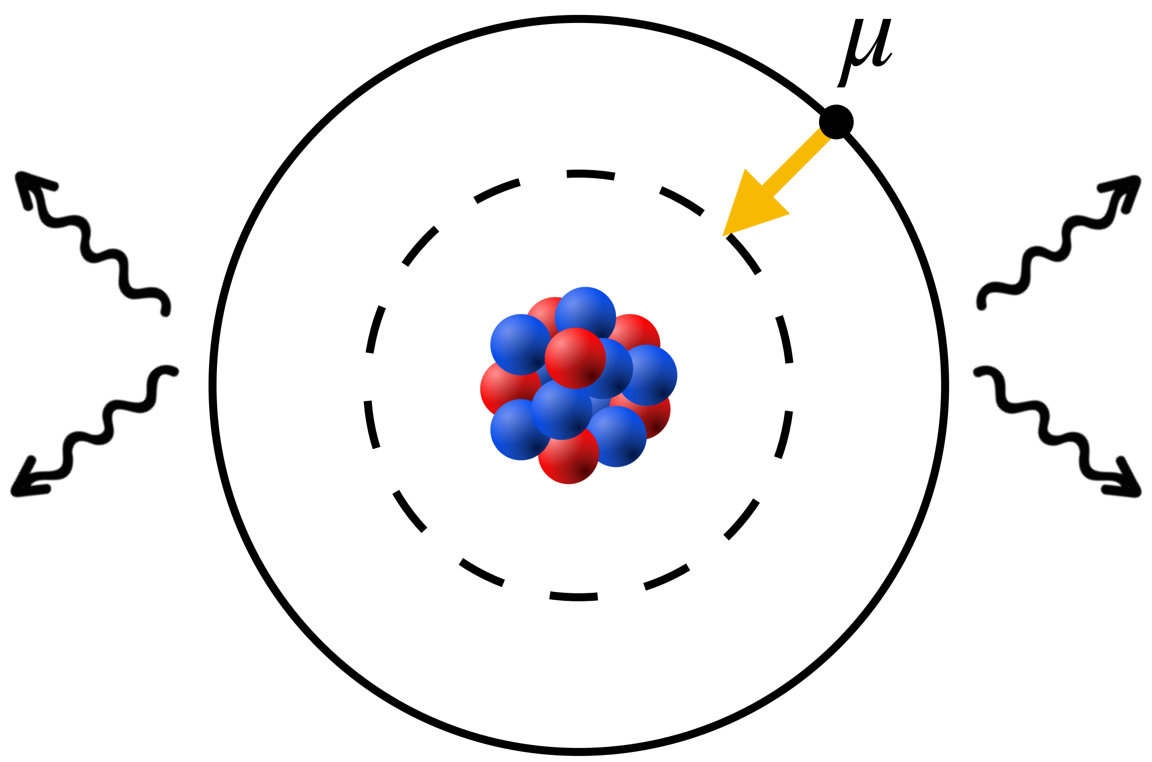
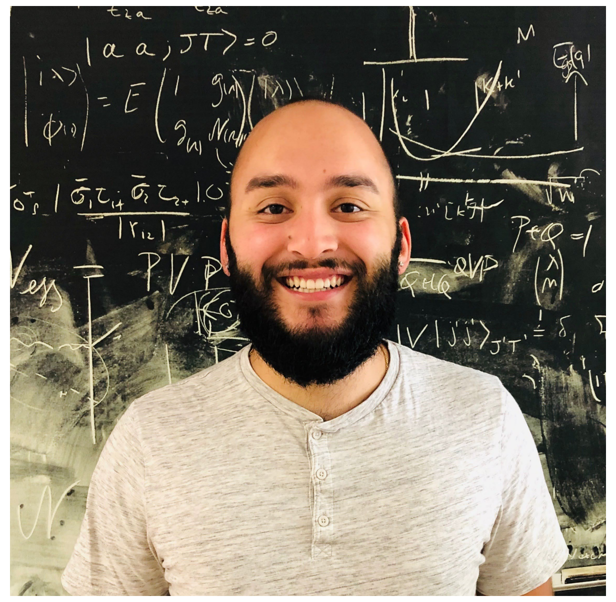
Nuclear corrections to muonic lithium atoms

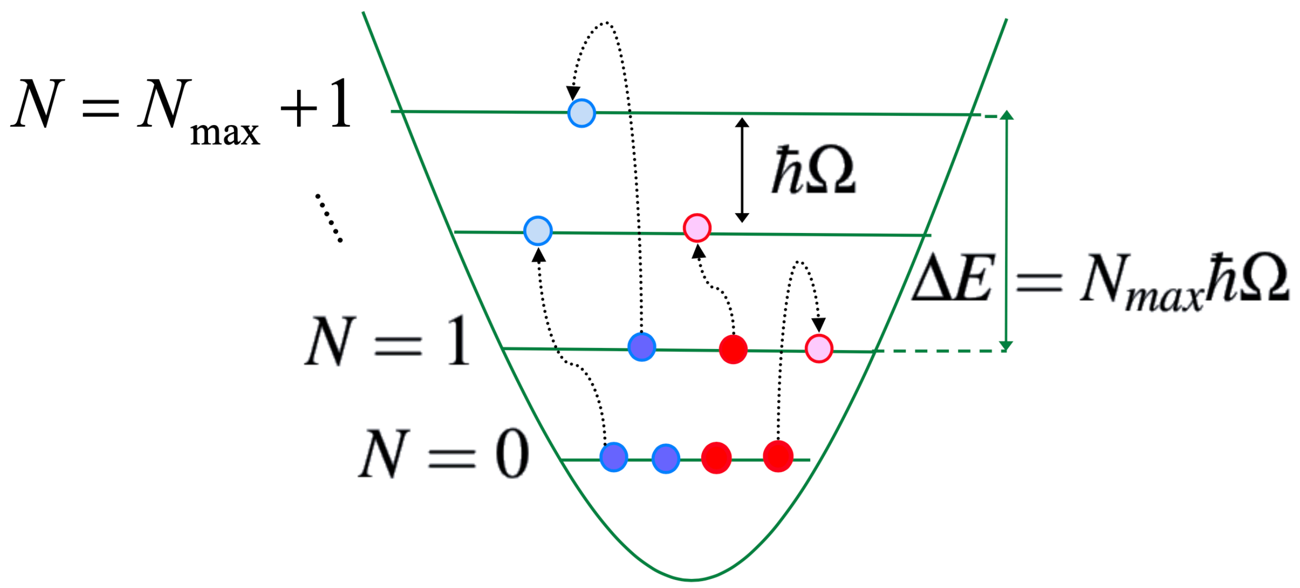
Ab initio calculations of polarizability of $^{6}\mathrm{Li}$ and $^{7}\mathrm{Li}$ atoms

TRIUMF

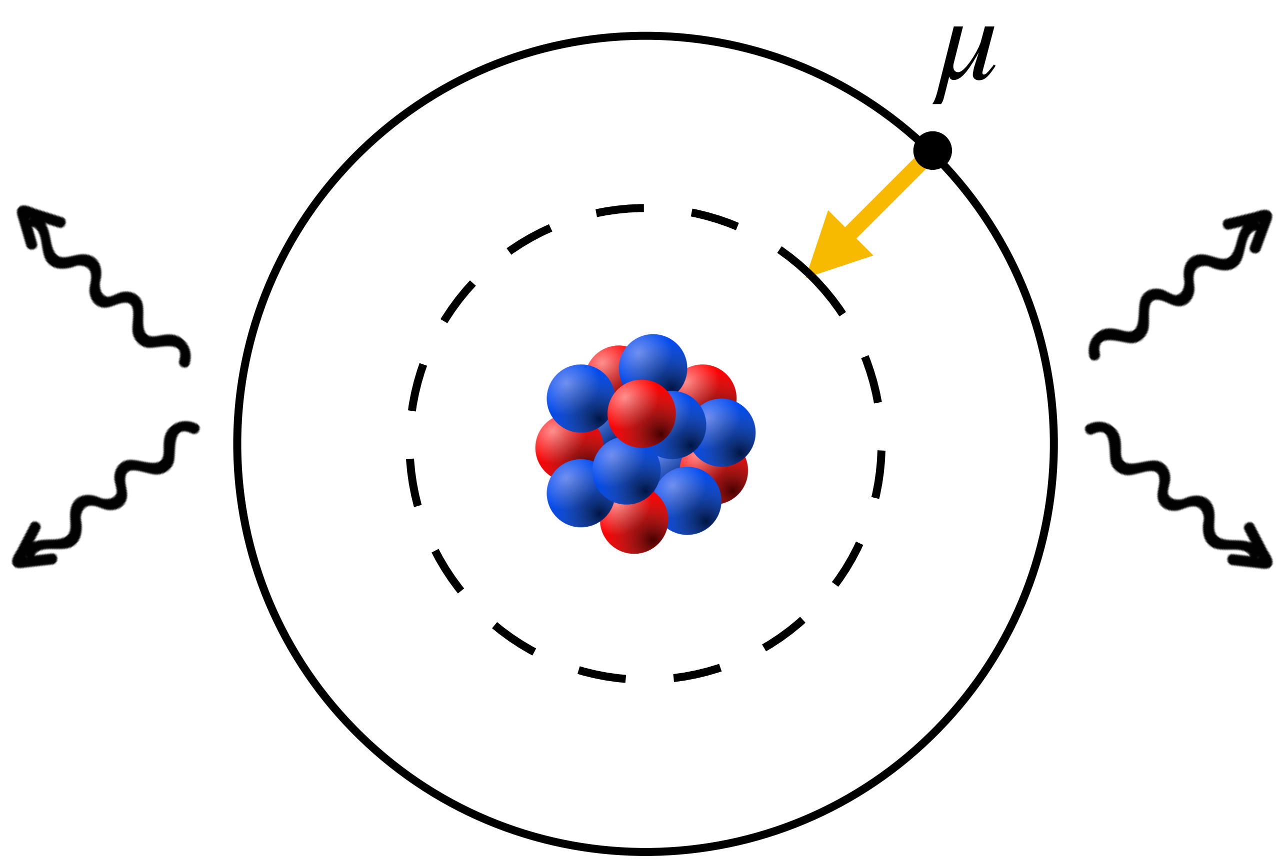





Michael Gennari Petr Navratil

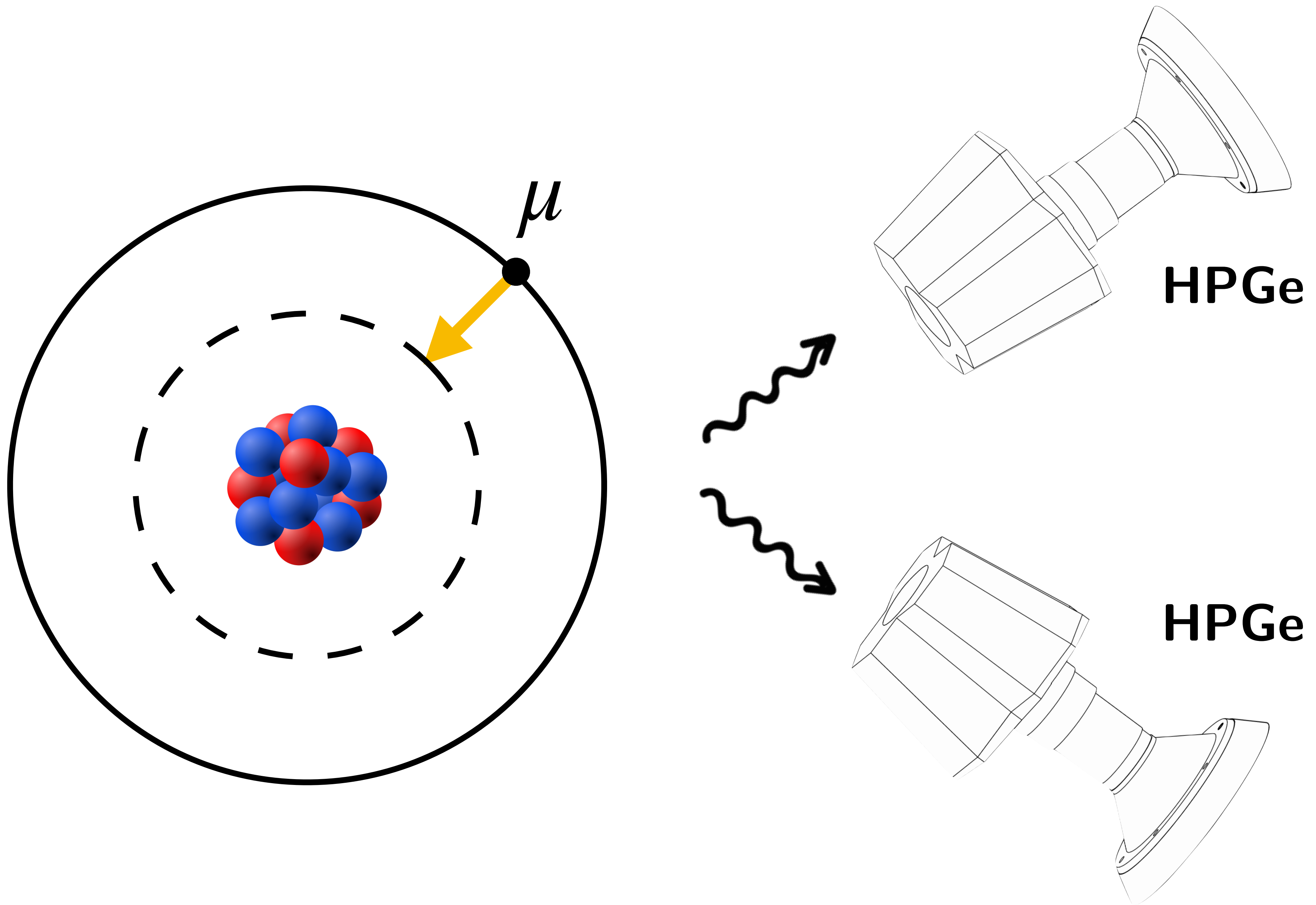


Muonic atoms and charge radii



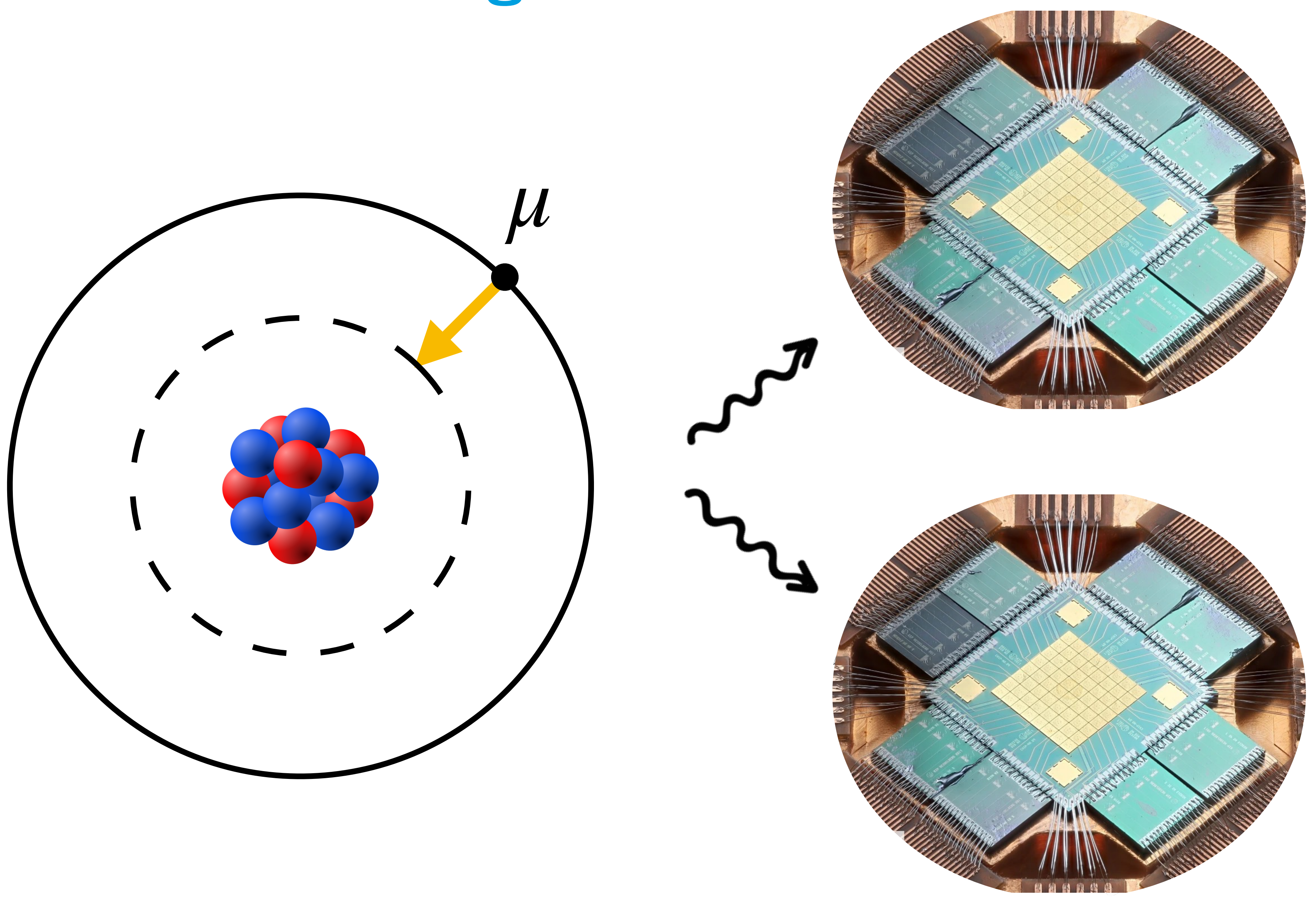
Muonic atoms as a precision probe

Observing muonic atoms



Muonic atoms as a precision probe

Observing muonic atoms



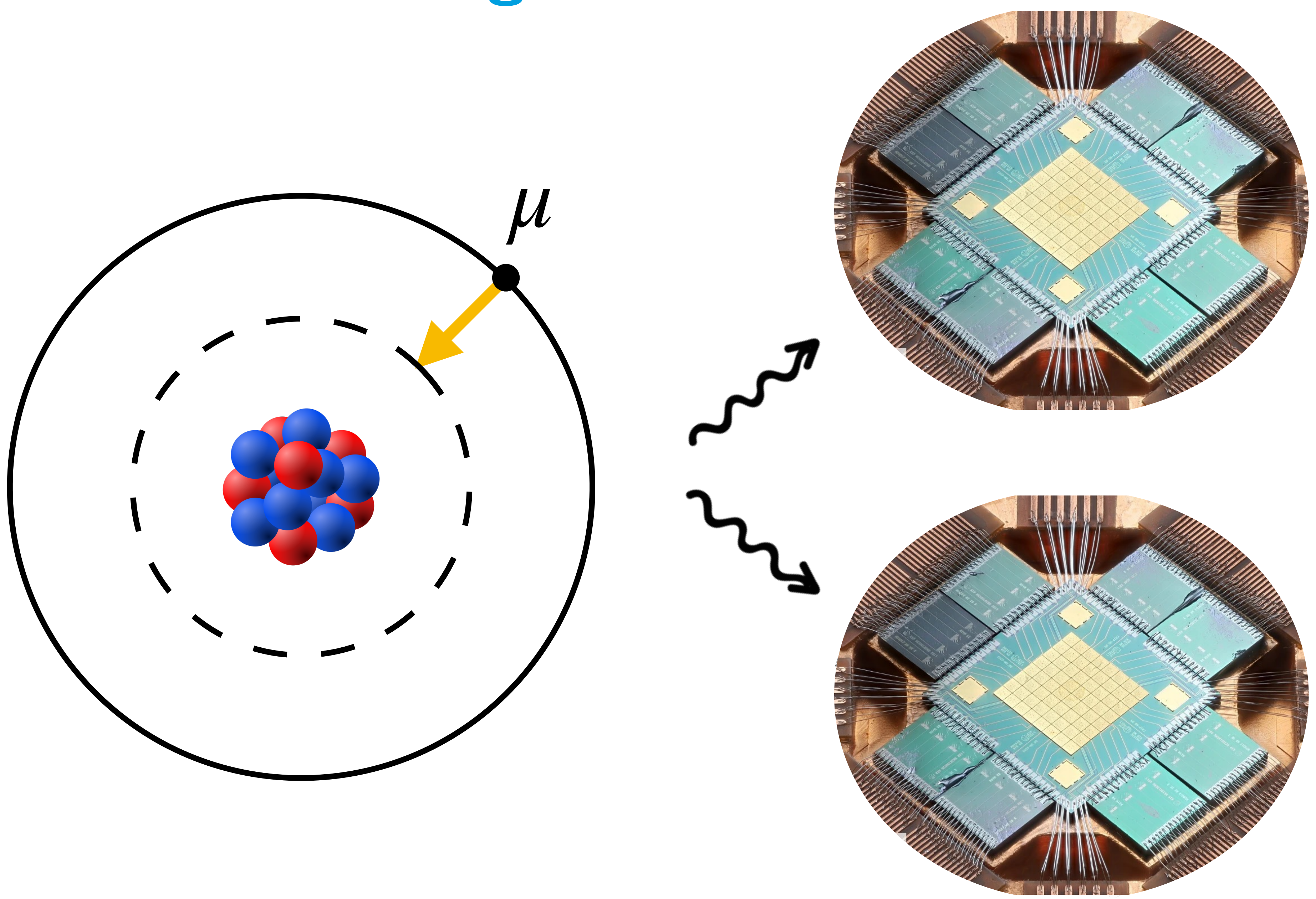
[Unger et al. J. Low Temp. Phys. (2024)]

