

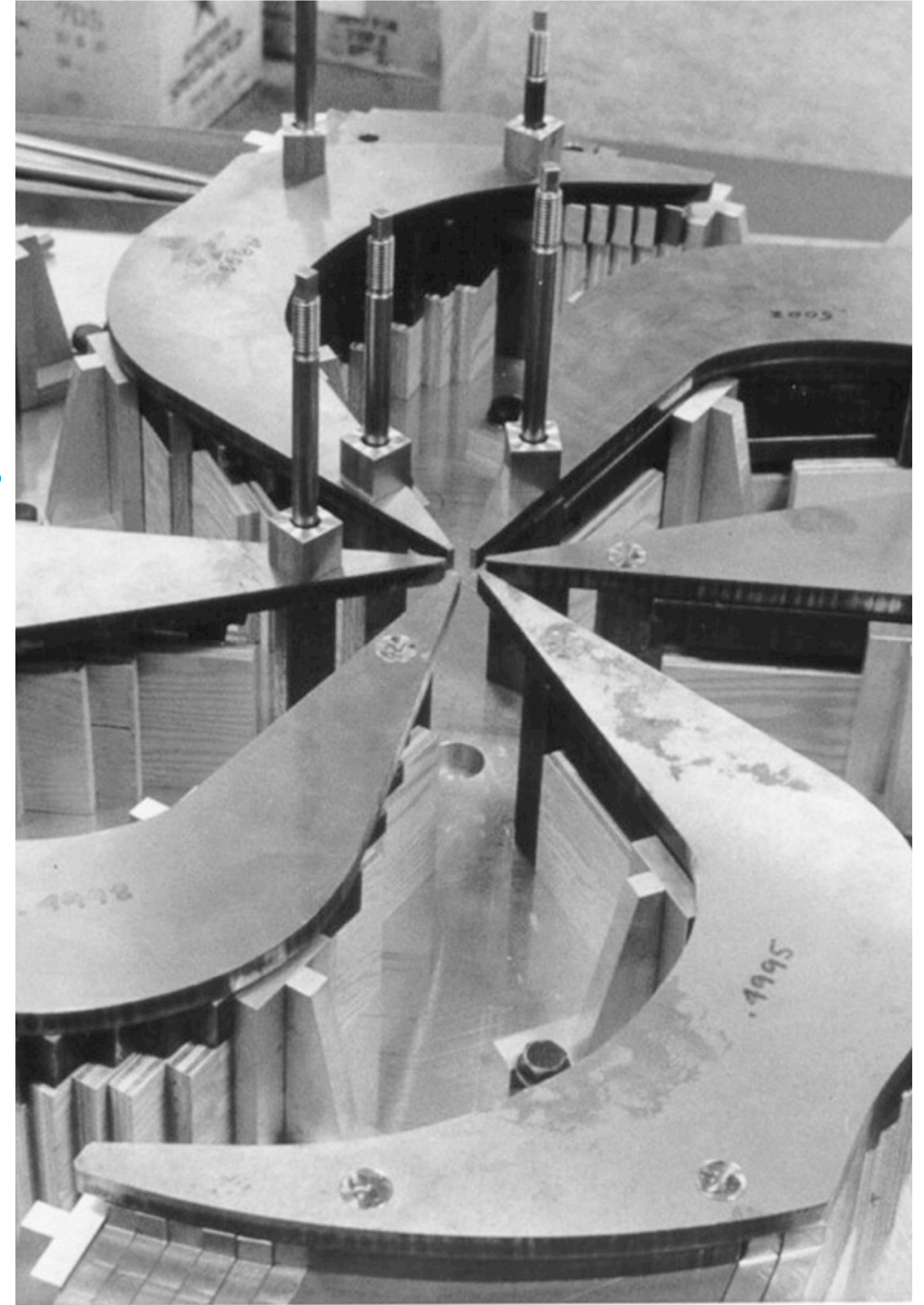
Ab initio nuclear corrections to muonic atoms

Extracting nuclear radii from precision spectroscopy

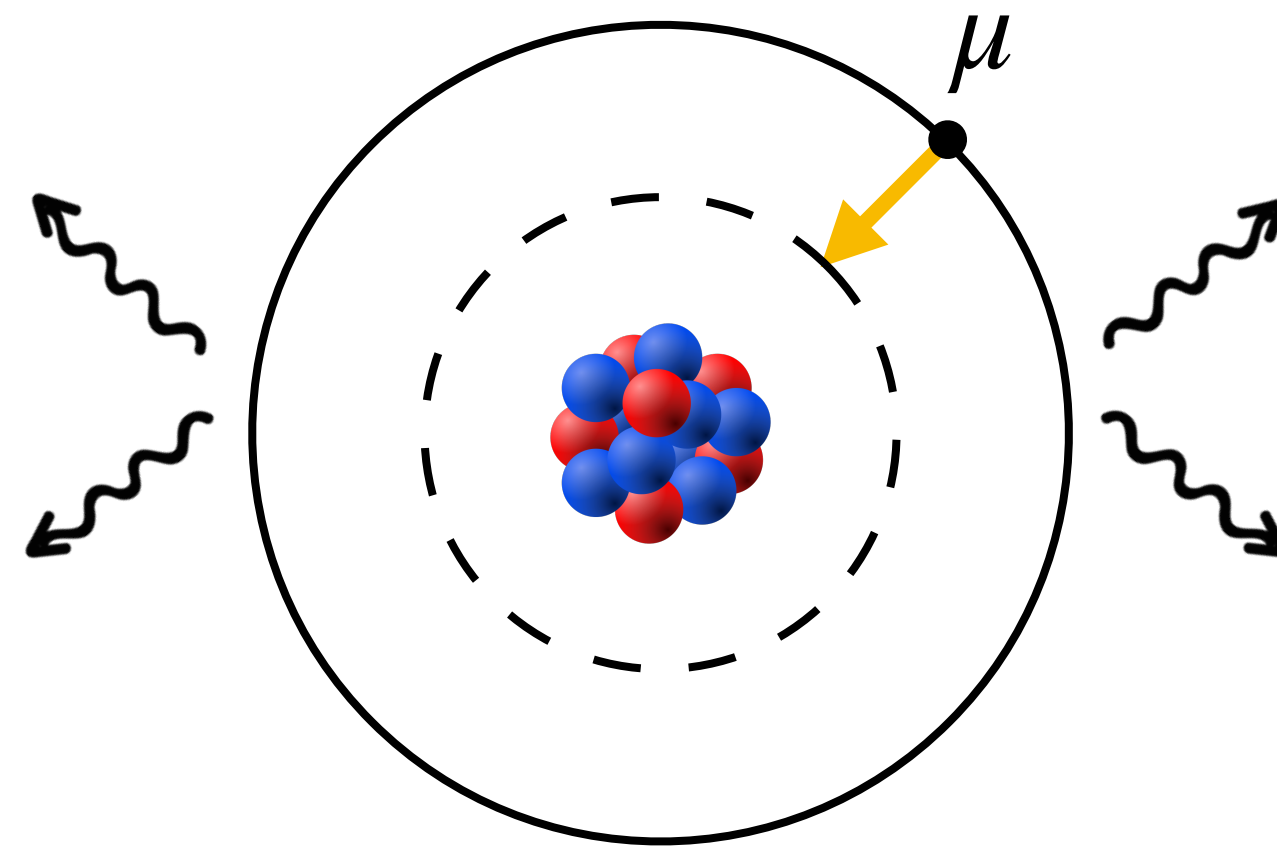
Collaborators: Petr Navratil, Michael Gennari

Mehdi Drissi
TRIUMF - Theory department

PAINT 2025
Vancouver - 25th of February 2025

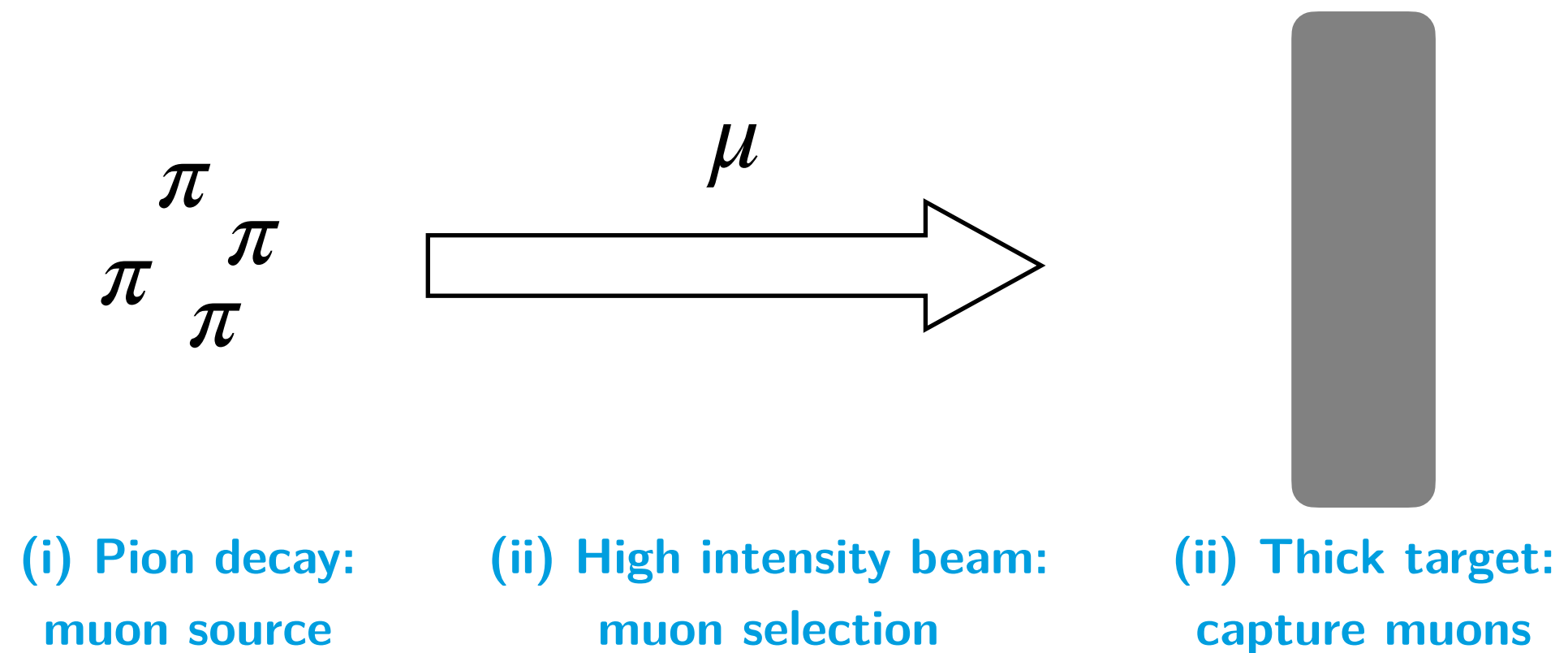


Muonic atoms and charge radii



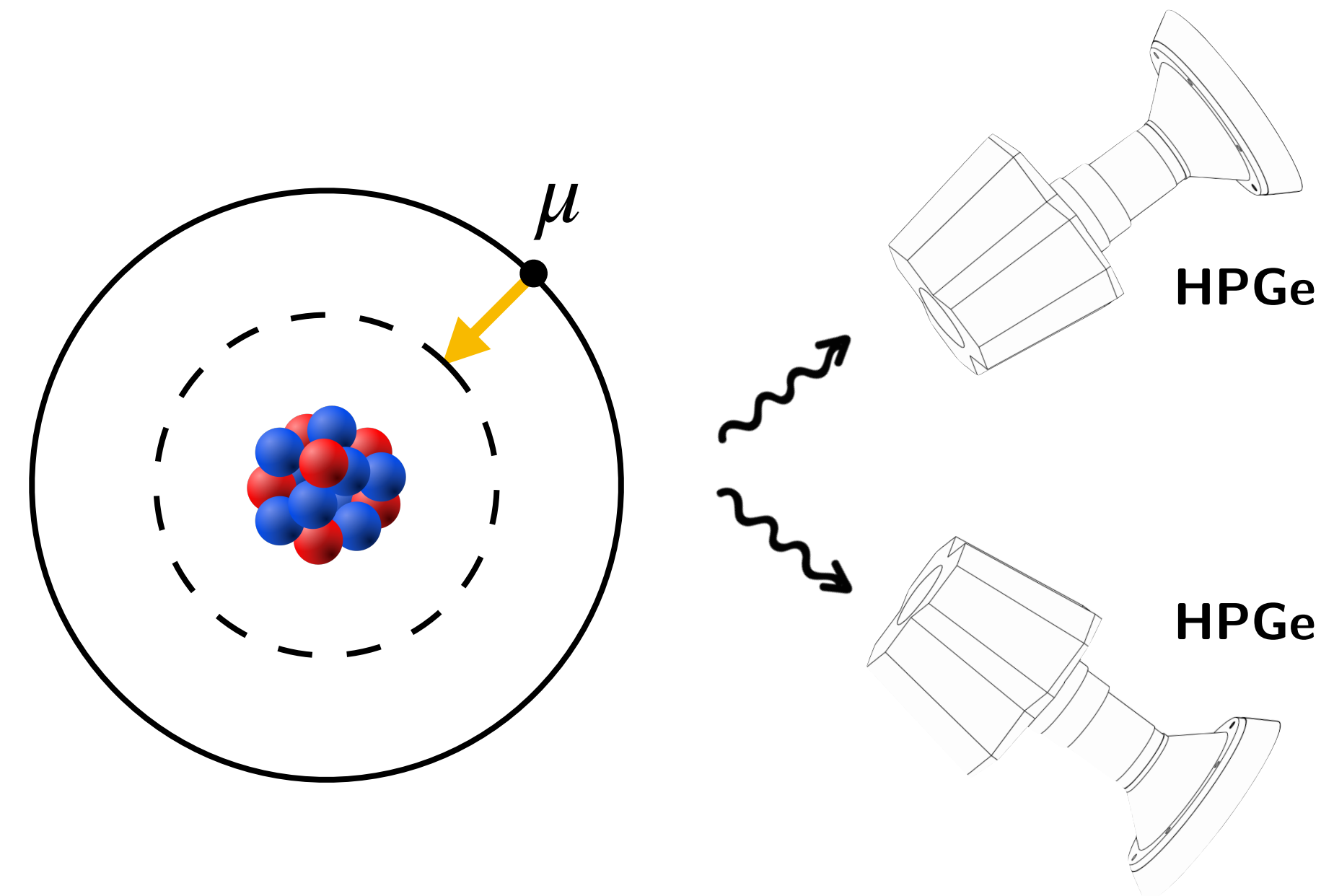
Observing muonic atoms with X-rays

How to make muonic atom



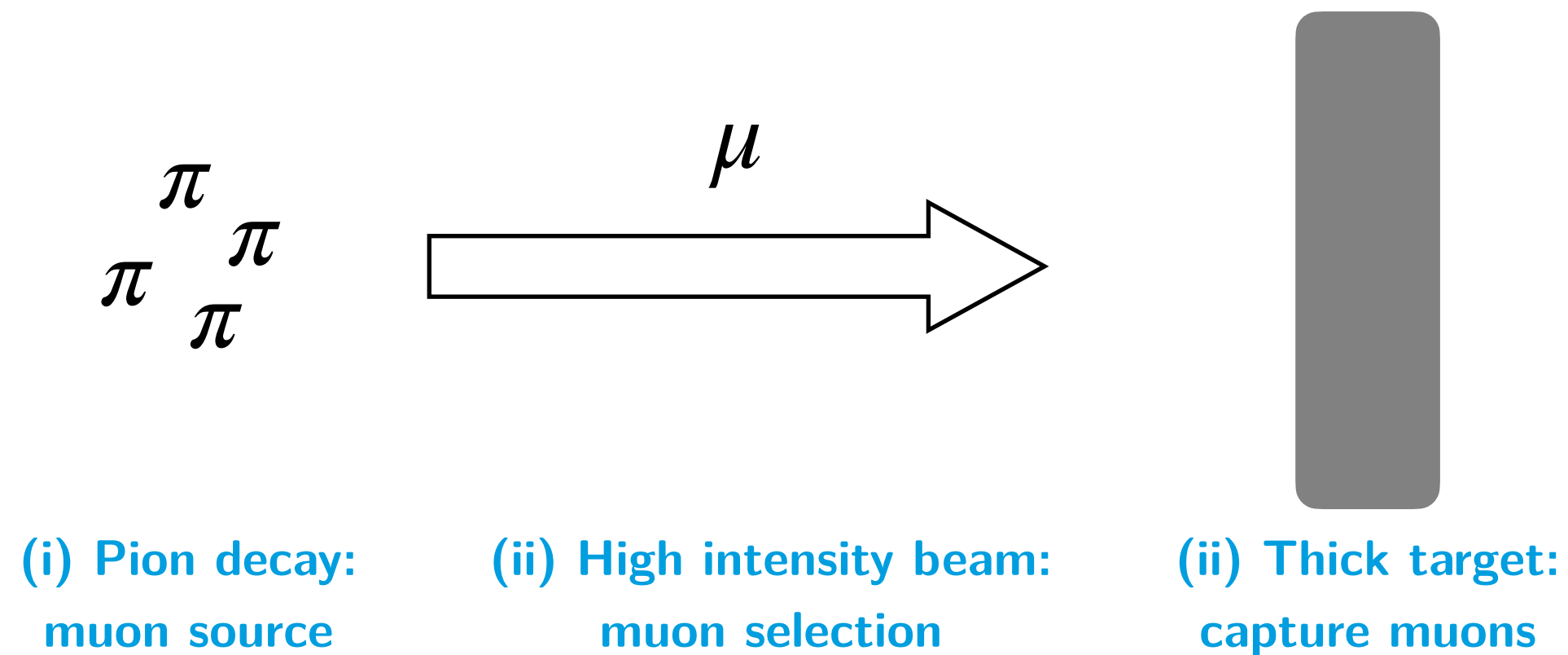
Typically muons captured on orbitals with $n \sim \sqrt{\frac{m_\mu}{m_e}} \sim 14$

Observing characteristic X-rays



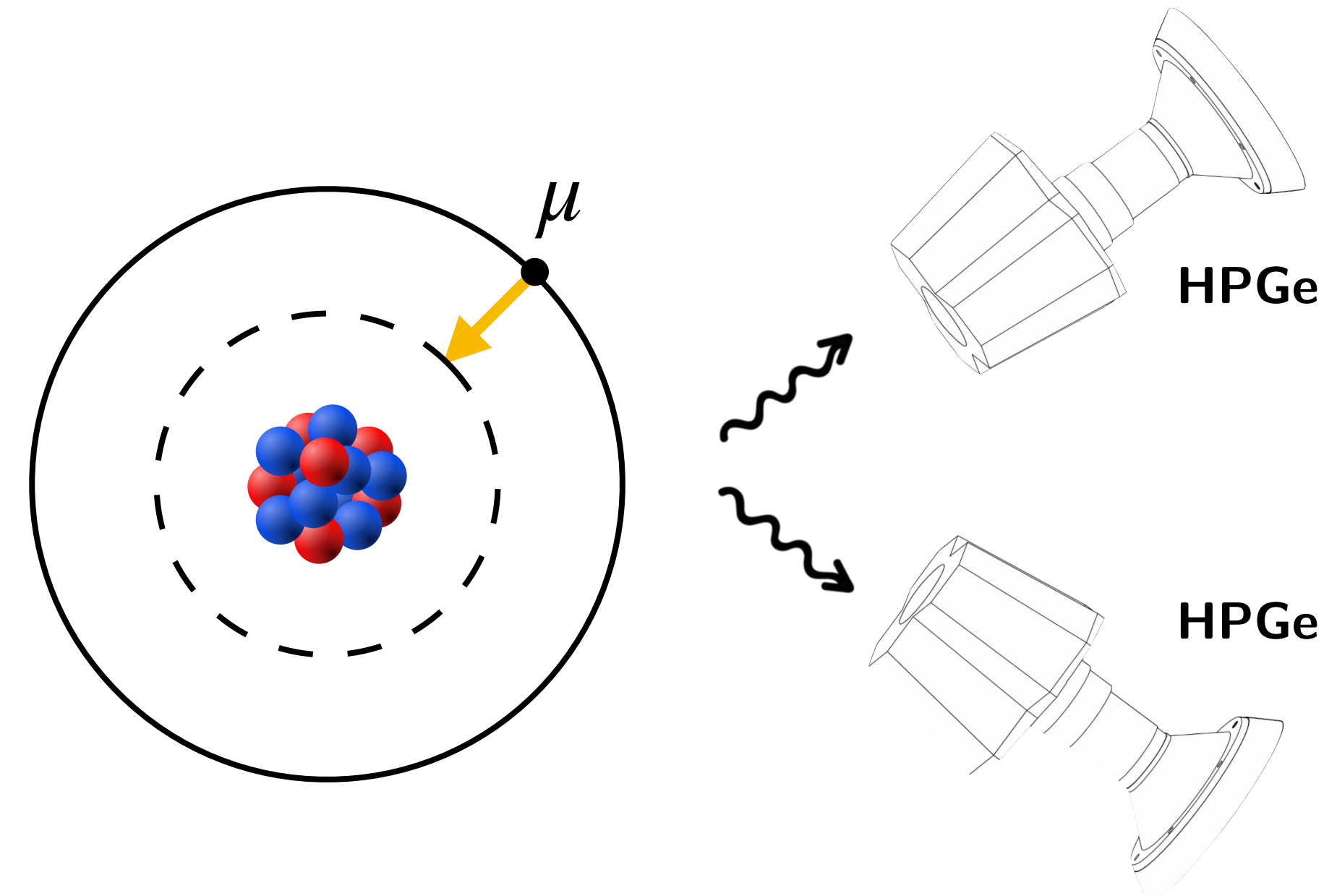
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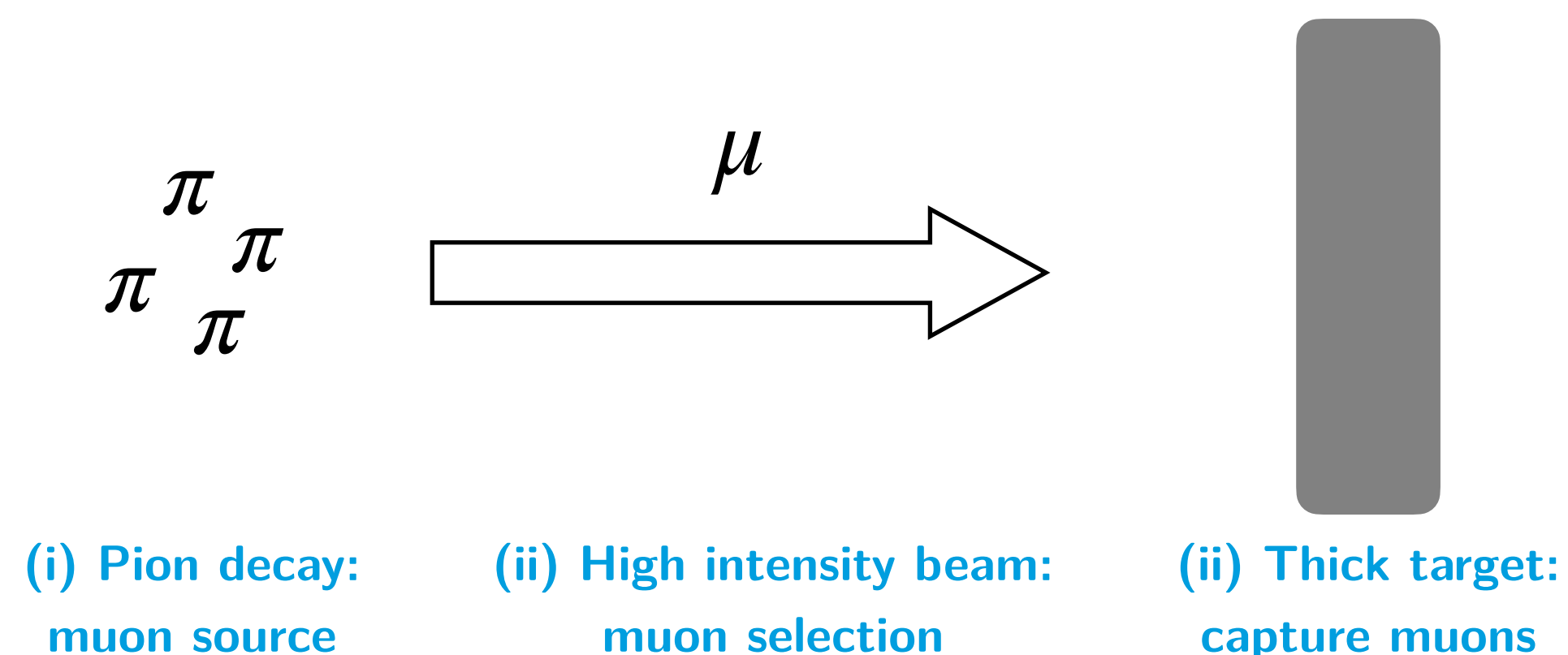
Muonic atom achievements

- Precise spectroscopy of almost all stable elements
- Charge radii extraction \Rightarrow **highest absolute accuracy**
- Combined with isotope-shift \Rightarrow **radii for unstable nuclei**

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

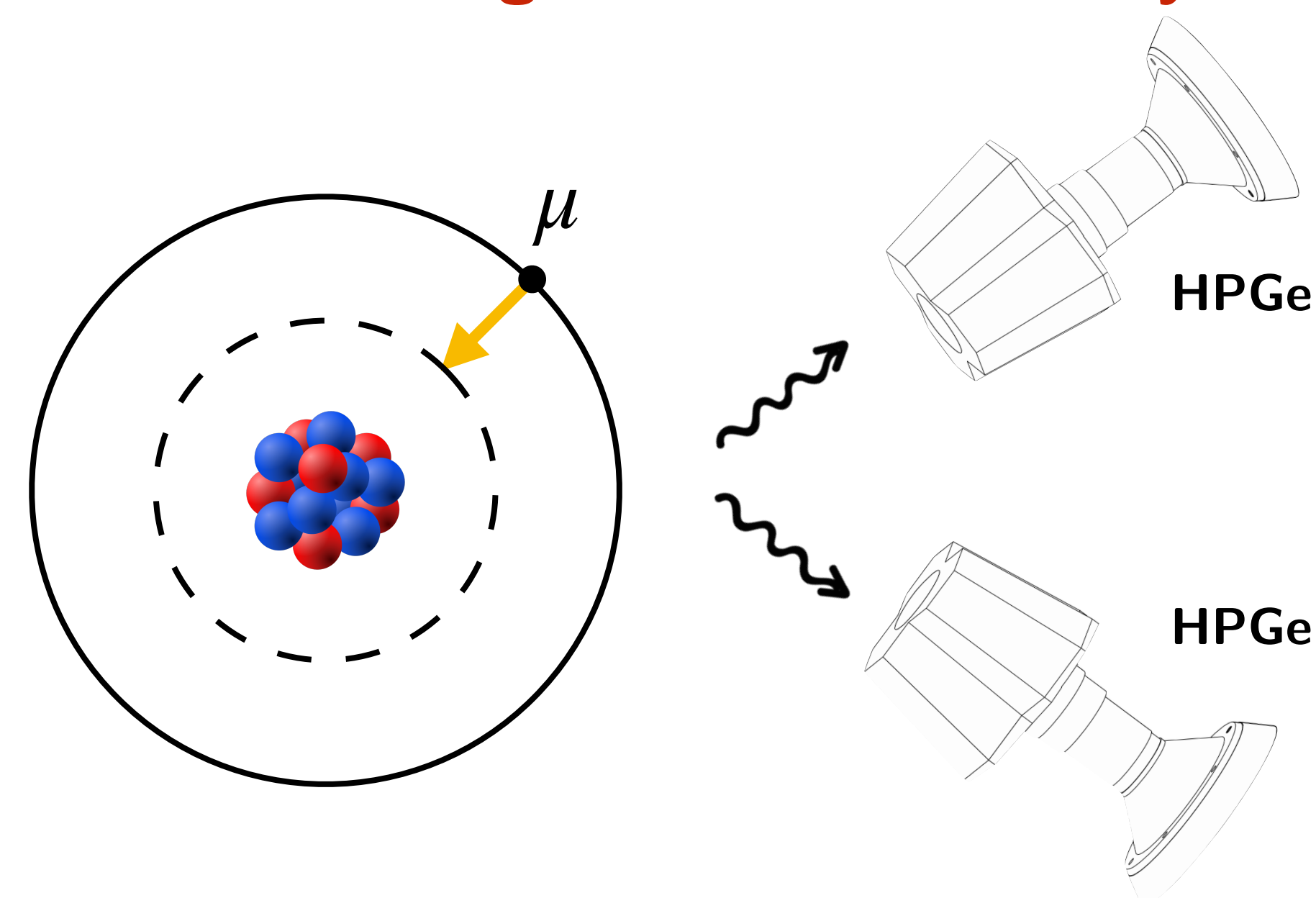
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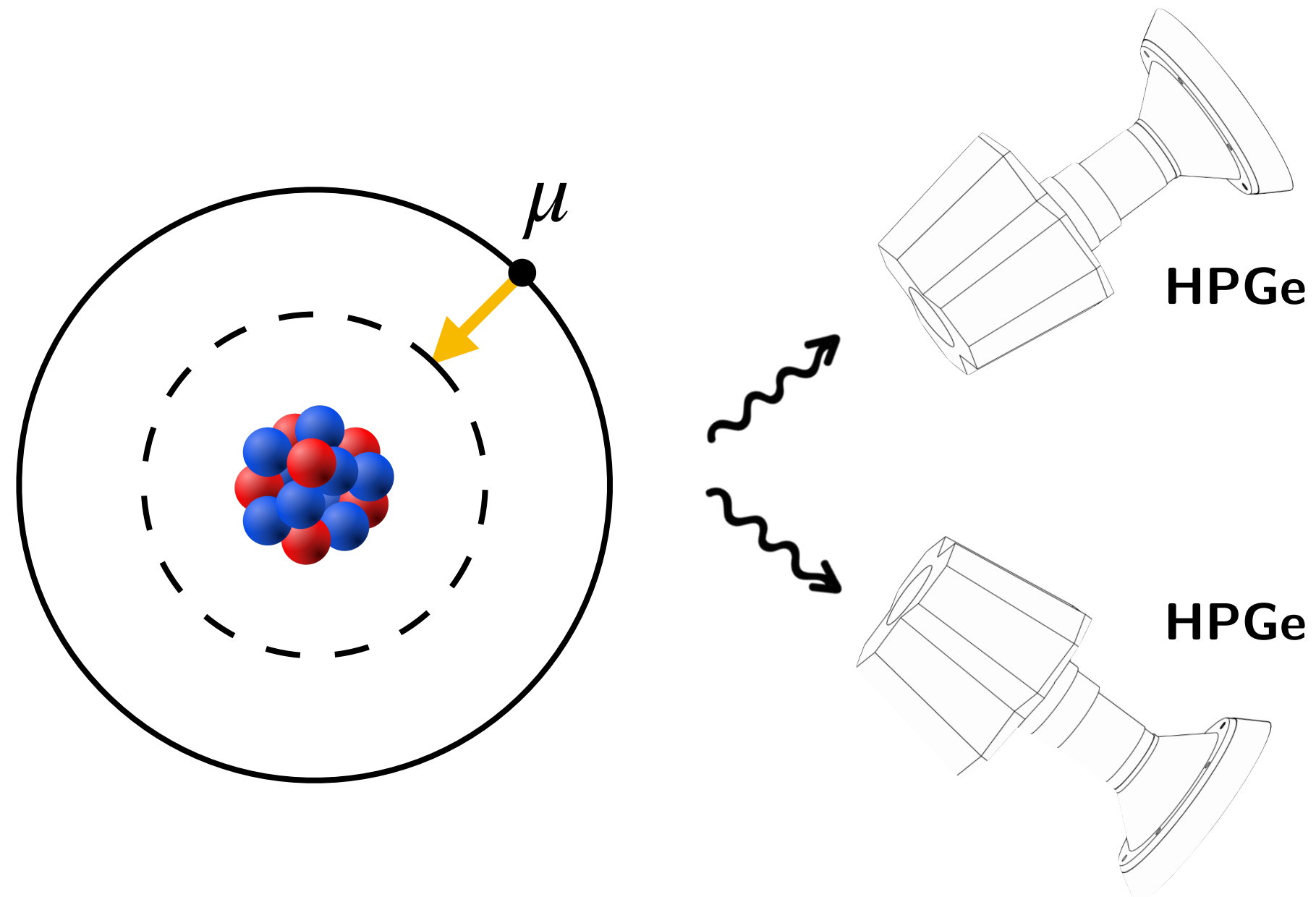
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Practical limitations

