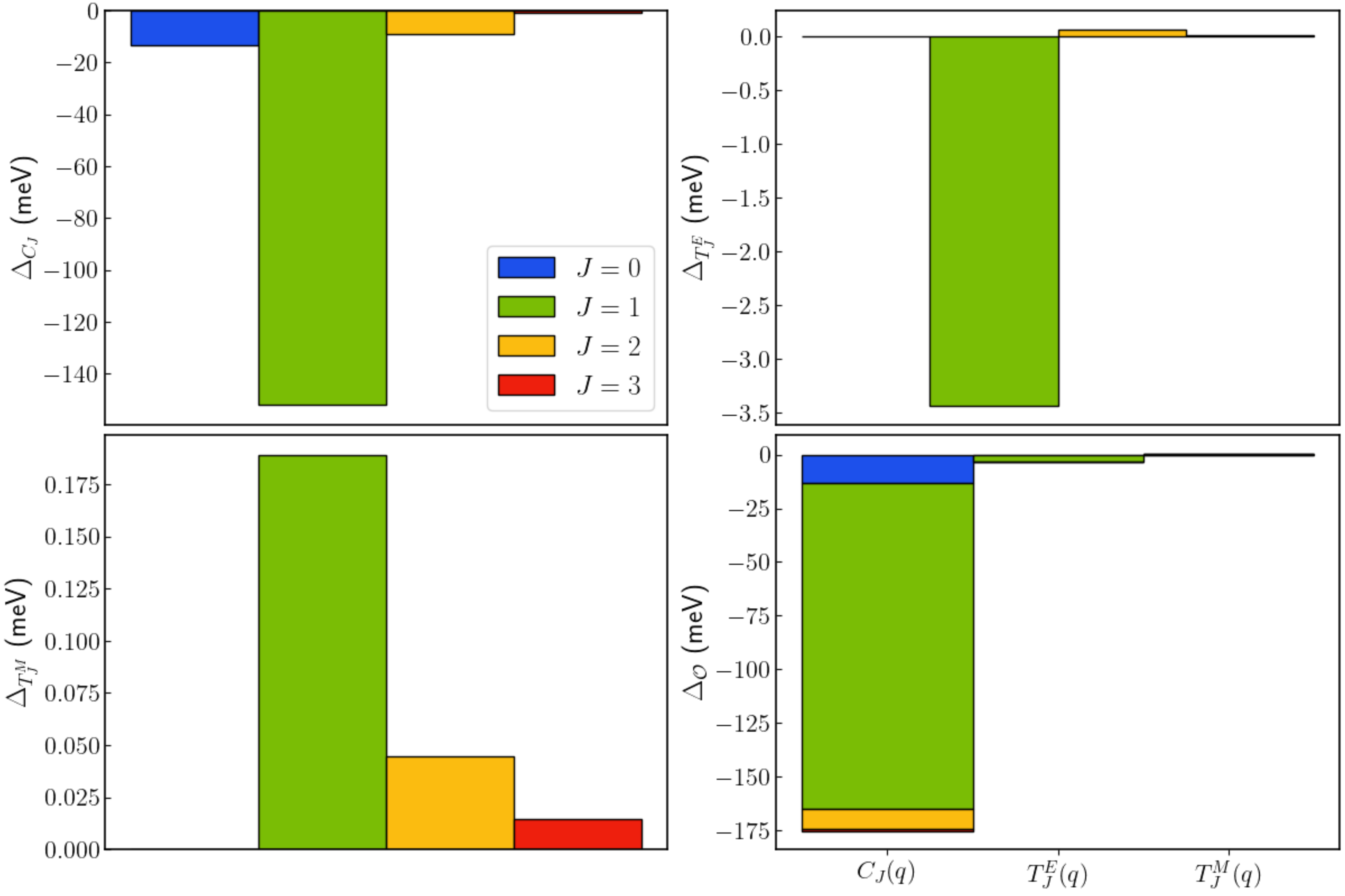

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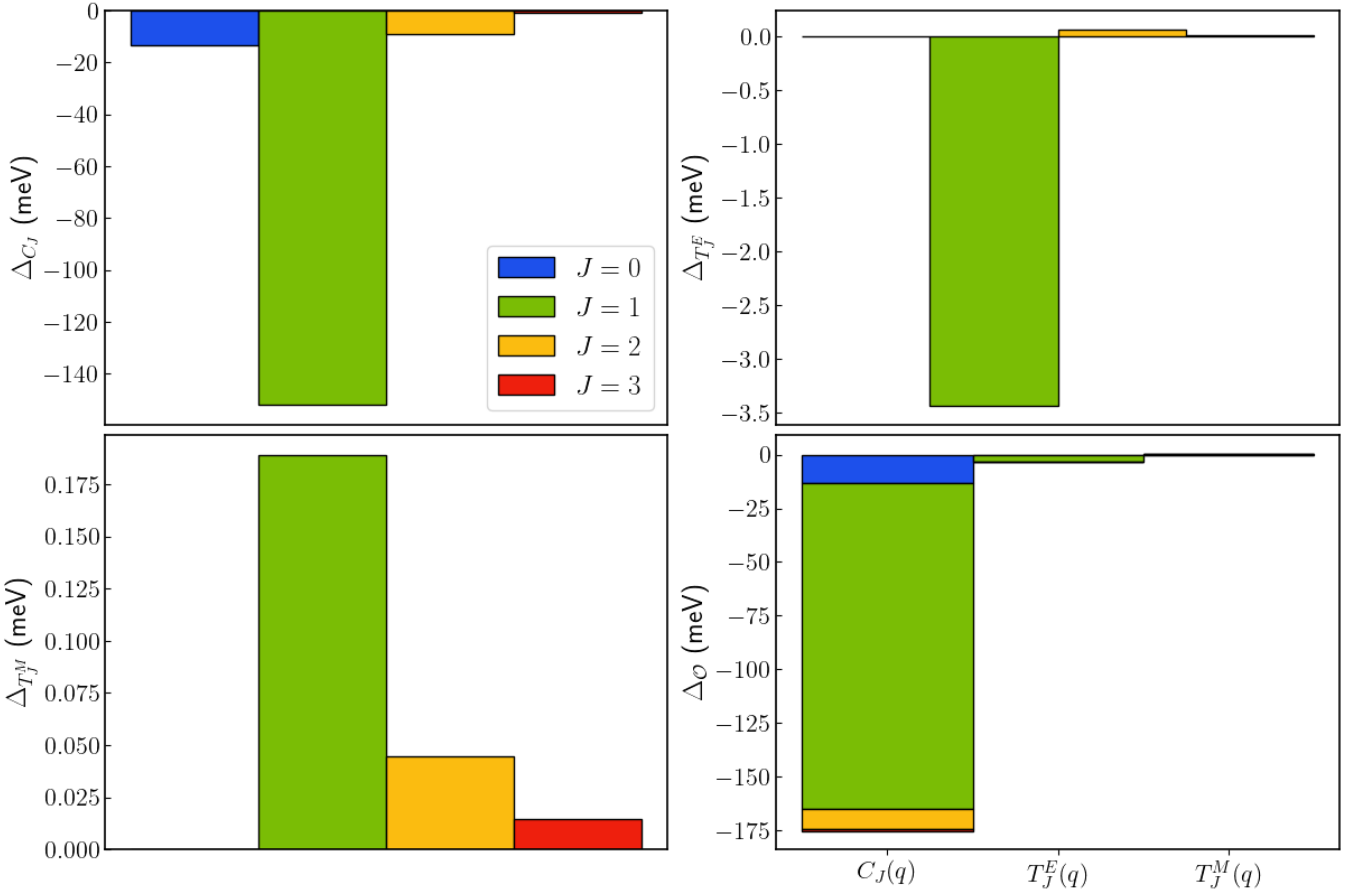