QUARTET collaboration

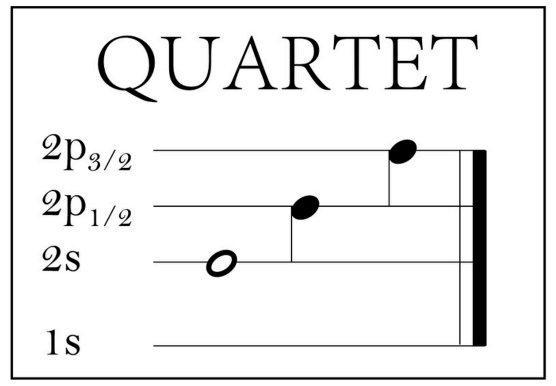
- Improving energy resolution with MMC
  - Quantum sensor detector to reach low-Z nuclei
  - **Data taken at PSI with** $\mathrm{Li}, \mathrm{Be}, \mathrm{B}$ **targets**

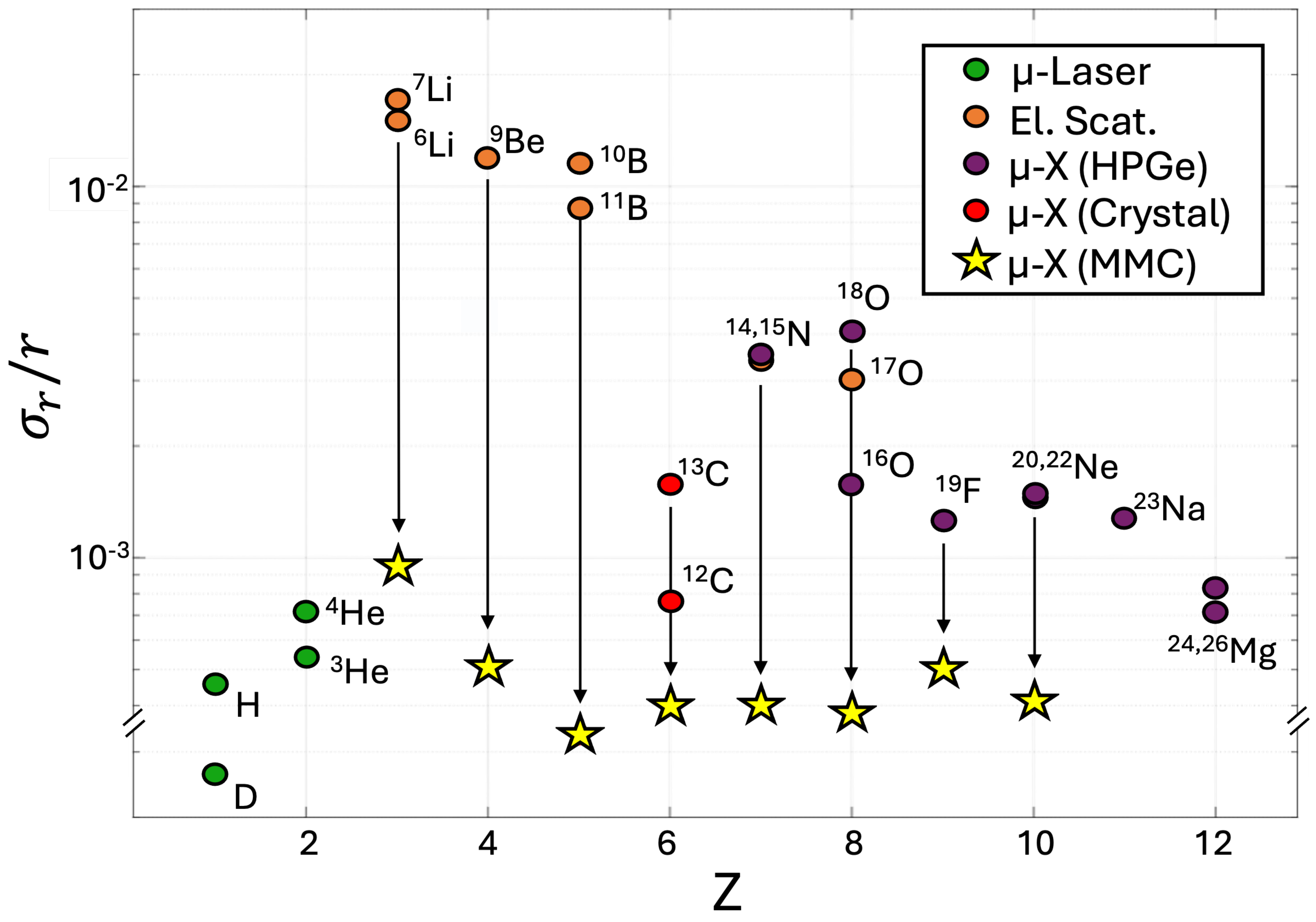
Muonic atoms as a precision probe

Observing muonic atoms



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





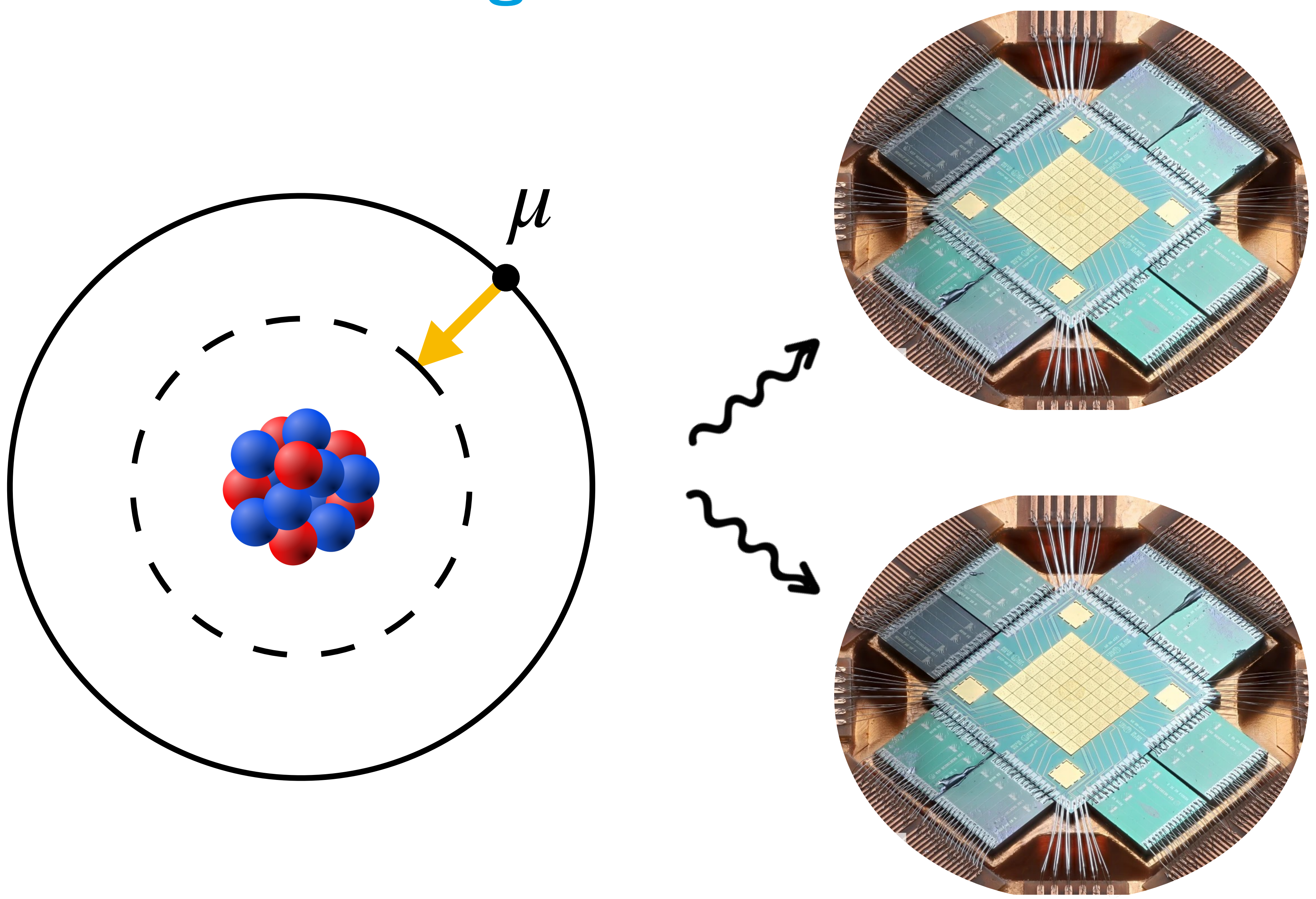
[QUARTET, Collaboration Meeting on Muonic X-ray (2025)]

QUARTET collaboration

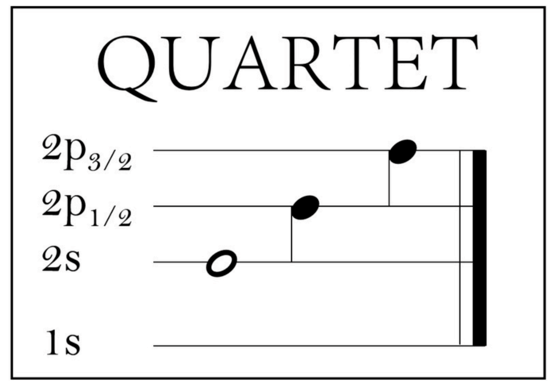
- Improving energy resolution with MMC
  - Quantum sensor detector to reach low-Z nuclei
  - **Data taken at PSI with Li, Be, B targets**

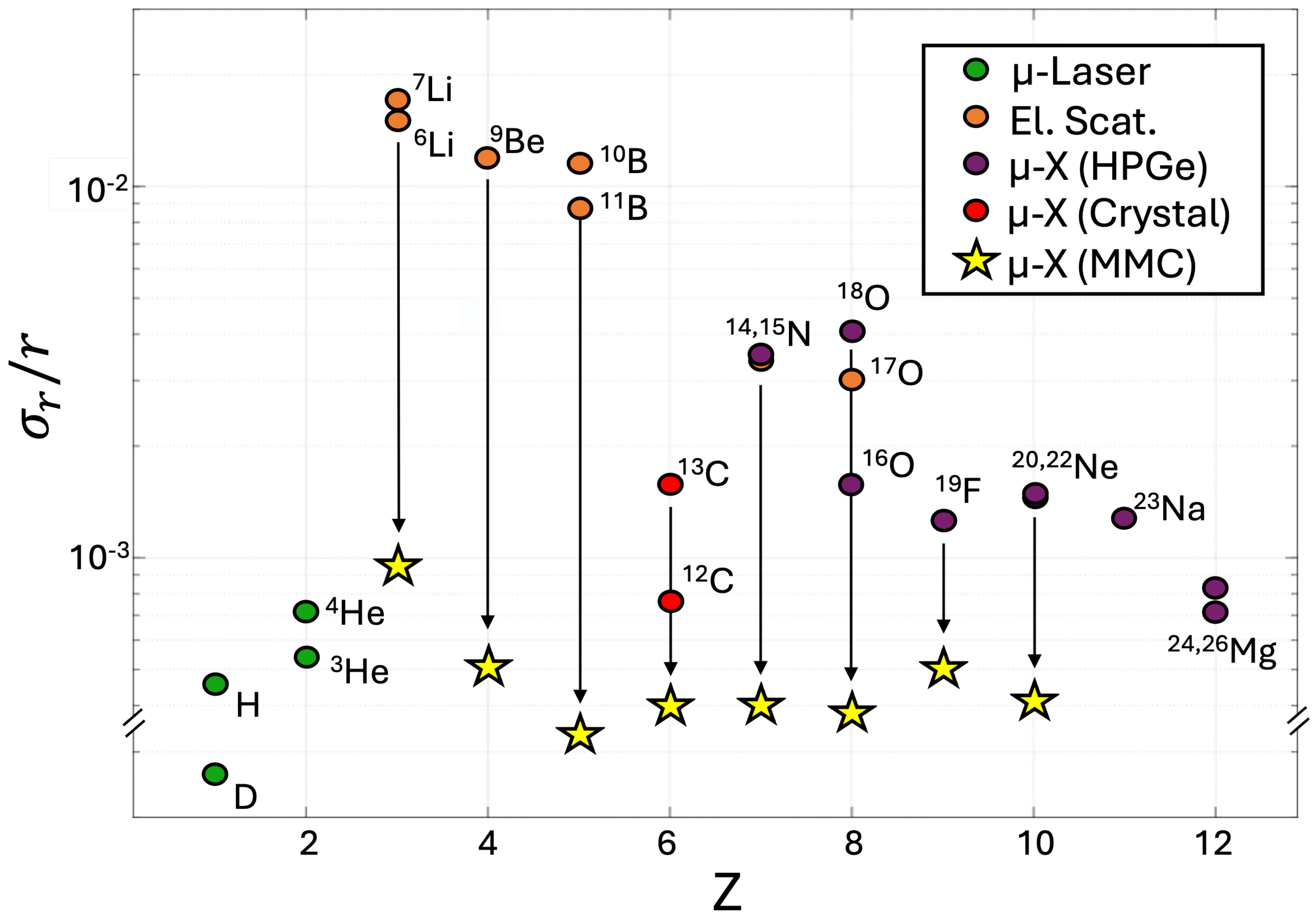
Muonic atoms as a precision probe

Observing muonic atoms



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





[QUARTET, Collaboration Meeting on Muonic X-ray (2025)]

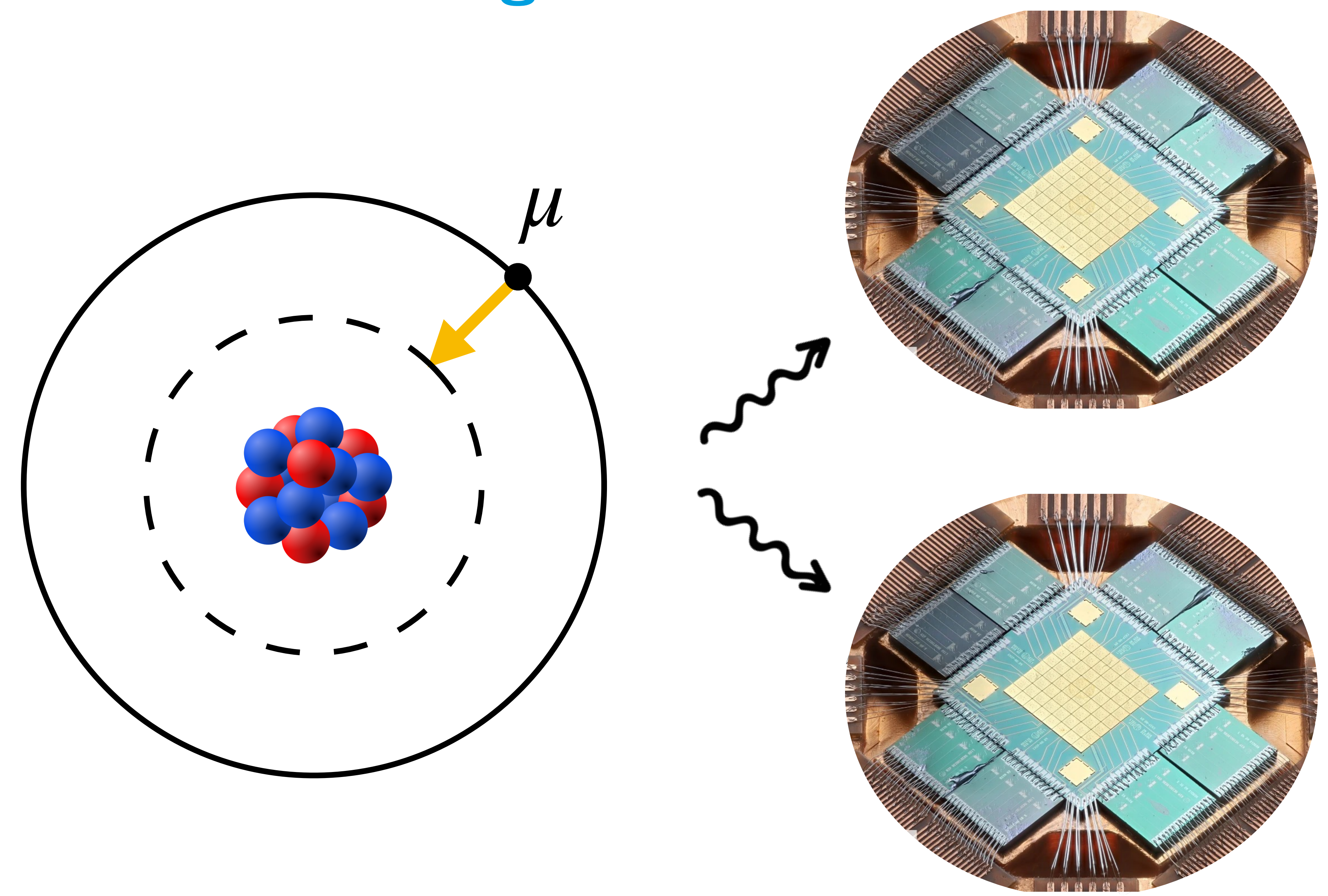
QUARTET collaboration

- Improving energy resolution with MMC
  - Quantum sensor detector to reach low-Z nuclei
  - **Data taken at PSI with $\mathrm{Li}, \mathrm{Be}, \mathrm{B}$ targets**