- × In general: limitations are very experiment dependent
 - × Never with a perfect energy resolution
- \Rightarrow **Many experimental challenges !**

Muonic atoms as a precision probe

Observing muonic atoms

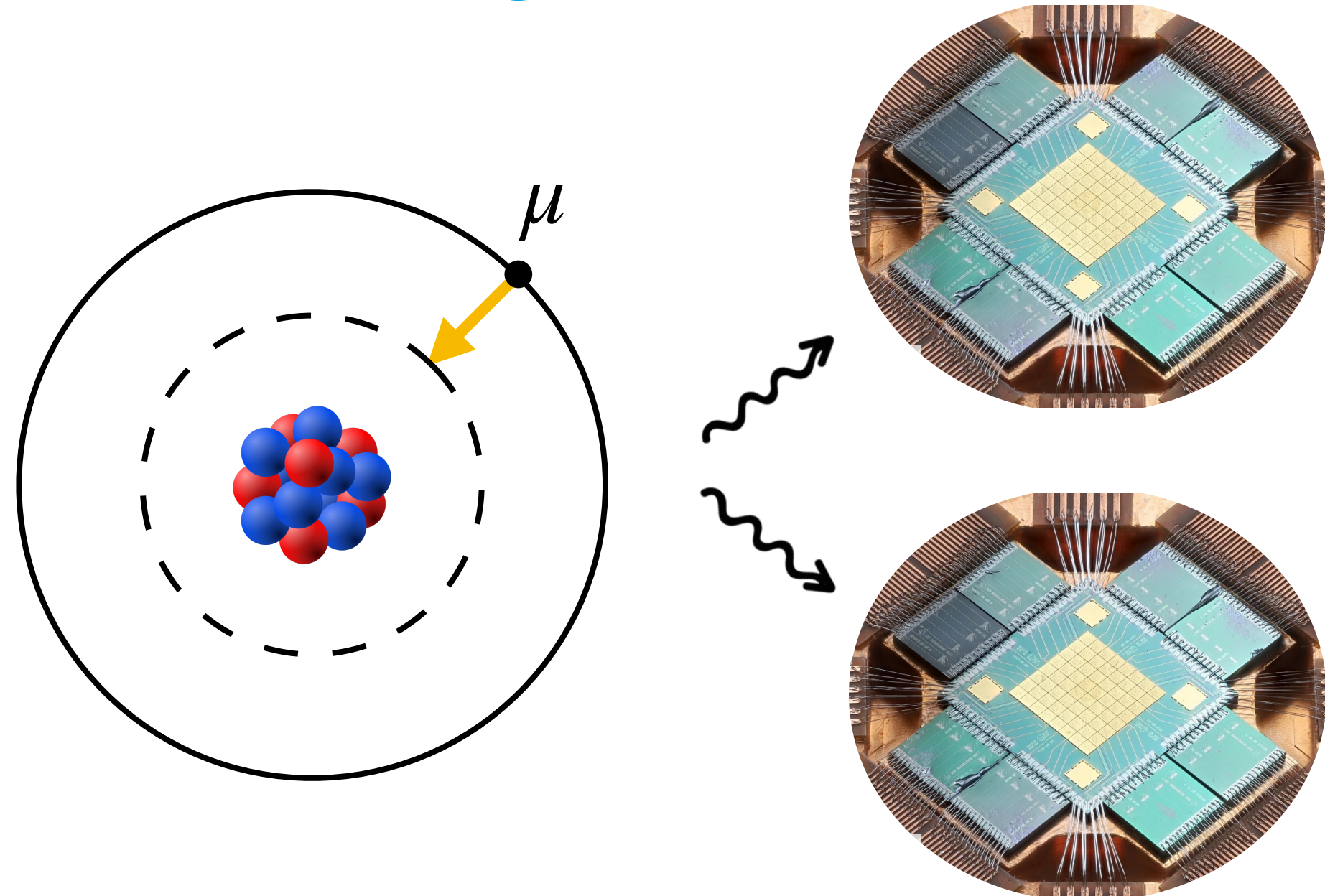


QUARTET collaboration

- Improving energy resolution
 - Quantum sensor detector to reach low-Z nuclei
 - **On-going work at PSI with ${}^6\text{Li}$ / ${}^7\text{Li}$ target**

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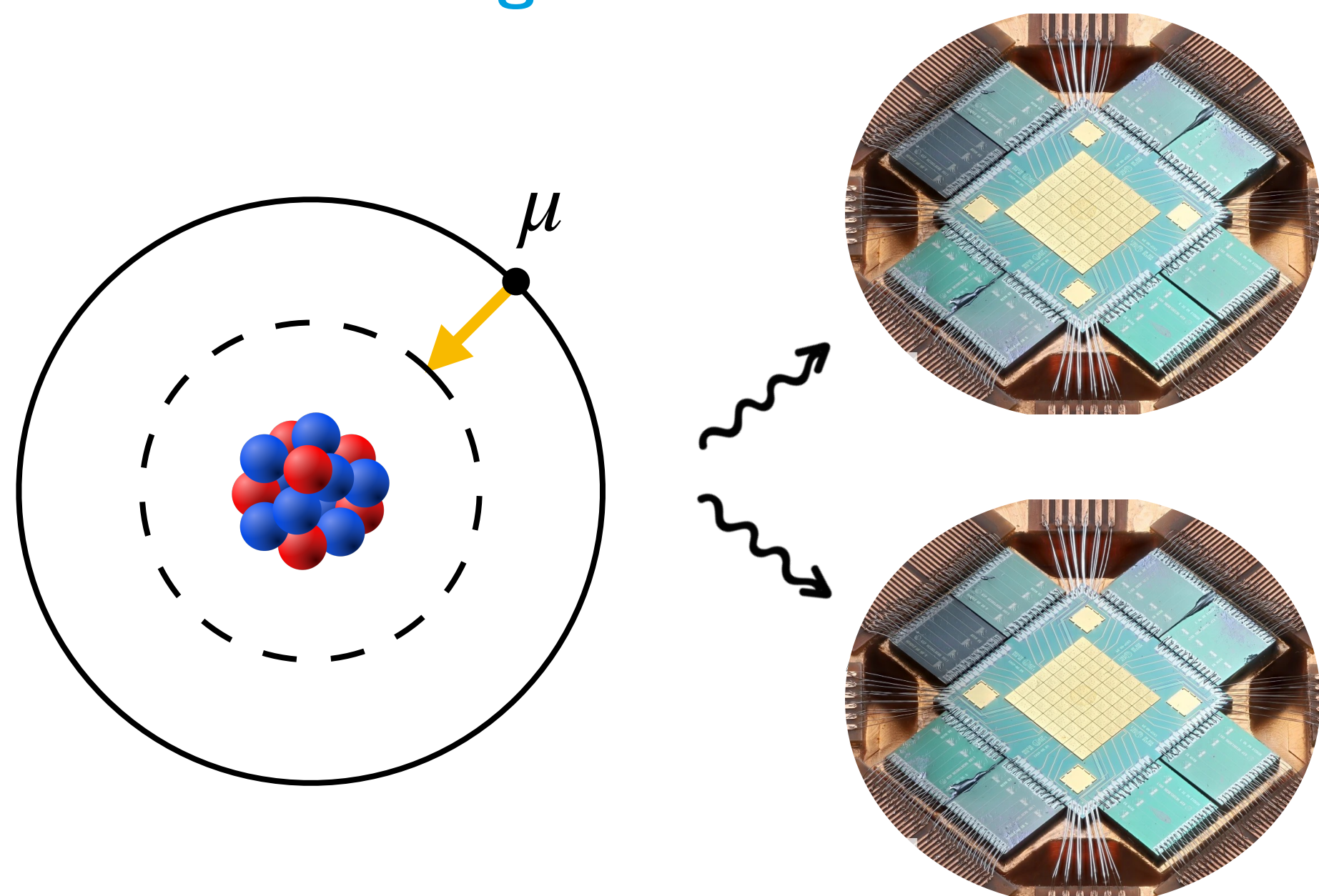
[Unger et al. J. Low Temp. Phys. (2024)]

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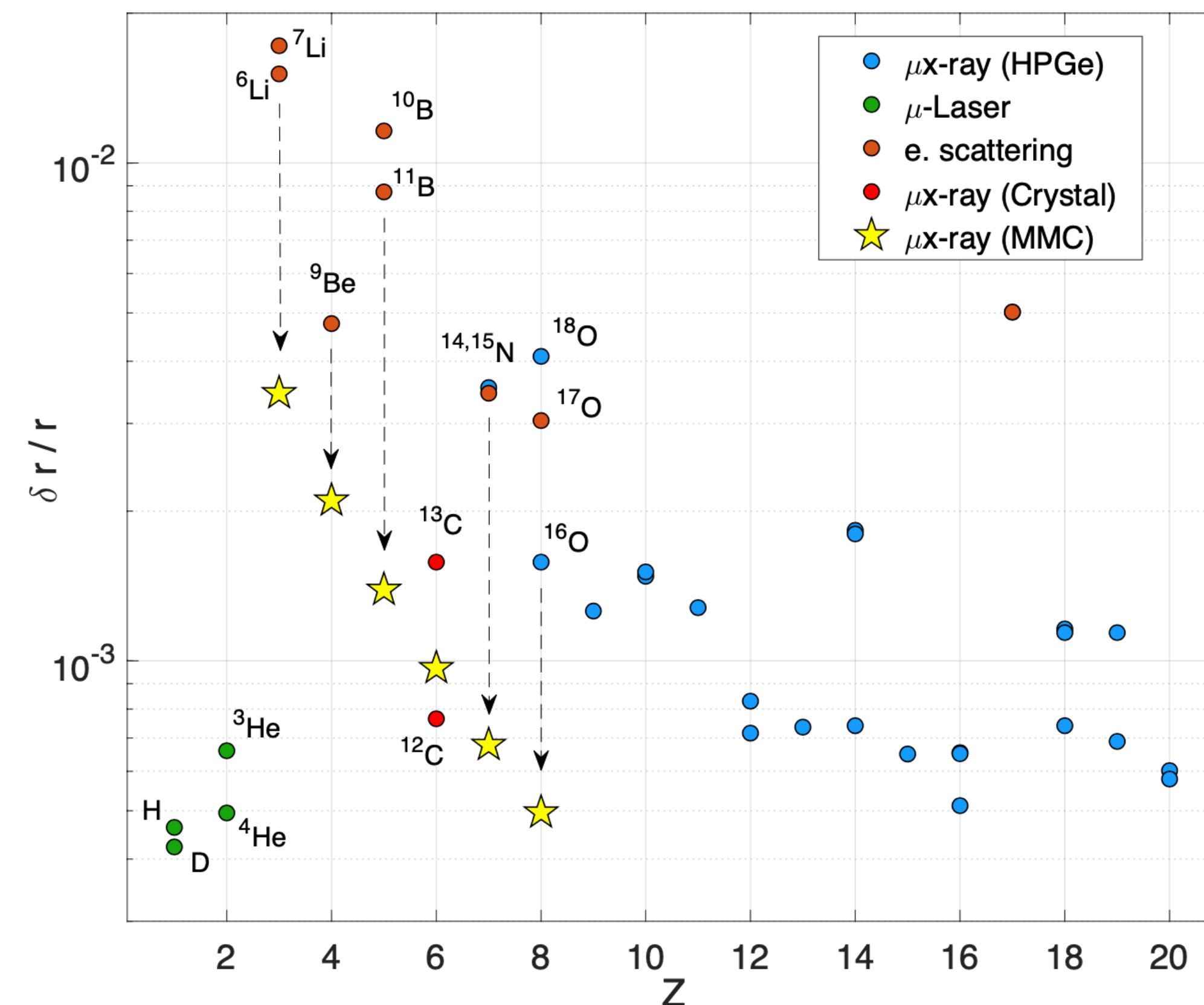
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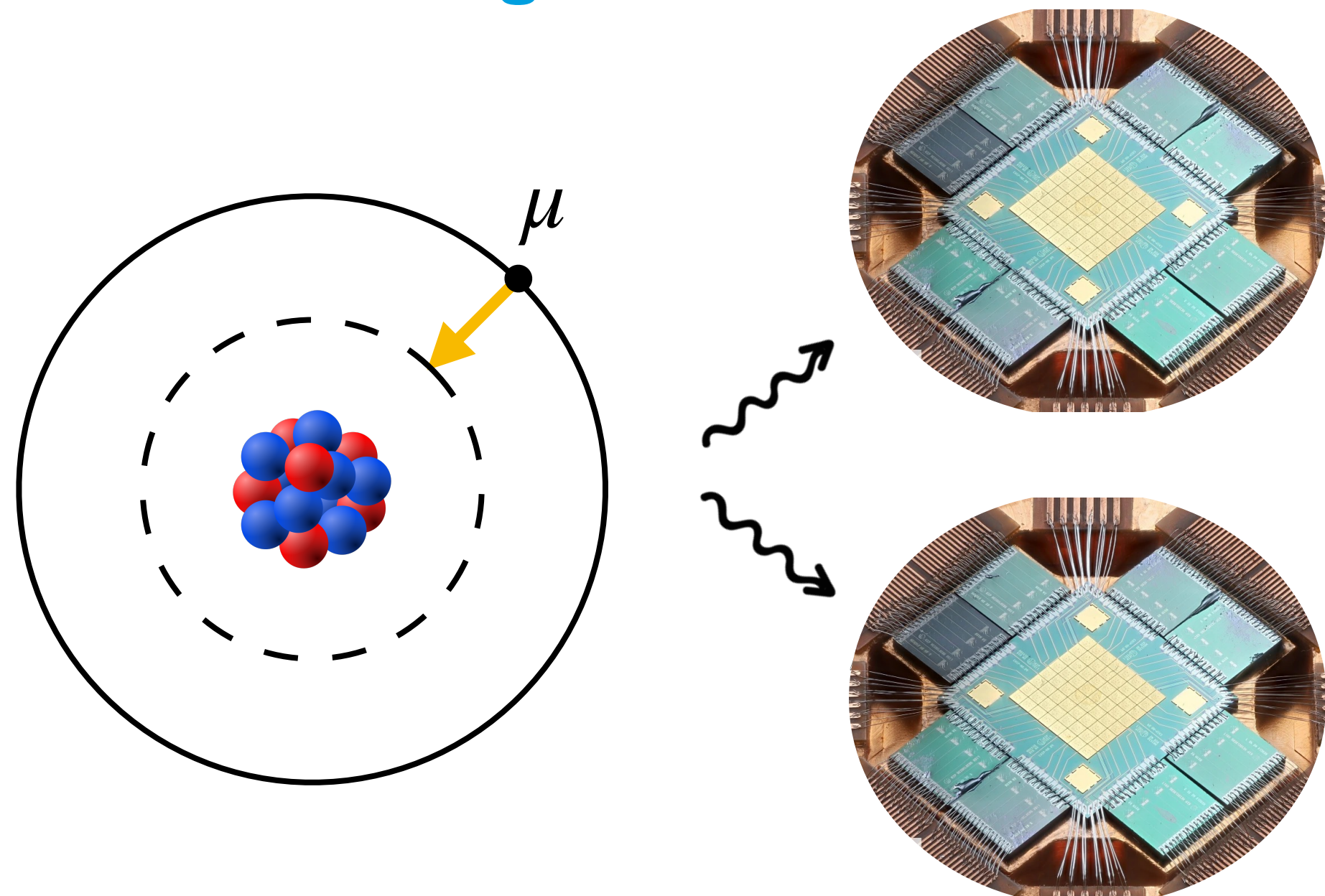
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[Antognini et al, arXiv:2210.16929] NuPECC Long Range Plan 2024

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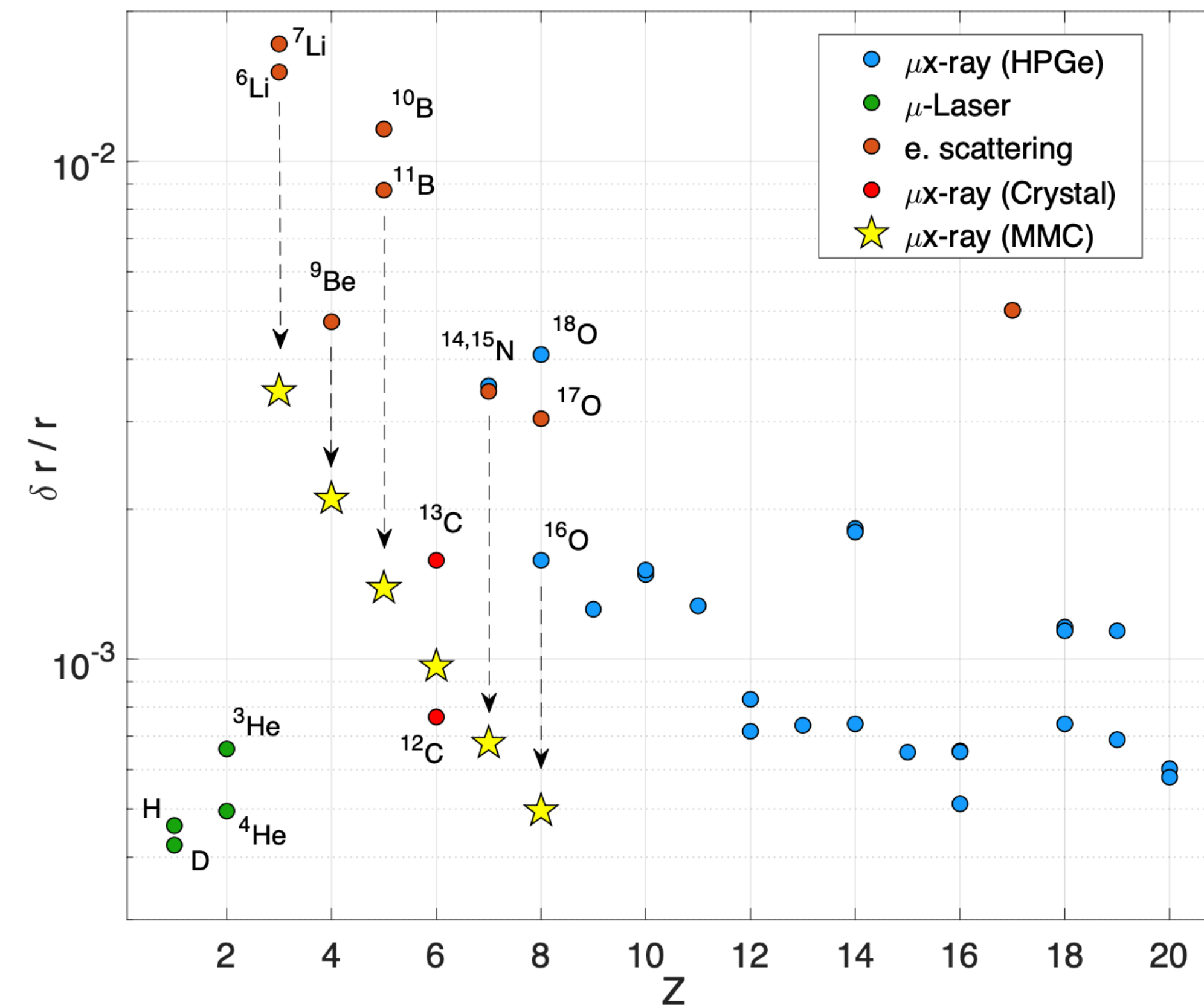
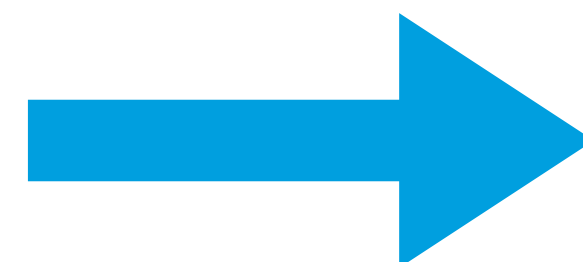
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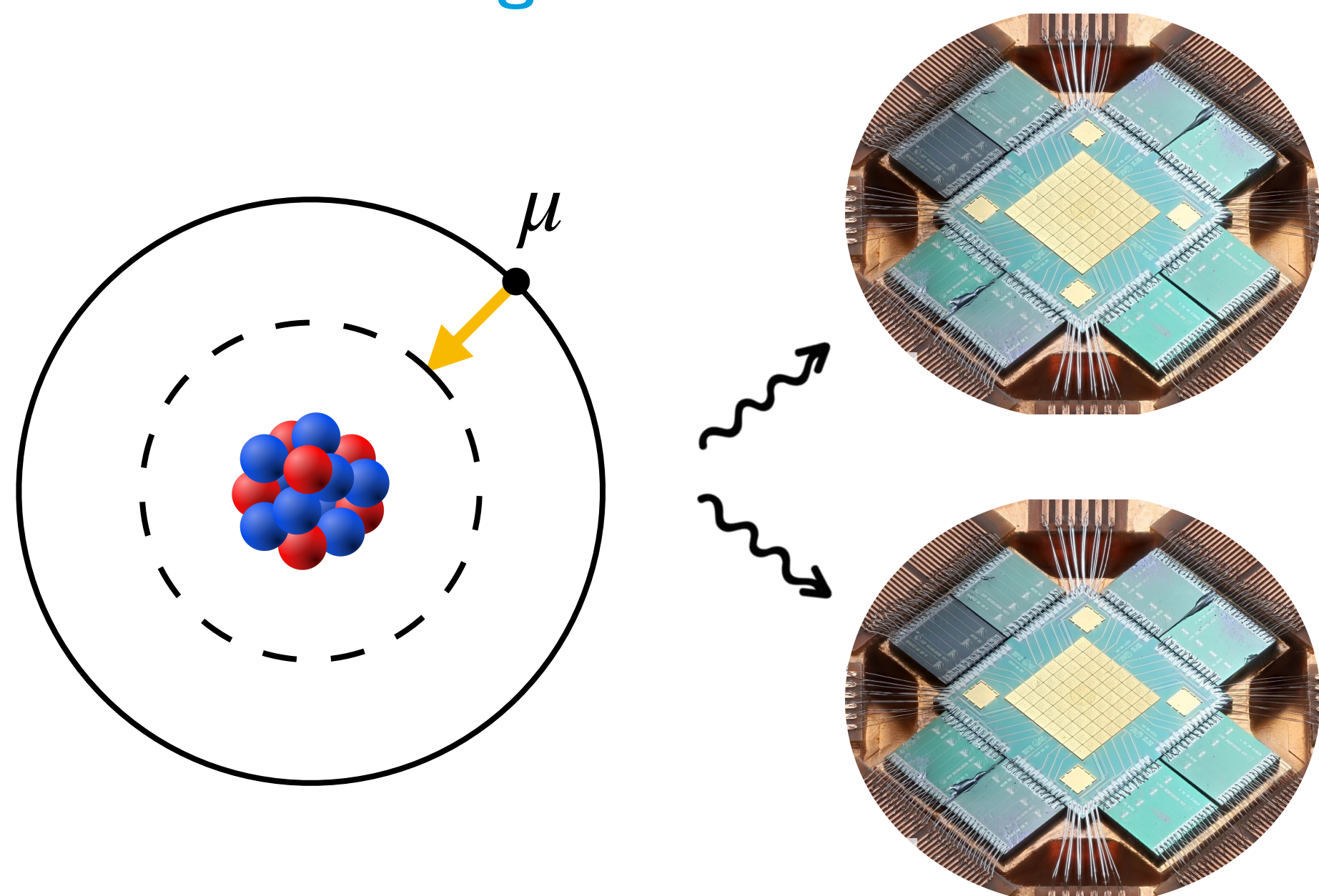


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Theoretical challenge: reach 10 meV uncertainty!