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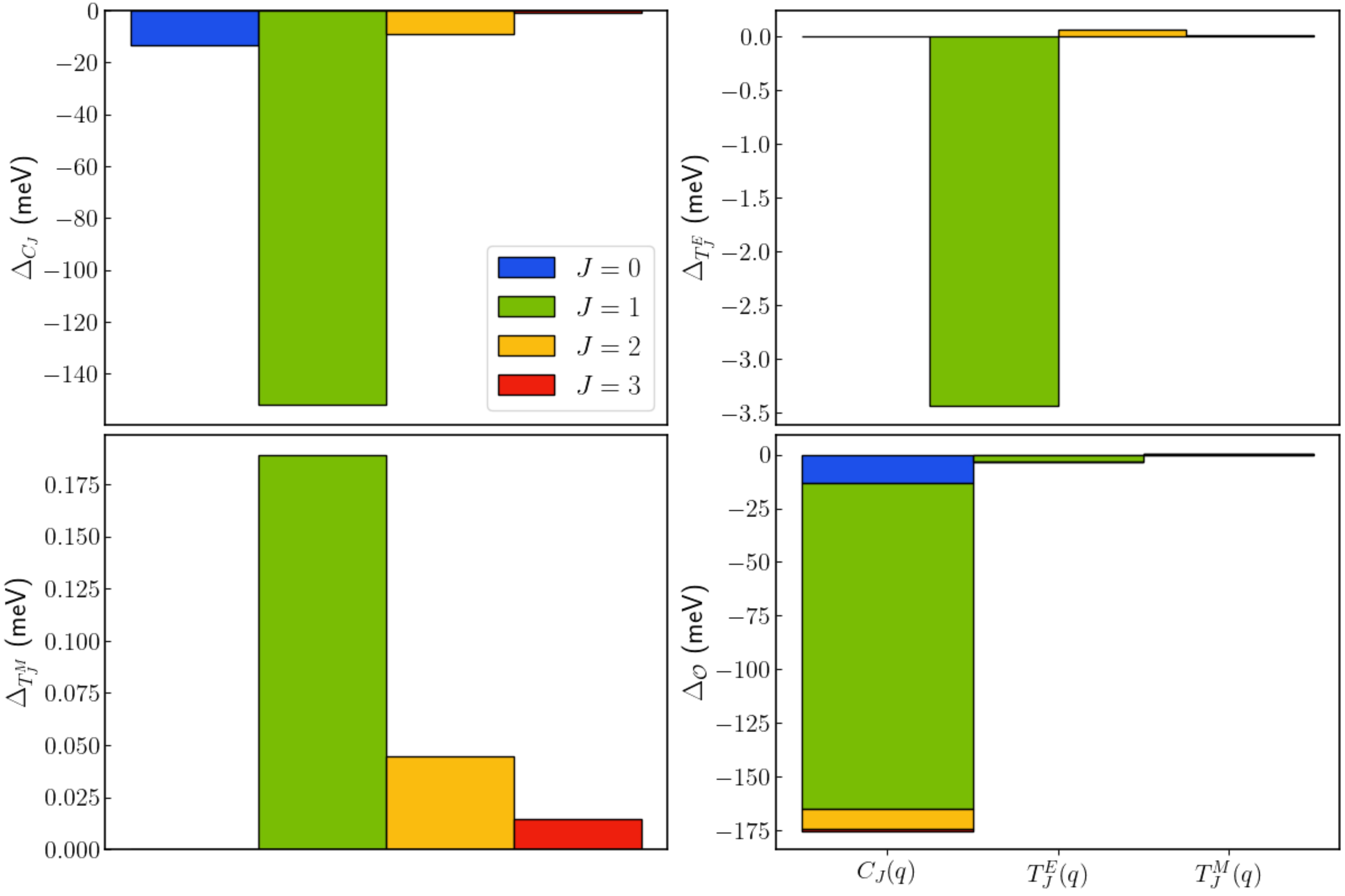