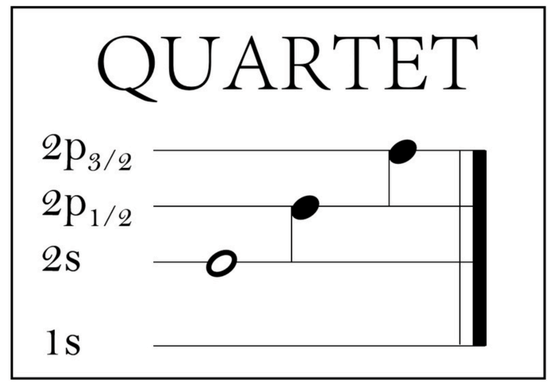
Theoretical challenge: $\sim$ **0.1 eV uncertainty on 1S**

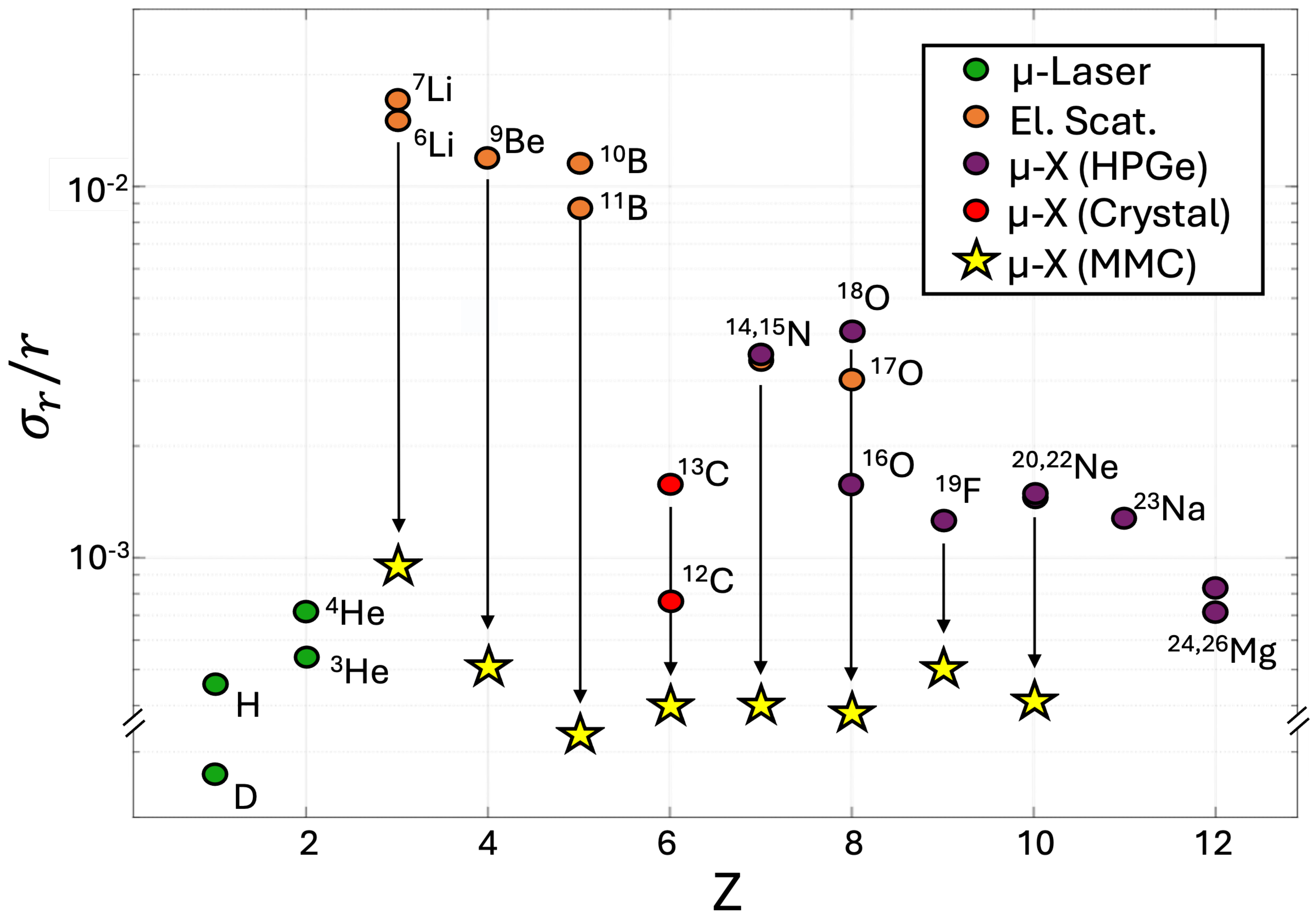
Muonic atoms as a precision probe

Observing muonic atoms



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





[QUARTET, Collaboration Meeting on Muonic X-ray (2025)]

QUARTET collaboration

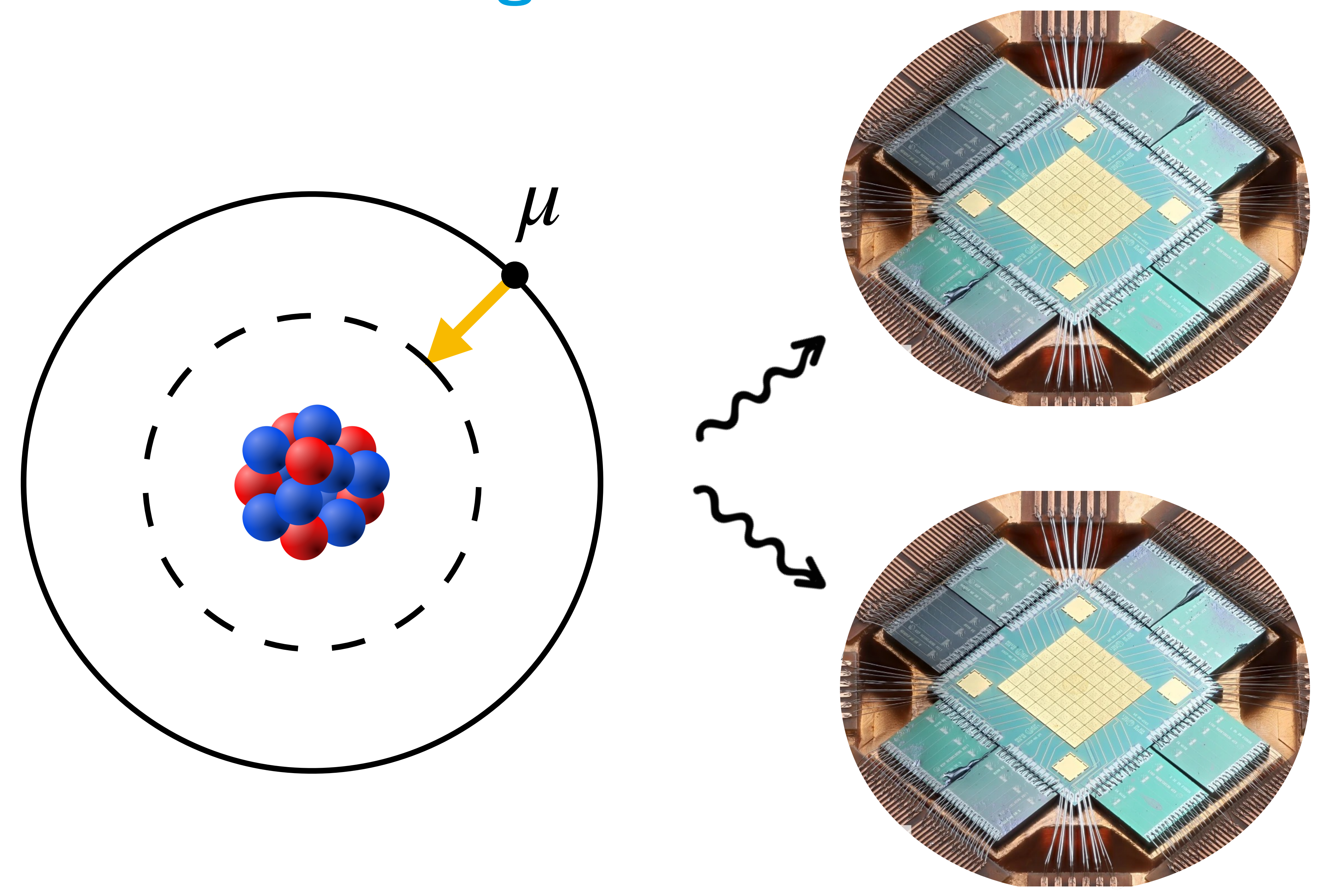
- Improving energy resolution with MMC
  - Quantum sensor detector to reach low-Z nuclei
  - **Data taken at PSI with Li, Be, B targets**

Theoretical challenge: $\sim$ **0.1 eV uncertainty on 1S**

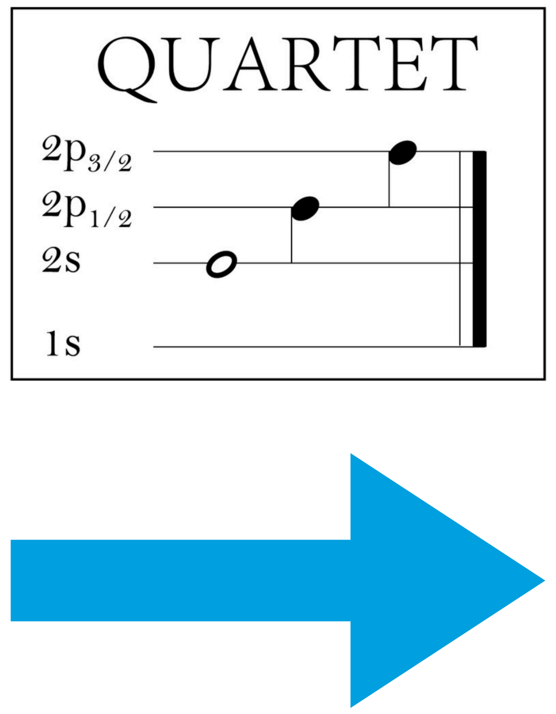
Nuclear physics: μ**-atom reference** $\Rightarrow$ **Isotopic chain**

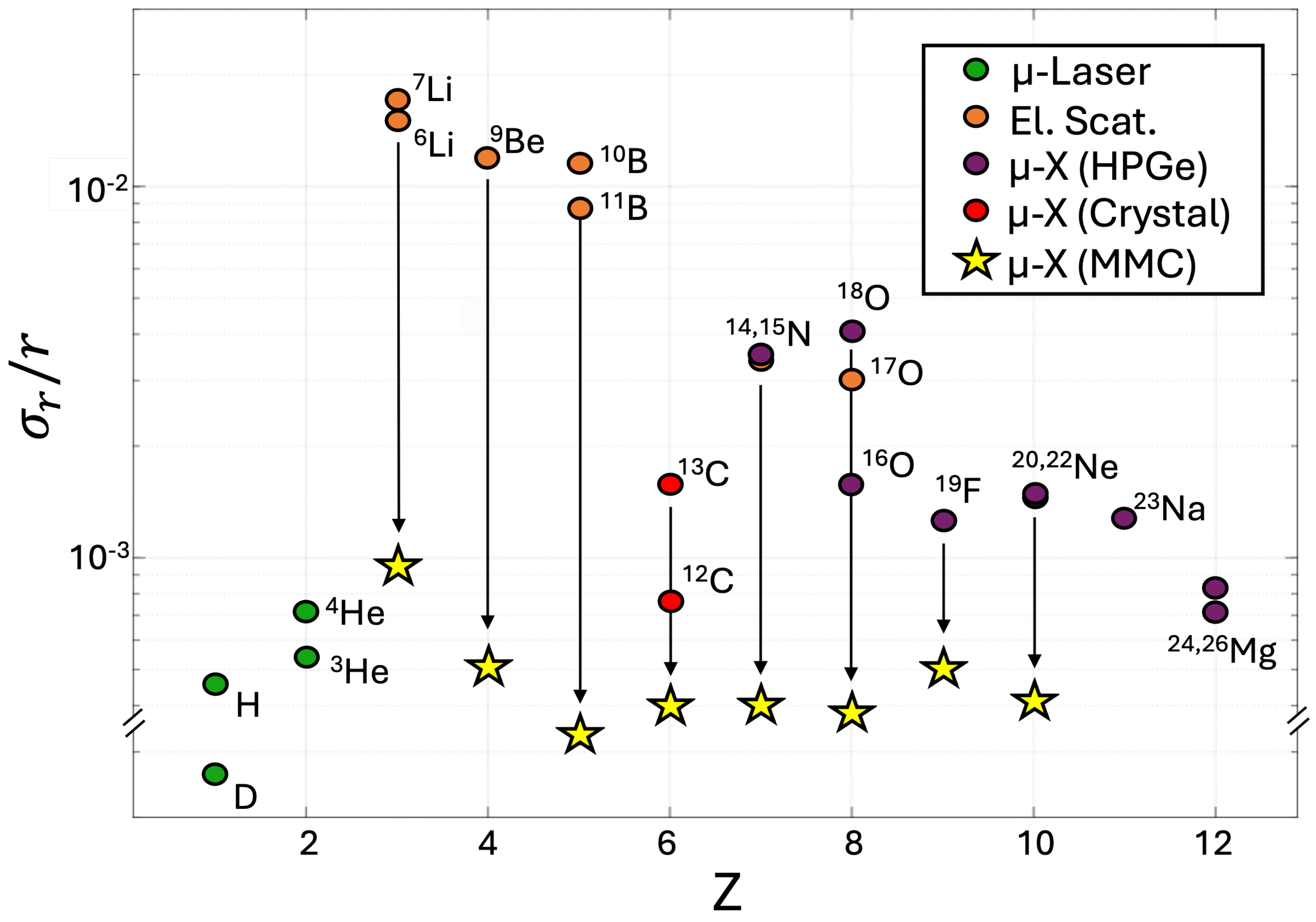
Muonic atoms as a precision probe

Observing muonic atoms



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





[QUARTET, Collaboration Meeting on Muonic X-ray (2025)]

QUARTET collaboration

- Improving energy resolution with MMC
  - Quantum sensor detector to reach low-Z nuclei
  - **Data taken at PSI with $\mathrm{Li}, \mathrm{Be}, \mathrm{B}$ targets**

Theoretical challenge: $\sim$ 0.1 eV uncertainty on 1S

Nuclear physics: μ-atom reference $\Rightarrow$ Isotopic chain

On-going puzzles: $\sim 3.5\sigma$ for $^{3-4}\mathrm{He}$ isotope shift

[Li Muli, Richardson, Bacca, PRL (2025)]

From energy levels to nuclear structure

From energy levels to nuclear structure

General many-body problem

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

From energy levels to nuclear structure

General many-body problem

- Main degrees of freedom
  - Nucleons → N ; photon → A ; Muon → ψ_μ
- Hamiltonian

[Friar, Rosen, Annals of Physics (1974)]

  - For simplicity assume non-relativistic nucleons of equal mass

$$H = H_{Nucl} + e \int \mathrm{d}^3x \; J_\mu(x) A^\mu(x) + \frac{e^2}{2m} \int \mathrm{d}^3x \mathrm{d}^3y \; f_{SG}(x,y) \; \vec{A}(x).\vec{A}(y) + H_{QED}$$

From energy levels to nuclear structure

General many-body problem

- Main degrees of freedom
  - Nucleons → N ; photon → A ; Muon → ψ_μ
- Hamiltonian

  [Friar, Rosen, Annals of Physics (1974)]
  - For simplicity assume non-relativistic nucleons of equal mass

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

- General approach to compute bound state of H
  - ✗ In principle use Bethe-Salpeter ⇒ bound states ≡ G_n poles
  - ✓ In practice use **effective external potential**

From energy levels to nuclear structure

General many-body problem

- Main degrees of freedom
  - Nucleons → N ; photon → A ; Muon → ψ_μ
- Hamiltonian

  [Friar, Rosen, Annals of Physics (1974)]

  - For simplicity assume non-relativistic nucleons of equal mass

$$H = H_{Nucl} + e \int \mathrm{d}^3x \; J_\mu(x) A^\mu(x) + \frac{e^2}{2m} \int \mathrm{d}^3x \mathrm{d}^3y \; f_{SG}(x,y) \; \vec{A}(x).\vec{A}(y) + H_{QED}$$

- General approach to compute bound state of H
  - ✗ In principle use Bethe-Salpeter ⇒ bound states ≡ G_n poles
  - ✓ In practice use **effective external potential**
- Main type of QED contributions
  - Electron vacuum polarization: $a_\mu \sim \lambda_e$ ⇒ **main one!**
  - Finite nuclear mass ⇒ recoil and relativistic corrections
  - Finite nuclear size contributions ⇒ Main one $\propto r_c^2$