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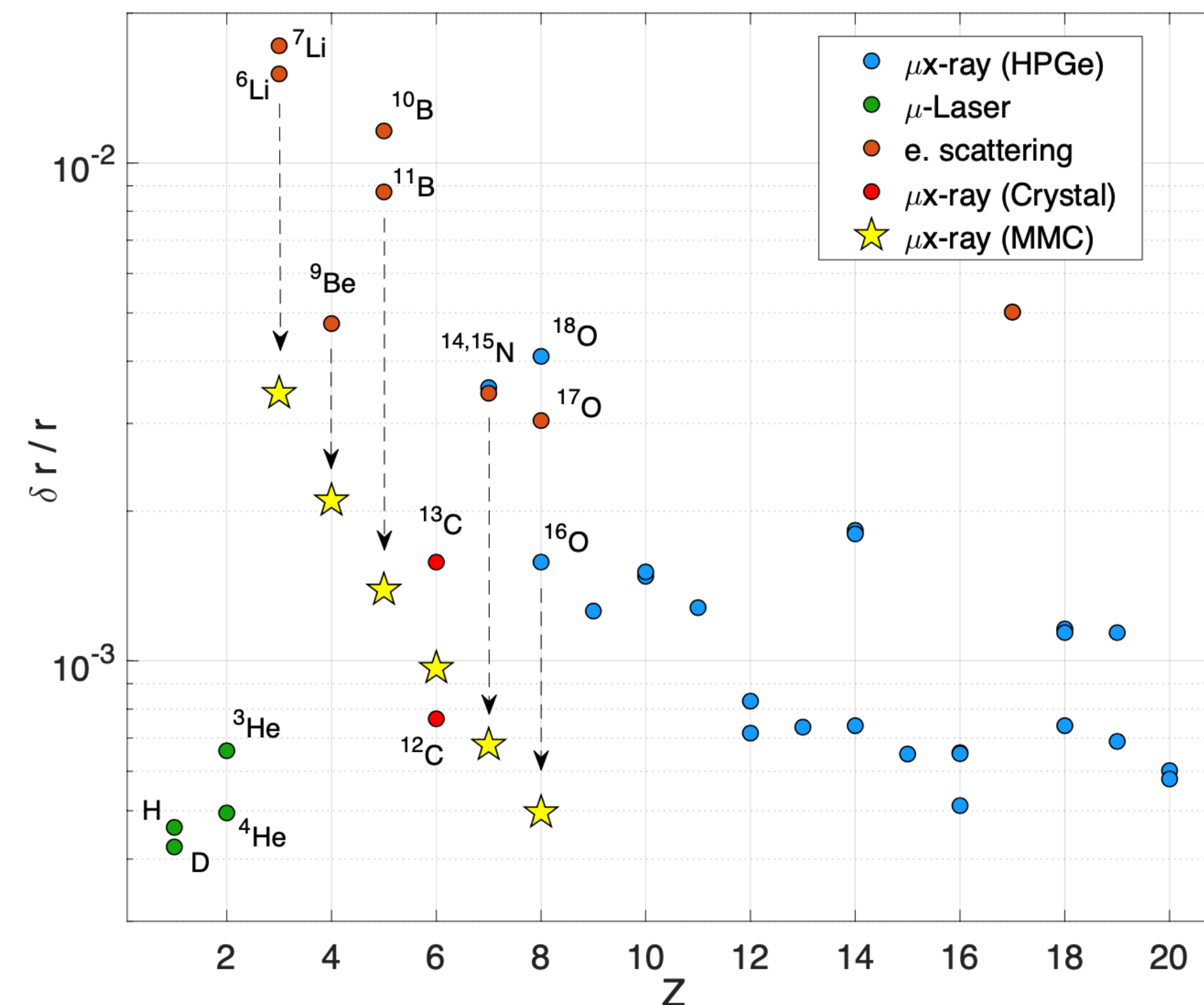
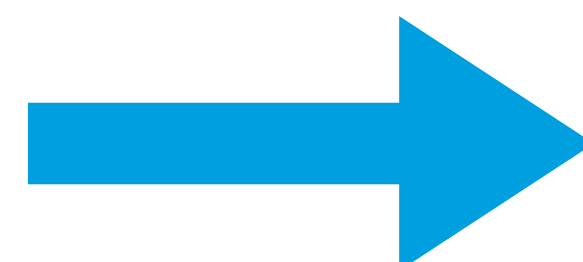
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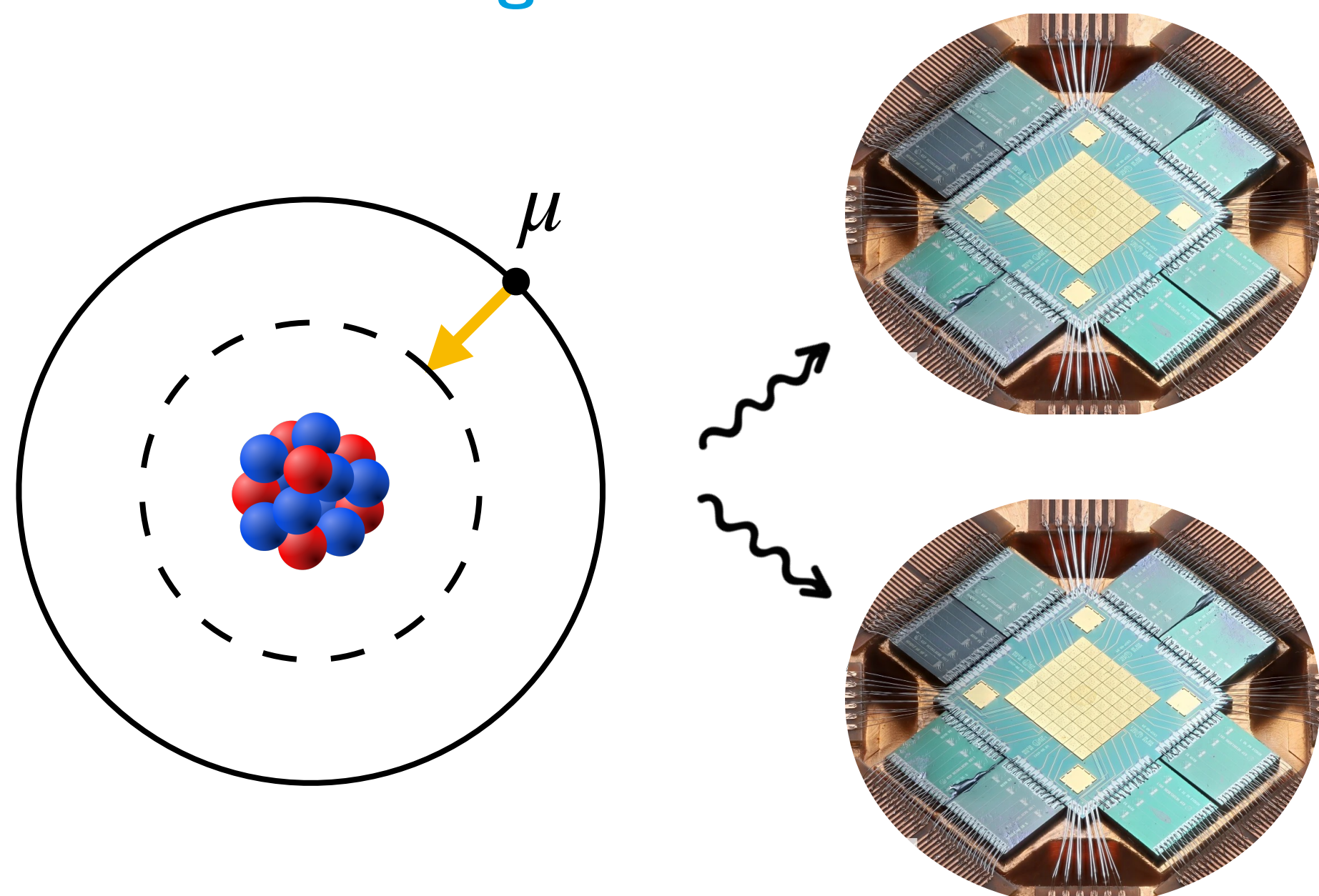


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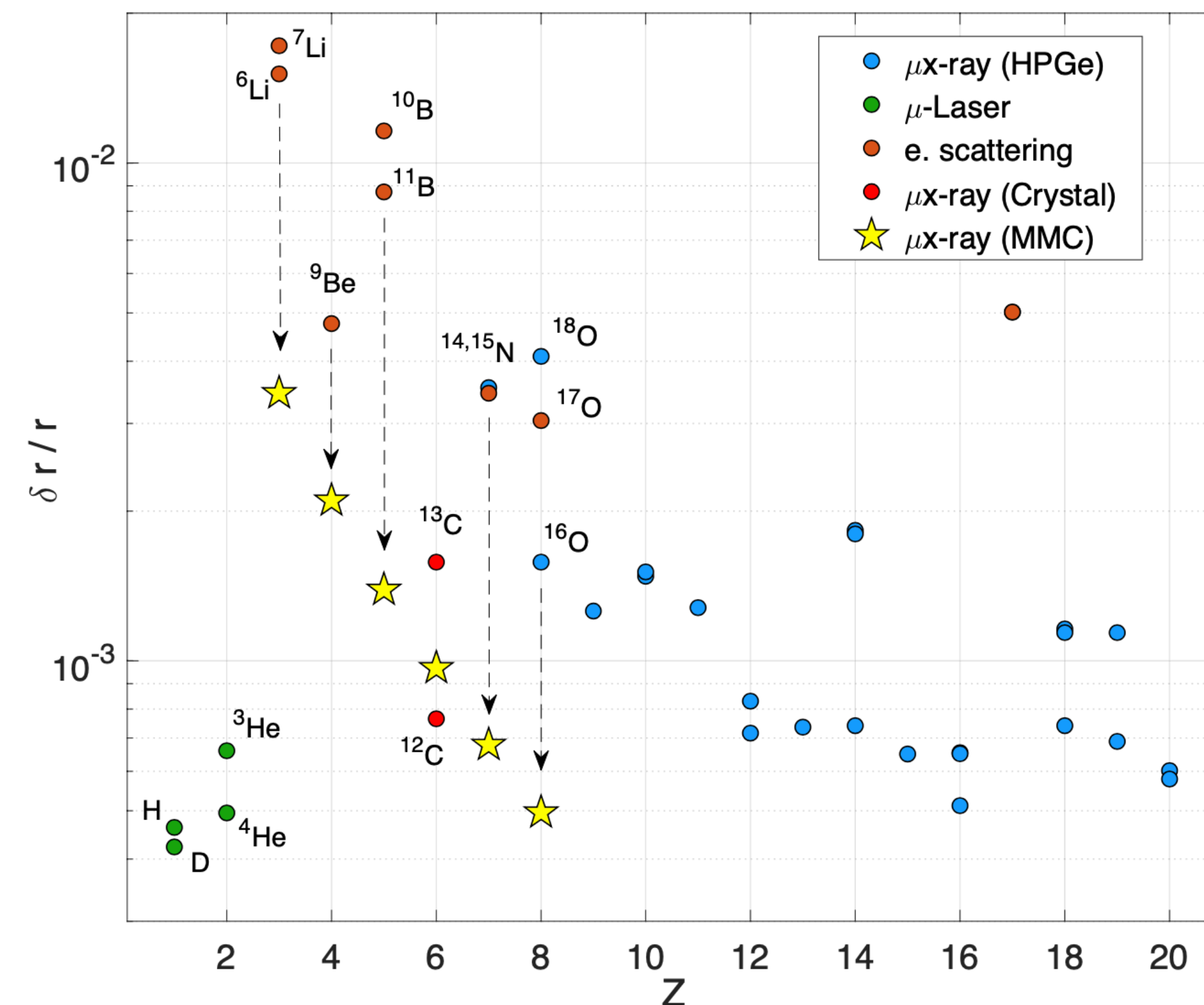
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- Theoretical challenge:** reach 10 meV uncertainty!
- Nuclear physics:** μ -atom reference \Rightarrow Isotopic chain
- On-going puzzles:** $\sim 3.5\sigma$ for ${}^{3-4}\text{He}$ isotope shift

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
 - Can be used to extract **nuclear structure information** like r_c
 - 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)

[Antognini et al, SciPost (2021)]

$$\Delta E(\mu\text{H}) = 206.0336(15) - 5.2275(10) \times r_p^2 + 0.0332(20)$$

$$\Delta E(\mu\text{D}) = 228.7767(10) - 6.1103(3) \times r_D^2 + 1.7449(200)$$

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General many-body problem

- Main degrees of freedom
 - Nucleons $\rightarrow N$; photon $\rightarrow A$; Muon $\rightarrow \psi_\mu$

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- For simplicity assume non-relativistic nucleons of equal mass

$$\begin{aligned} H = & H_{Nucl} + e \int d^3x J_\mu(x) A^\mu(x) \\ & + \frac{e^2}{2m} \int d^3x d^3y f_{SG}(x, y) \vec{A}(x) \cdot \vec{A}(y) \\ & + H_{QED} \end{aligned}$$

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- General approach to compute bound state of H

- ✗ In principle use Bethe-Salpeter \Rightarrow bound states $\equiv G_n$ poles

- ✓ In practice use **effective external potential**

- Corrections up to $(Z\alpha)^5$ to match exp accuracy

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Radius extraction master formula

$$\delta_{\text{LS}} = \delta_{\text{QED}} + \mathcal{C} r_c^2 + \delta_{\text{NS}}$$

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Simple point-like nucleus

Finite nucleus size effect

Nuclear structure dependent

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Bound states QED contributions

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Bound muon within potential

- Zero-order: external Coulomb potential

- Solve exactly for $H_0 = \frac{\vec{p}^2}{2m_r} - \frac{Z\alpha}{r}$
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● What effective potential to apply on muon ?

- **Effective potential** as perturbation away from Coulomb
- Defined to **match QED** scattering at a given order
- Bound-state \Rightarrow **Distorted Wave Born approximation**

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

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● Main type of QED contributions

- Electron vacuum polarization: $a_\mu \sim \lambda_e \Rightarrow$ **main one!**
- Finite nuclear mass \Rightarrow recoil and relativistic corrections
- Finite nuclear size contributions \Rightarrow Main one $\propto r_c^2$

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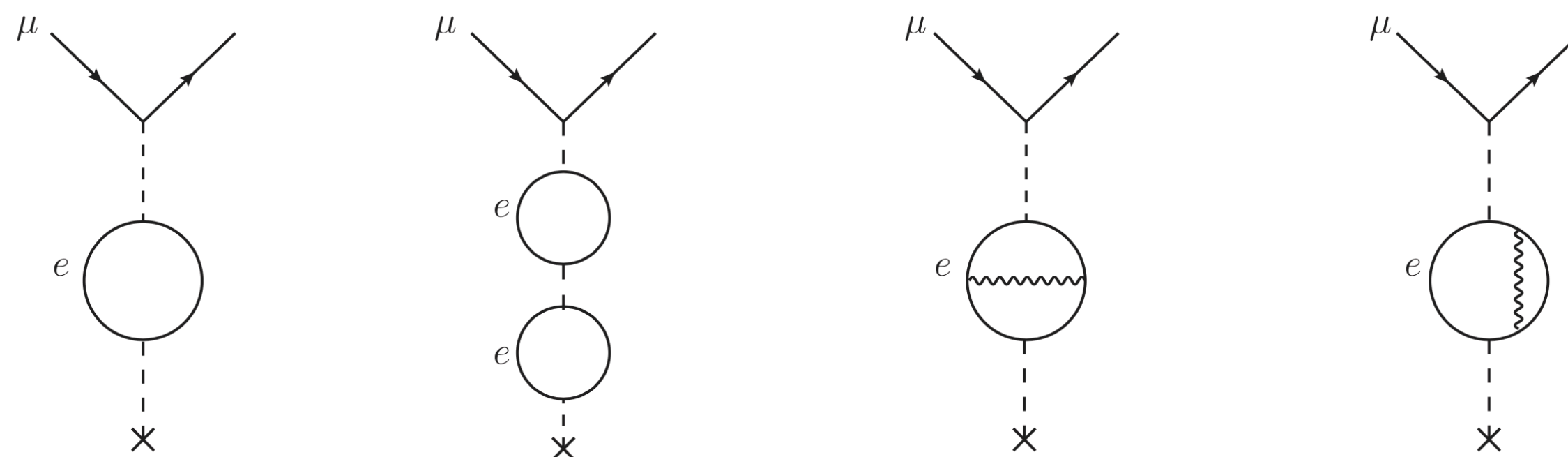
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Example: electron vacuum polarization corrections

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

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$\Rightarrow \delta_{\text{QED}}$ term in δ_{LS}

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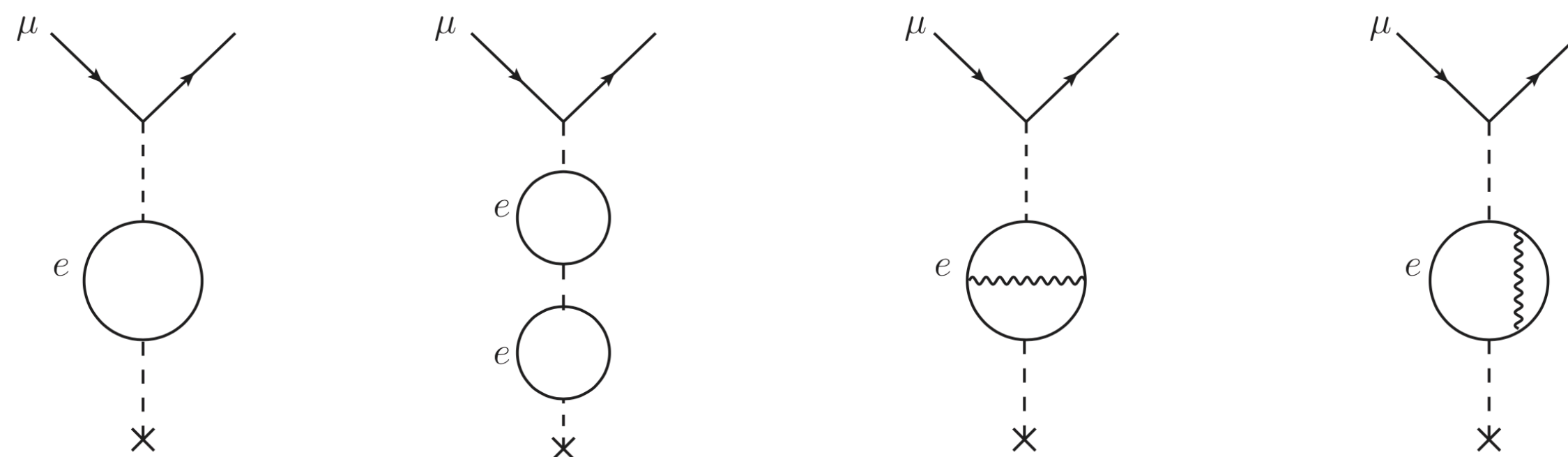
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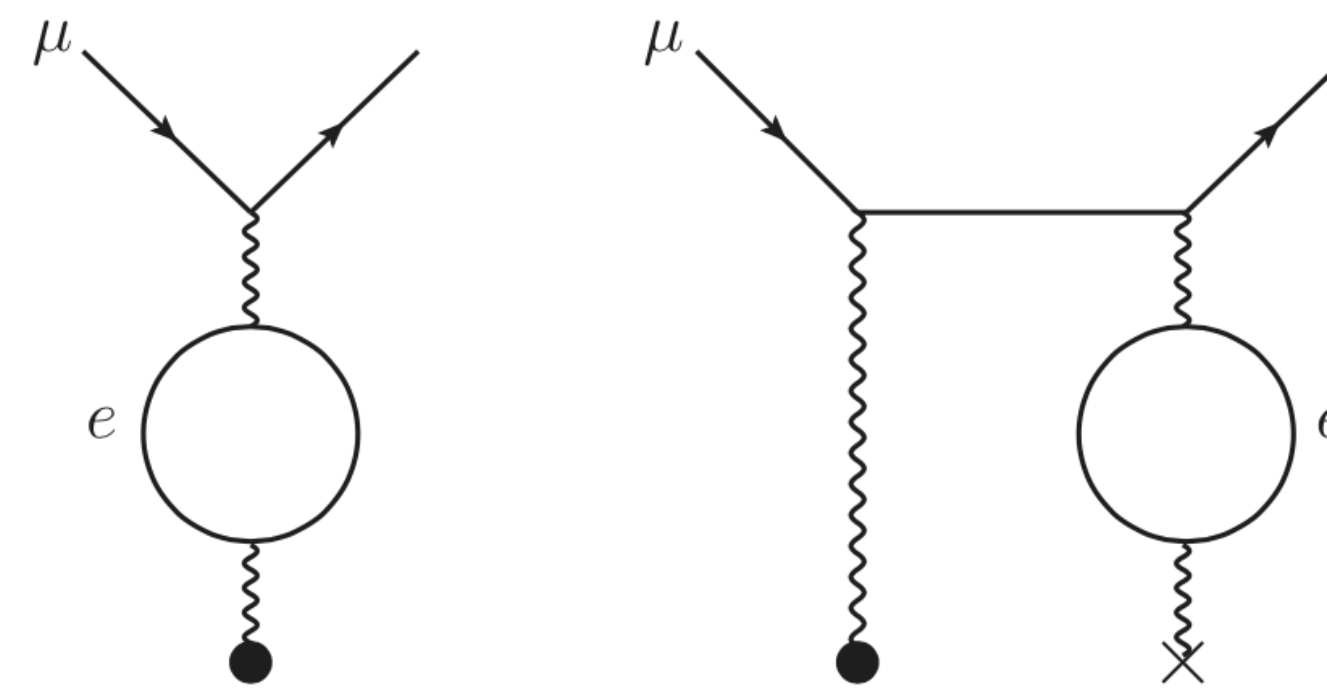
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$\Rightarrow \delta_{\text{QED}}$ term in δ_{LS}

Example: finite-size corrections

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



$\Rightarrow \mathcal{O}r_c^2$ term in δ_{LS}

Bound states QED contributions

7

Section	Order	Correction	μH	μD	$\mu^3\text{He}^+$	$\mu^4\text{He}^+$
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
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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	$\alpha(Z\alpha)^4$	$\mu\text{SE}^{(1)} + \mu\text{VP}^{(1)}$, LO	-0.663 45	-0.769 43	-10.652 5	-10.926 0
III.G	$\alpha(Z\alpha)^5$	$\mu\text{SE}^{(1)} + \mu\text{VP}^{(1)}$, NLO	-0.004 43	-0.005 18	-0.174 9	-0.179 7
III.H	$\alpha^2(Z\alpha)^4$	$\mu\text{VP}^{(1)}$ with eVP ⁽¹⁾	0.000 13	0.000 15	0.003 8	0.003 9
III.I	$\alpha^2(Z\alpha)^4$	$\mu\text{SE}^{(1)}$ 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	$\alpha^2(Z\alpha)^4$	$\mu F_1^{(2)}, \mu F_2^{(2)}, \mu\text{VP}^{(2)}$	-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)


The two-photon exchange nuclear correction

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NS correction: $\delta_{\text{NS}} = \delta_{\text{TPE}} + \delta_{\text{3PE}} + \dots$

The two-photon exchange nuclear correction

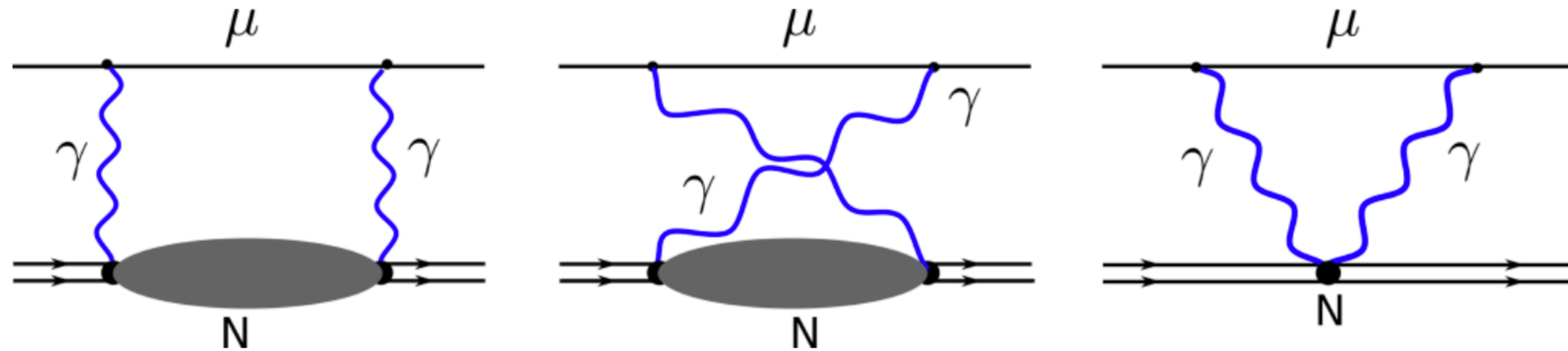
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$$\delta_{LS} = \delta_{QED} + \mathcal{O}(r_c^2) + \delta_{NS}$$



NS correction: $\delta_{NS} = \delta_{TPE} + \delta_{3PE} + \dots$

Two photon exchanges contributions



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

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The two-photon exchange nuclear correction

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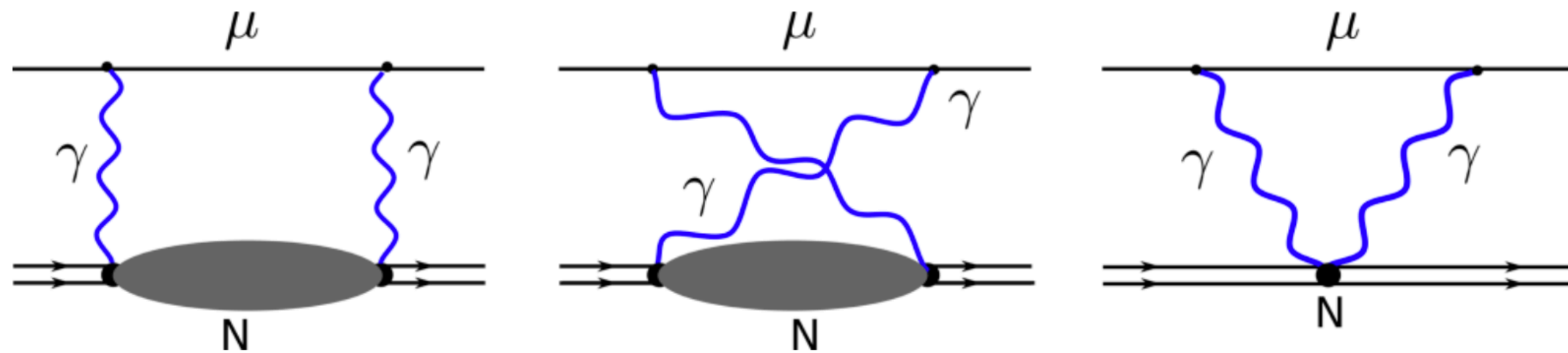
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$$T_{\mu\nu}(q) = \delta_{\mu\nu} \left\langle \Psi \left| \int d^3x e^{iq \cdot x} f_{SG}(x, 0) \right| \Psi \right\rangle + \sum_{N \neq 0} \left[\frac{\langle \Psi | J_\mu(0) | N \vec{q} \rangle \langle N \vec{q} | J_\nu(0) | \Psi \rangle}{E_0 - E_N + q_0 + i\epsilon} + \frac{\langle \Psi | J_\nu(0) | N - \vec{q} \rangle \langle N - \vec{q} | J_\mu(0) | \Psi \rangle}{E_0 - E_N - q_0 + i\epsilon} \right]$$