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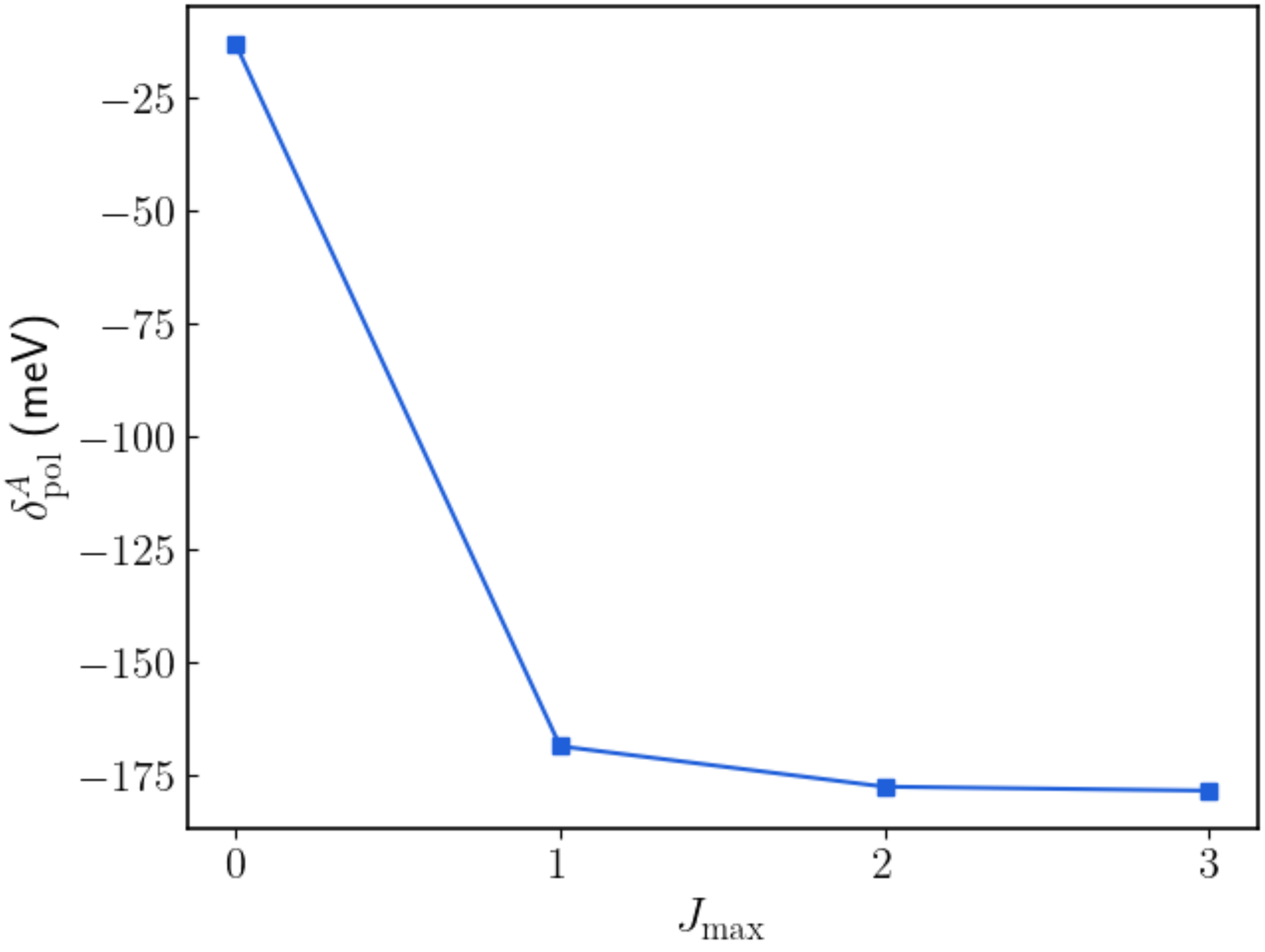
  - Well-known **dipole** dominance
  - **Charge** contributions are dominant
- Negligible contributions
  - TM is negligible for any J
  - TE is relevant only for $J = 1$