From energy levels to nuclear structure

General many-body problem

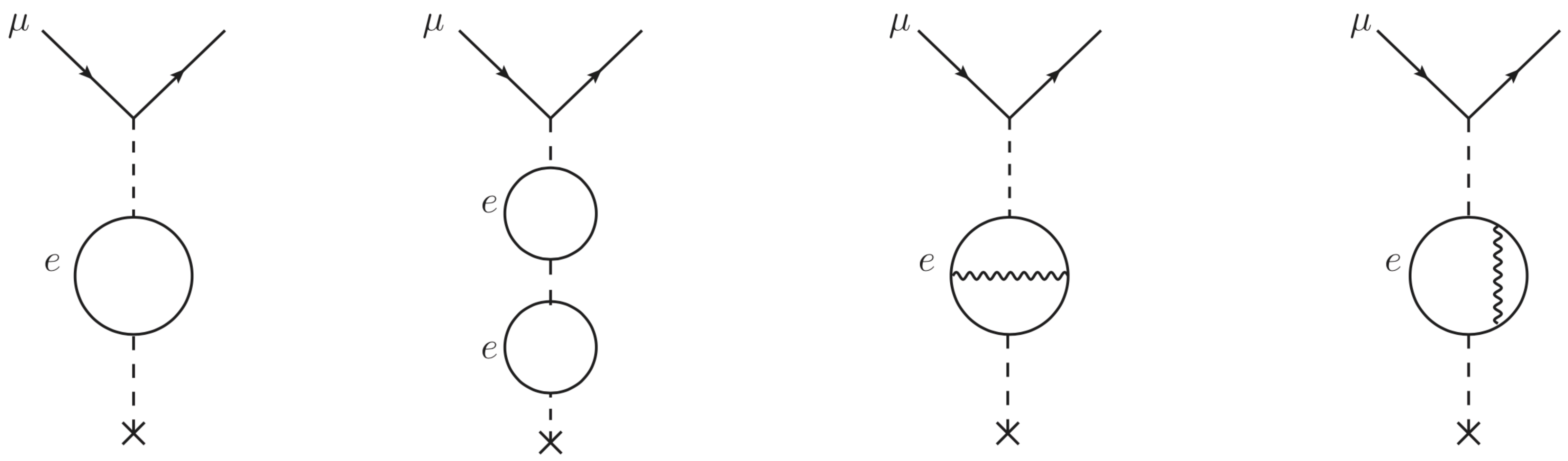
- Main degrees of freedom
  - Nucleons → N ; photon → A ; Muon → ψ_μ
- Hamiltonian [Friar, Rosen, Annals of Physics (1974)]
  - For simplicity assume non-relativistic nucleons of equal mass

$$H = H_{Nucl} + e\int \mathrm{d}^3x\; J_\mu(x)A^\mu(x) + \frac{e^2}{2m}\int \mathrm{d}^3x\mathrm{d}^3y\; f_{SG}(x,y)\; \vec{A}(x).\vec{A}(y) + H_{QED}$$

- General approach to compute bound state of H
  - ✗ In principle use Bethe-Salpeter ⇒ bound states ≡ G_n poles
  - ✓ In practice use **effective external potential**
- Main type of QED contributions
  - Electron vacuum polarization: $a_\mu \sim \lambda_e$ ⇒ **main one!**
  - Finite nuclear mass ⇒ recoil and relativistic corrections
  - Finite nuclear size contributions ⇒ Main one ∝ r_c^2

Example: electron vacuum polarization corrections

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



⇒ δ_{QED} term in δ_{E}

From energy levels to nuclear structure

General many-body problem

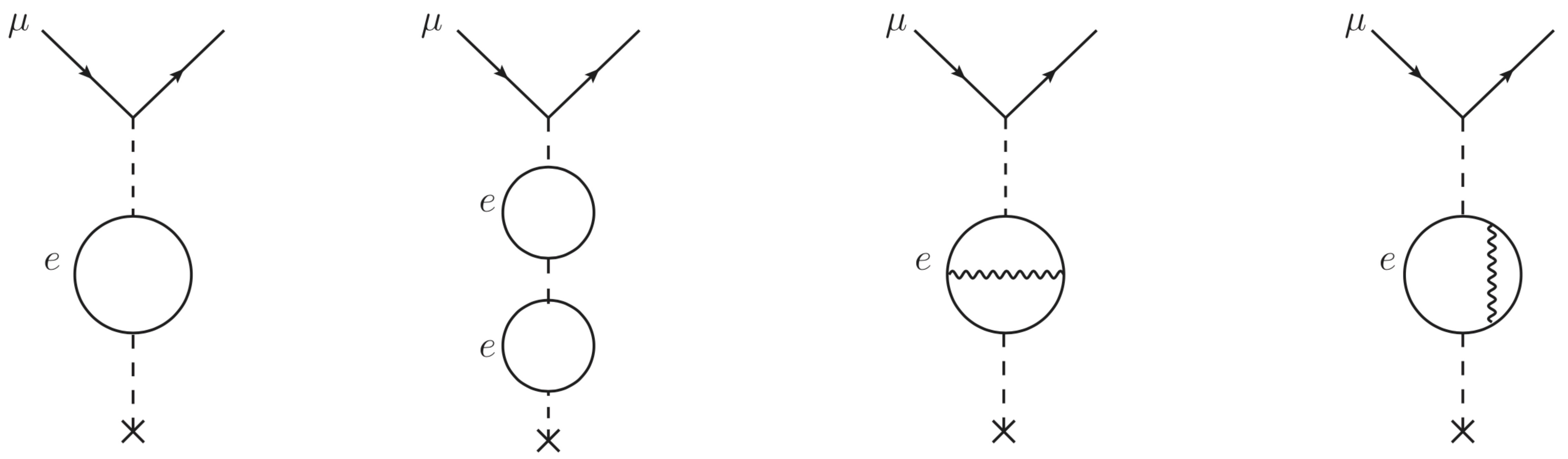
- Main degrees of freedom
  - Nucleons $\rightarrow N$; photon $\rightarrow A$; Muon $\rightarrow \psi_\mu$
- Hamiltonian [Friar, Rosen, Annals of Physics (1974)]
  - For simplicity assume non-relativistic nucleons of equal mass

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

- General approach to compute bound state of H
  - ✗ In principle use Bethe-Salpeter ⇒ bound states ≡ G_n poles
  - ✓ In practice use **effective external potential**
- Main type of QED contributions
  - Electron vacuum polarization: $a_\mu \sim \lambda_e$ ⇒ **main one!**
  - Finite nuclear mass ⇒ recoil and relativistic corrections
  - Finite nuclear size contributions ⇒ Main one $\propto r_c^2$

Example: electron vacuum polarization corrections

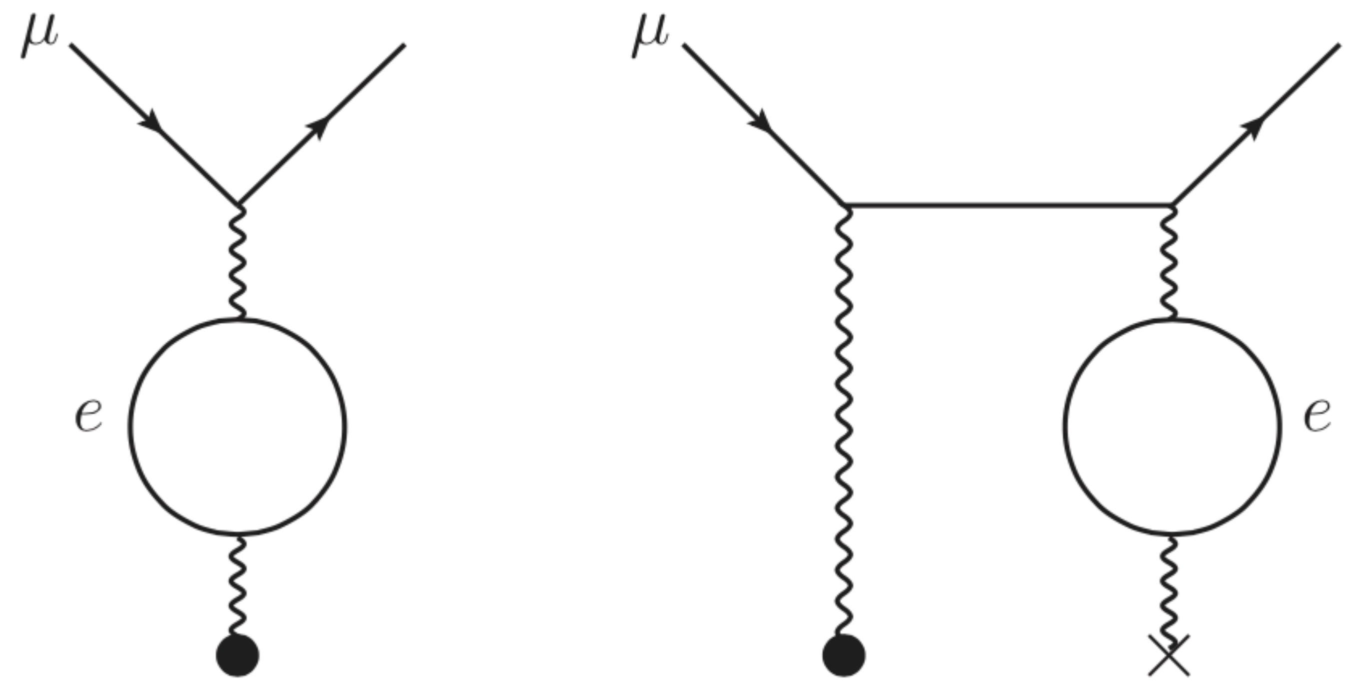
[Pachucki et al. Review of Modern Physics (2024)]



$\Rightarrow\ \delta_{\mathrm{QED}}$ term in δ_{E}

Example: finite-size corrections

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



$\Rightarrow\ \mathscr{C} r_c^2$ term in δ_{E}

The two-photon exchange nuclear correction

Radius extraction master formula

$$\delta_{\mathrm{E}} = \delta_{\mathrm{QED}} + \mathscr{C}\ r_c^2 + \delta_{\mathrm{NS}}$$

The two-photon exchange nuclear correction

Radius extraction master formula

$$\delta_{\mathrm{E}} = \delta_{\mathrm{QED}} + \mathscr{C}\ r_c^2 + \delta_{\mathrm{NS}}$$

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

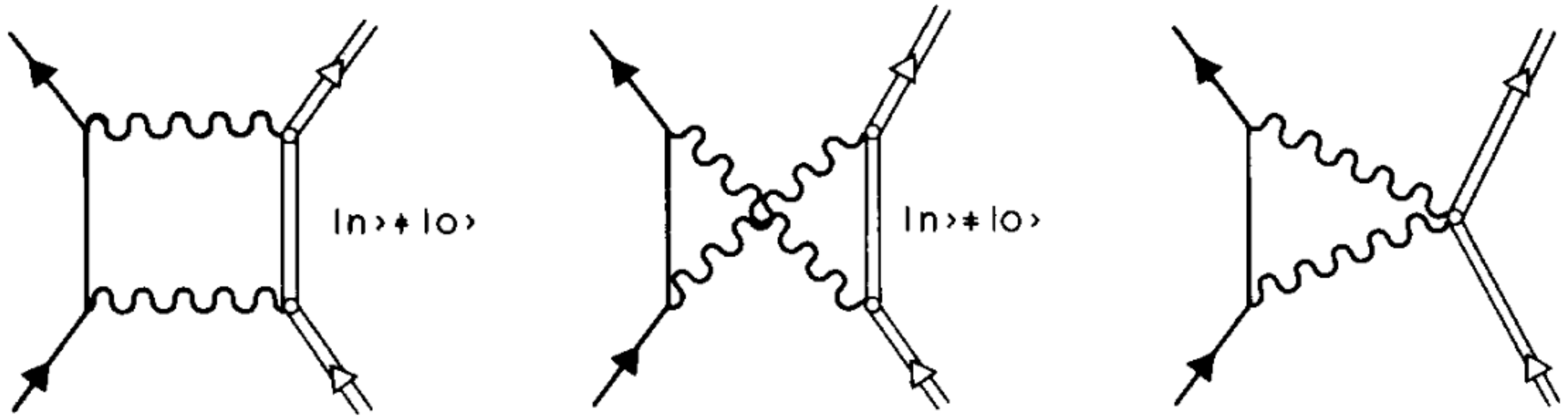
The two-photon exchange nuclear correction

Radius extraction master formula

$$\delta_{\mathrm{E}} = \delta_{\mathrm{QED}} + \mathscr{C}\ r_c^2 + \delta_{\mathrm{NS}}$$

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

Two-photon polarizability contributions



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

[Bernabeu et al, Nuclear Physics A (1974)] [Rosenfelder Nuclear Physics A (1983)]

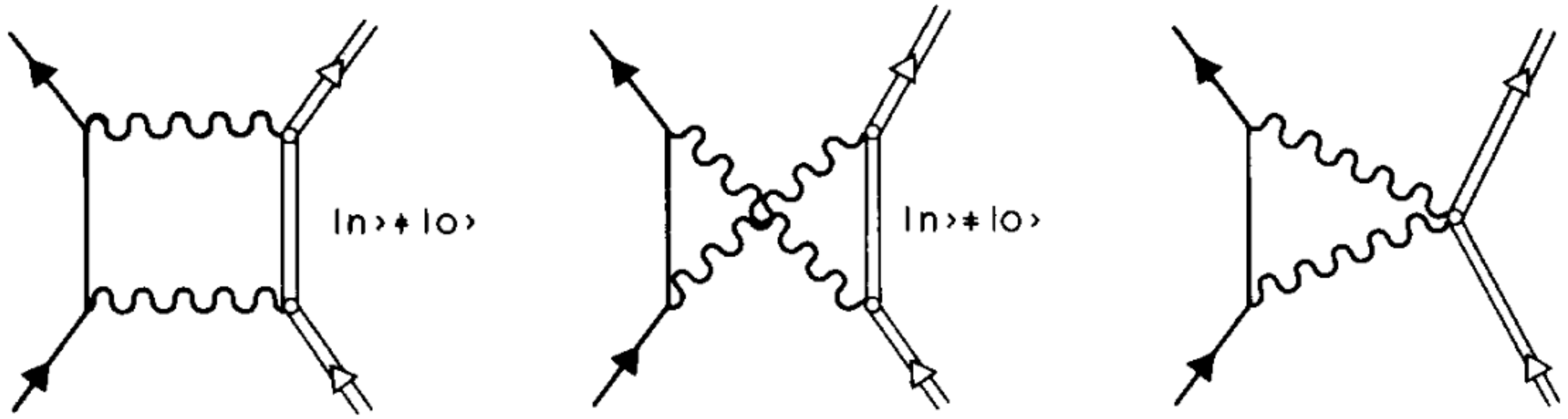
The two-photon exchange nuclear correction

Radius extraction master formula

$$\delta_{\mathrm{E}} = \delta_{\mathrm{QED}} + \mathscr{C}\, r_c^2 + \delta_{\mathrm{NS}}$$

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

Two-photon polarizability contributions



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

[Bernabeu et al, Nuclear Physics A (1974)] [Rosenfelder Nuclear Physics A (1983)]

Hadronic tensor [Friar, Annals of Physics (1976)]

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

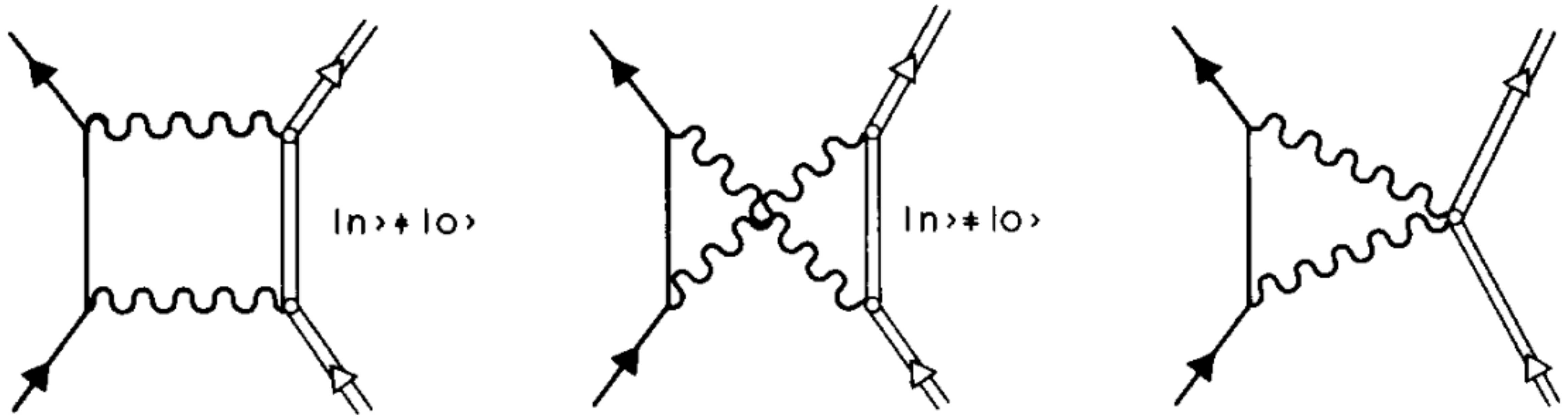
The two-photon exchange nuclear correction

Radius extraction master formula

$$\delta_E = \delta_{QED} + \mathscr{C}\, r_c^2 + \delta_{NS}$$

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

Two-photon polarizability contributions



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

[Bernabeu et al, Nuclear Physics A (1974)] [Rosenfelder Nuclear Physics A (1983)]

Hadronic tensor [Friar, Annals of Physics (1976)]

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

Nuclear polarizability [Hernandez et al. PRC (2019)]

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

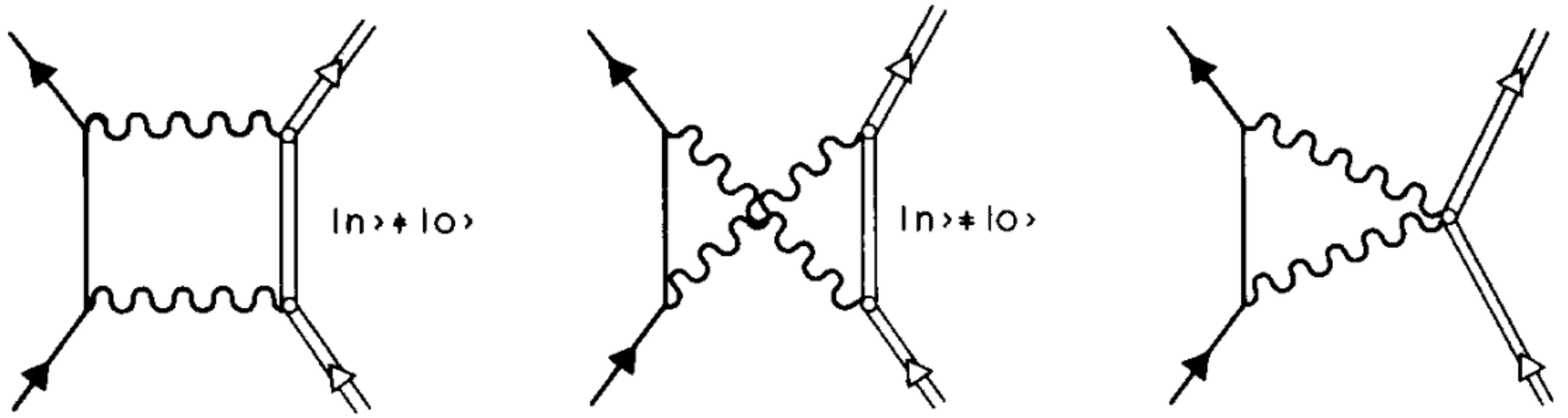
The two-photon exchange nuclear correction

Radius extraction master formula

$$\delta_{\mathrm{E}} = \delta_{\mathrm{QED}} + \mathscr{C}\ r_c^2 + \delta_{\mathrm{NS}}$$