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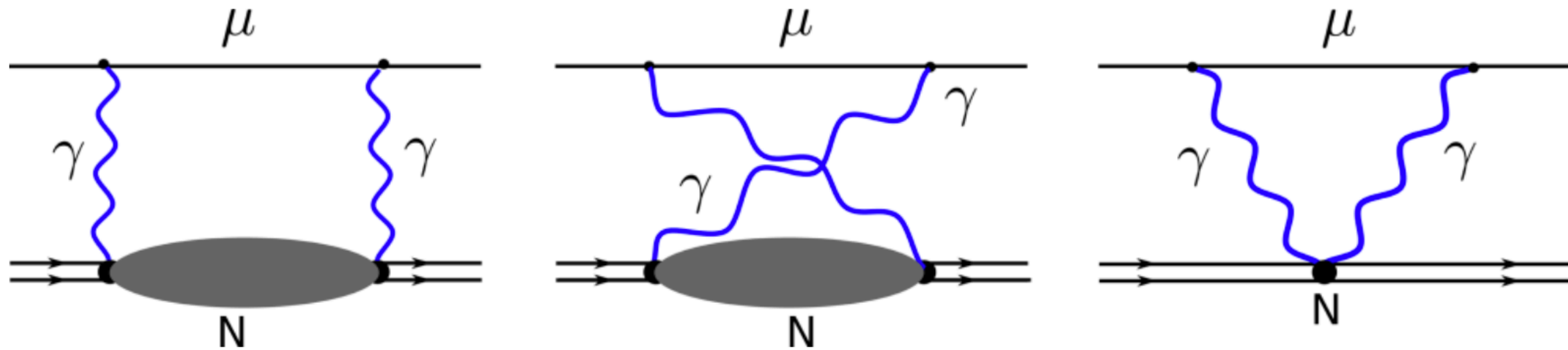
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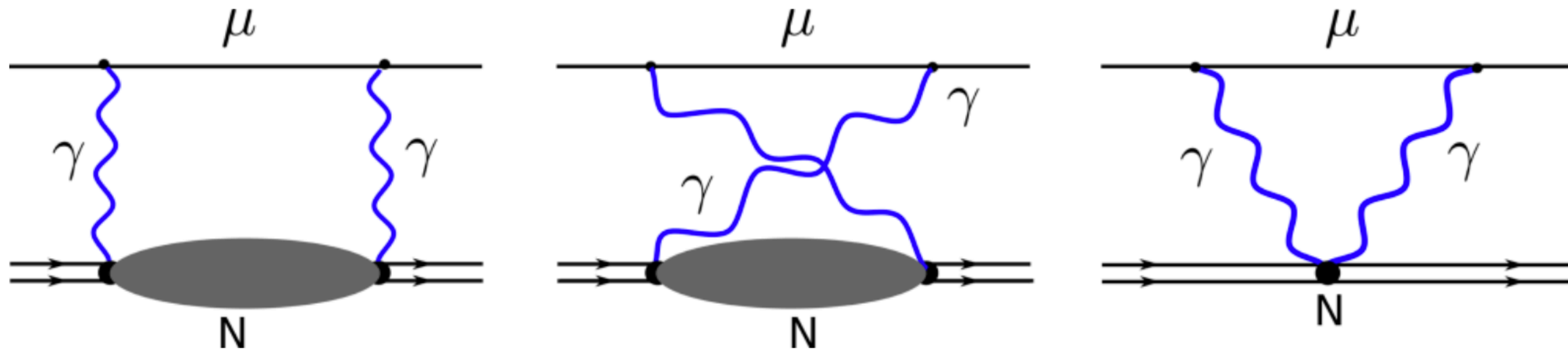
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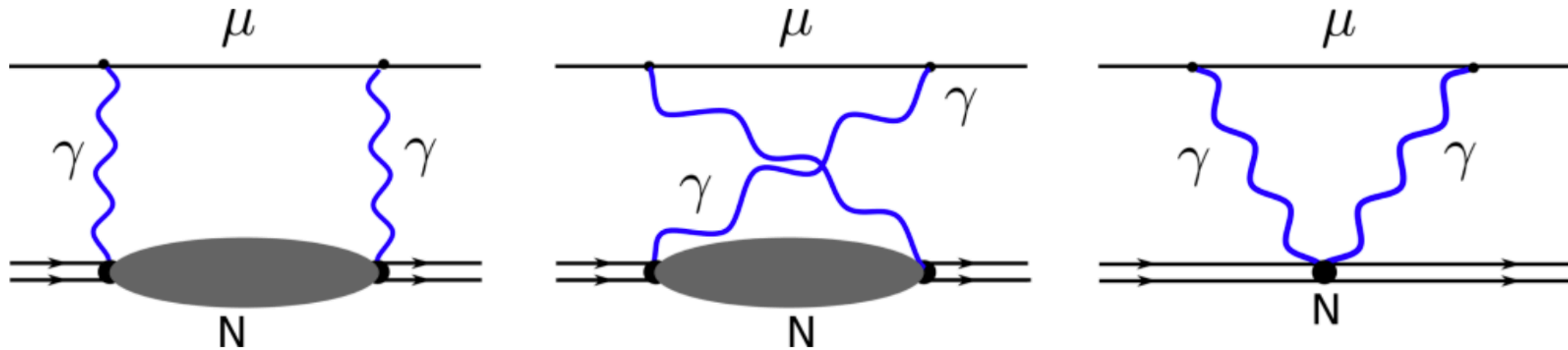
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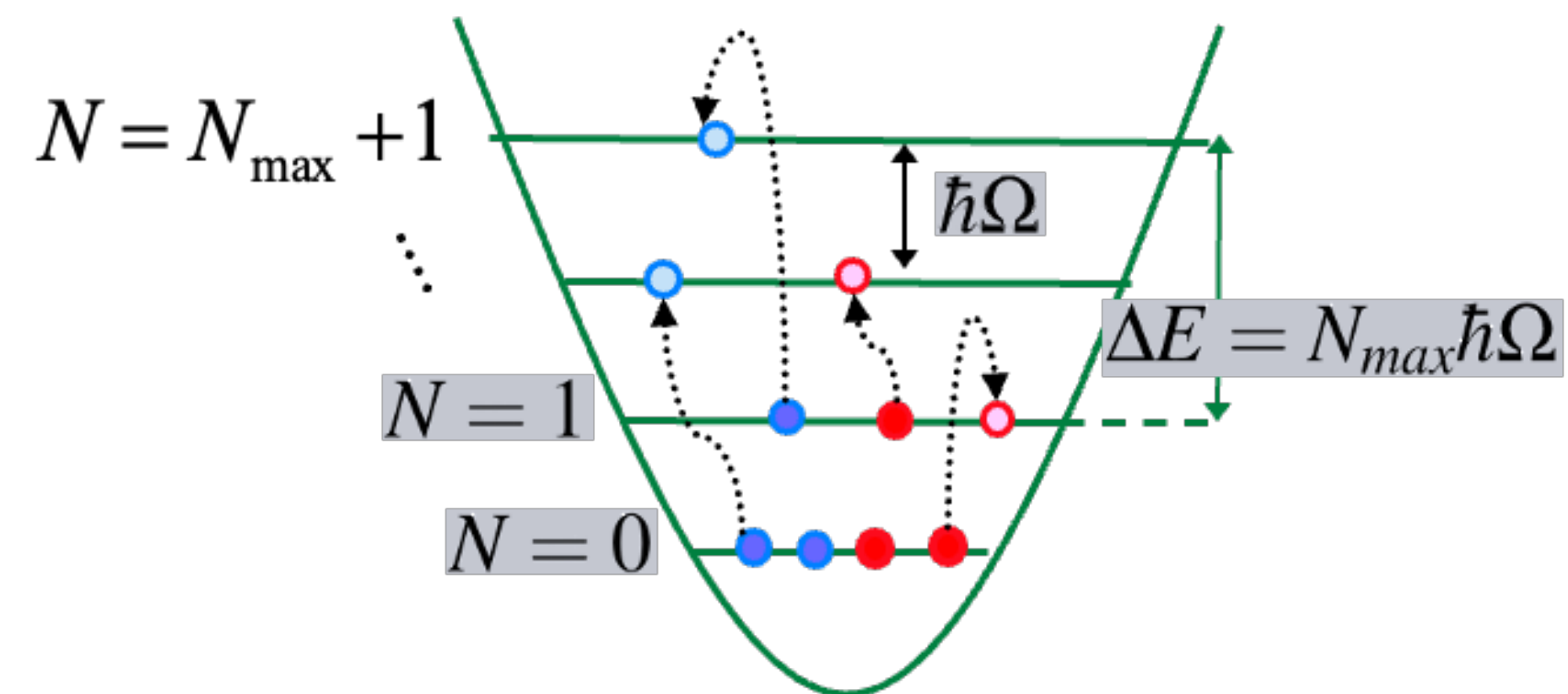
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Ab initio nuclear corrections



Nuclear physics modelling

Model used for nuclear currents

● Electromagnetic current modelling

- General one-body current for point-like particles
- Form factors given by the isovector dipole model

- $f_{SN}(q) = \left(1 + \frac{q^2}{M_V^2}\right)^{-2}$, $F_{1,2}^{(T)}(q) = F_{1,2}^{(T)}(0) f_{SN}(q)$

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- Vary many-body basis: (Ω, N_{\max})

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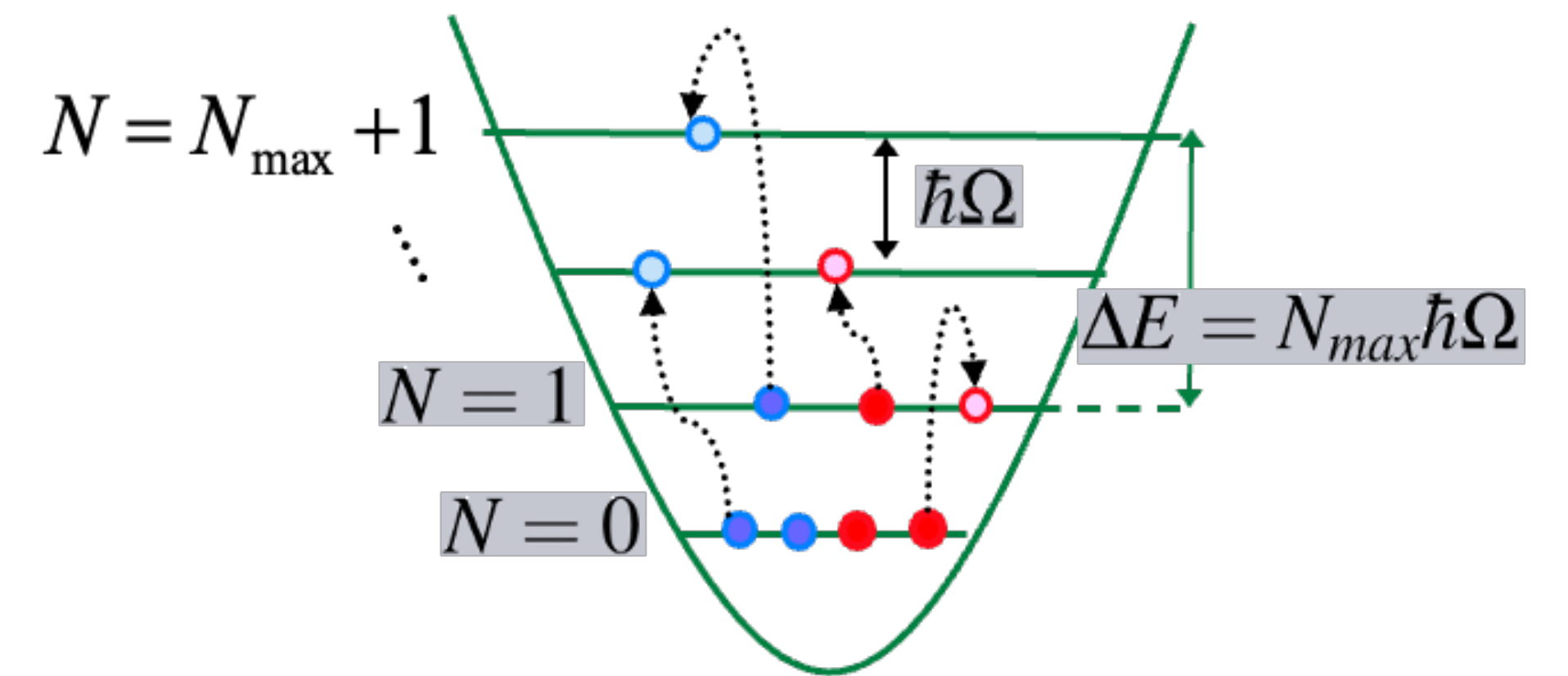
Many-body approximation

- No-Core Shell Model
- More details in next section

➔ Negligible many-body approximation uncertainty

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 $\langle\phi_{i+1}|\phi_{i+1}\rangle = 1$

● Output:

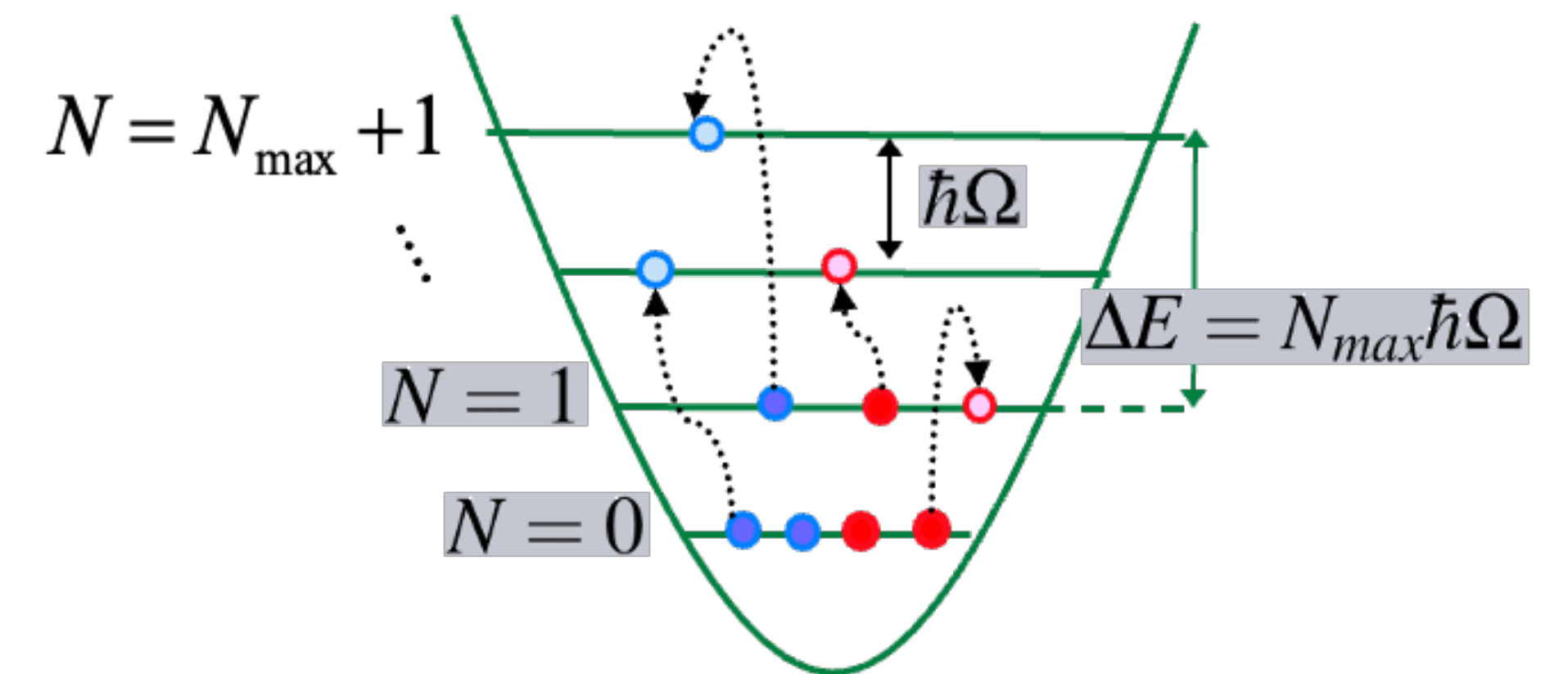
○ Lanczos basis and coefficients $\{|\phi_i\rangle, \alpha_i, \beta_i\}$

→ **H in Lanczos basis**

○ Lanczos basis \equiv orthonormal basis in Krylov space $\{|\phi_1\rangle, H|\phi_1\rangle, \dots, H^{N_L}|\phi_1\rangle\}$

$$\begin{pmatrix} \alpha_1 & \beta_2 & & & & & \\ \beta_2 & \alpha_2 & \beta_3 & & & & \\ & \beta_3 & \alpha_3 & \ddots & & & \\ & & \ddots & \ddots & \beta_{k-1} & & \\ & & & & \beta_{k-1} & \alpha_{k-1} & \beta_k \\ & & & & & \beta_k & \alpha_k \end{pmatrix}$$

Anti-symmetrized products of many-body HO states



The No-Core Shell Model

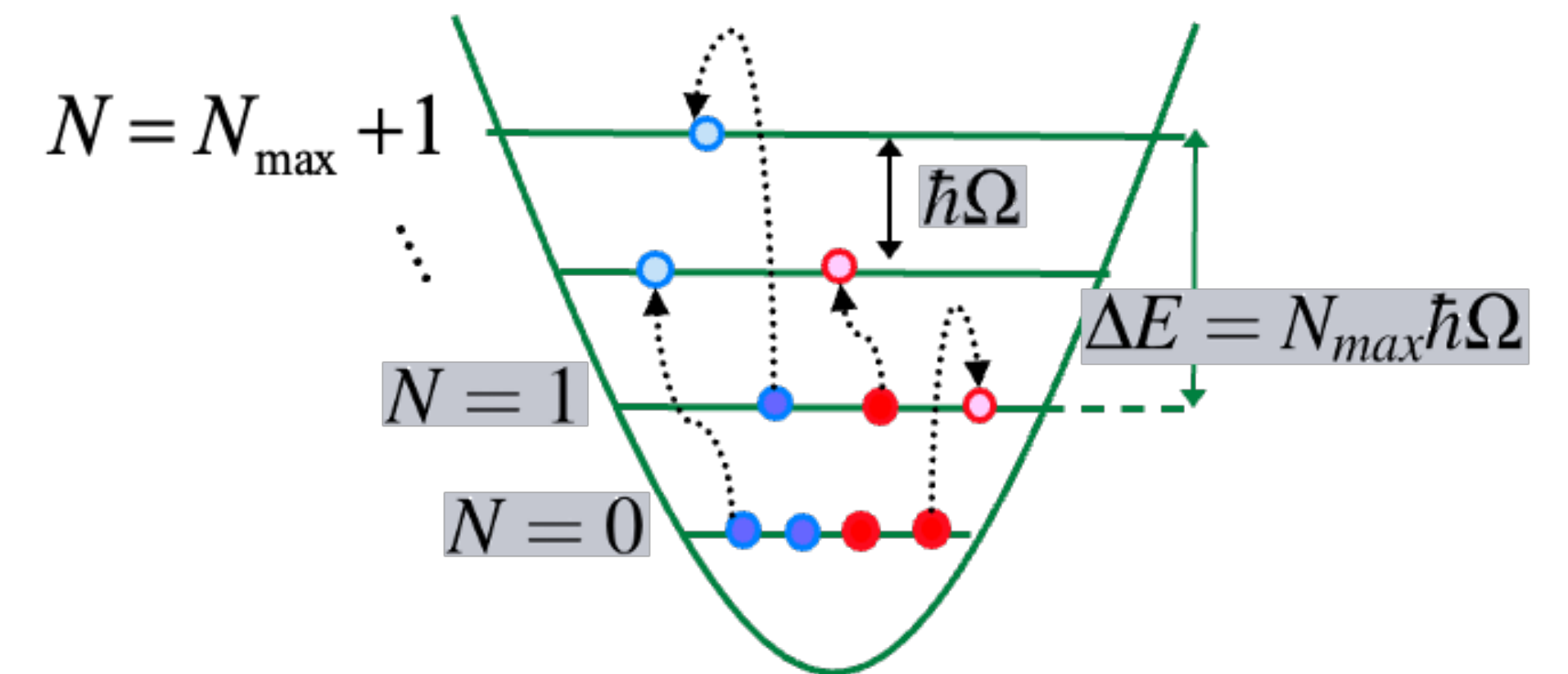
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Application to nuclear structure

- Efficient calculation of spectra
 - Selection rules sparsity \Rightarrow **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

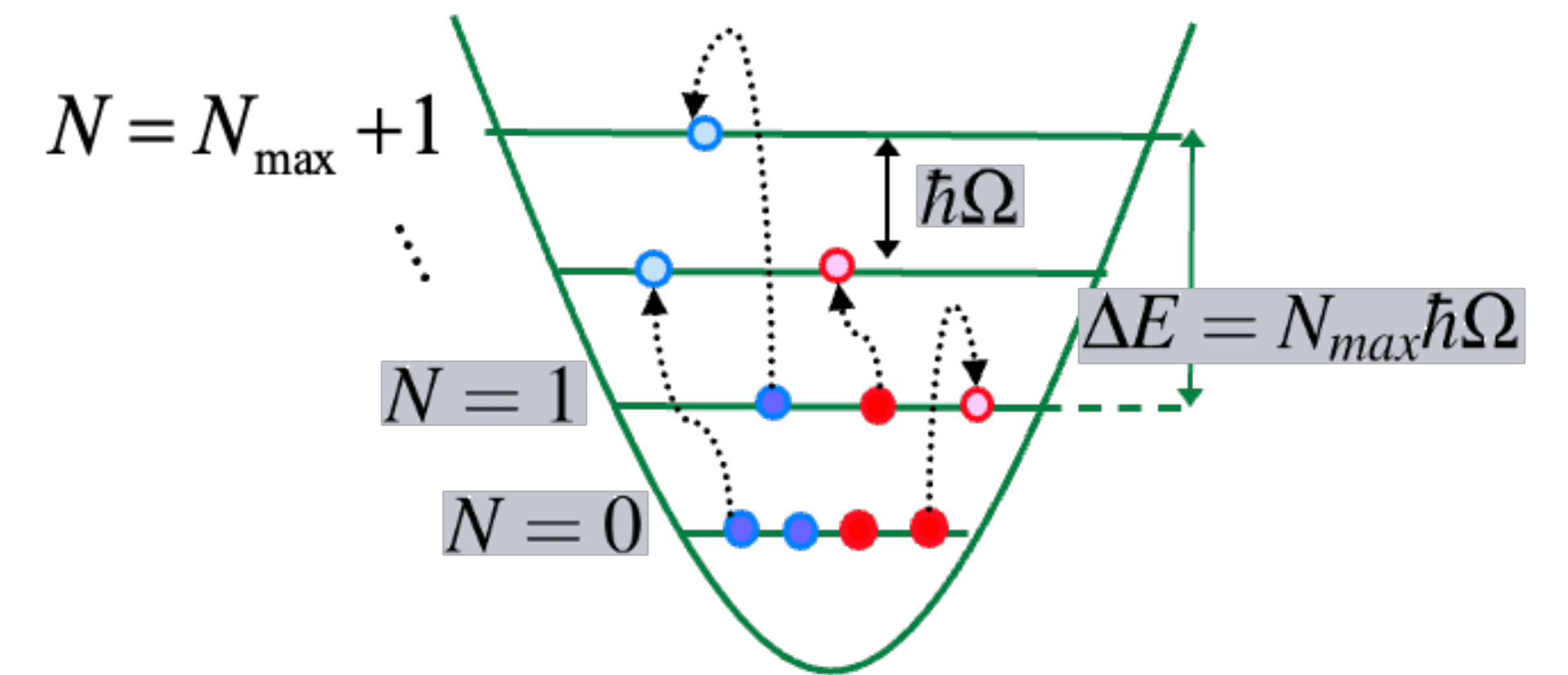
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Application to ${}^7\text{Li}$

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

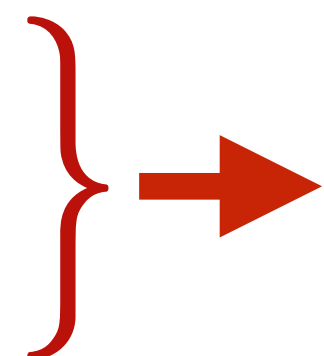
The Lanczos strength algorithm

Computing strength functions

• We need to compute for each eigenstate and operator:

• Eigenvalues: E_N

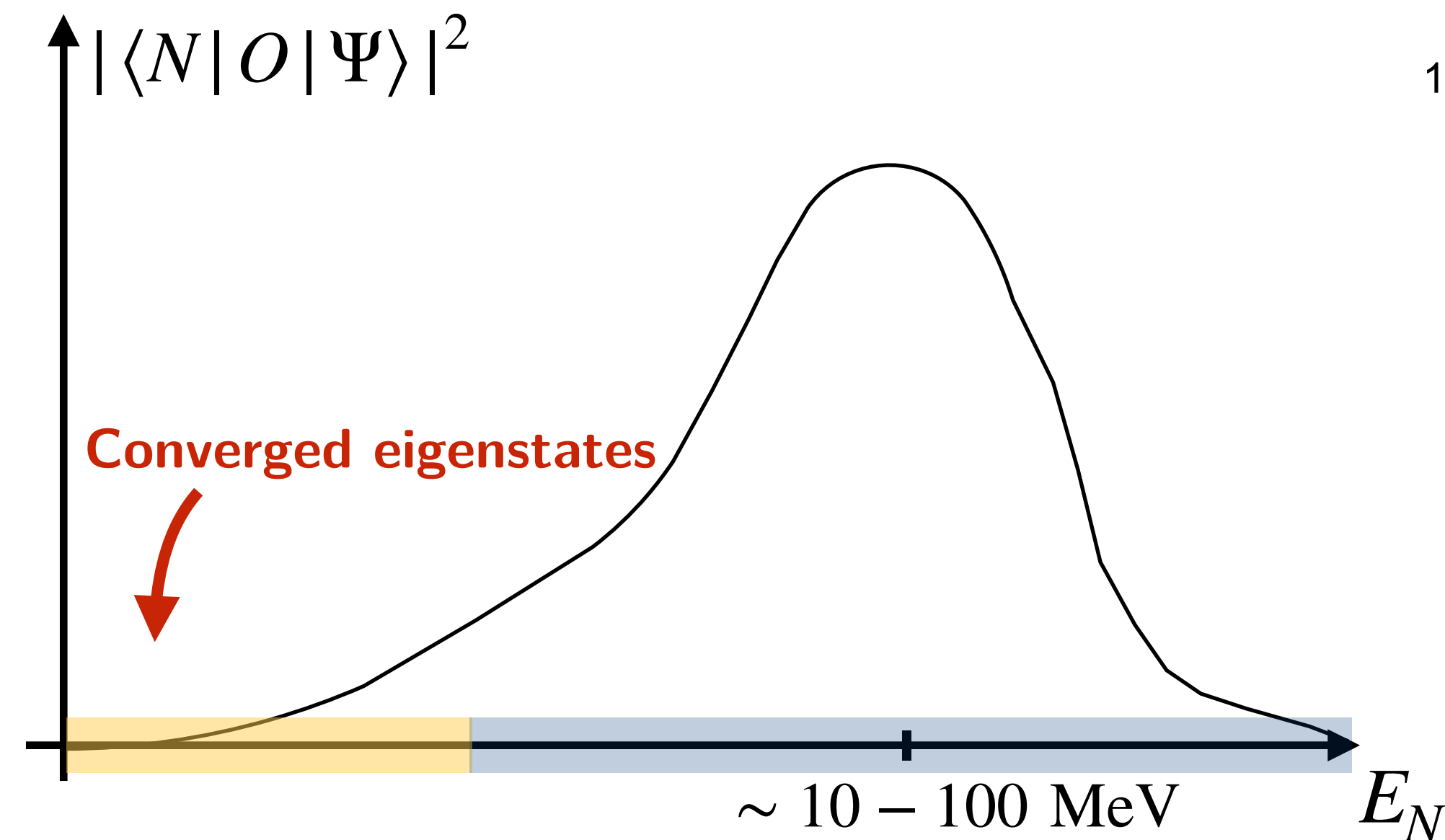
• Overlaps: $|\langle N|O|\Psi\rangle|^2$



Too expensive
to converge all of them !!