➡ **Only half the operators are relevant**

Checking convergence in $J_{\max}$



Results

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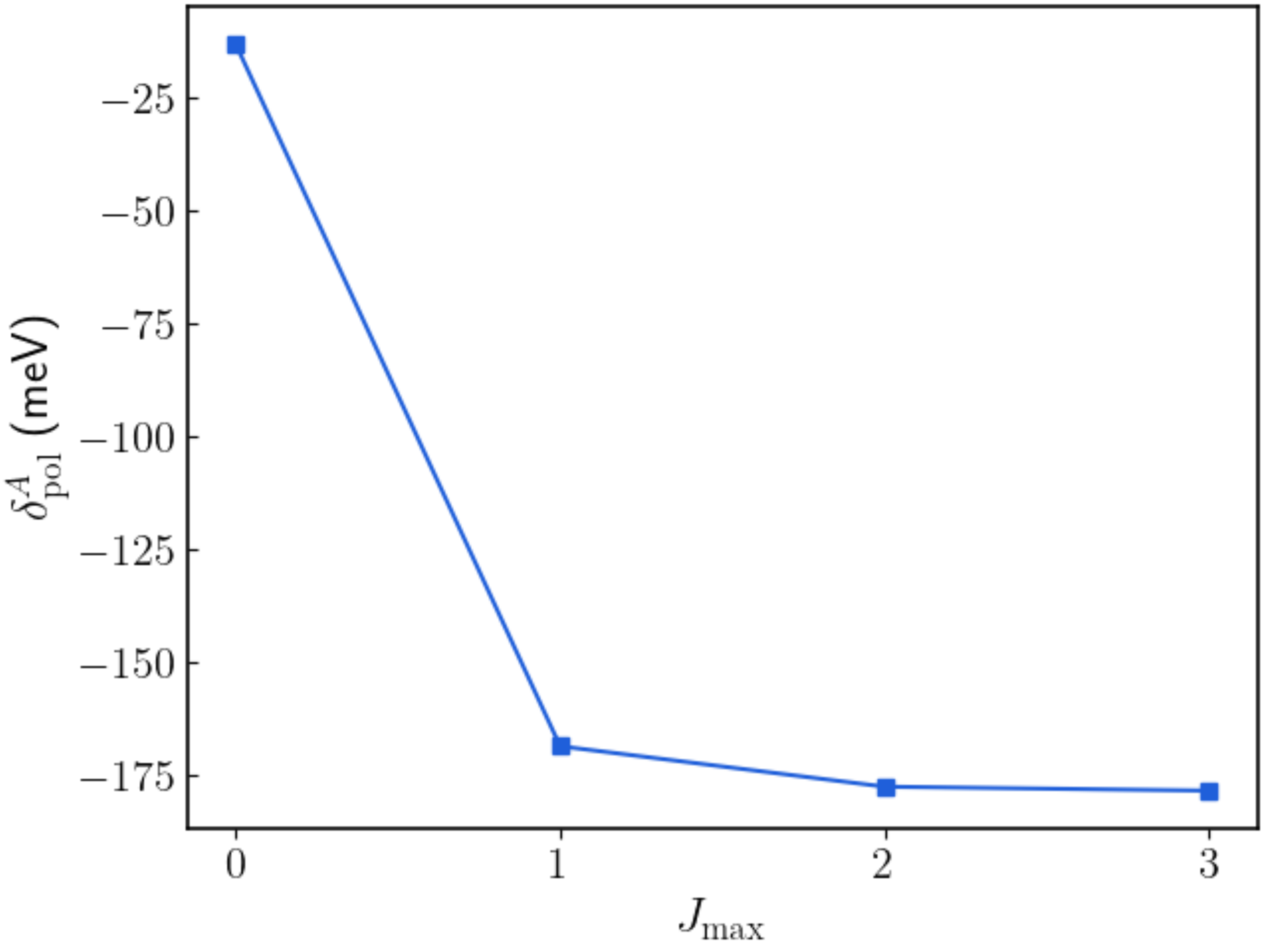