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

Two-photon polarizability contributions



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

[Bernabeu et al, Nuclear Physics A (1974)] [Rosenfelder Nuclear Physics A (1983)]

Hadronic tensor [Friar, Annals of Physics (1976)]

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

Nuclear polarizability [Hernandez et al. PRC (2019)]

- TPE decomposition: $\delta_{\mathrm{TPE}} = \delta^A_{\mathrm{pol}} + \delta^N_{\mathrm{pol}}\ (+\delta_{\mathrm{el}})$
- Multipole decomposition: $\delta^A_{\mathrm{pol}} = \Delta_C + \Delta_{T,E} + \Delta_{T,M}$

➡ $\Delta_X \equiv \int \mathrm{d}q \int \mathrm{d}\omega\ K_X(\omega, q)\ S_X(\omega, q)$

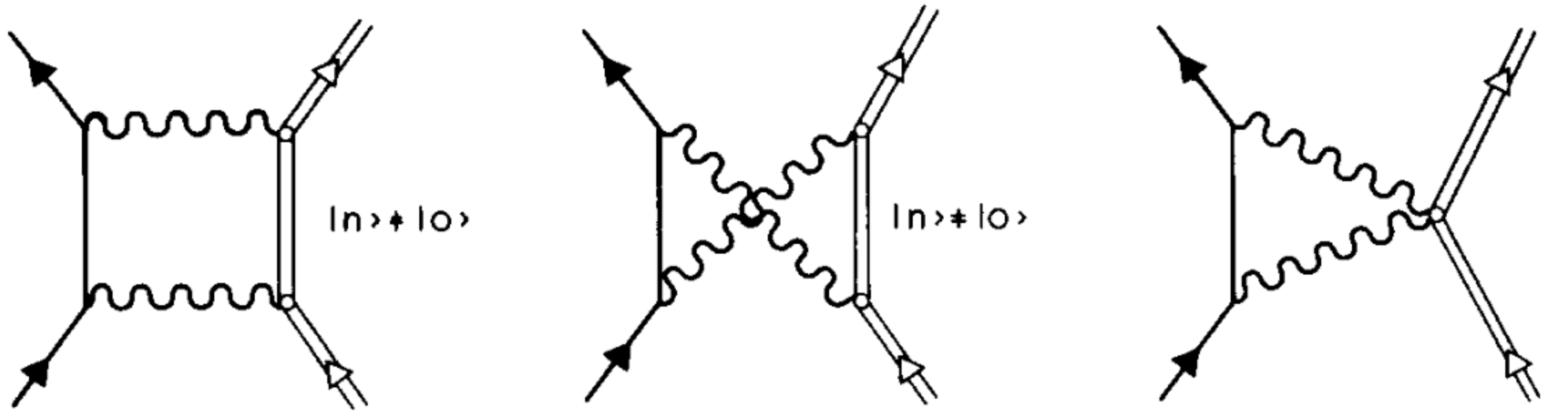
The two-photon exchange nuclear correction

Radius extraction master formula

$$\delta_E = \delta_{QED} + \mathscr{C}\ r_c^2 + \delta_{NS}$$

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

Two-photon polarizability contributions



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

[Bernabeu et al, Nuclear Physics A (1974)] [Rosenfelder Nuclear Physics A (1983)]

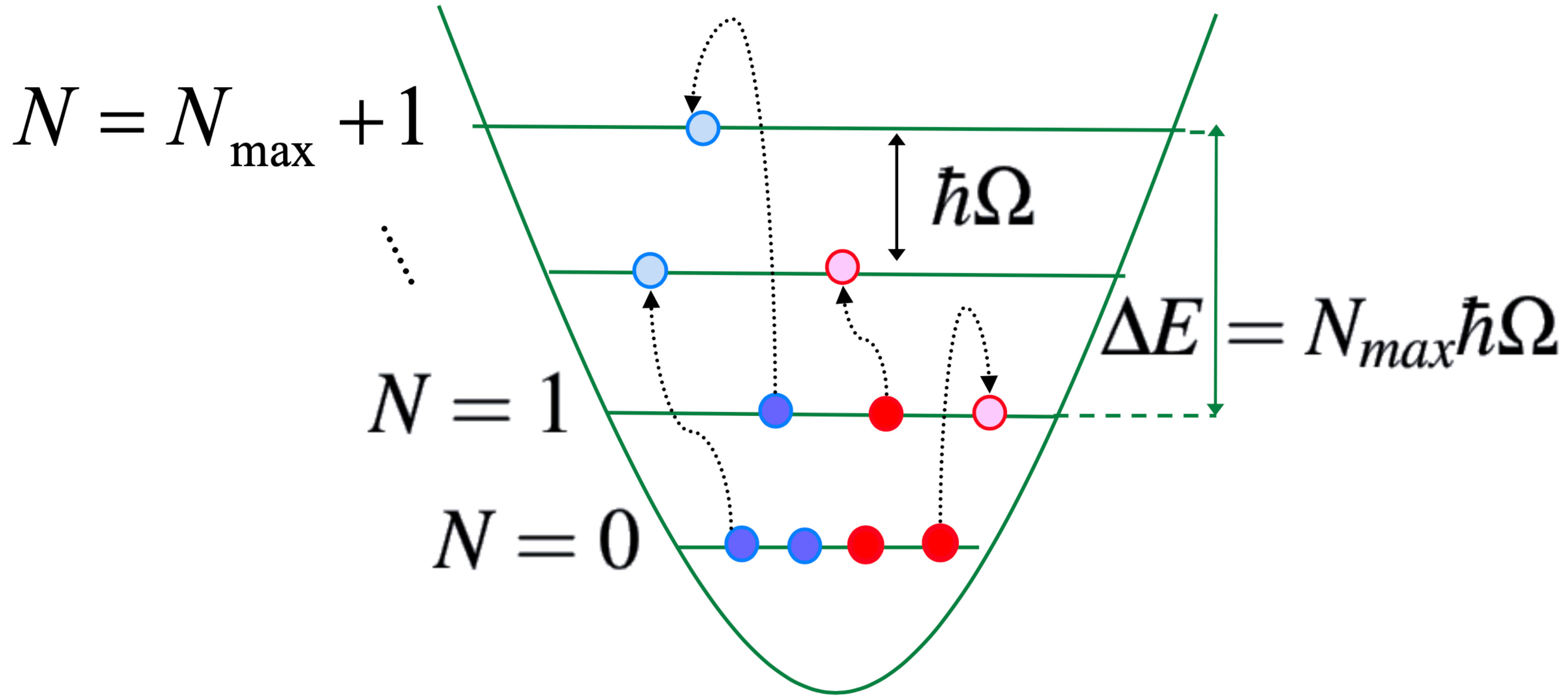
Hadronic tensor [Friar, Annals of Physics (1976)]

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

Nuclear polarizability [Hernandez et al. PRC (2019)]

- TPE decomposition: $\delta_{TPE} = \delta^A_{pol} + \delta^N_{pol}\ (+\delta_{el})$
- Multipole decomposition: $\delta^A_{pol} = \Delta_C + \Delta_{T,E} + \Delta_{T,M}$
  - ➡ $\Delta_X \equiv \int dq \int d\omega\ K_X(\omega,q)\ S_X(\omega,q)$
- Spectral functions:
  - ➡ $S_X(\omega,q) \equiv \sum_{J\geq 0}\sum_{N\neq 0} |\langle N | O_{X,J}(q) | \Psi\rangle|^2 \delta(E_N - E_0 - \omega)$

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
  - Non-relativistic reduction:
    - ➡ $\vec{j} \equiv$ charge convection $+$ magnetic moment rotational

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
  - Non-relativistic reduction:
    - ➡ $\vec{j} \equiv$ charge convection + magnetic moment rotational

- Multipole decomposition of nuclear currents

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

  - $M_{JM_J;TM_T}(q) \equiv \int d^3x \, \mathbf{M}_J^{M_J}(qx) J_0(x)_{TM_T}$
  - $T^E_{JM_J;TM_T}(q) \equiv \int d^3x \left[\frac{1}{q} \nabla \times \vec{\mathbf{M}}^{M_J}_{JJ}(qx) \right] . \vec{J}(x)_{TM_T}$
  - $T^M_{JM_J;TM_T}(q) \equiv \int d^3x \vec{\mathbf{M}}^{M_J}_{JJ}(qx) \, . \, \vec{J}(x)_{TM_T}$

➡ **Truncation at $J = 3$**

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
  - Non-relativistic reduction:

    ➡ $\vec{j} \equiv$ charge convection + magnetic moment rotational

- Multipole decomposition of nuclear currents

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

  - $M_{JM_J;TM_T}(q) \equiv \int d^3x \, \mathbf{M}_J^{M_J}(qx) J_0(x)_{TM_T}$
  - $T^E_{JM_J;TM_T}(q) \equiv \int d^3x \left[\frac{1}{q}\nabla \times \vec{\mathbf{M}}^{M_J}_{JJ}(qx)\right] . \vec{J}(x)_{TM_T}$
  - $T^M_{JM_J;TM_T}(q) \equiv \int d^3x \vec{\mathbf{M}}^{M_J}_{JJ}(qx) . \vec{J}(x)_{TM_T}$

➡ **Truncation at $J = 3$**

Model used for 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**

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
  - Non-relativistic reduction:
    ➡ $\vec{j} \equiv$ charge convection + magnetic moment rotational

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

➡ **Truncation at $J = 3$**

Model used for 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 many-body basis: $(\Omega, N_{\max})$

  ➡ **Estimate model space truncation uncertainty**

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
  - Non-relativistic reduction:

    ➡ $\vec{j} \equiv$ charge convection + magnetic moment rotational

- Multipole decomposition of nuclear currents

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

  - $M_{JM_J;TM_T}(q) \equiv \int d^3x \, \mathbf{M}_J^{M_J}(qx) J_0(x)_{TM_T}$
  - $T^E_{JM_J;TM_T}(q) \equiv \int d^3x \left[\frac{1}{q}\nabla \times \vec{\mathbf{M}}^{M_J}_{JJ}(qx)\right] . \vec{J}(x)_{TM_T}$
  - $T^M_{JM_J;TM_T}(q) \equiv \int d^3x \vec{\mathbf{M}}^{M_J}_{JJ}(qx) \, . \, \vec{J}(x)_{TM_T}$

  ➡ **Truncation at $J = 3$**

Model used for 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 many-body basis: $(\Omega, N_{\max})$

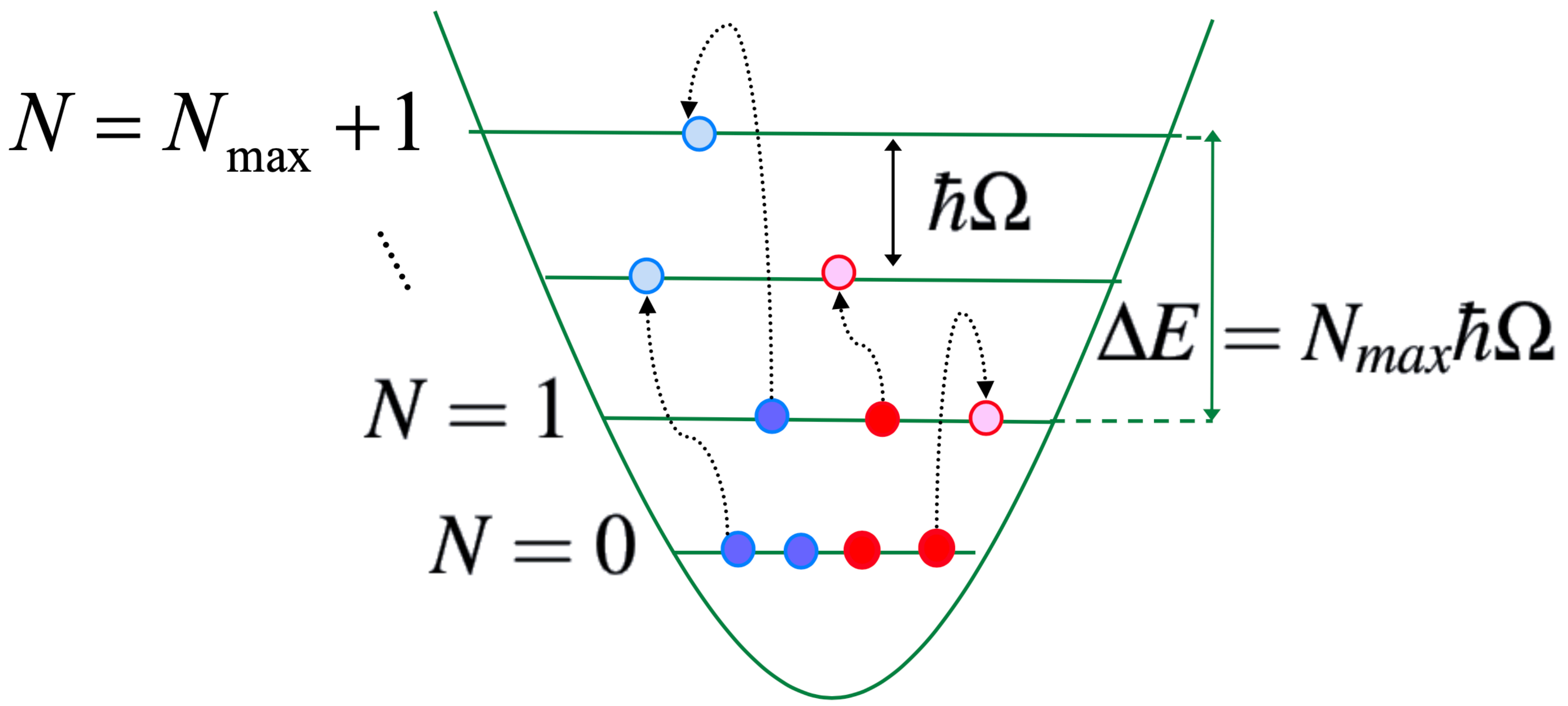
  ➡ **Estimate model space truncation uncertainty**

- 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

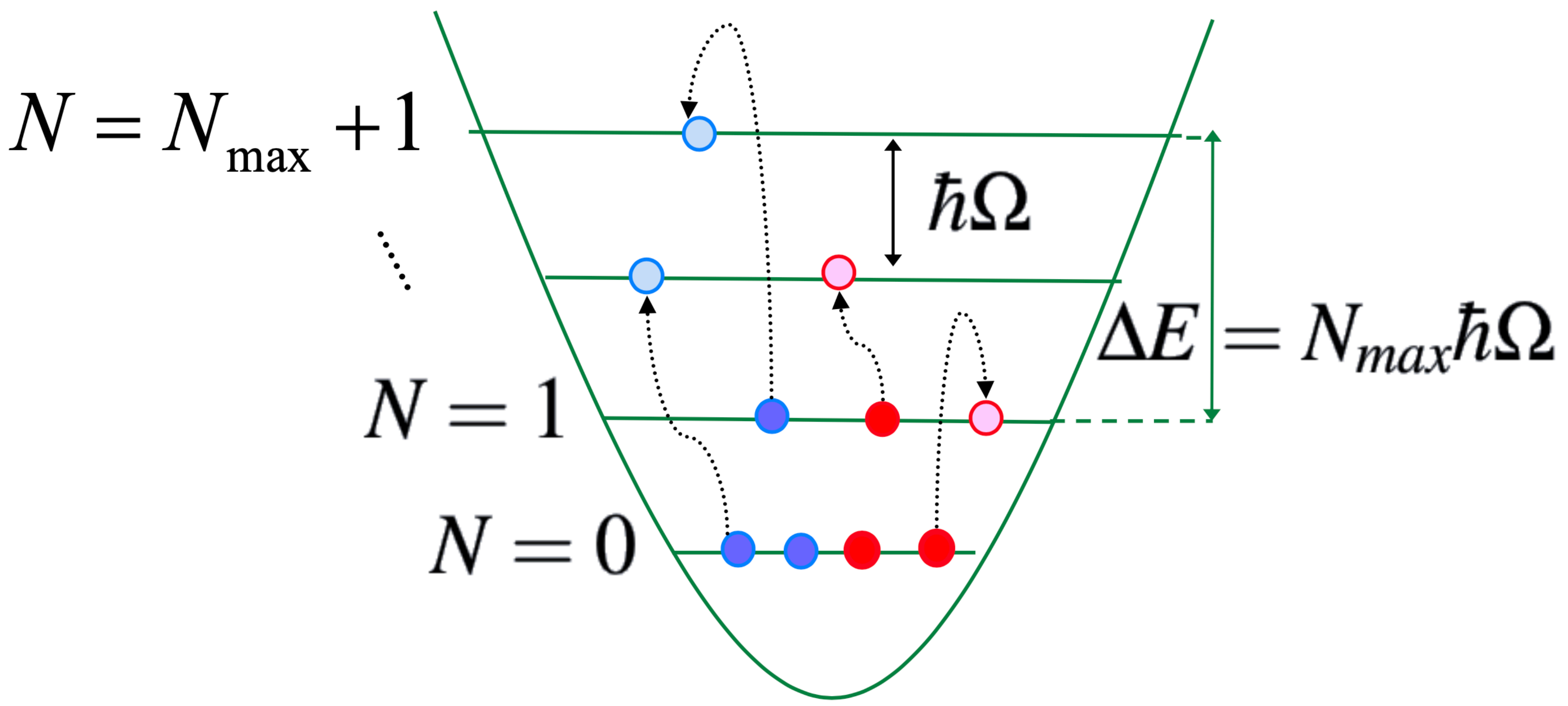
Lanczos tridiagonalization algorithm [Lanczos (1950)]