• Lanczos strength algorithm

• Variant of Lanczos: ensure convergence of **sum rules**



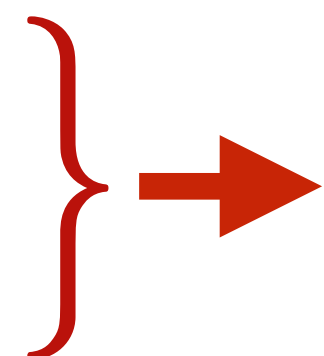
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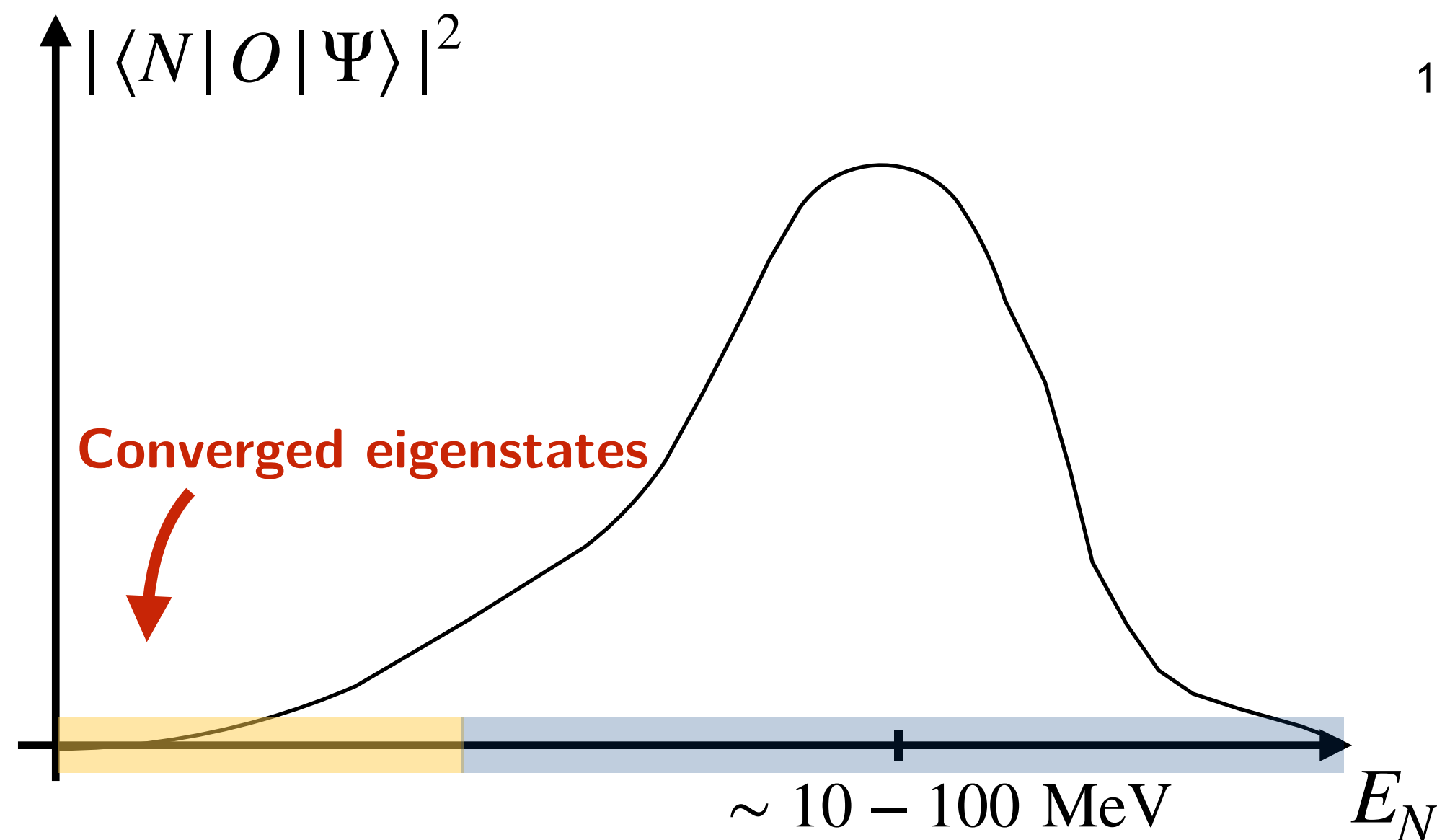
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Sum rules convergence

• Convergence problem

• Often the **strength is fragmented**

• Only low-lying states converged in general

• Lanczos strength algorithm

• Recover exactly $\int d\omega \omega^n S_O(\omega)$ for any $n \leq 2N_L$

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

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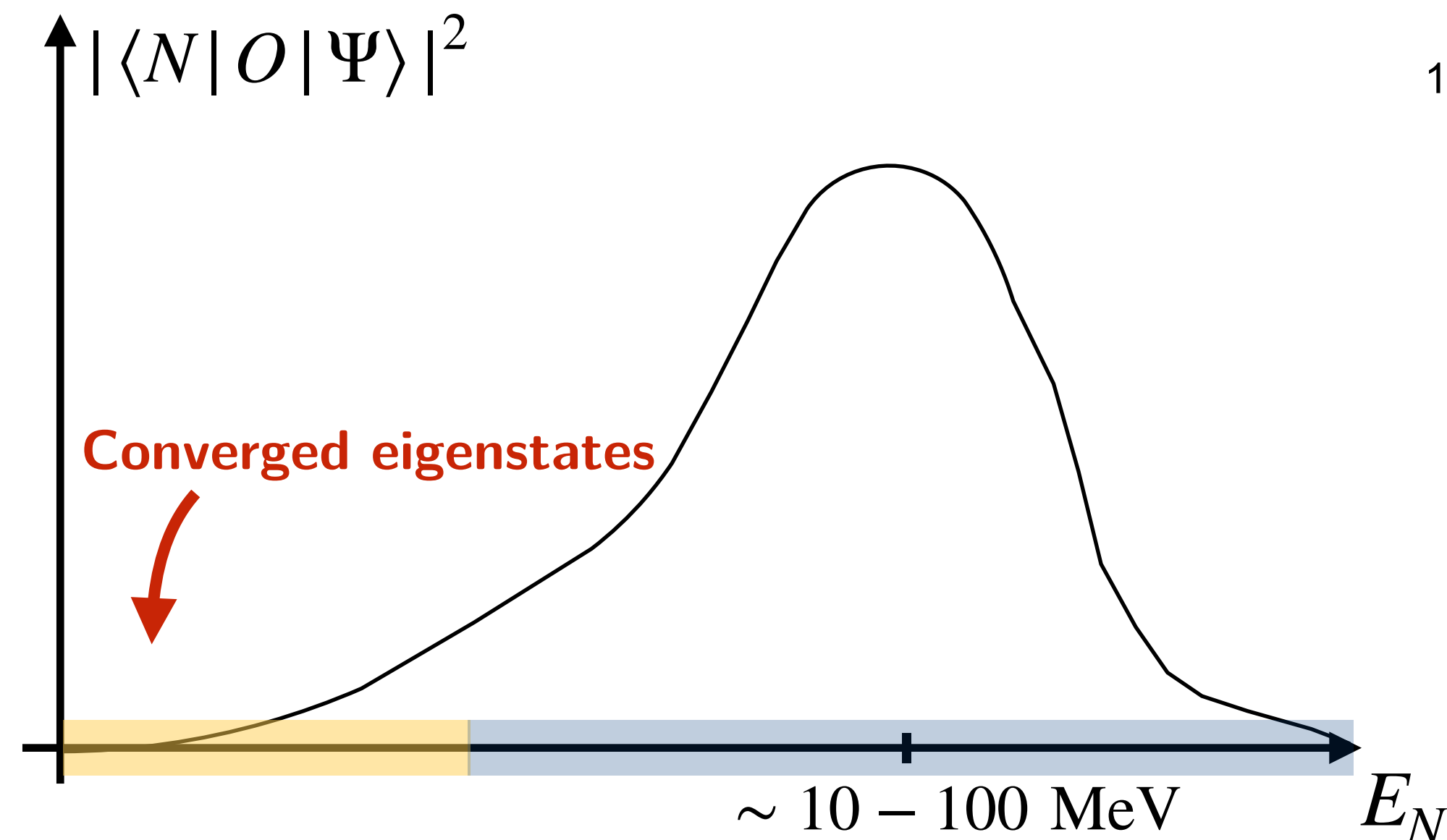
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Main idea of the algorithm

• For each operator O

• Compute $\frac{O|\Psi\rangle}{\sqrt{\langle\Psi|O^\dagger O|\Psi\rangle}} \Rightarrow$ **Pivot** $|\phi'_1\rangle$ for 2nd Lanczos

• Extract strength from orthonormality of Lanczos basis

• $|\langle\Psi|O|N\rangle|^2 = \langle\Psi|O^\dagger O|\Psi\rangle \times |\langle\phi'_1|N\rangle|^2$

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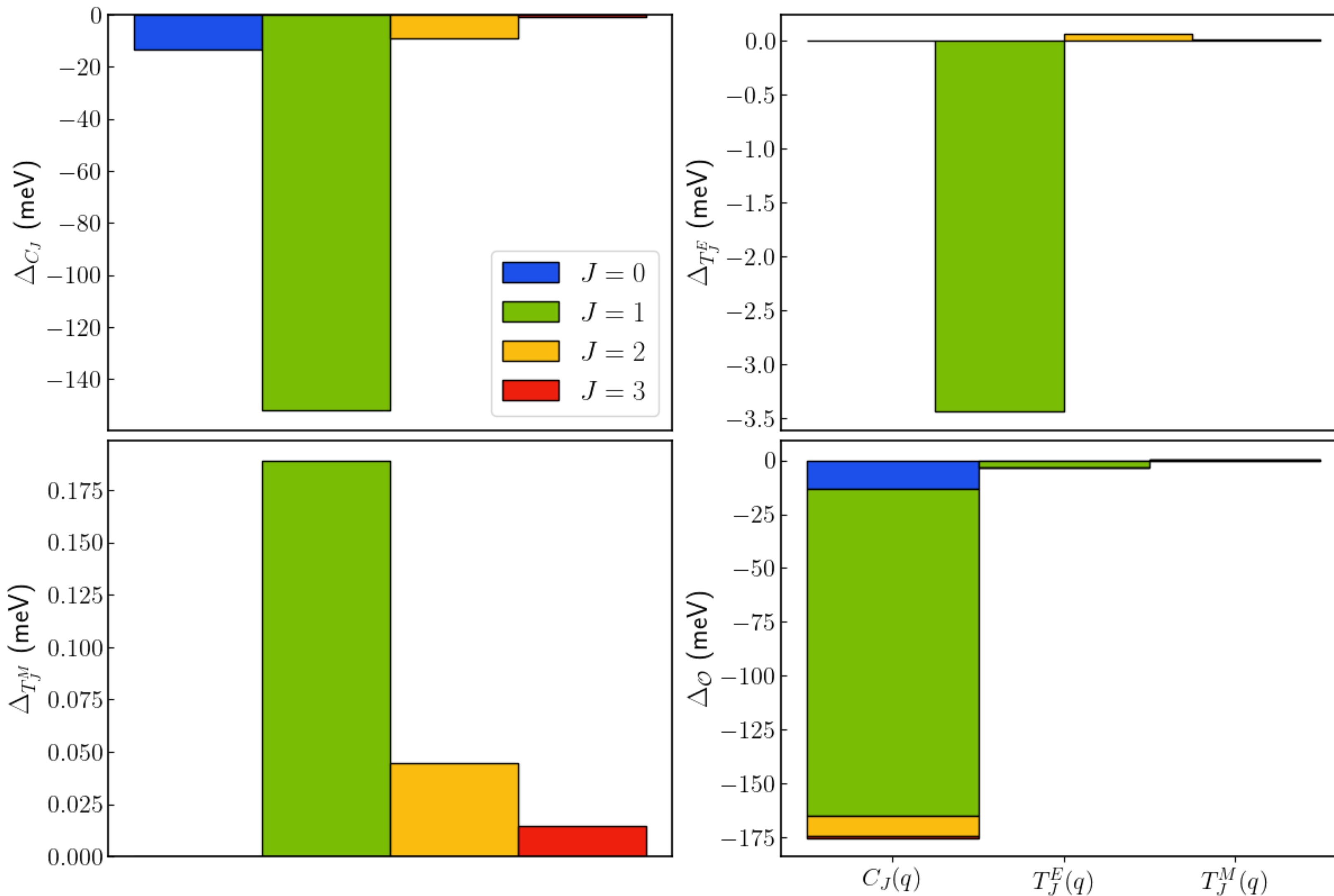
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A first test case for N4LO-E7 and $N_{\max} = 7$

Numerical calculations

- ⦿ $q_{\max} = 700$ MeV and $\Delta q = 10$ MeV
- ⦿ 10 different operators for $J_{\max} = 3$
- ➔ **700 NCSM calculations at $N_{\max} = 7$**

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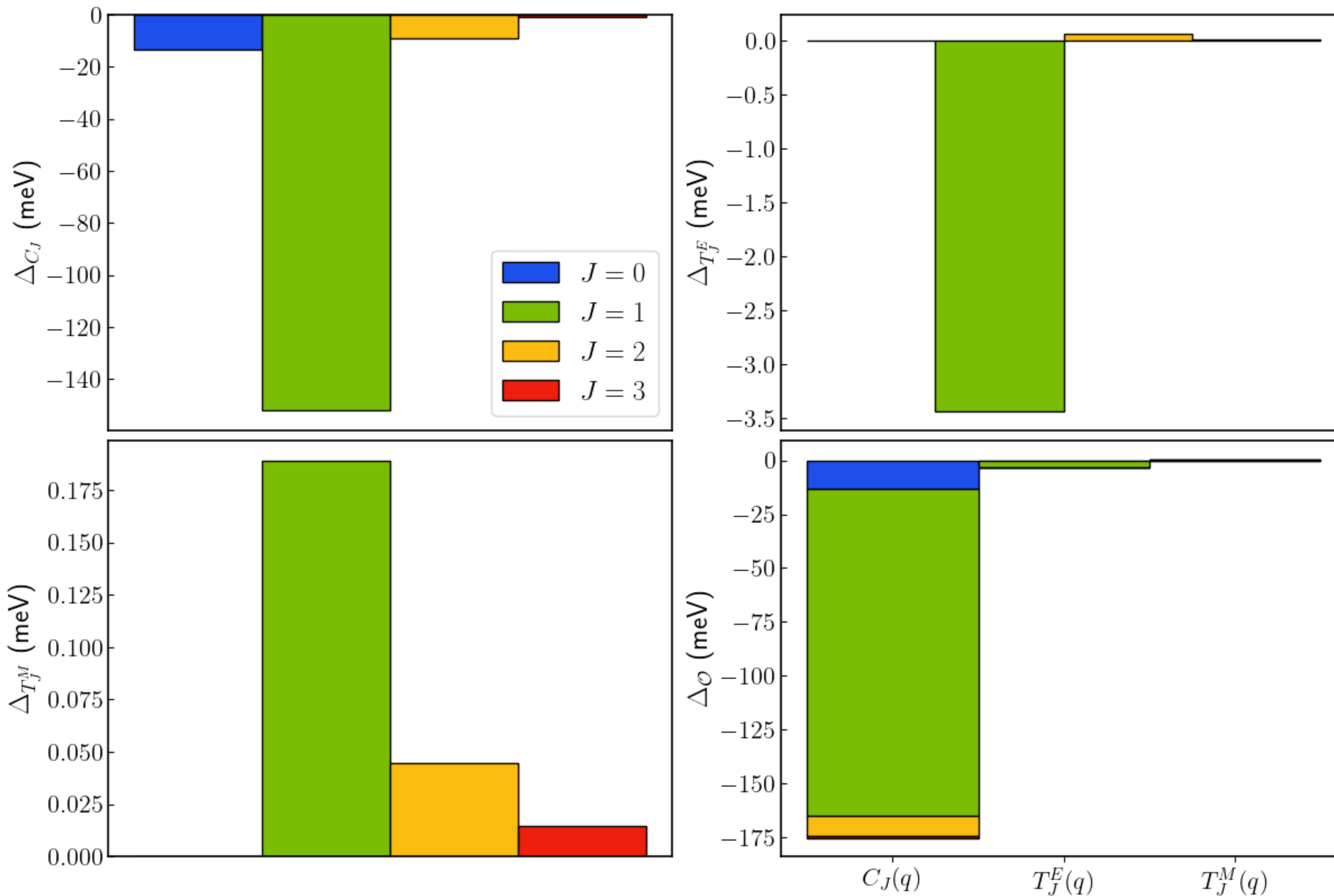


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13



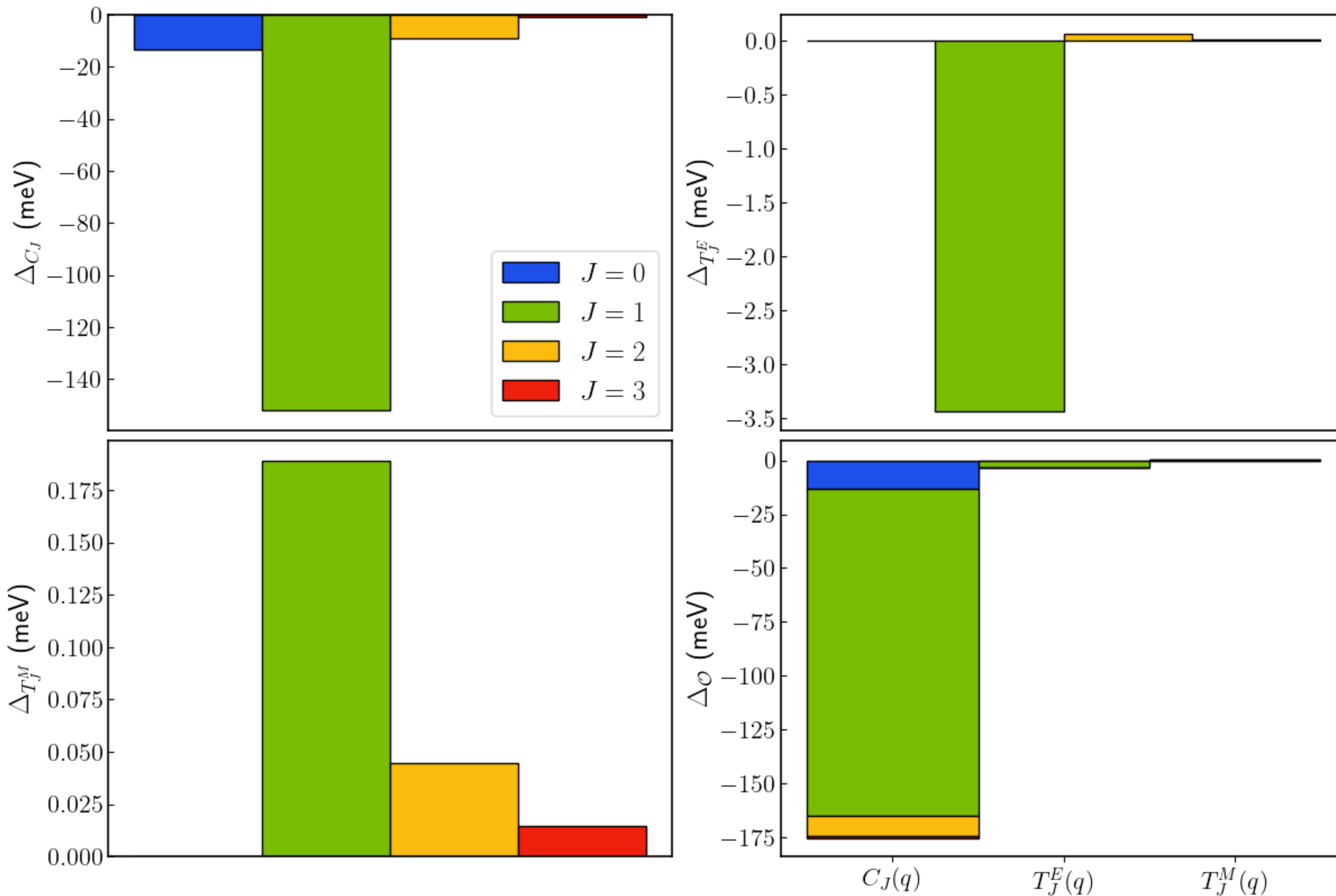
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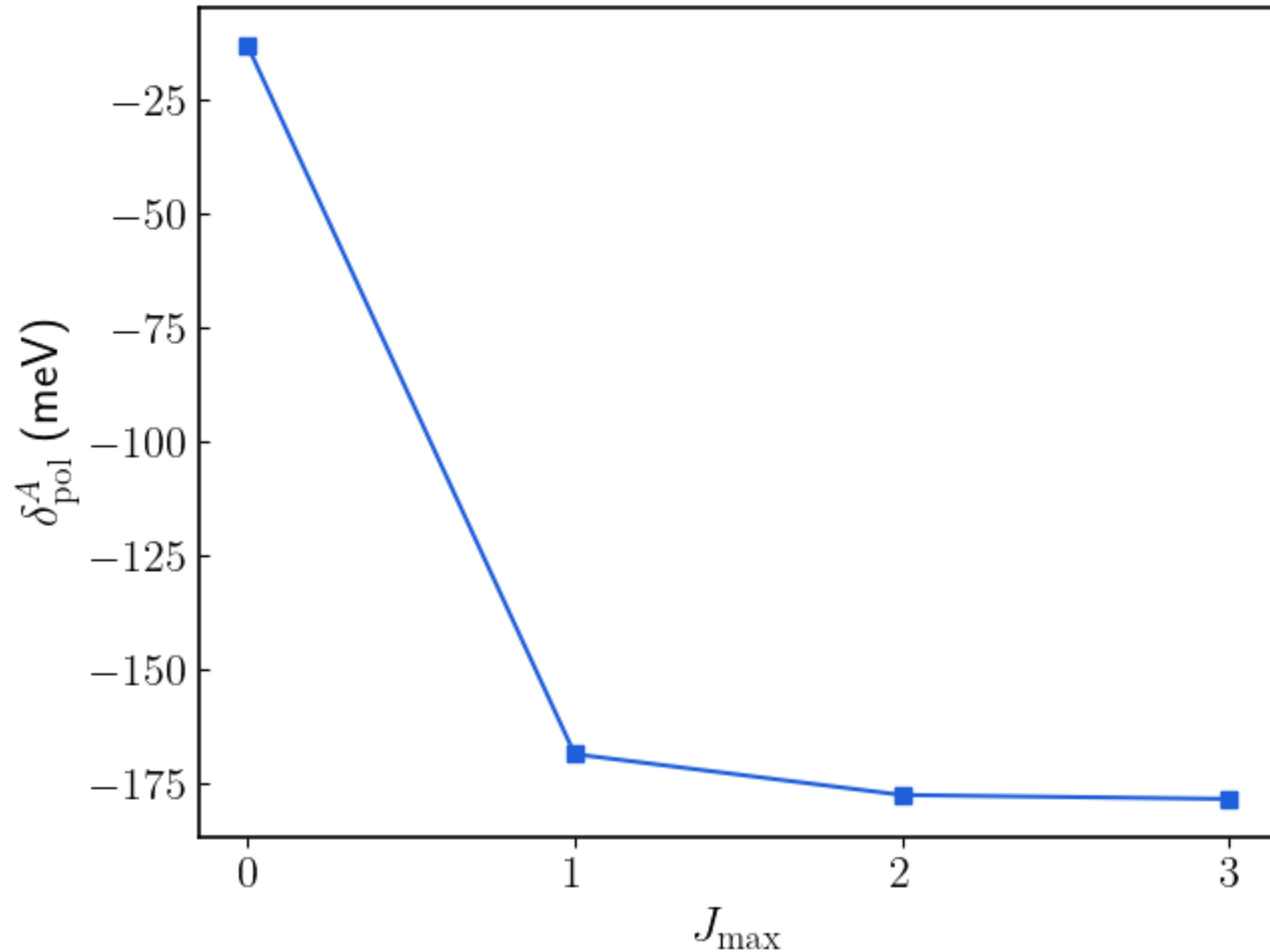
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 - Well-known **dipole** dominance
 - **Charge** contributions are dominant
- Negligible contributions
 - TM is negligible for any J
 - TE is relevant only for $J = 1$
- ➔ **Only half the operators are relevant**

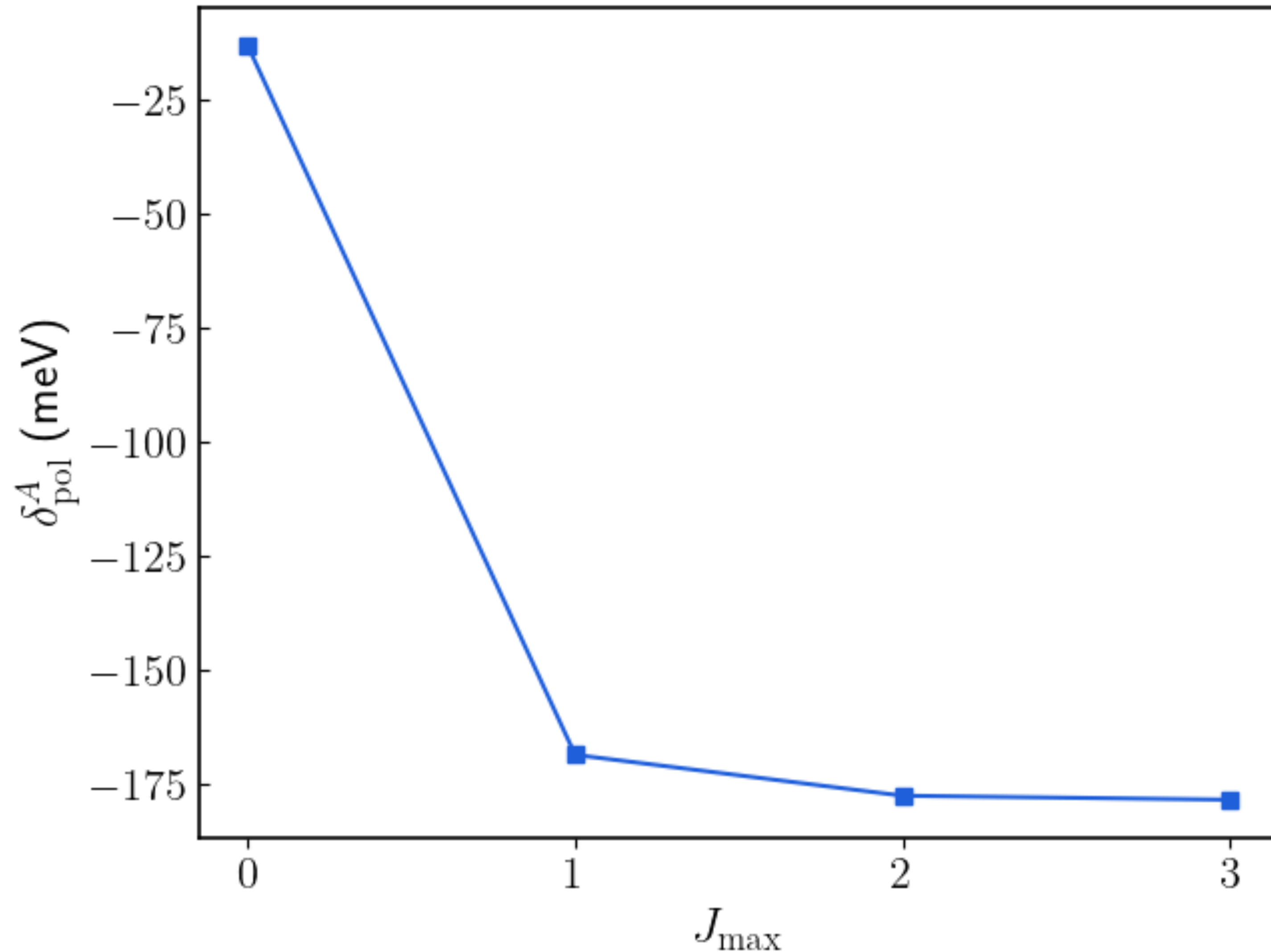
Checking convergence in J_{\max}



Results

- ⦿ Here shown for $N_{\max} = 7$ and N4LO-E7
- ⦿ All other cases are similar
- ➔ **Fast exponential convergence**

Checking convergence in J_{\max}



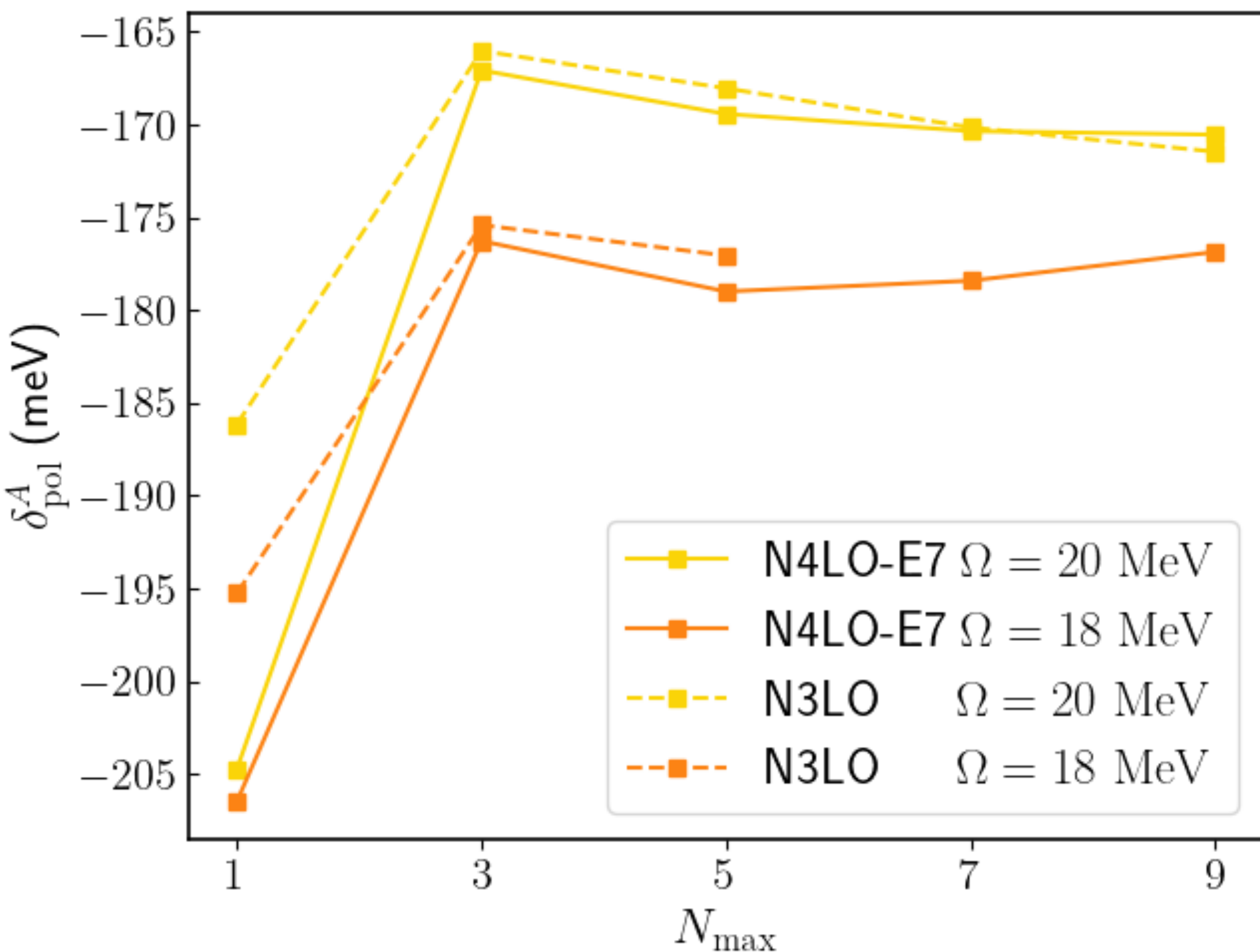
Results

- Here shown for $N_{\max} = 7$ and N4LO-E7
- All other cases are similar
- ➔ **Fast exponential convergence**