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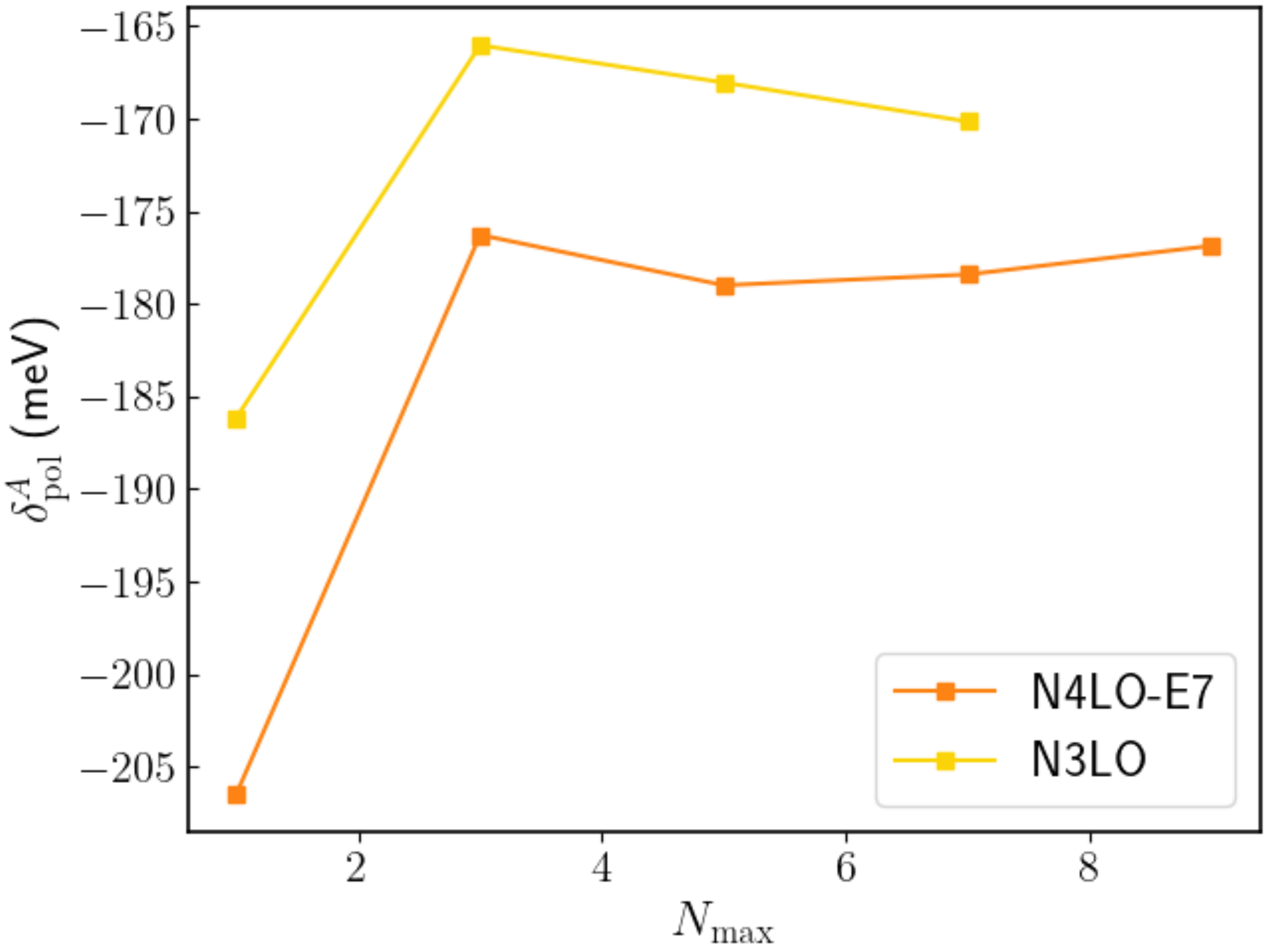
➡ **Fast exponential convergence**