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

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

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

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

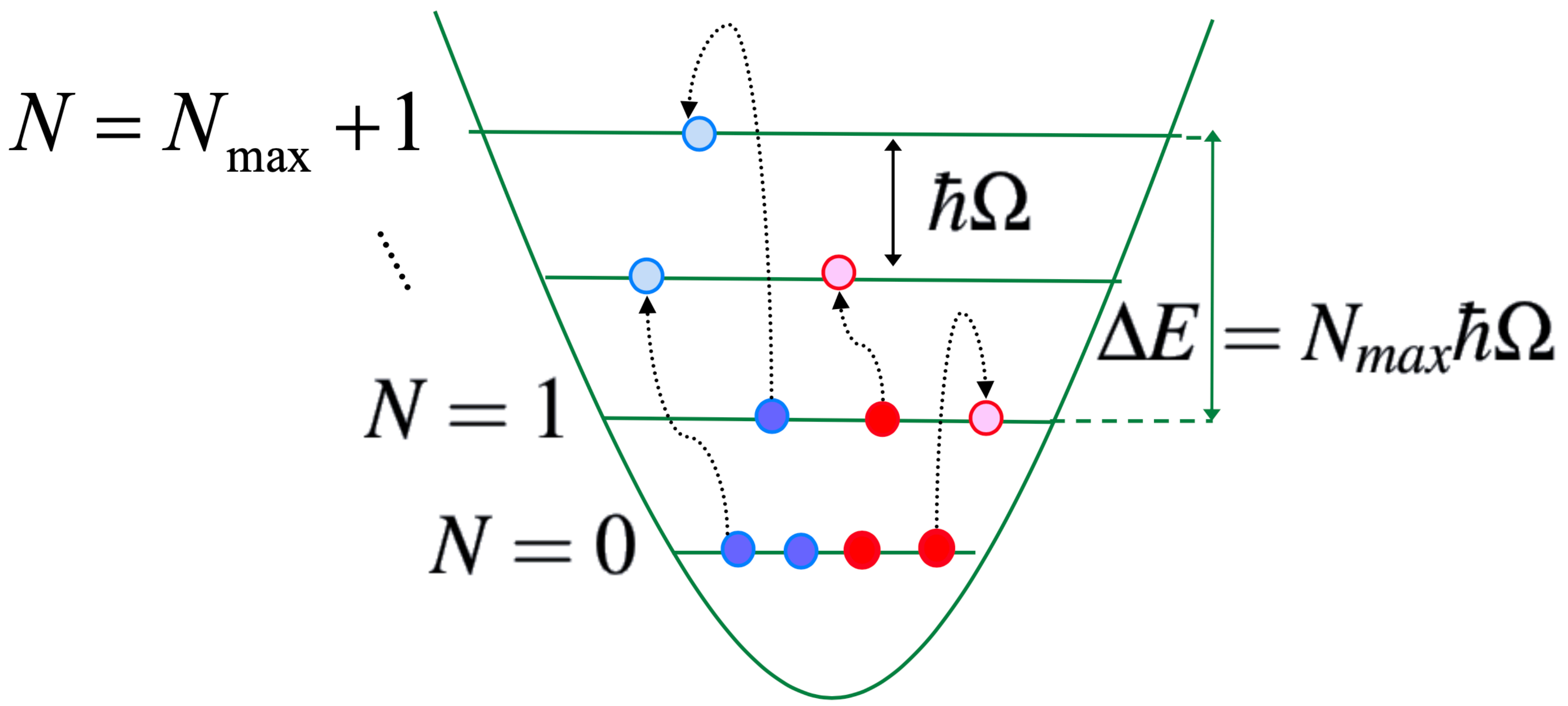
$$\begin{pmatrix} \alpha_1 & \beta_2 & & & & \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \beta_3 & \alpha_3 & \ddots & & \\ & & \ddots & \ddots & \beta_{k-1} & \\ & & & \beta_{k-1} & \alpha_{k-1} & \beta_k \\ & & & & \beta_k & \alpha_k \end{pmatrix}$$

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

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

Anti-symmetrized products of many-body HO states



The No-Core Shell Model

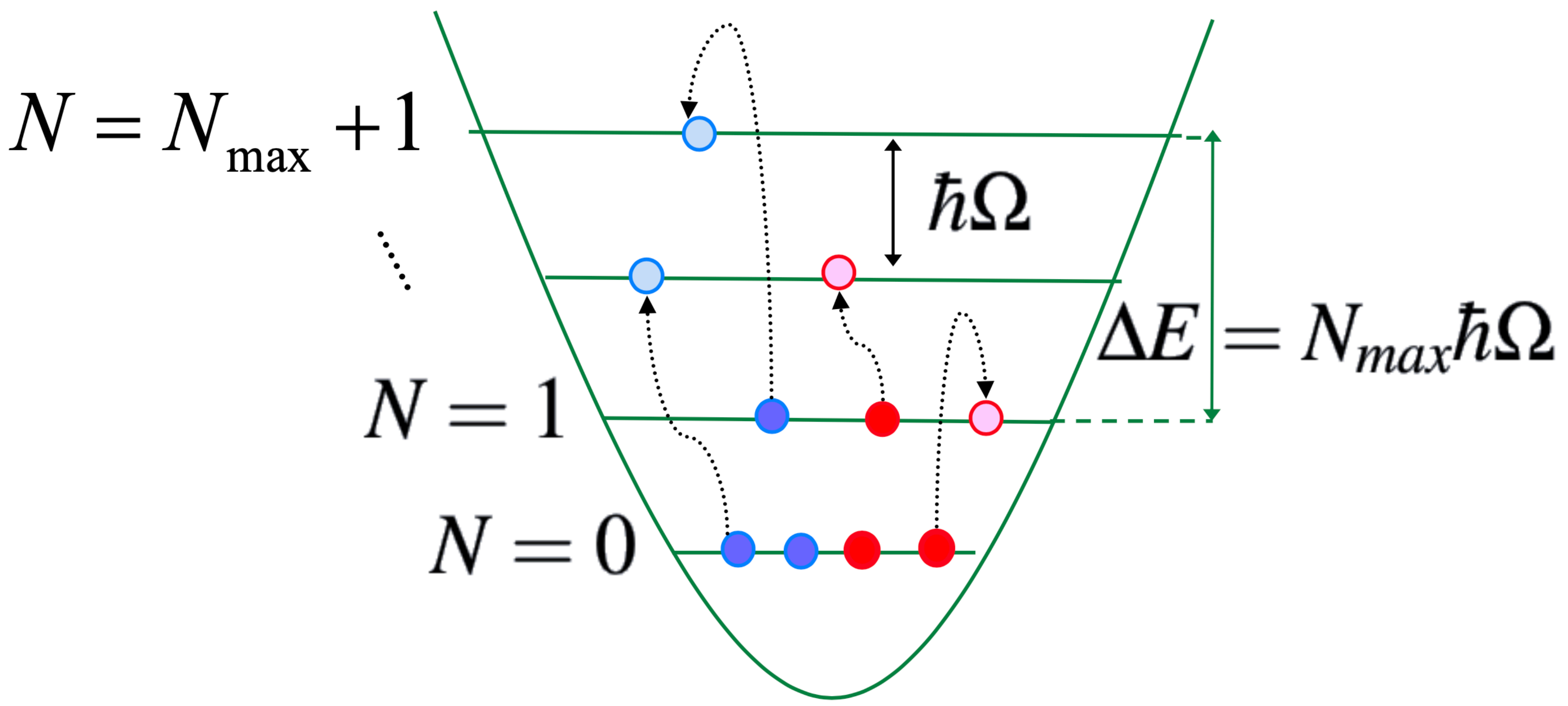
Lanczos tridiagonalization algorithm [Lanczos (1950)]

- 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 ≡ orthonormal basis in Krylov space $\left\{|\phi_1\rangle, H|\phi_1\rangle, \ \ldots, H^{N_L}|\phi_1\rangle\right\}$

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

H **in Lanczos basis**

Anti-symmetrized products of many-body HO states



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

Application to lithium isotopes

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

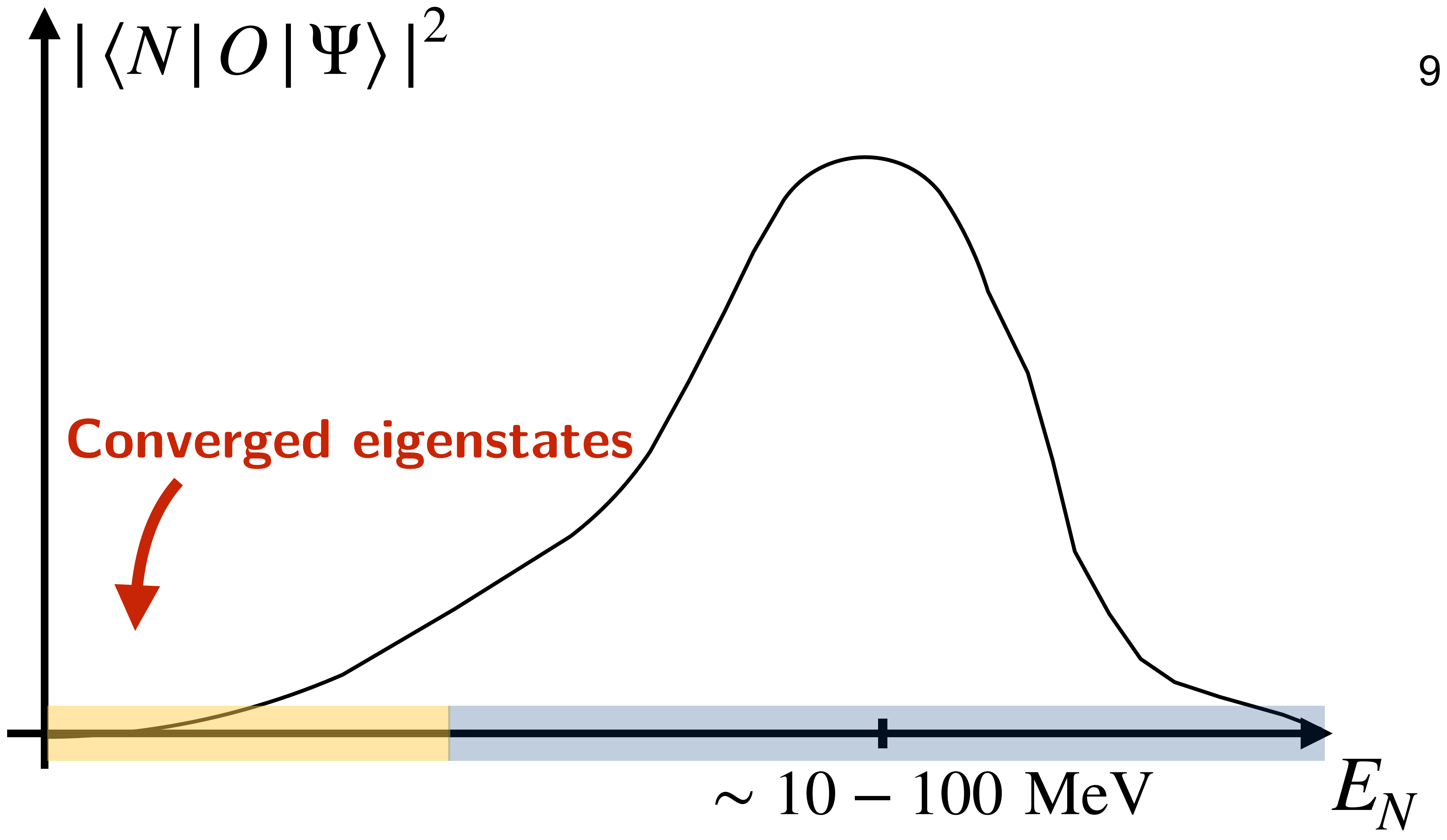
The Lanczos strength algorithm

Computing strength functions

- We need to compute for each eigenstate and operator:
  - Eigenvalues: E_N
  - Overlaps: $|\langle N|O|\Psi\rangle|^2$

  → **Too expansive to converge all of them !!**

- Lanczos strength algorithm
  - Variant of Lanczos: ensure convergence of **sum rules**



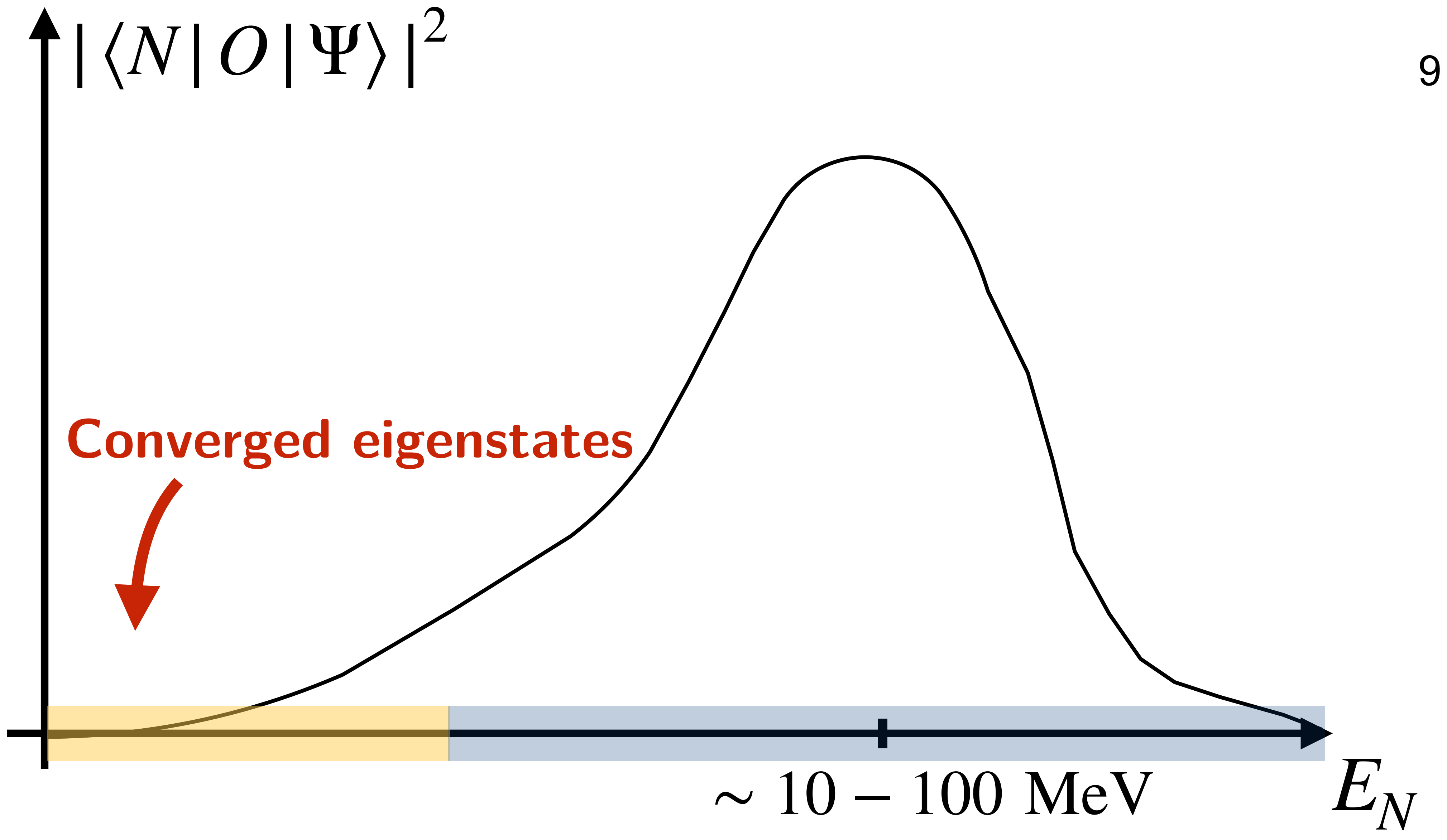
The Lanczos strength algorithm

Computing strength functions

- We need to compute for each eigenstate and operator:
  - Eigenvalues: E_N
  - Overlaps: $|\langle N|O|\Psi\rangle|^2$

  → **Too expansive to converge all of them !!**

- Lanczos strength algorithm
  - Variant of Lanczos: ensure convergence of **sum rules**



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 $\sim P_{100}(\omega)$)

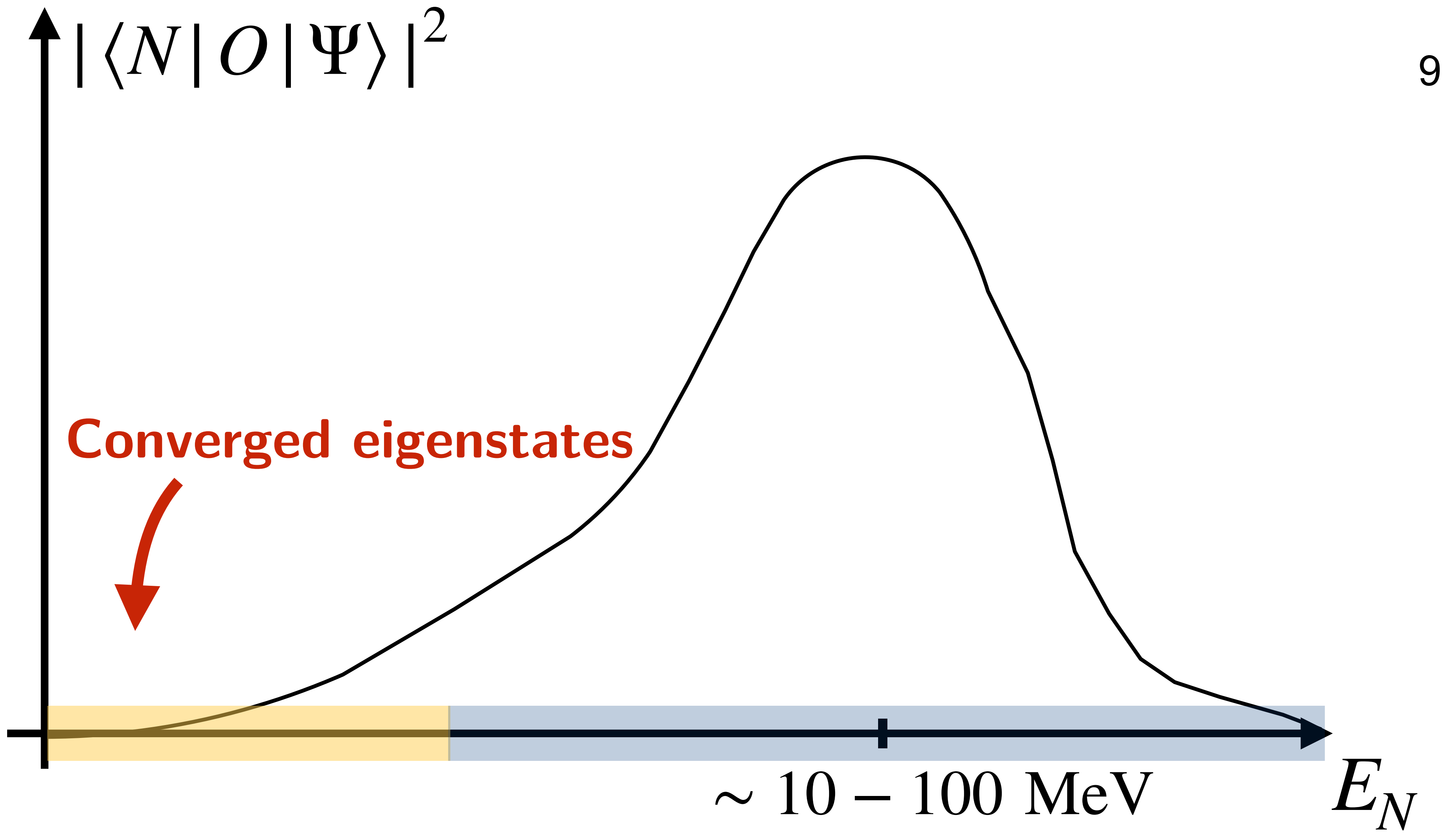
The Lanczos strength algorithm

Computing strength functions

- We need to compute for each eigenstate and operator:
  - Eigenvalues: E_N
  - Overlaps: $|\langle N|O|\Psi\rangle|^2$

  → **Too expansive to converge all of them !!**

- Lanczos strength algorithm
  - Variant of Lanczos: ensure convergence of **sum rules**