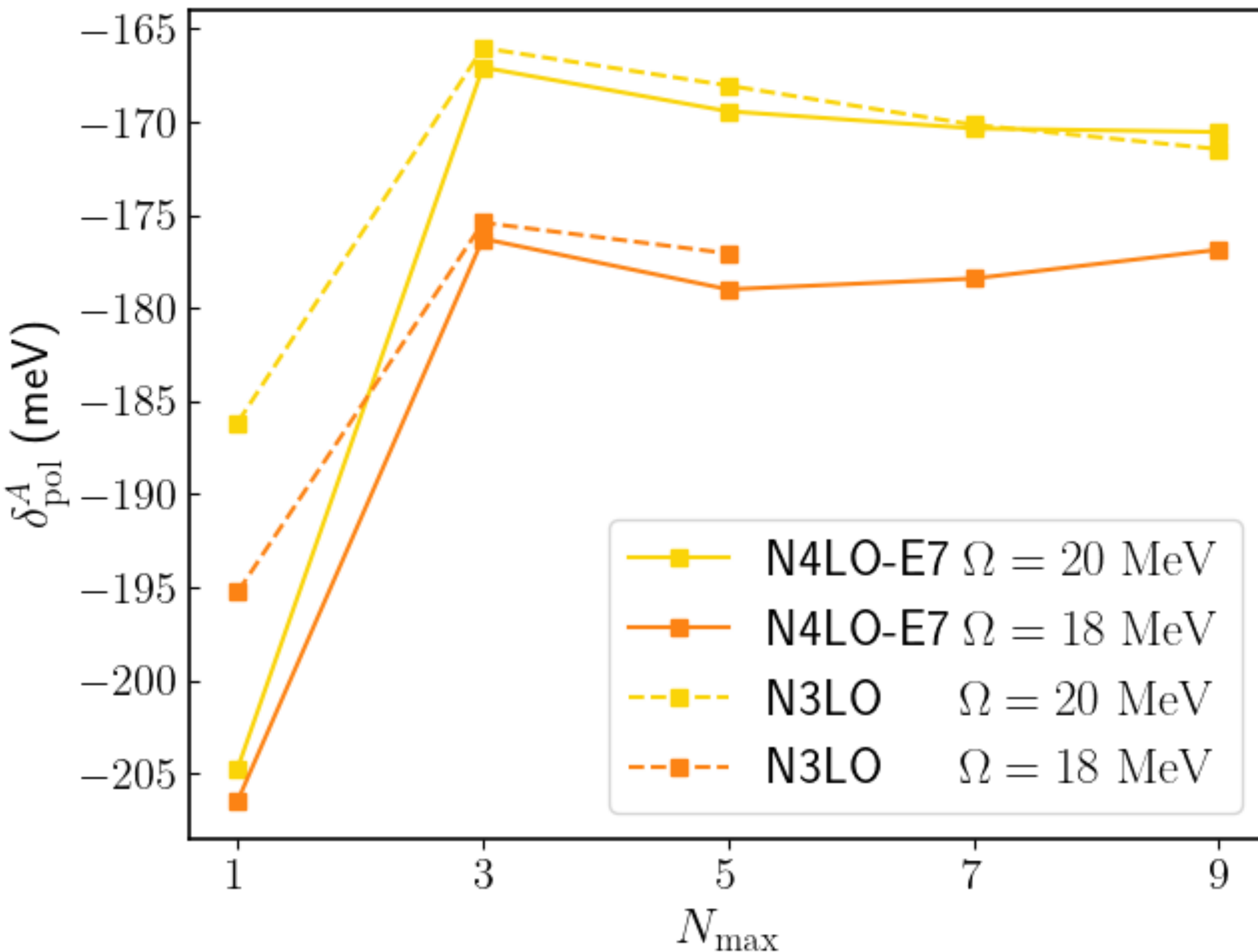
$$\epsilon_{J_{\max}} \lesssim 0.1 \text{ meV}$$

Multipole truncation \Rightarrow Negligible uncertainty

Dependence on (Ω, N_{\max}) and the interaction



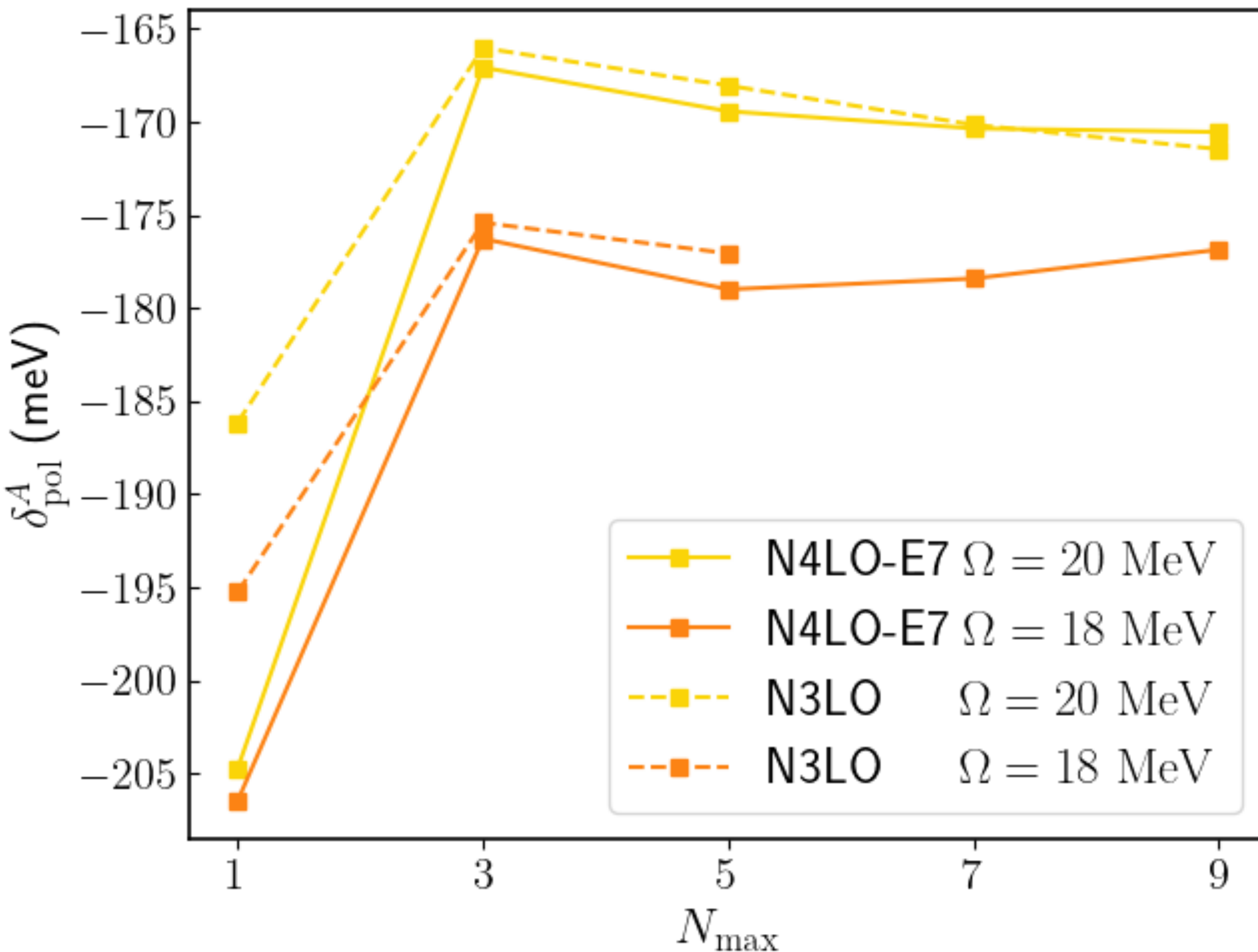
Dependence on (Ω, N_{\max}) and the interaction



Numerical results

- Model-space dependence
 - Optimal frequency around 20 MeV
 - Run calculations for $\Omega = 18, 20$ MeV
 - Truncations for $N_{\max} = 1 - 9$
- On-going (Ω, N_{\max}) dependence: $\epsilon_{(\Omega, N_{\max})} \simeq 5$ meV

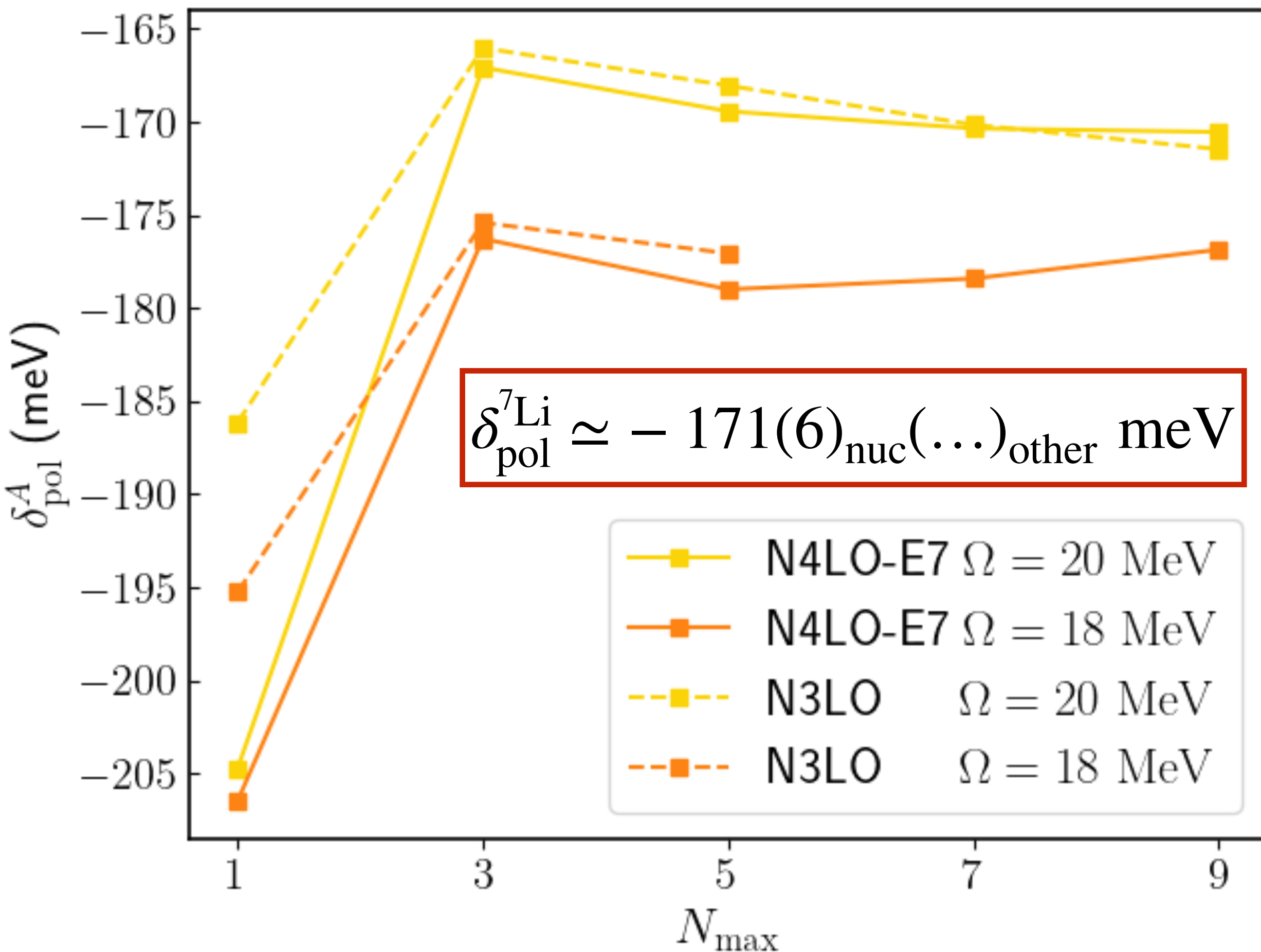
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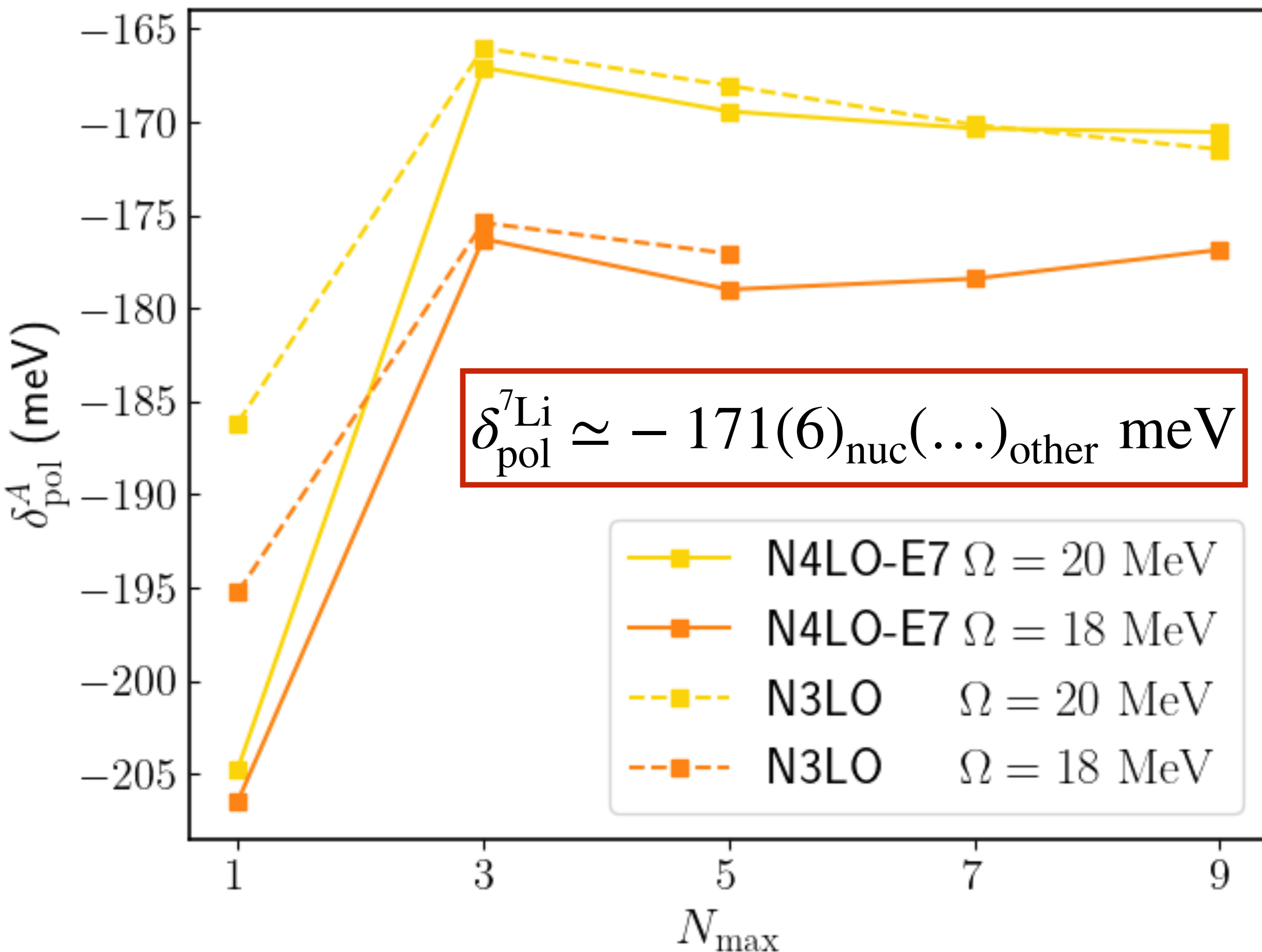
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A 10 meV precision for nuclear structure corrections seems doable in the near future!

Conclusion

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 - Elastic component: δ_{el}^A with NCSMC
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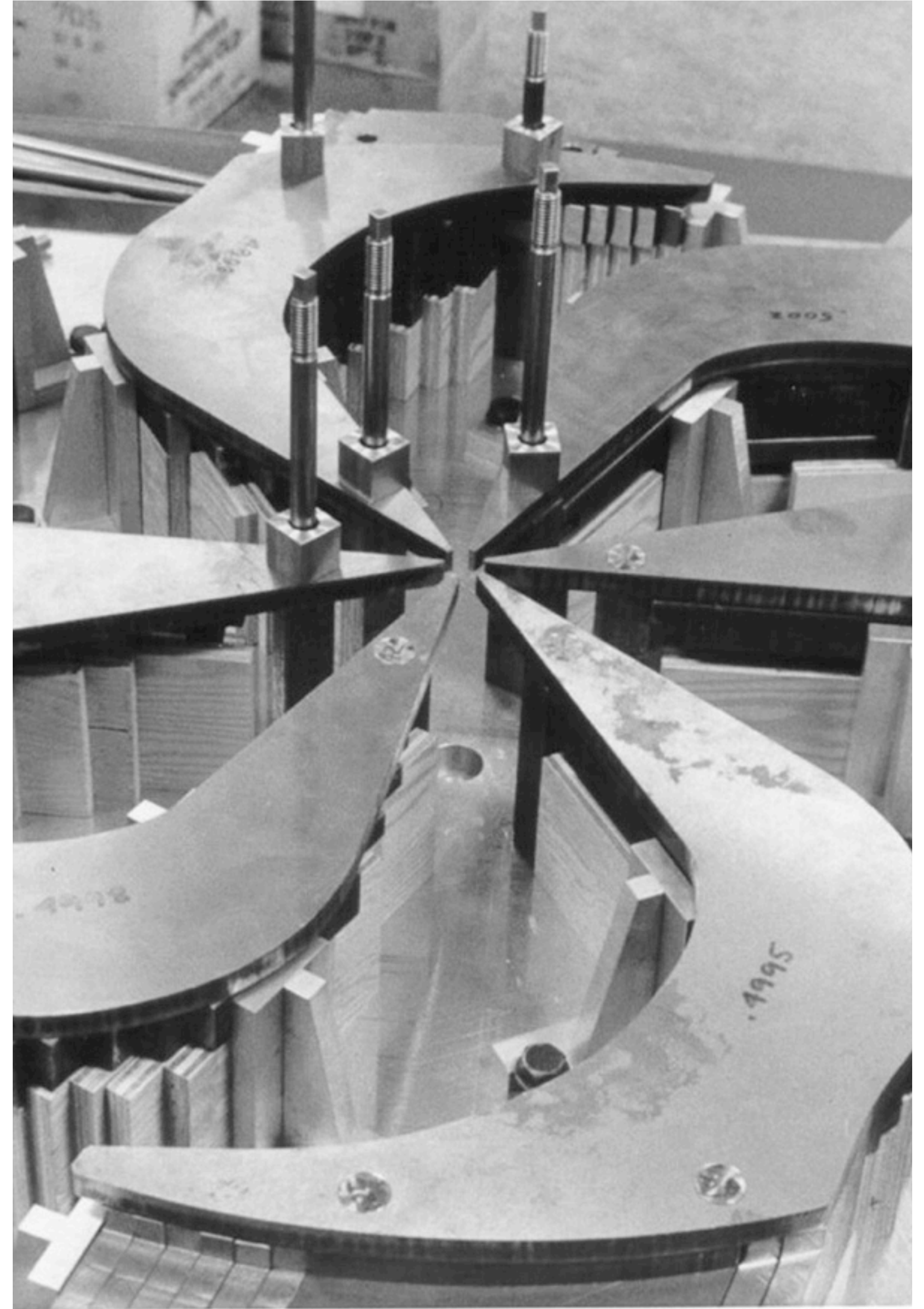
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 - Hadronic physics: more realistic model
- Towards better controlling theoretical uncertainty
 - Shifting from pheno towards EFT approach
 - EFT based on **potential-NRQED** for $Z > 1$

Thank you
Merci

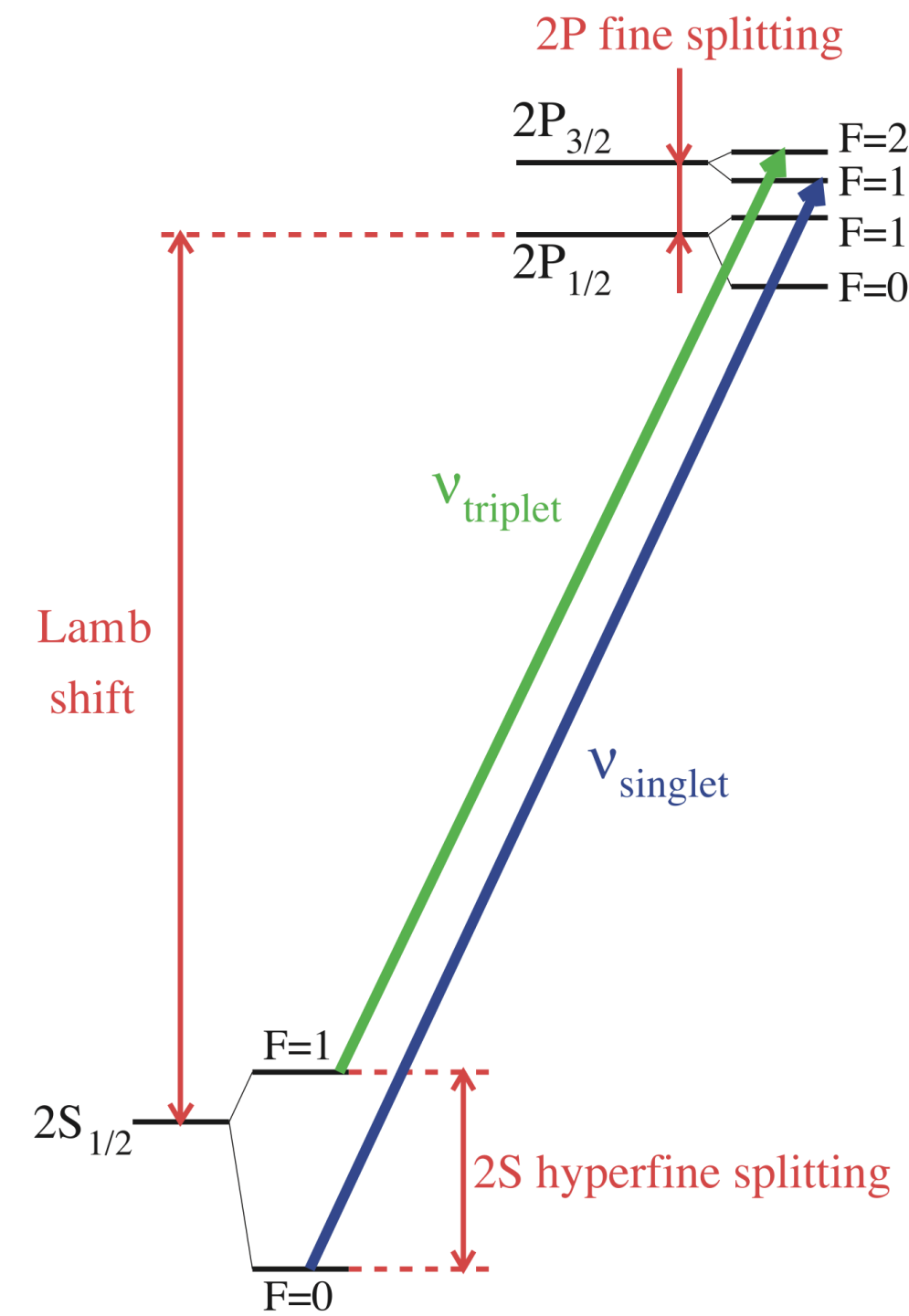
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Backup slides

The muonic Lamb shift as a precision probe

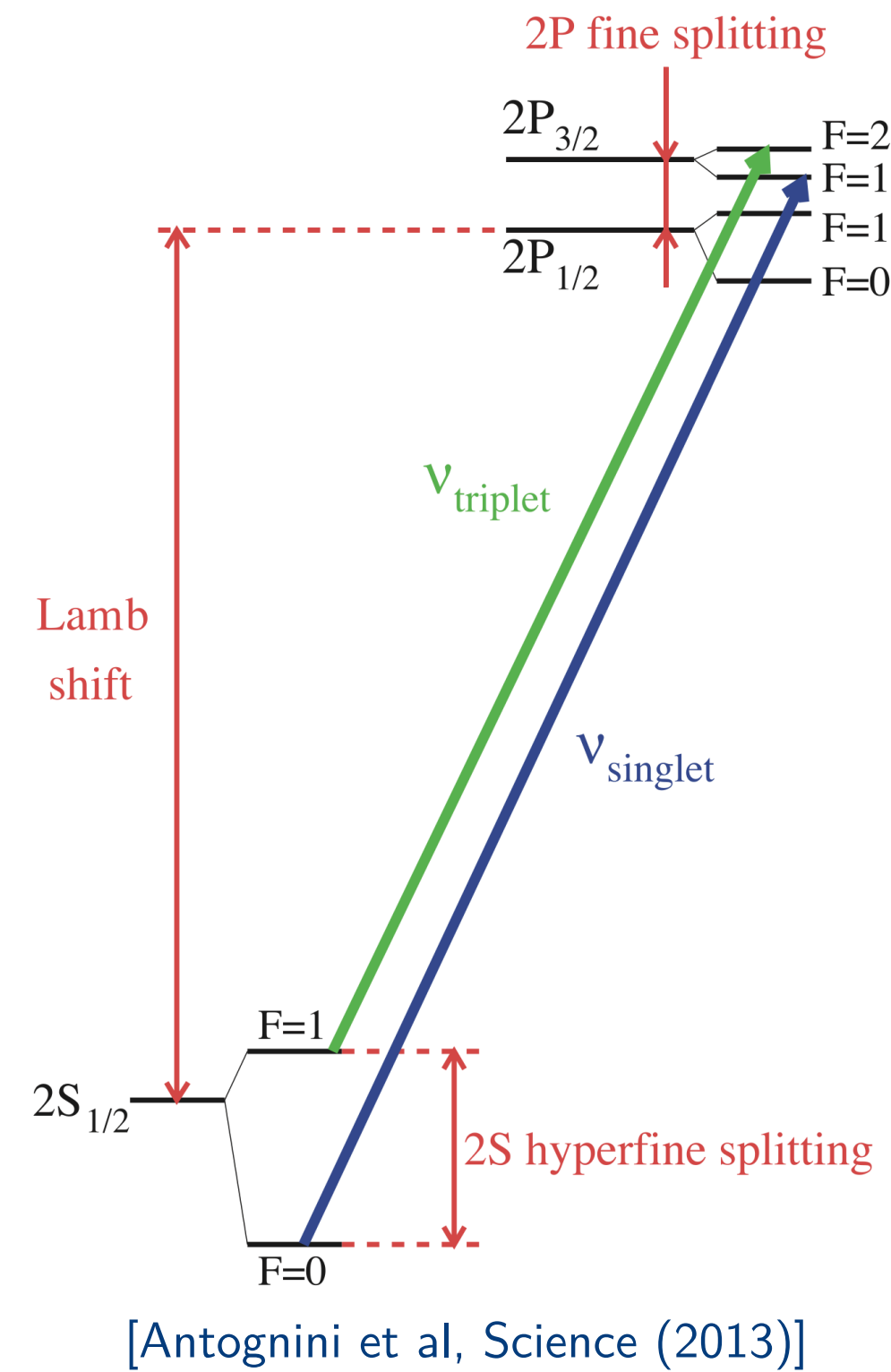
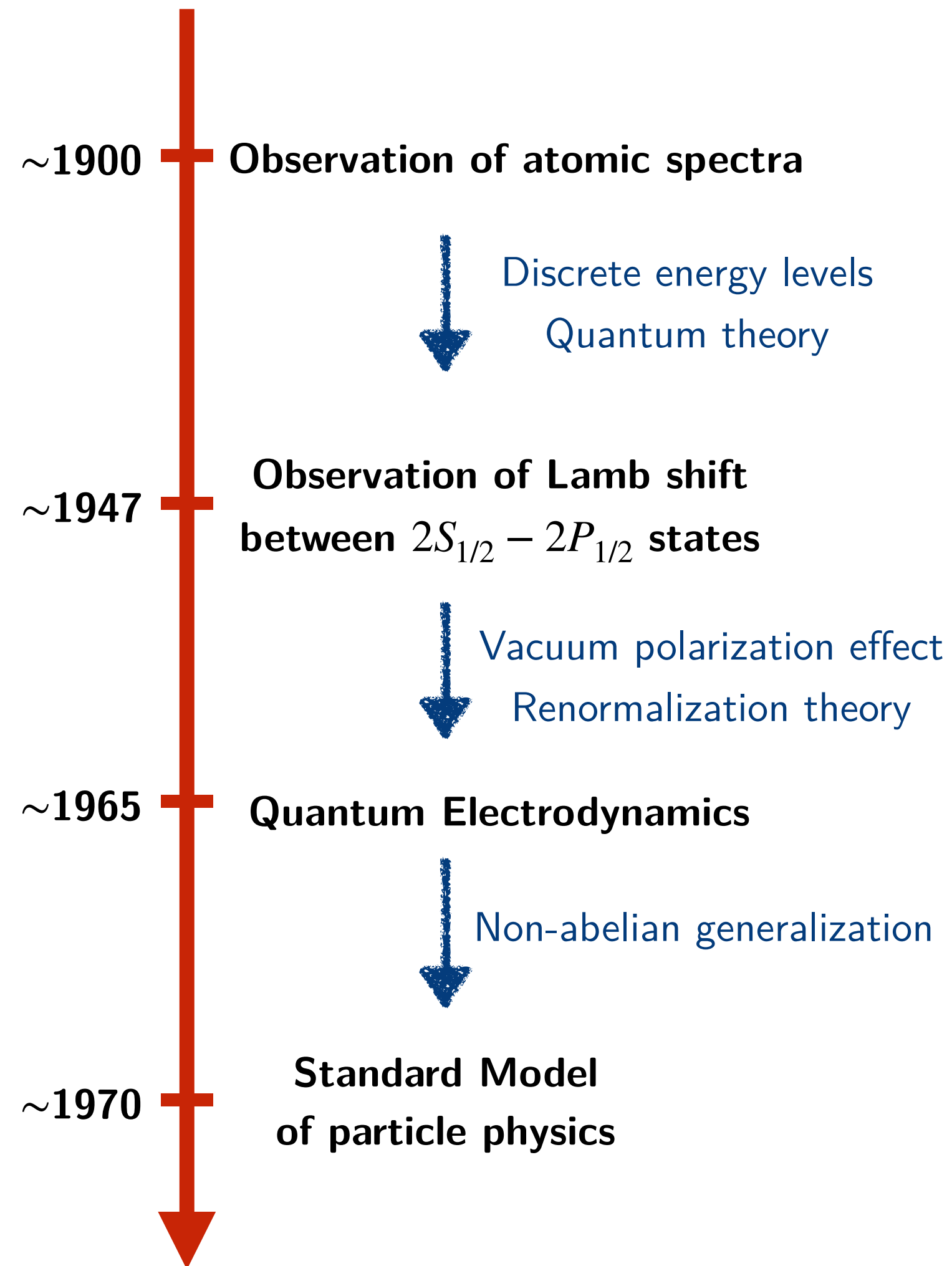