$$\epsilon_{J_{\max}} \lesssim 0.1 \text{ meV}$$

Multipole truncation $\Rightarrow$ negligible uncertainty

Convergence in $N_{\max}$ and interaction dependence



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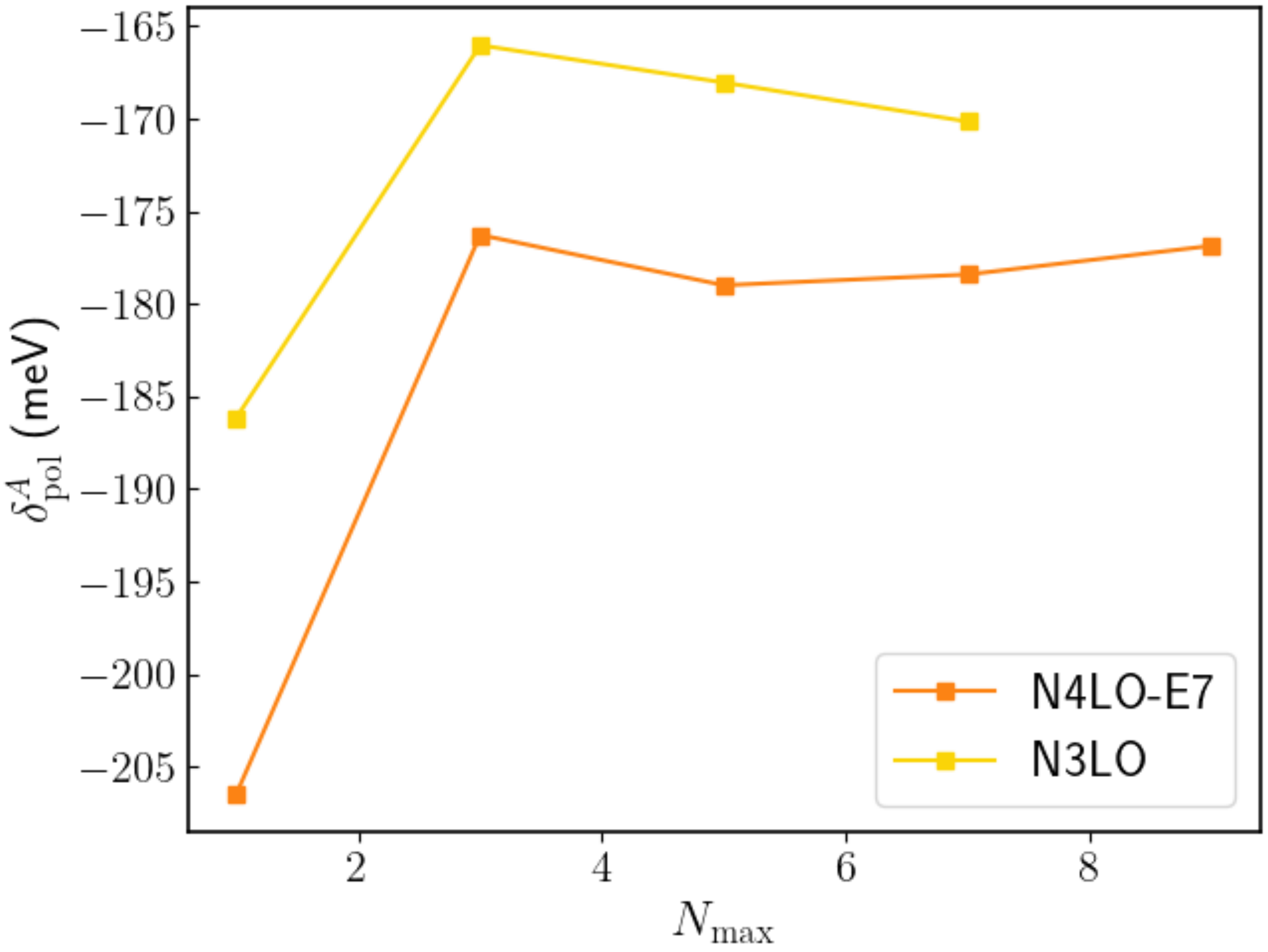

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- <u>N4LO-E7 interaction</u>
  - $N_{\max}$ fluctuation $\simeq 1 - 2$ meV
  - Multiple frequencies still to be run

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- <u>N3LO interaction</u>
  - $N_{\max} = 9$ still to be completed
  - Heavy calculations $\Rightarrow$ run on Frontiers

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- Overall consistent with previous estimation!