Main idea of the algorithm

- For each operator O
  - Compute $\dfrac{O|\Psi\rangle}{\sqrt{\langle\Psi|O^\dagger O|\Psi\rangle}}$ $\Rightarrow$ **Pivot** $|\phi_1'\rangle$ **for** 2^{nd} **Lanczos**
- Why first $2N_L$ moments are exact
  - $\int d\omega\, \omega^{2N_L}\, S_O(\omega) = \langle\phi_1'|H^{2N_L}|\phi_1'\rangle = \langle\phi_1'|H^{N_L}H^{N_L}|\phi_1'\rangle$

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 $\sim P_{100}(\omega)$)

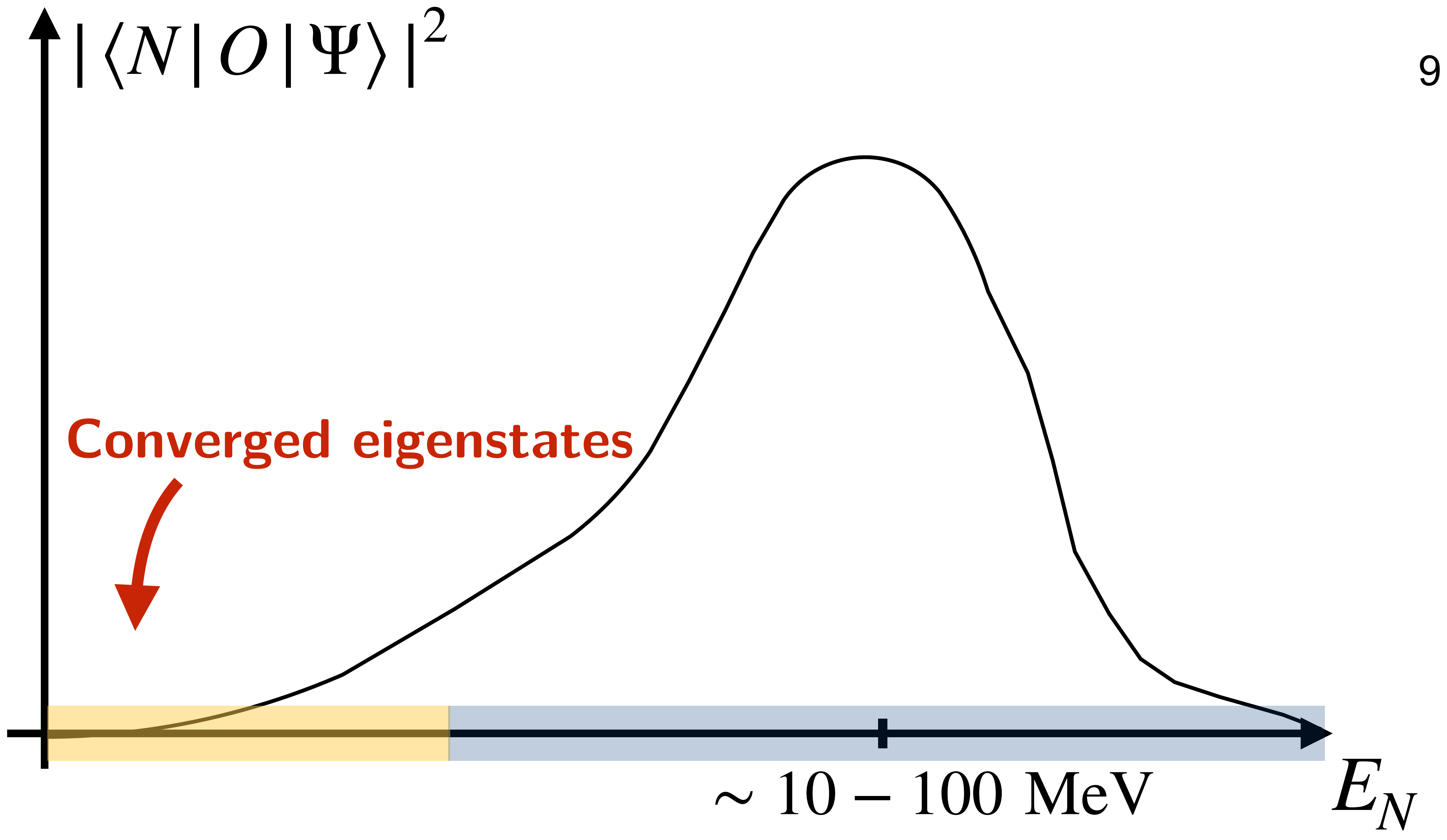
The Lanczos strength algorithm

Computing strength functions

- We need to compute for each eigenstate and operator:
  - Eigenvalues: E_N
  - Overlaps: $|\langle N|O|\Psi\rangle|^2$

  → **Too expansive to converge all of them !!**

- Lanczos strength algorithm
  - Variant of Lanczos: ensure convergence of **sum rules**



Main idea of the algorithm

- For each operator O
  - Compute $\dfrac{O|\Psi\rangle}{\sqrt{\langle\Psi|O^\dagger O|\Psi\rangle}}$ $\Rightarrow$ **Pivot** $|\phi_1'\rangle$ **for** 2^{nd} **Lanczos**
- Why first $2N_L$ moments are exact
  - $\int d\omega\, \omega^{2N_L} S_O(\omega) = \langle\phi_1'|H^{2N_L}|\phi_1'\rangle = \langle\phi_1'|H^{N_L}H^{N_L}|\phi_1'\rangle$, with $H^{N_L}|\phi_1'\rangle \in \text{Span}\left\{|\phi_1'\rangle, \dots, |\phi_{N_L}'\rangle\right\}$

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 $\sim P_{100}(\omega)$)

Numerical results for $^{6-7}\mathrm{Li}$ isotopes

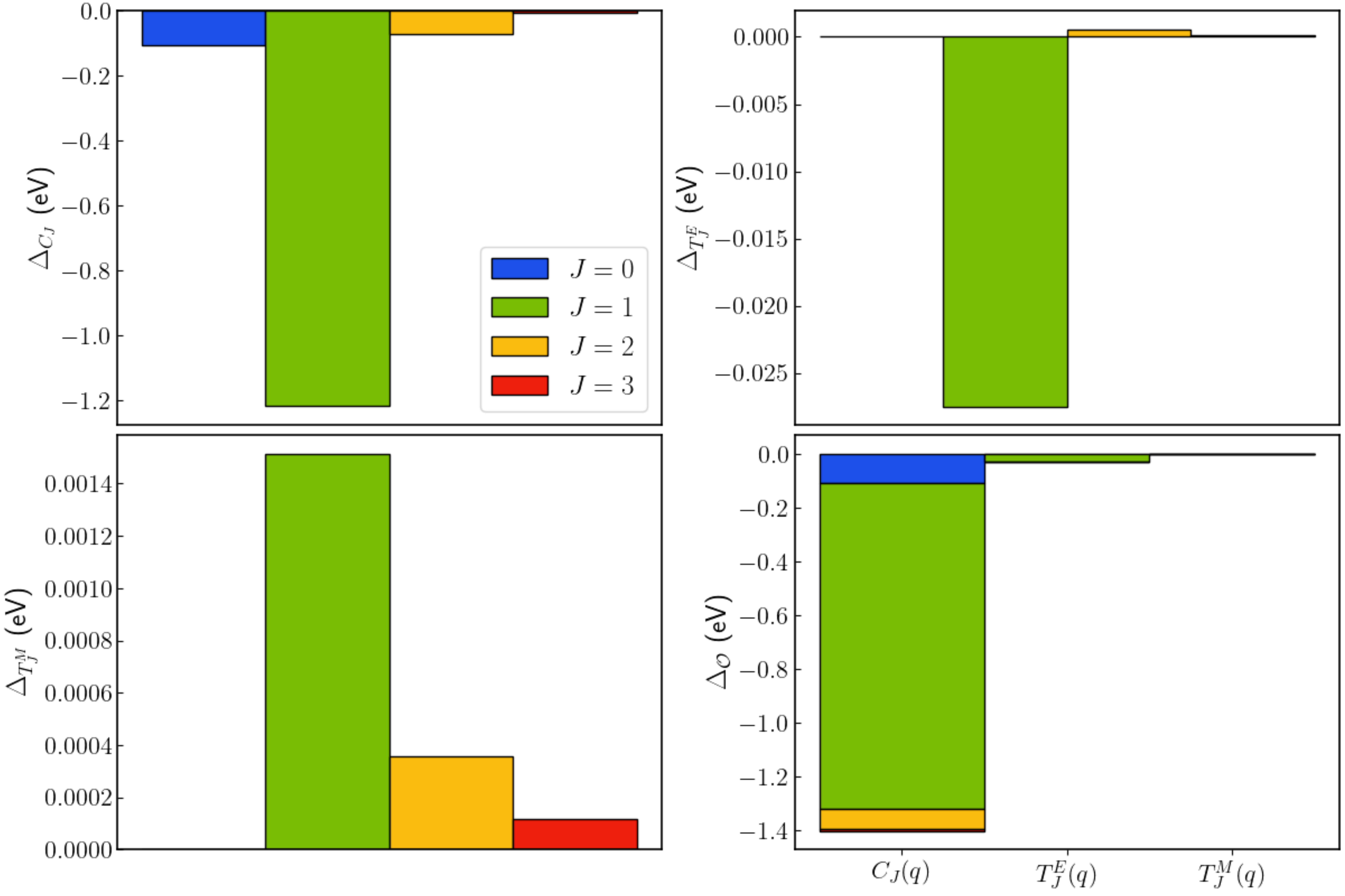
A first test case for N4LO-E7 and $N_{\max} = 7$

Numerical calculations

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

➡ **700 NCSM calculations at $N_{\max} = 7$**

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

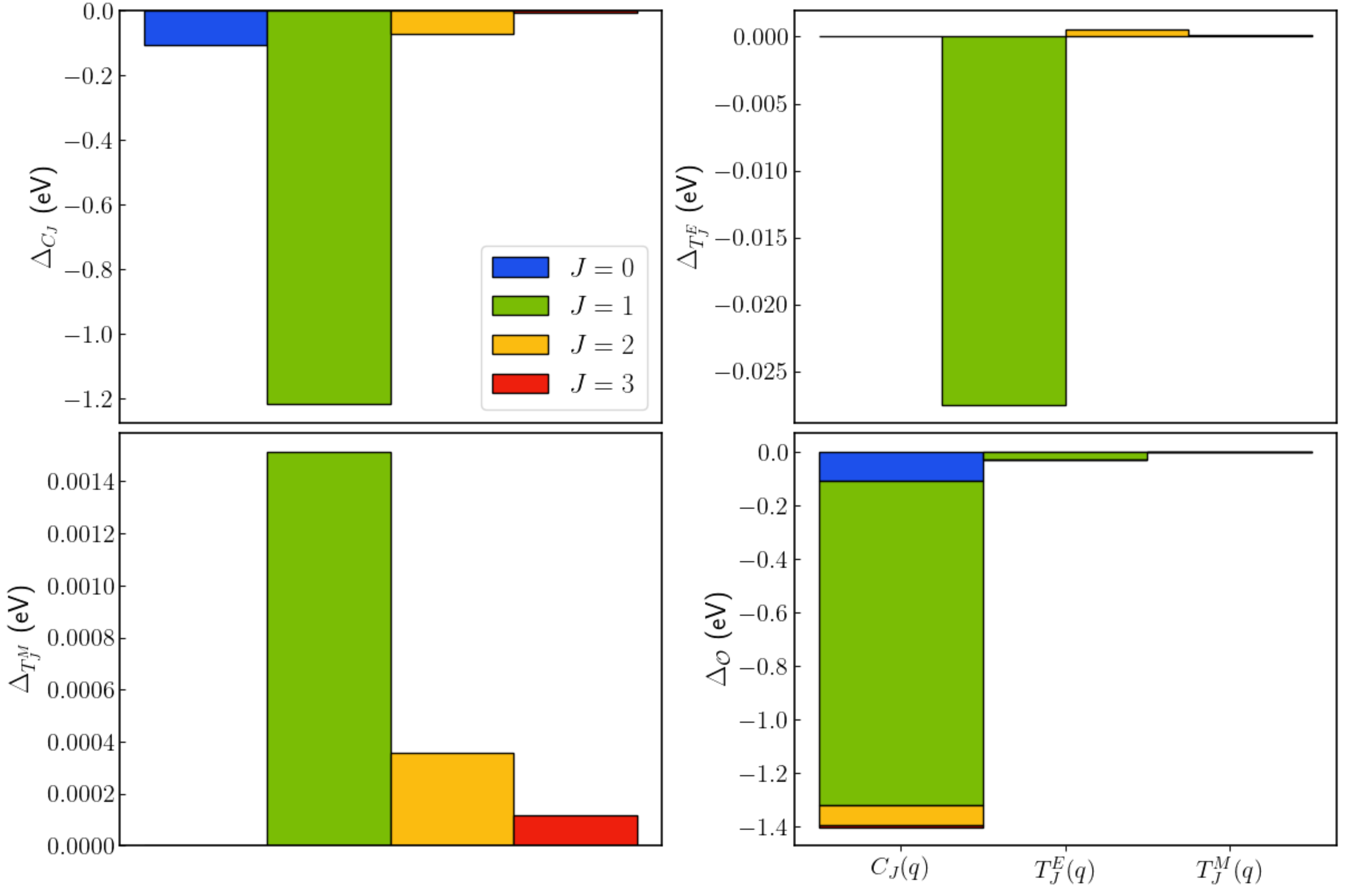


Numerical calculations

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

➡ **700 NCSM calculations at $N_{\max} = 7$**

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 $J_{\max} = 3$

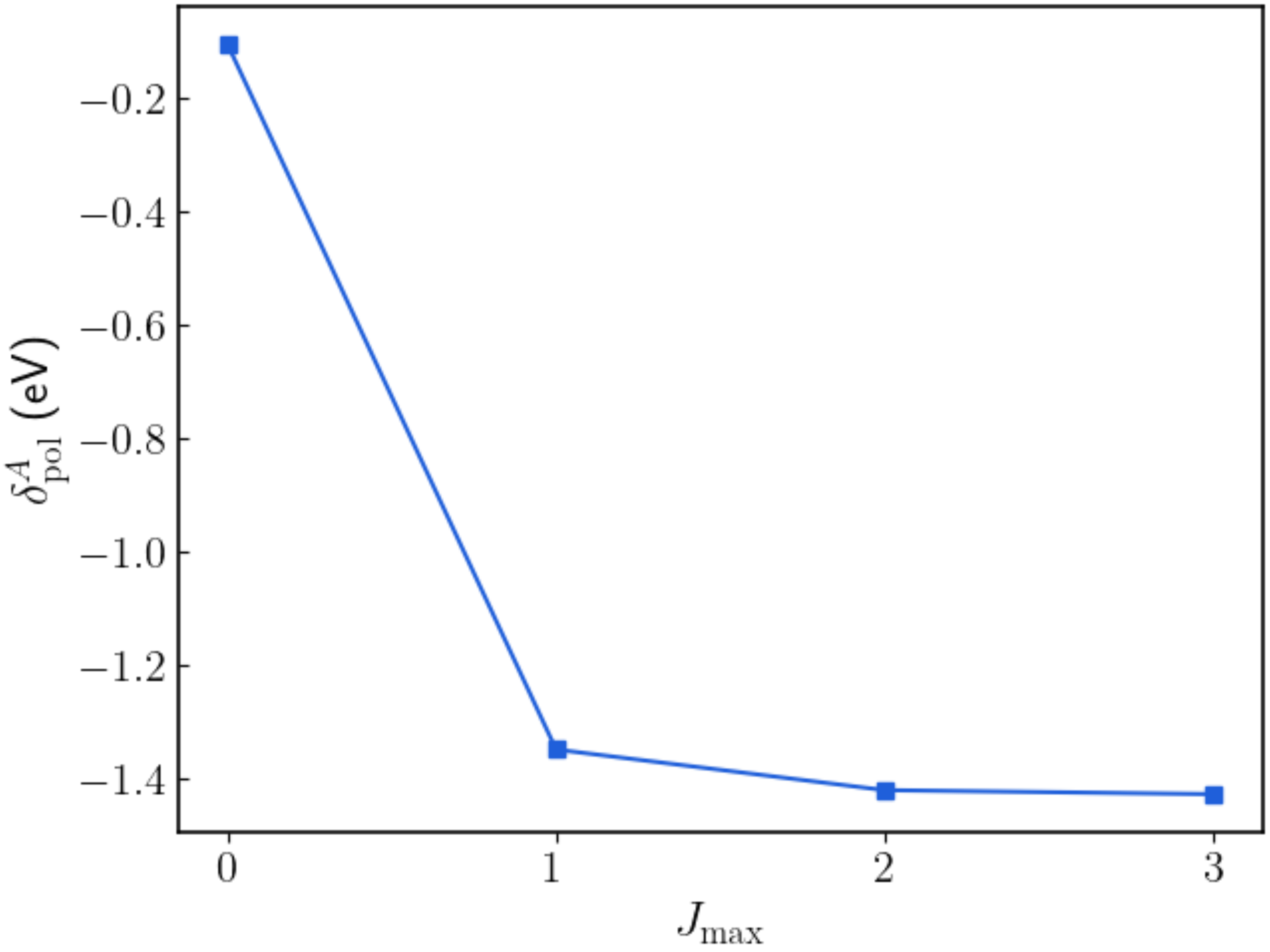
➡ **700 NCSM calculations at $N_{\max} = 7$**

Observations

- Contribution repartitions
  - 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 $J_{\max}$