[Antognini et al, Science (2013)]

The muonic Lamb shift as a precision probe

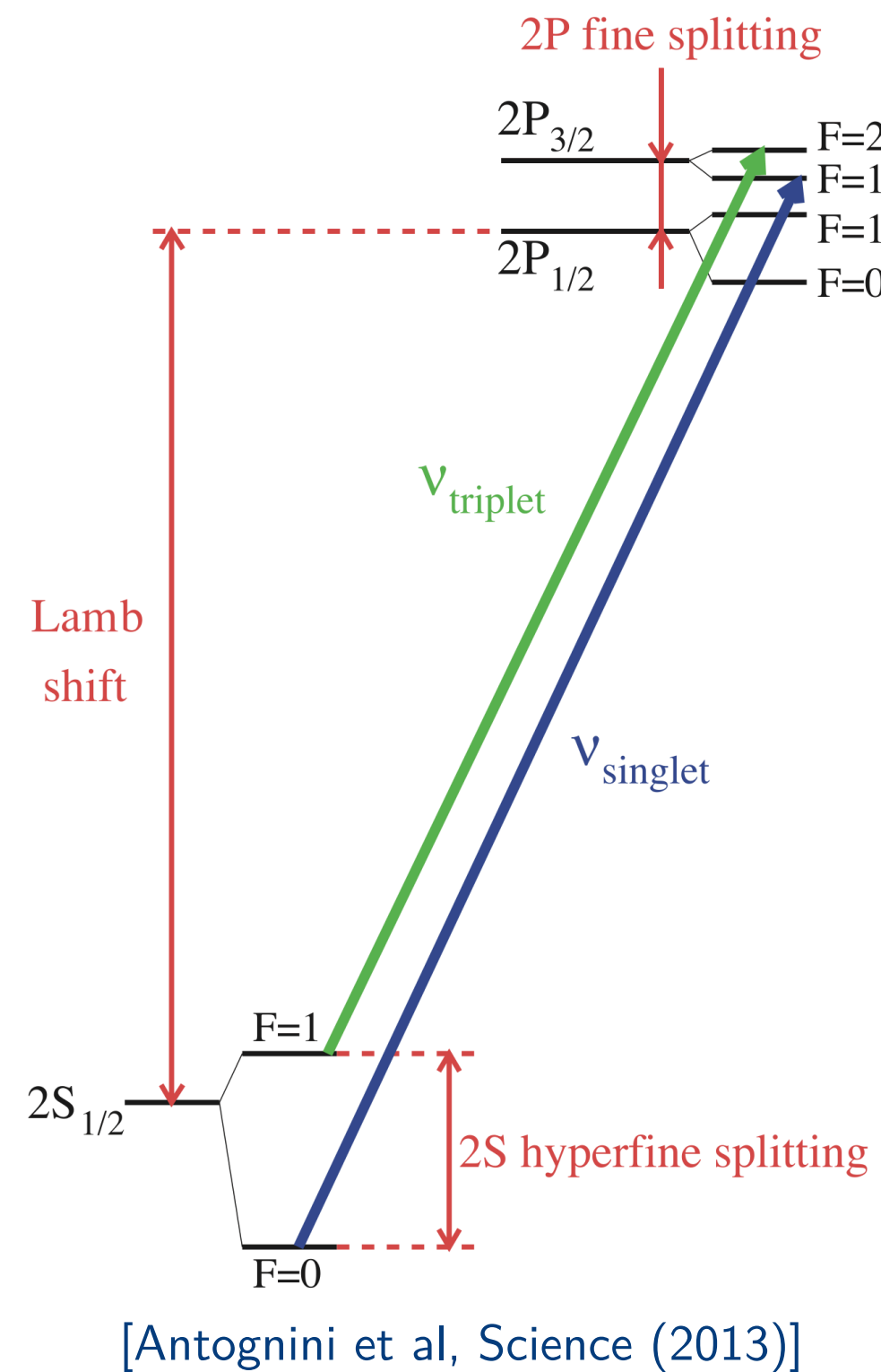
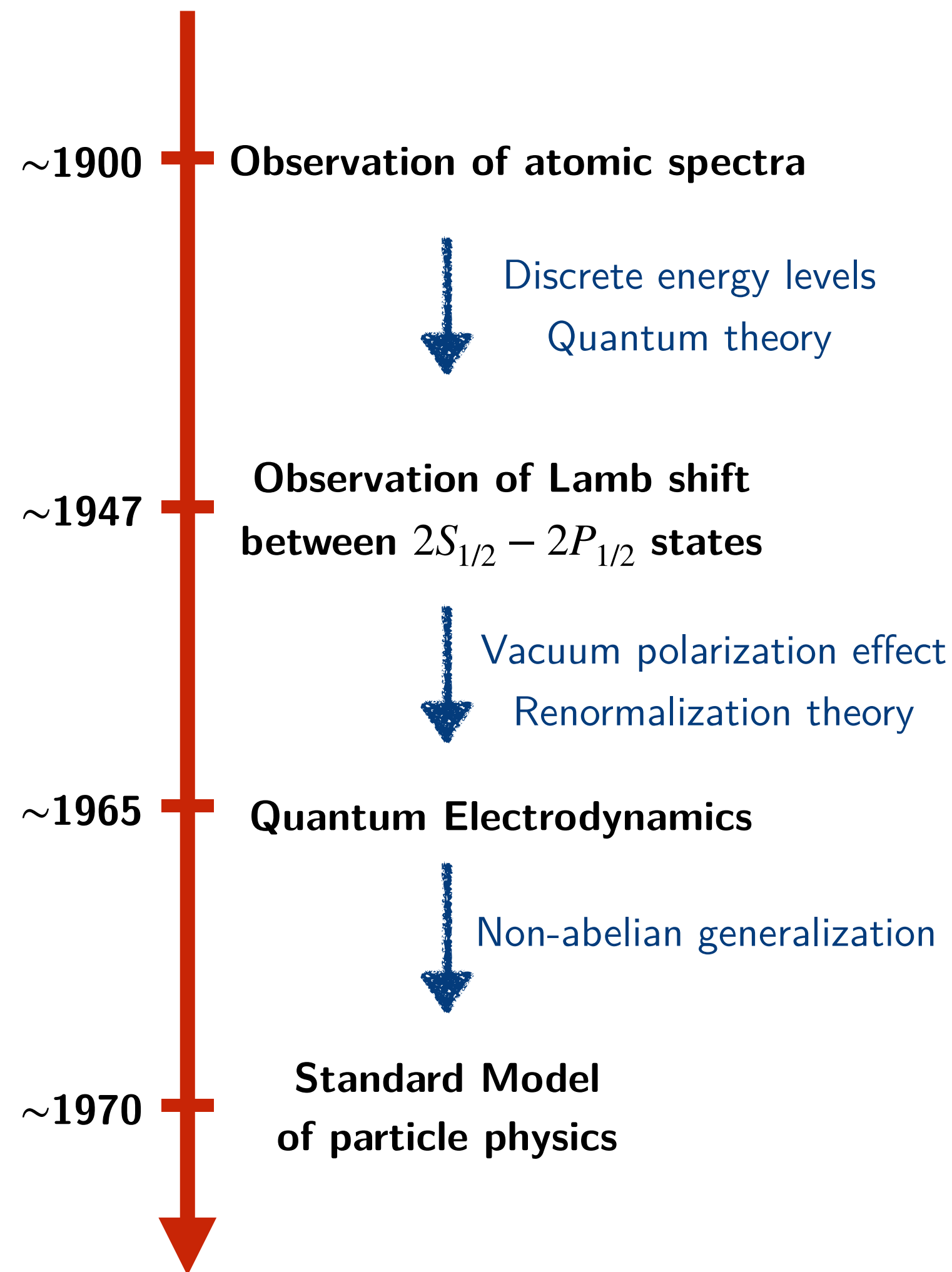
A key probe to develop the Standard Model...

19

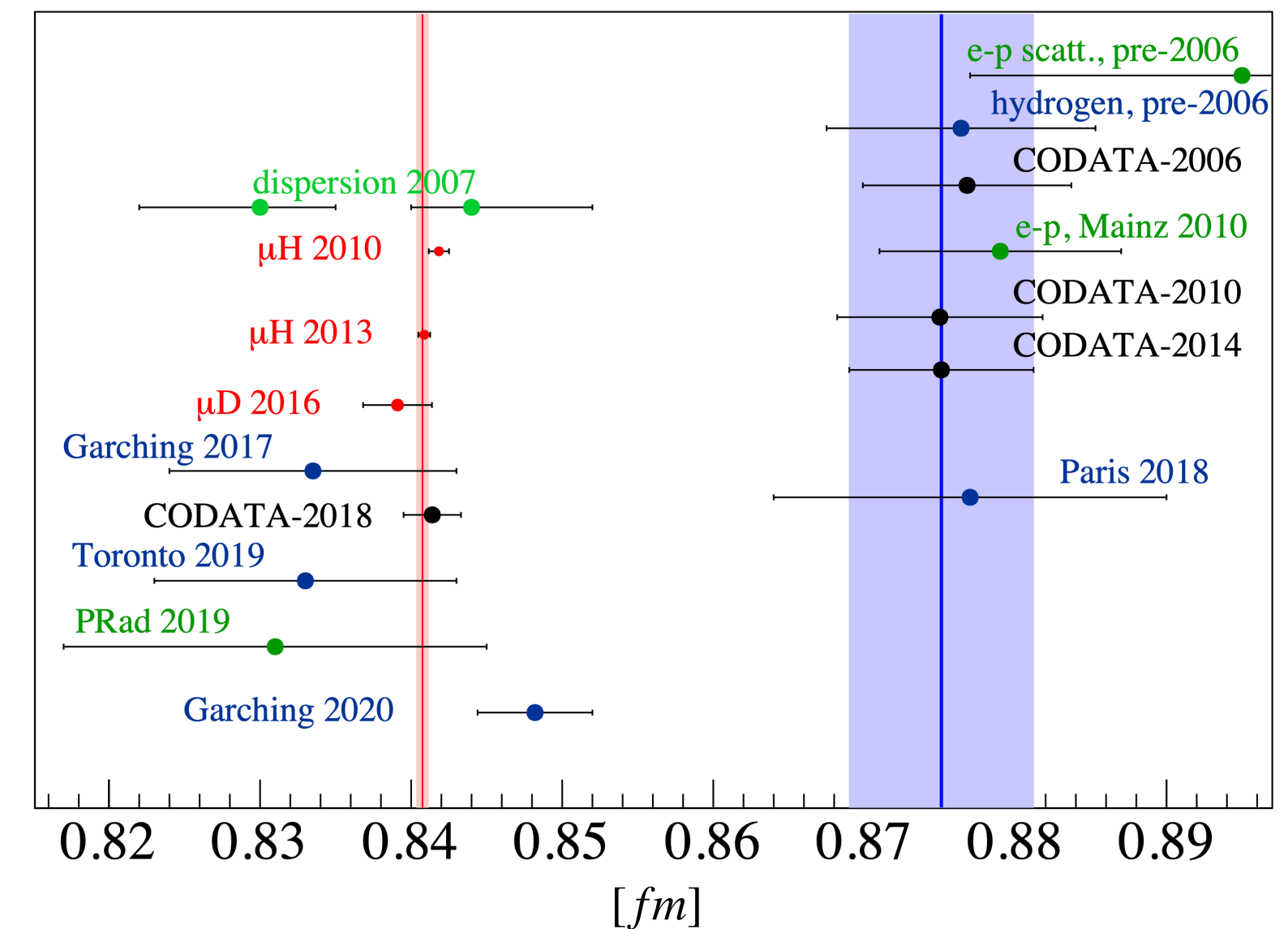


The muonic Lamb shift as a precision probe

A key probe to develop the Standard Model...



... and pushing the precision frontier further



- Precise measurement of proton radius: [CODATA 2018]

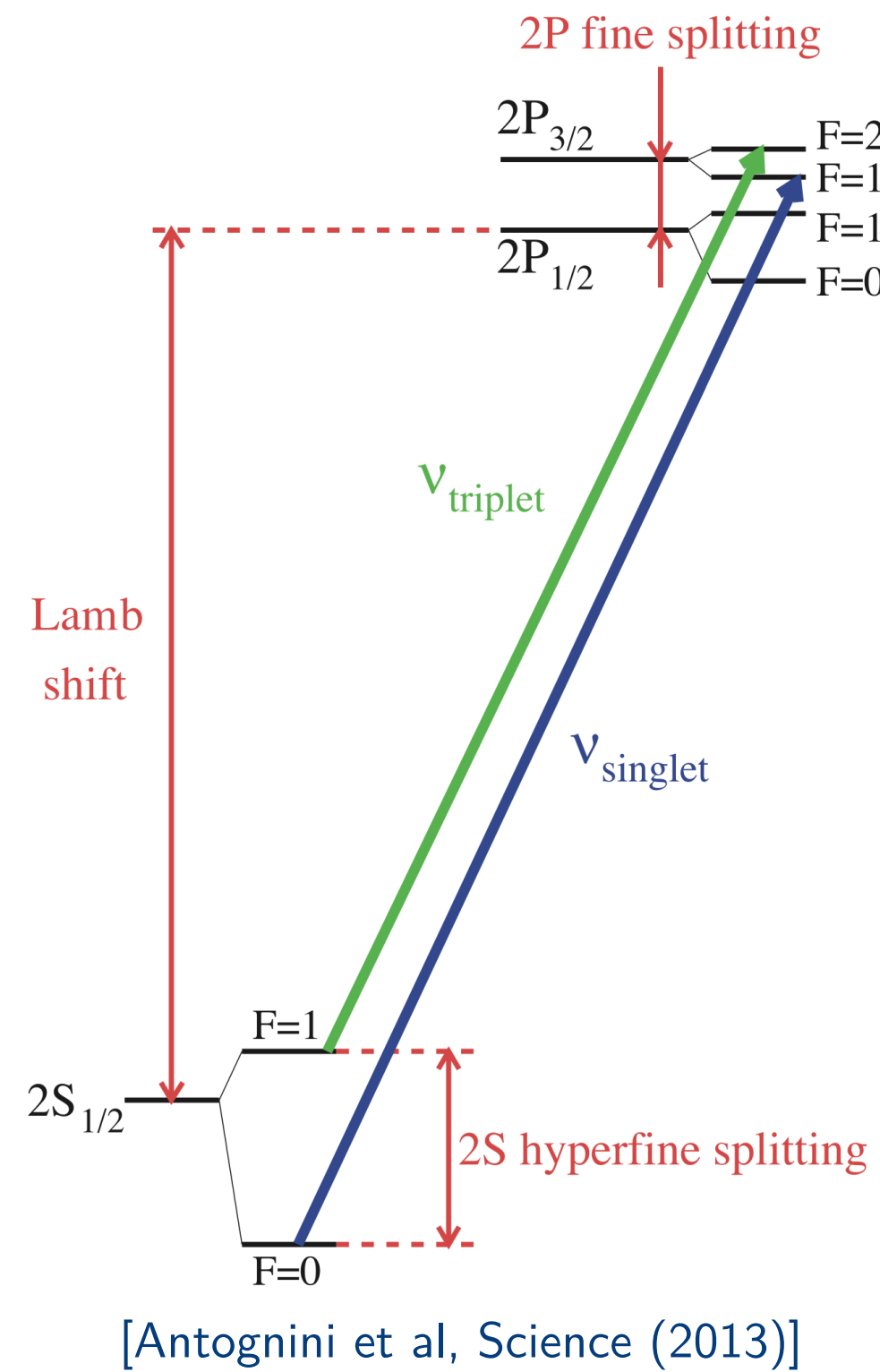
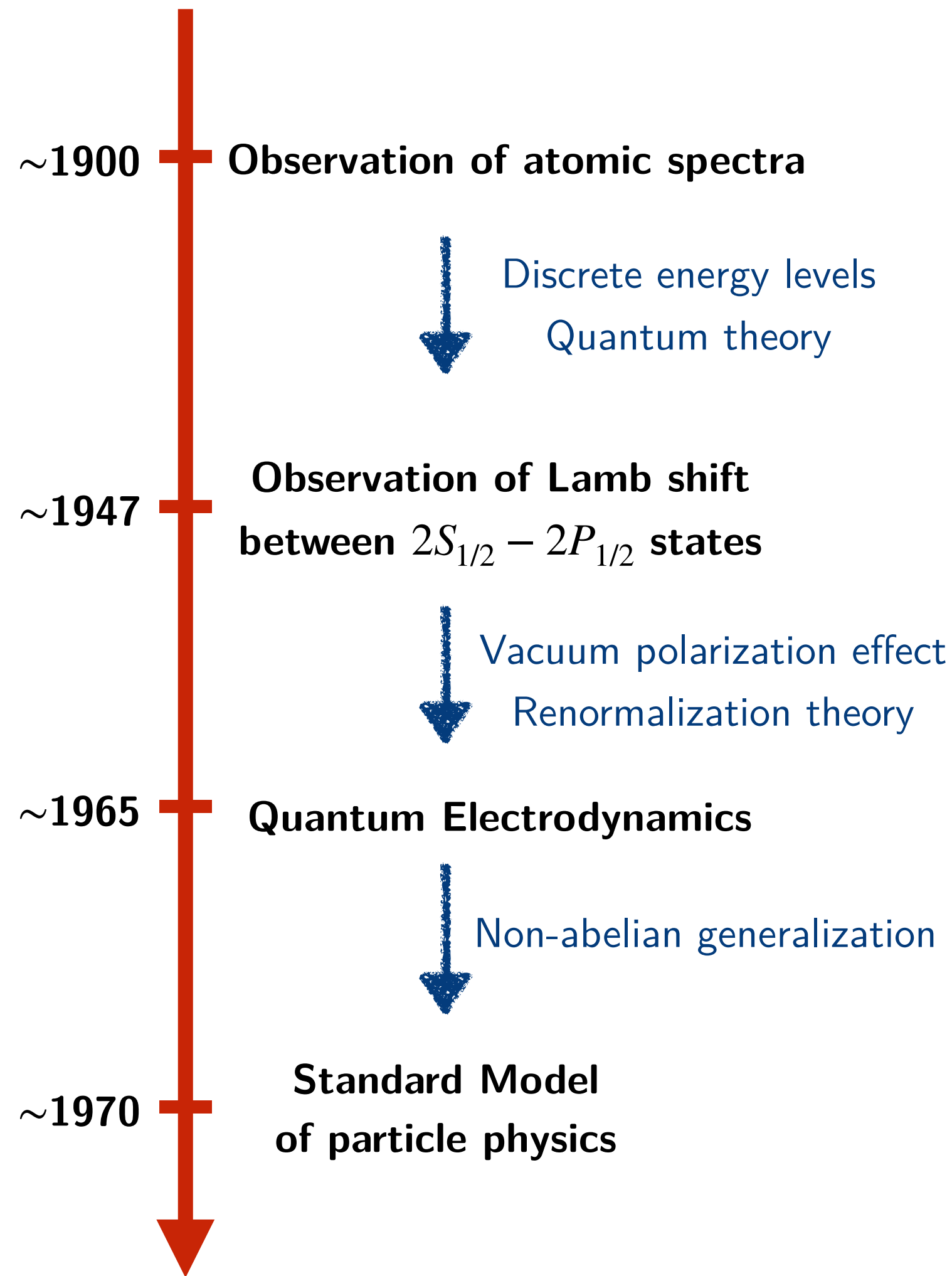
$$r_p = 8.414(19) \times 10^{-16} \text{m}$$

- Rydberg constant re-evaluation: [CODATA 2018]

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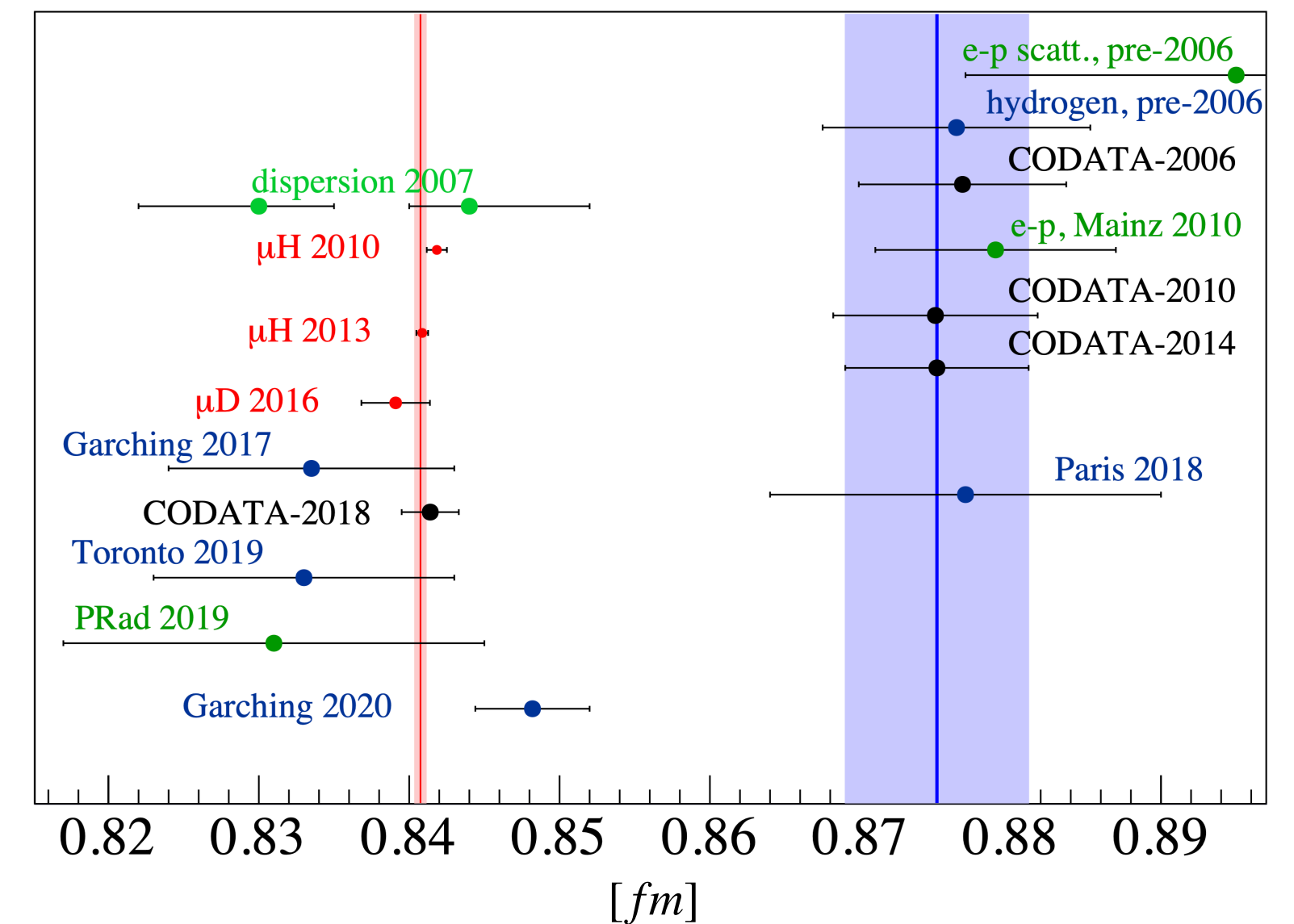
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And much more !!

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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
 - CREMA = on-going attempt to measure **HFS for proton!**

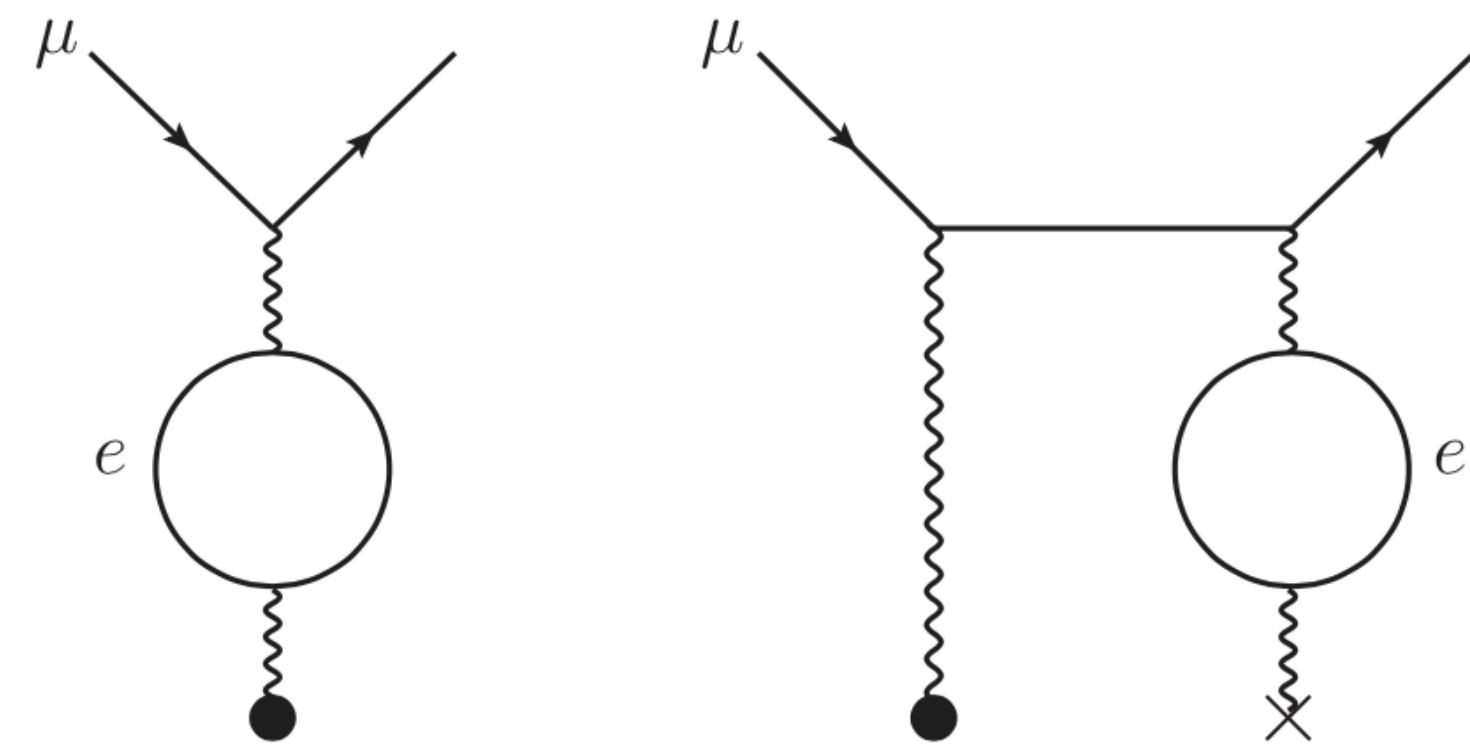
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Examples with electron vacuum polarization

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⇒ $\mathcal{O}(r_c^2)$ term in δ_{LS}