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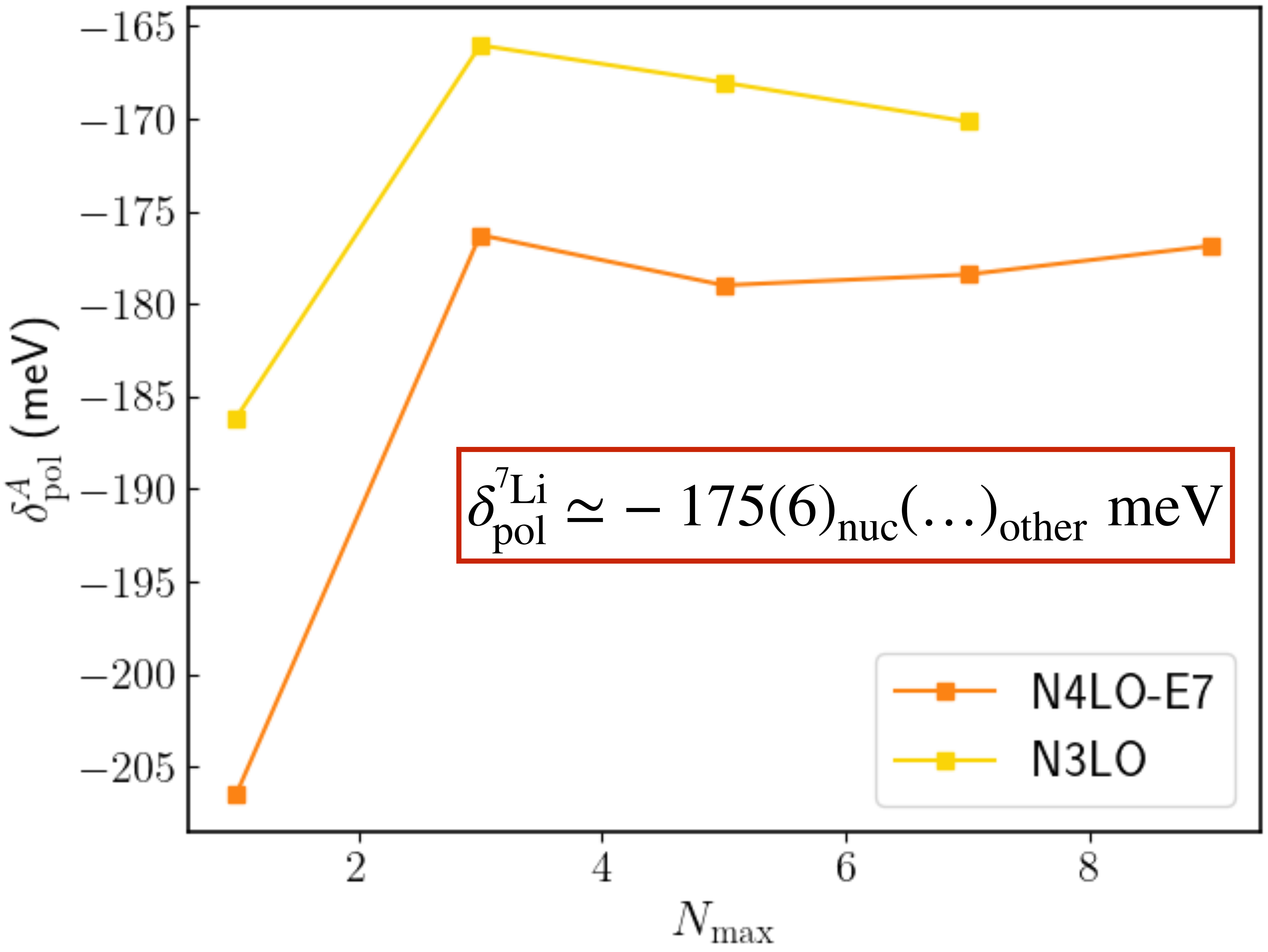

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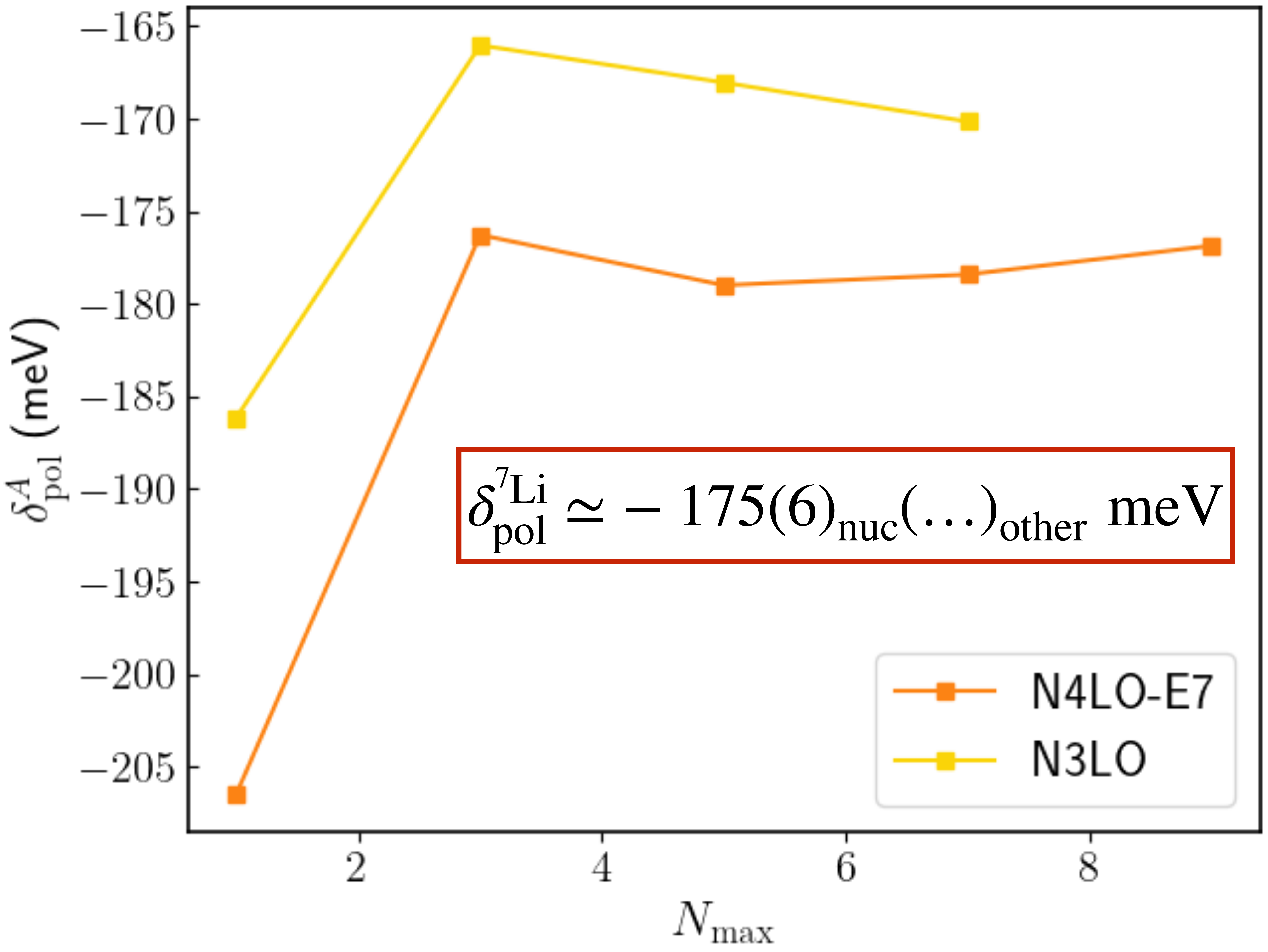

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A 10 meV precision for nuclear structure corrections seems doable in the near future !

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  - Is there already a standard tower of EFTs to use ?
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Thank you
Merci

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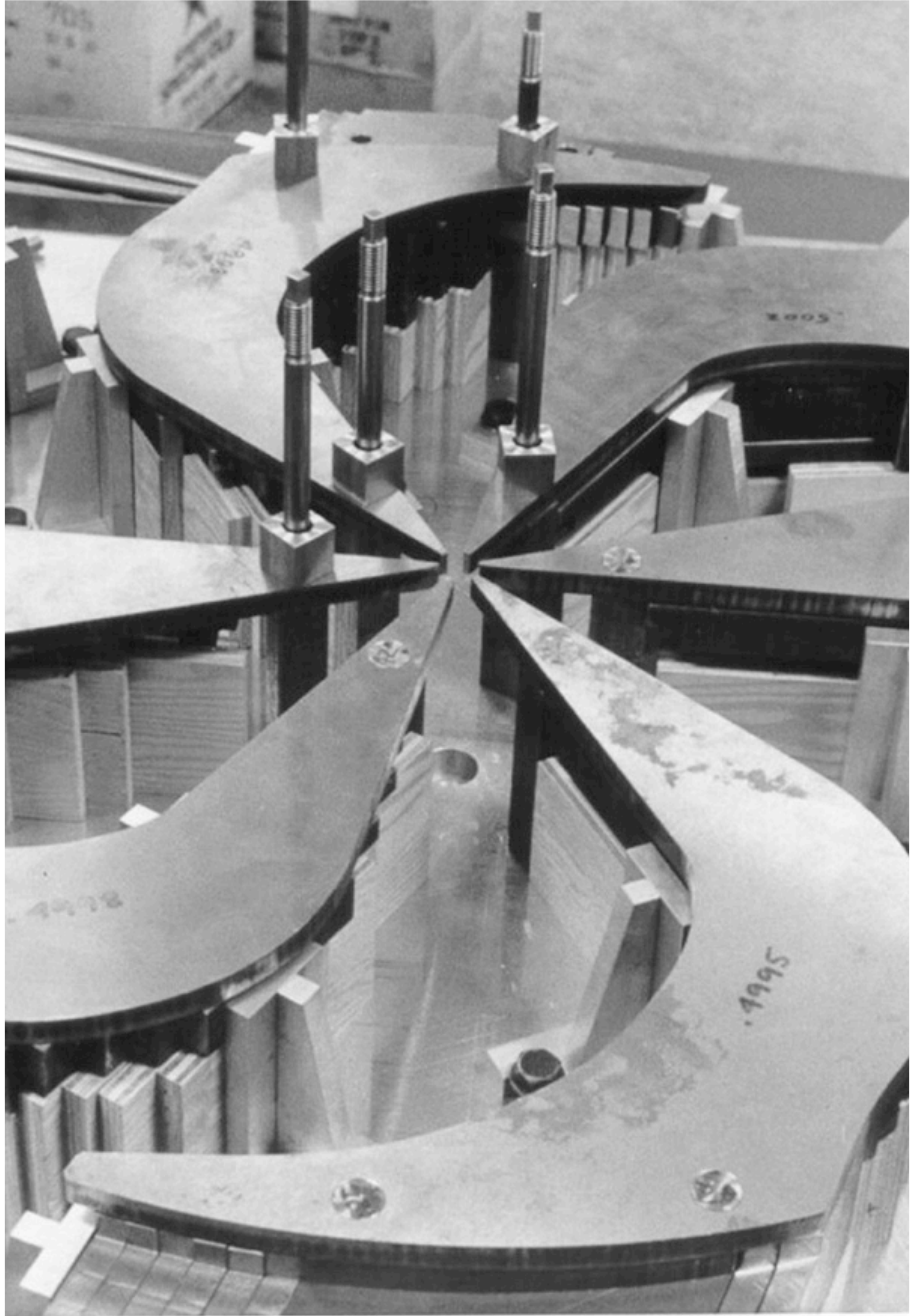

Discovery, accelerated