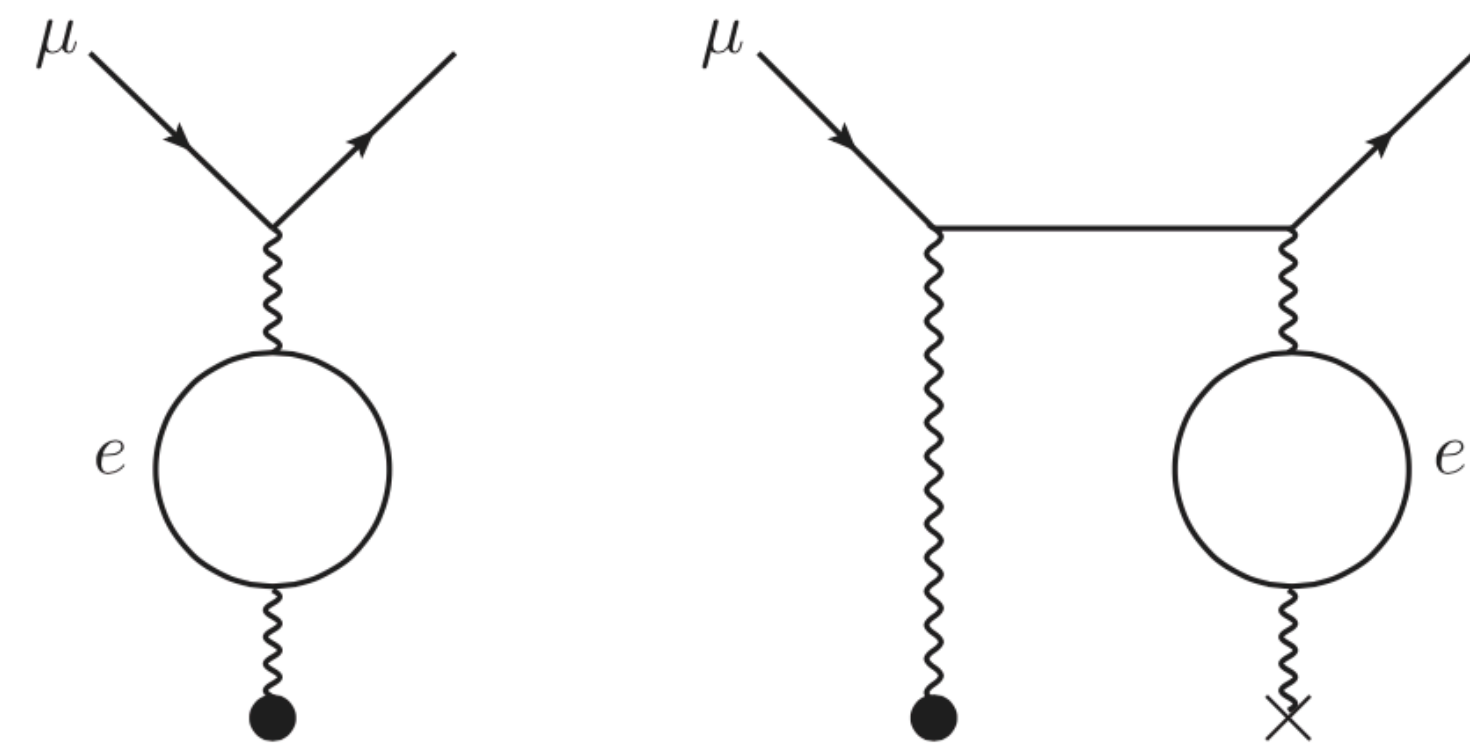
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[Pachucki et al. Review of Modern Physics (2024)]

Section	Order	Correction	μH	μD	$\mu^3\text{He}^+$	$\mu^4\text{He}^+$
IV.A	$(Z\alpha)^4$	r_c^2	$-5.1975 r_p^2$	$-6.0732 r_d^2$	$-102.523 r_h^2$	$-105.322 r_\alpha^2$
IV.B	$\alpha(Z\alpha)^4$	eVP ⁽¹⁾ with r_c^2	$-0.0282 r_p^2$	$-0.0340 r_d^2$	$-0.851 r_h^2$	$-0.878 r_\alpha^2$
IV.C	$\alpha^2(Z\alpha)^4$	eVP ⁽²⁾ with r_c^2	$-0.0002 r_p^2$	$-0.0002 r_d^2$	$-0.009(1) r_h^2$	$-0.009(1) r_\alpha^2$

Nuclear structure dependent corrections

Nuclear structure effects

- ① Corrections accounting for non static effects
 - Nucleus is no longer treated as a structureless particle
 - Main contribution from **two-photon exchange** δ_{TPE}
 - **Nuclear excited states** become necessary

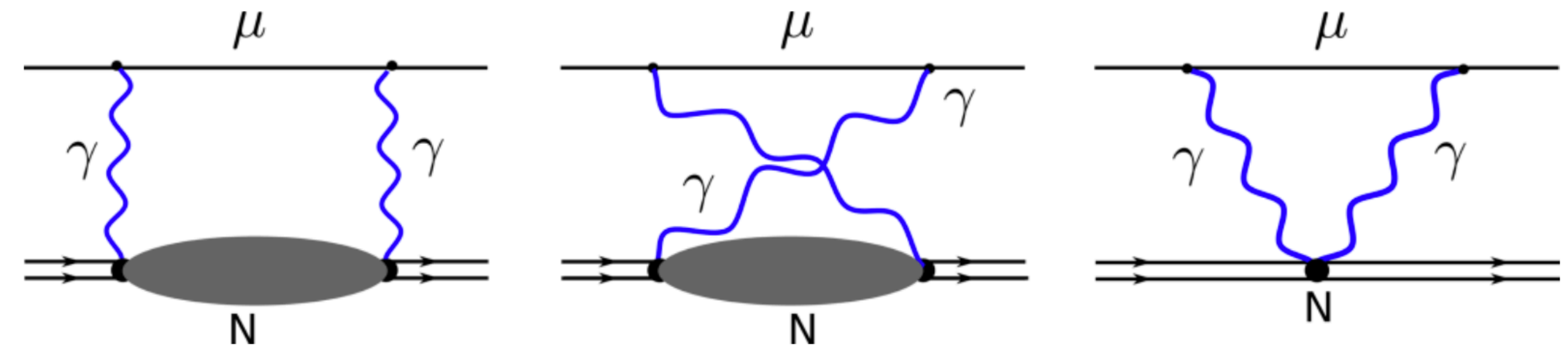
➔ δ_{TPE} contributes at $(Z\alpha)^5$
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Two photon exchanges contributions



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

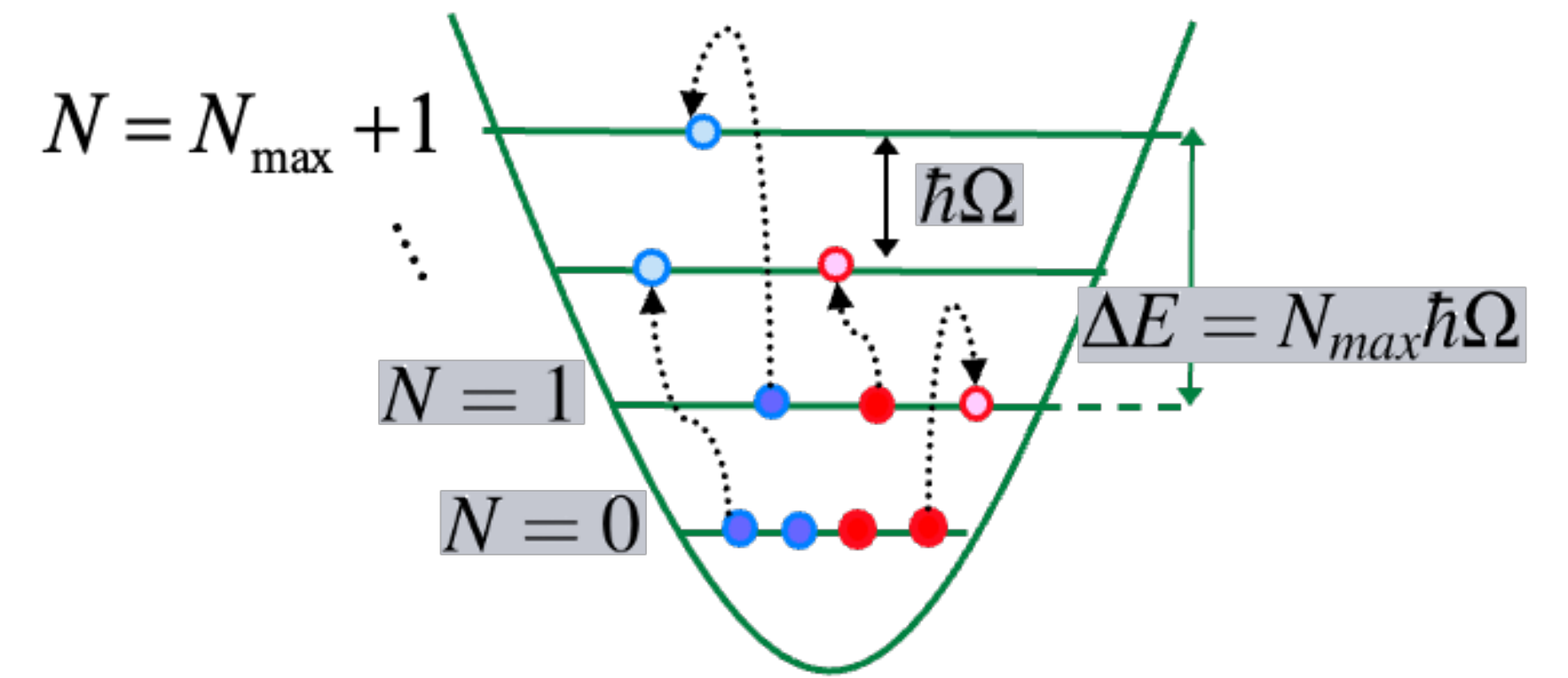
with:

- $D^{\mu\nu}(q) \equiv$ the photon propagator
- $t_{\mu\nu} \equiv$ the leptonic tensor
- $T_{\mu\nu} \equiv$ the hadronic tensor [Bernabeu et al, Nuclear Physics A (1974)]
[Rosenfelder Nuclear Physics A (1983)]
- $k \equiv (m_r, 0)$ [Hernandez et al. Physical Review C (2019)]

Ab initio No-Core Shell Model calculations

Anti-symmetrized products of many-body HO states

22



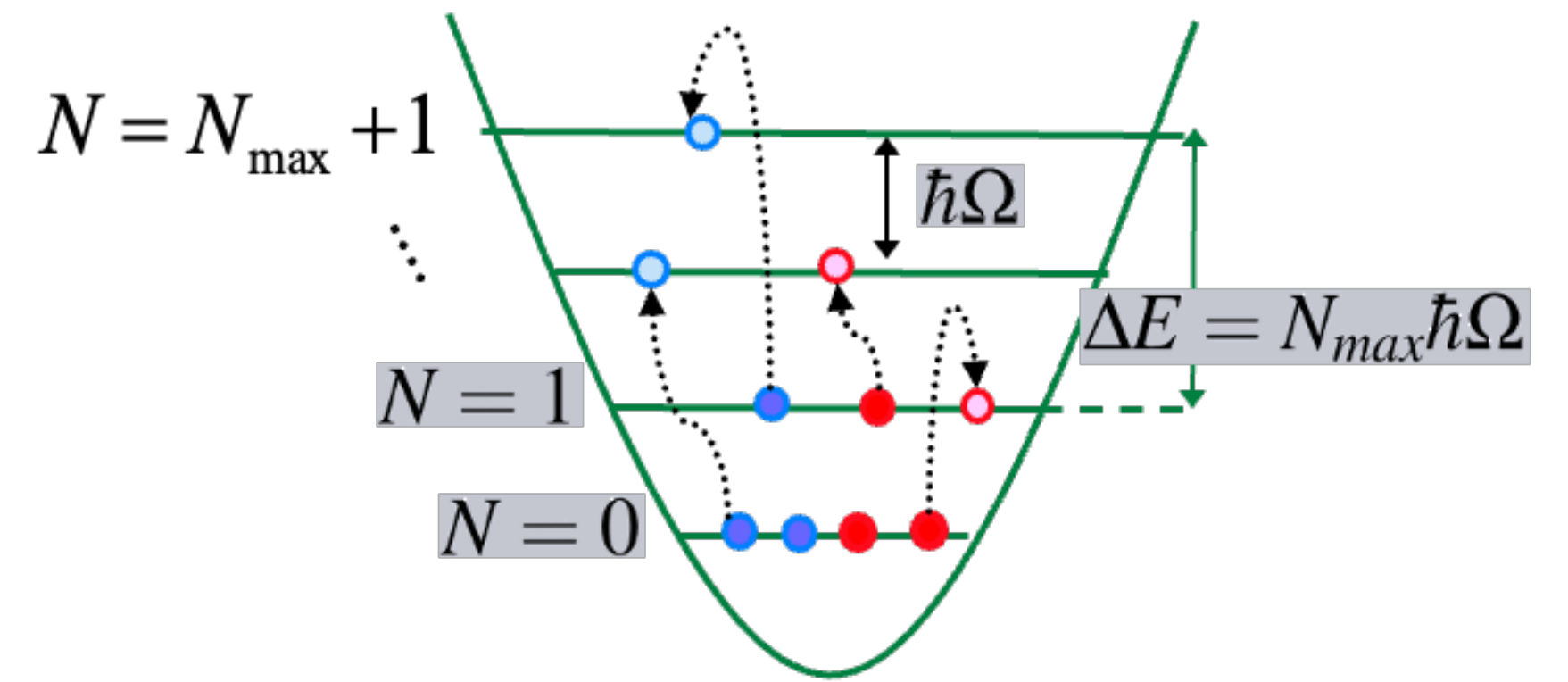
Ab initio No-Core Shell Model calculations

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 $\langle\phi_{i+1}|\phi_{i+1}\rangle = 1$
- Output:
 - Lanczos basis and coefficients $\{|\phi_i\rangle, \alpha_i, \beta_i\}$ \rightarrow **H in Lanczos basis**

$$\begin{pmatrix} \alpha_1 & \beta_2 & & & & & \\ \beta_2 & \alpha_2 & \beta_3 & & & & \\ & \beta_3 & \alpha_3 & \ddots & & & \\ & & \ddots & \ddots & \beta_{k-1} & & \\ & & & & \beta_{k-1} & \alpha_{k-1} & \beta_k \\ & & & & & \beta_k & \alpha_k \end{pmatrix}$$

Anti-symmetrized products of many-body HO states



Application to nuclear structure

- Efficient calculation of spectra
 - Selection rules \Rightarrow **Fast matrix-vector multiplication**
 - In practice: $N_L \sim 100 - 200$ is sufficient
- Application to ${}^7\text{Li}$
 - $N_L = 200$ for $N_{\max} = 1$ to 9
 - Ground-state of ${}^7\text{Li}$ $|\Psi\rangle \Rightarrow$ **Starting point for δ_{pol}^A**

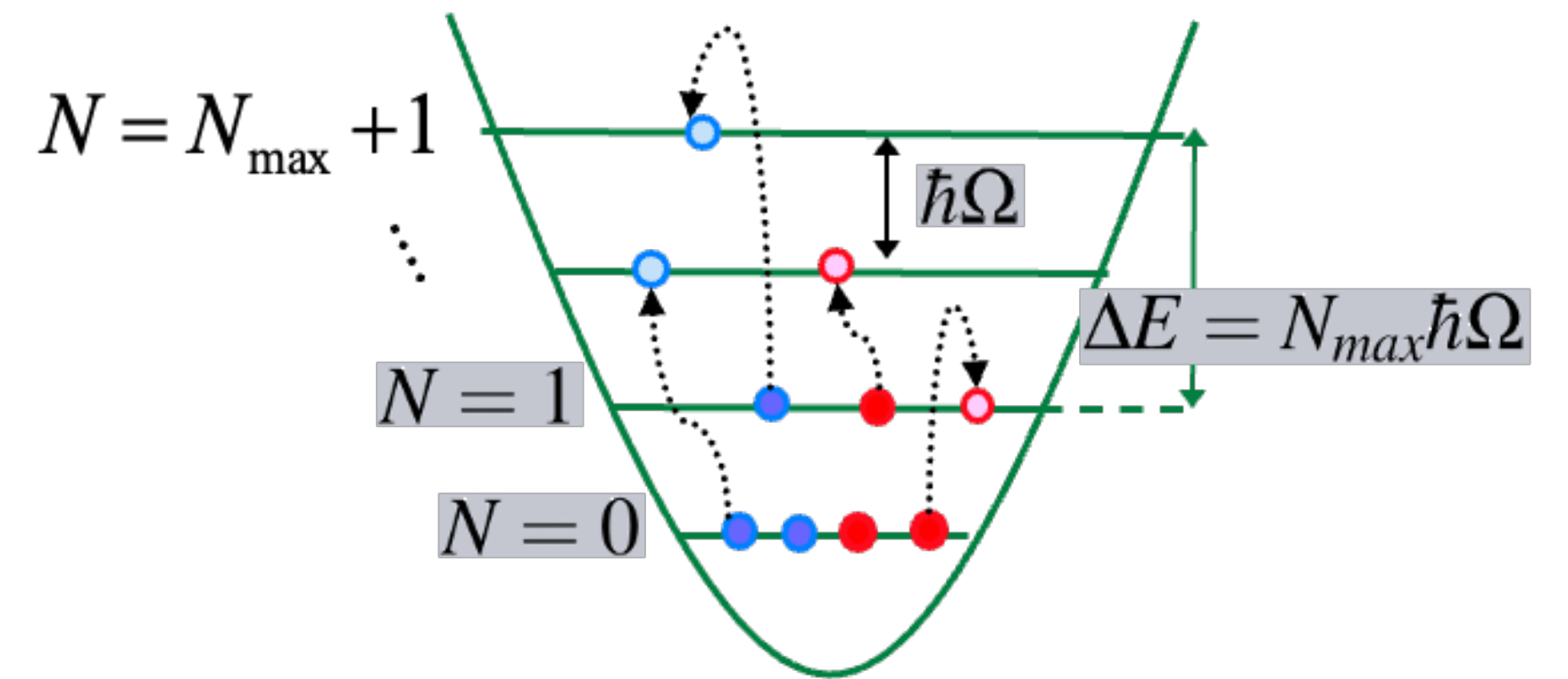
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Lanczos-strength algorithm for δ_{pol}^A

- Spectral function obtained with a second Lanczos:
 - Pivot based on 1st Lanczos output: $|\phi'_1\rangle = \frac{O|\Psi^{J\pi T}\rangle}{\sqrt{\langle\Psi^{J\pi T}|O^\dagger O|\Psi^{J\pi T}\rangle}}$
 - \Rightarrow **Strengths:** $|\langle\Psi_n^{J\pi T}|O|\Psi^{J\pi T}\rangle|^2 = |\langle\phi'_1|\Psi_n^{J\pi T}\rangle|^2 \langle\Psi^{J\pi T}|O^\dagger O|\Psi^{J\pi T}\rangle$
- Convergence properties:
 - Recovers **exactly** the first $2n$ moments for n Lanczos steps!
 - \Rightarrow **One additional NCSM run per operator**

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

First tests of sum rule convergence

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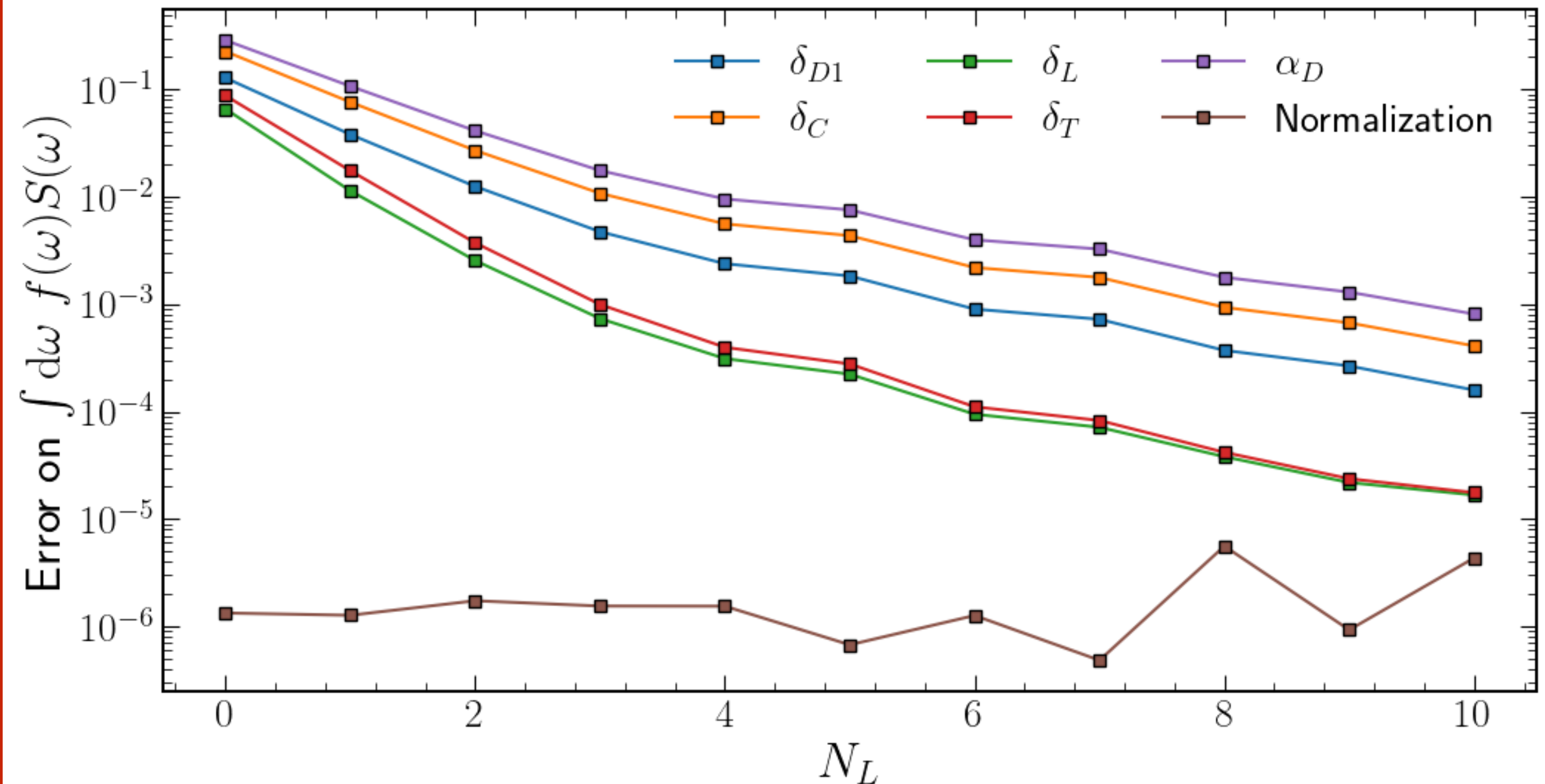
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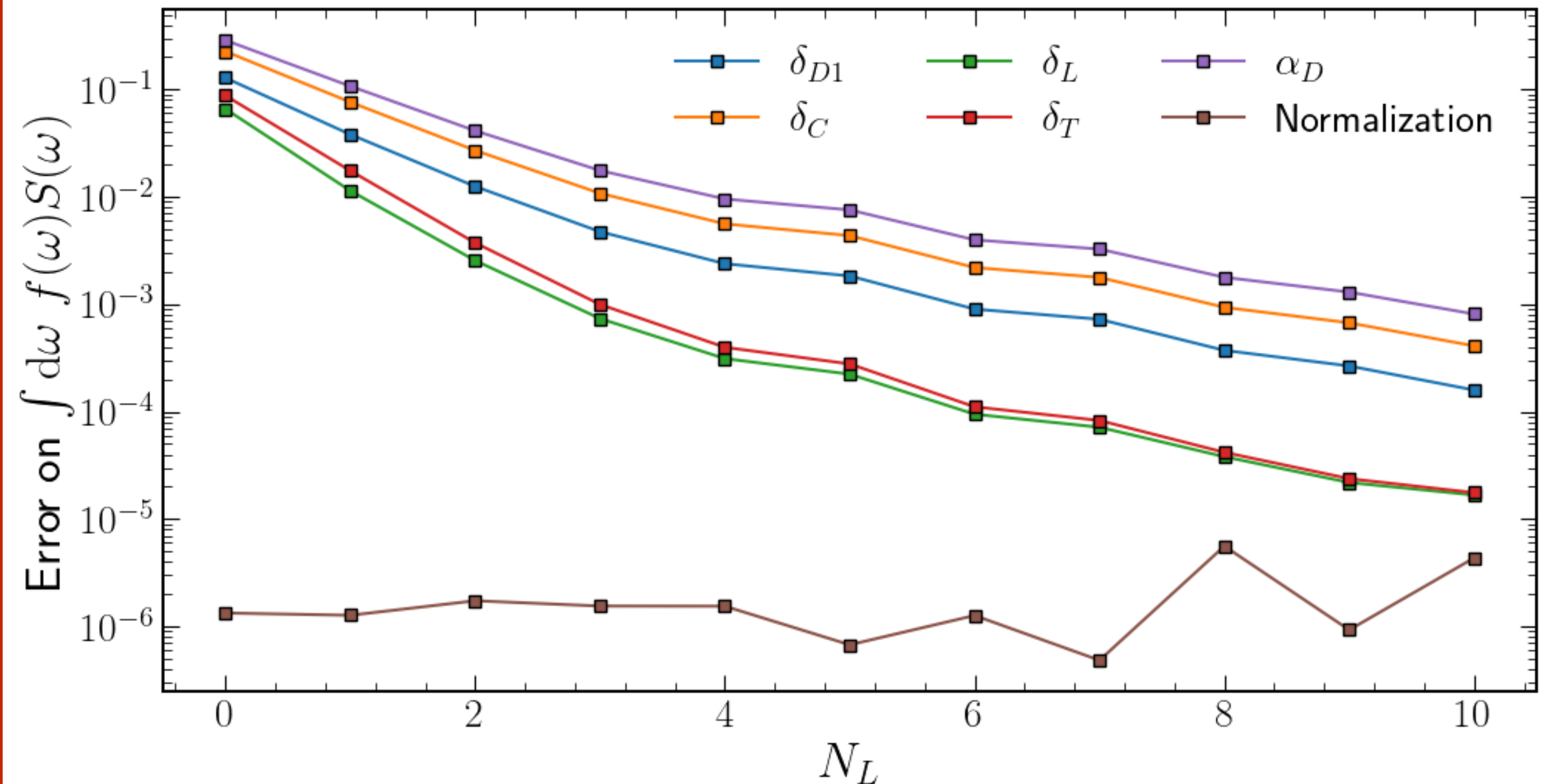
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- Sum rules converge quickly $\Rightarrow N_L = 50$ is sufficient
- Reaches plateau around $\sim 10^{-5}$ relative error

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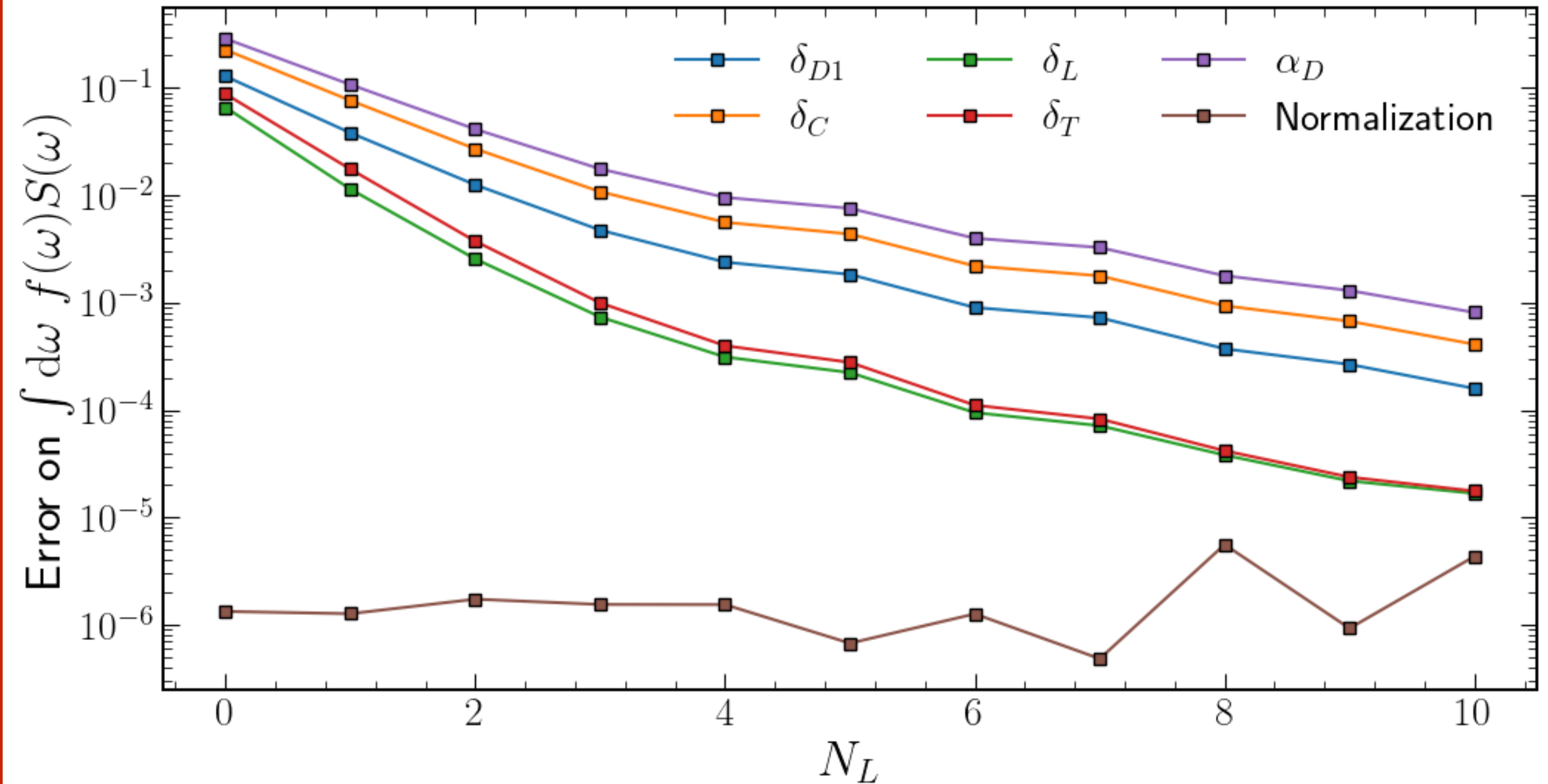


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First conclusion: numerical noise from Lanczos algo is negligible

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