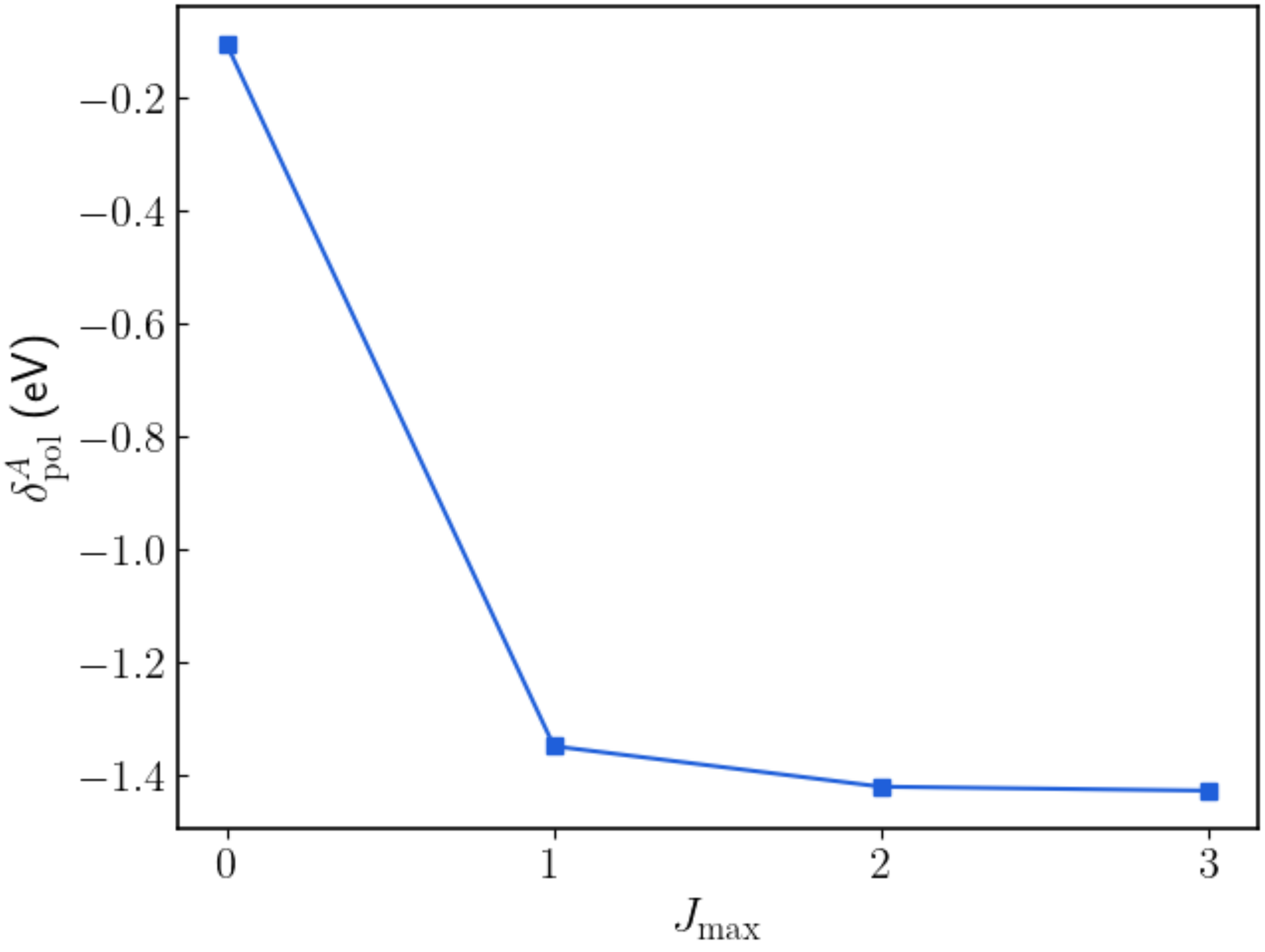


Results

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

➡ **Fast exponential convergence**

Checking convergence in $J_{\max}$



Results

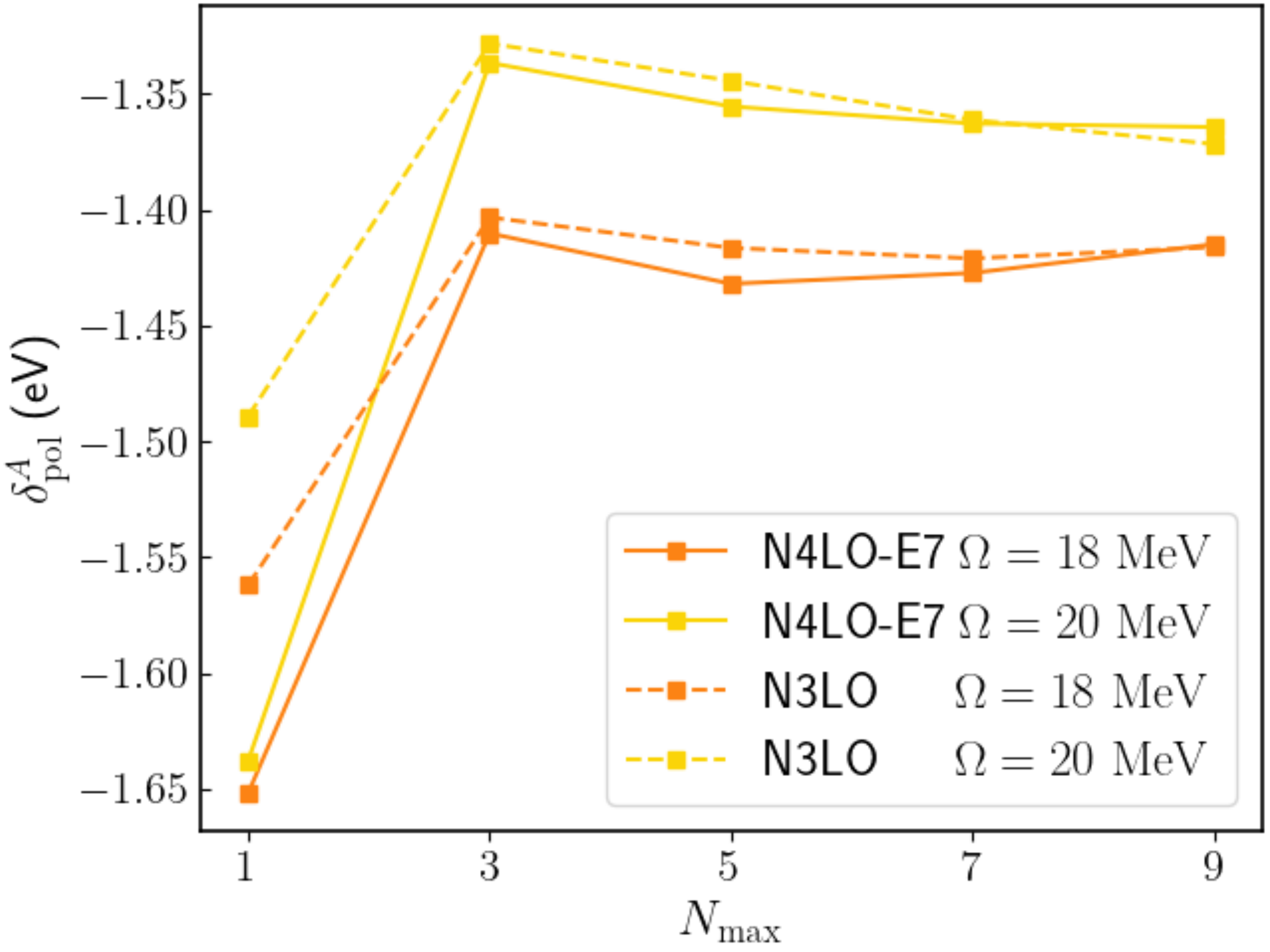
- Here shown for $N_{\max} = 7$ and N4LO-E7
- All other cases are similar

➡ **Fast exponential convergence**

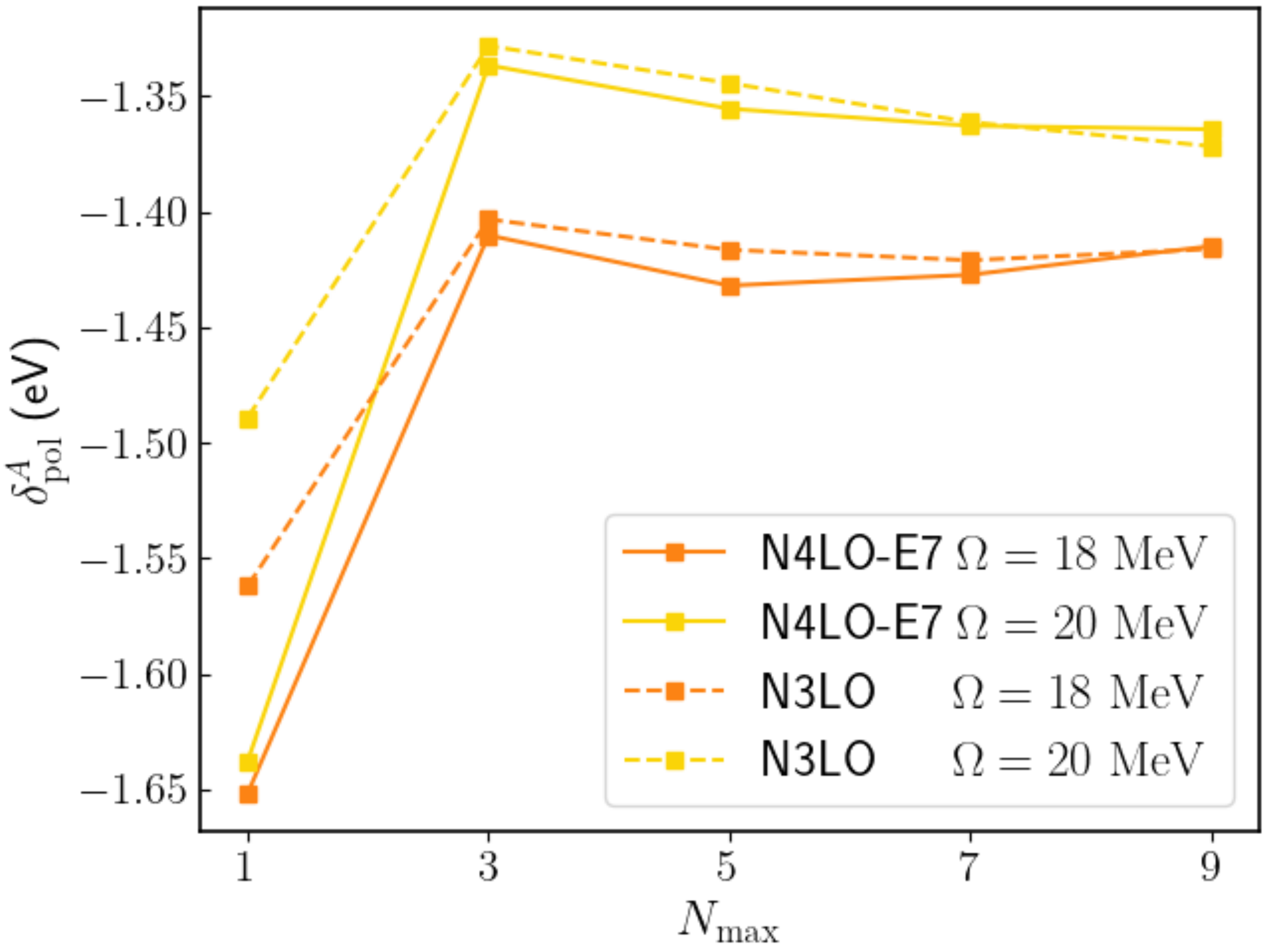
$$\epsilon_{J_{\max}} \lesssim 1 \text{ meV}$$

Multipole truncation $\Rightarrow$ Negligible uncertainty

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



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

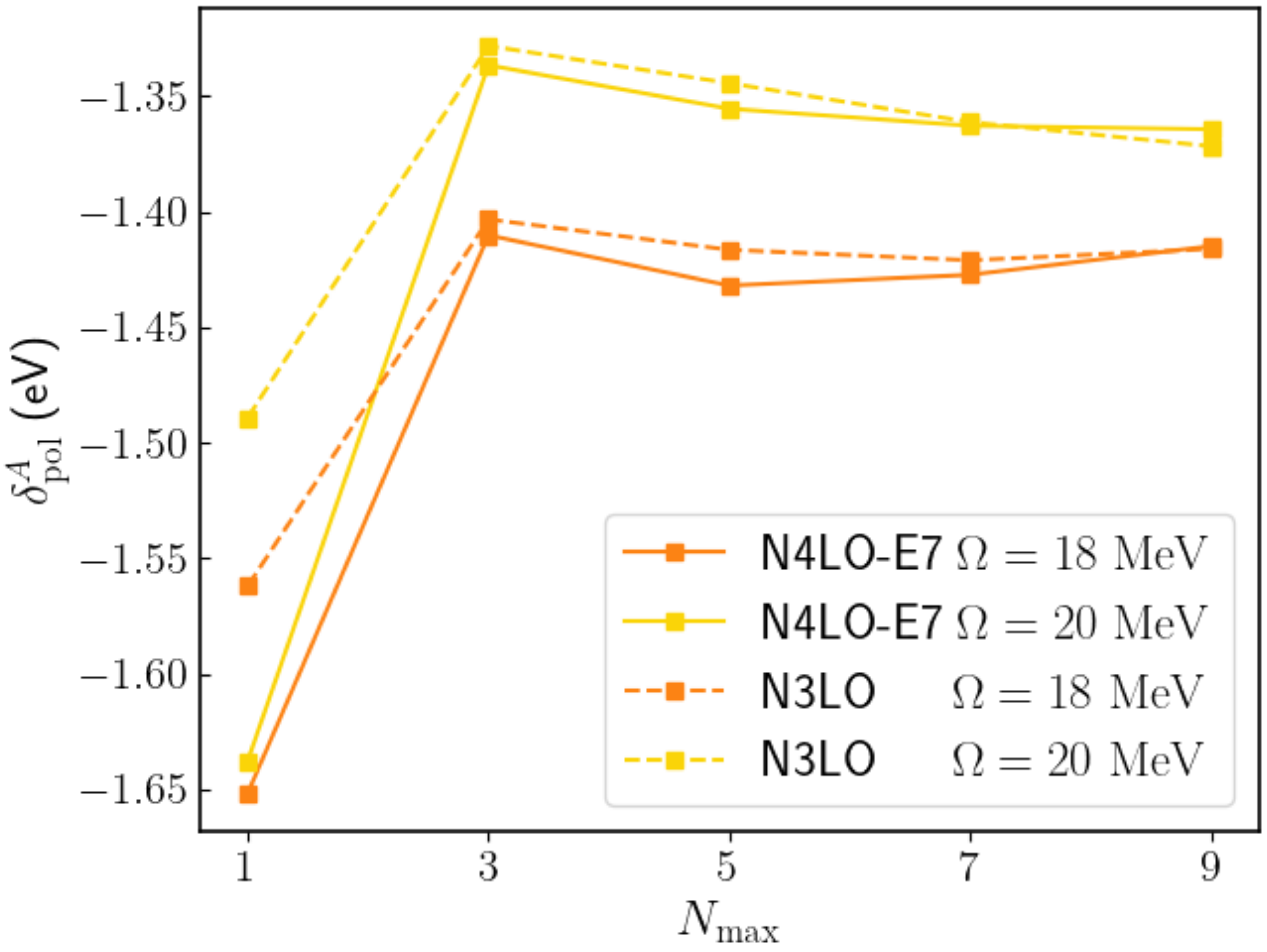


Numerical results

- Model-space dependence
  - Optimal frequency around 20 MeV
  - Run calculations for $\Omega = 18,\ 20$ MeV
  - Truncations for $N_{\max} = 1 - 9$

➡ $(\Omega, N_{\max})$ dependence: $\epsilon_{(\Omega, N_{\max})} \simeq 0.05$ eV

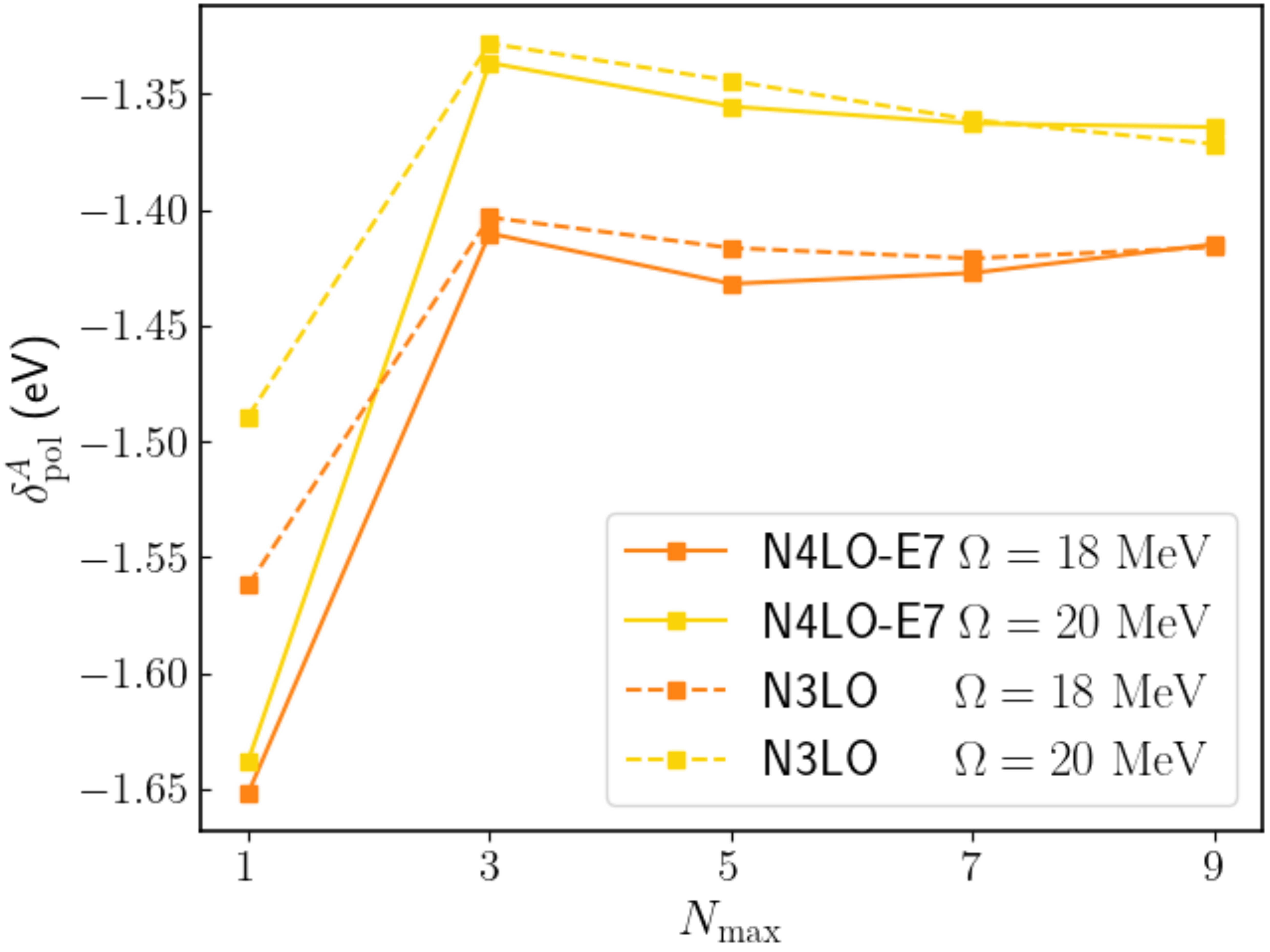
Dependence on $(\Omega, N_{\max})$ and the interaction



Numerical results

- Model-space dependence
  - Optimal frequency around 20 MeV
  - Run calculations for $\Omega = 18,\ 20$ MeV
  - Truncations for $N_{\max} = 1 - 9$
  - ➡ $(\Omega, N_{\max})$ dependence: $\epsilon_{(\Omega, N_{\max})} \simeq 0.05$ eV
- Interaction dependence
  - N3LO ≡ 2N-N3LO(500) + 3N-lnl
  - N4LO-E7 ≡ 2N-N4LO(500) + 3N-lnl-E7
  - ➡ interaction dependence: $\epsilon_{\rm int} \simeq 0.01 - 0.02$ eV

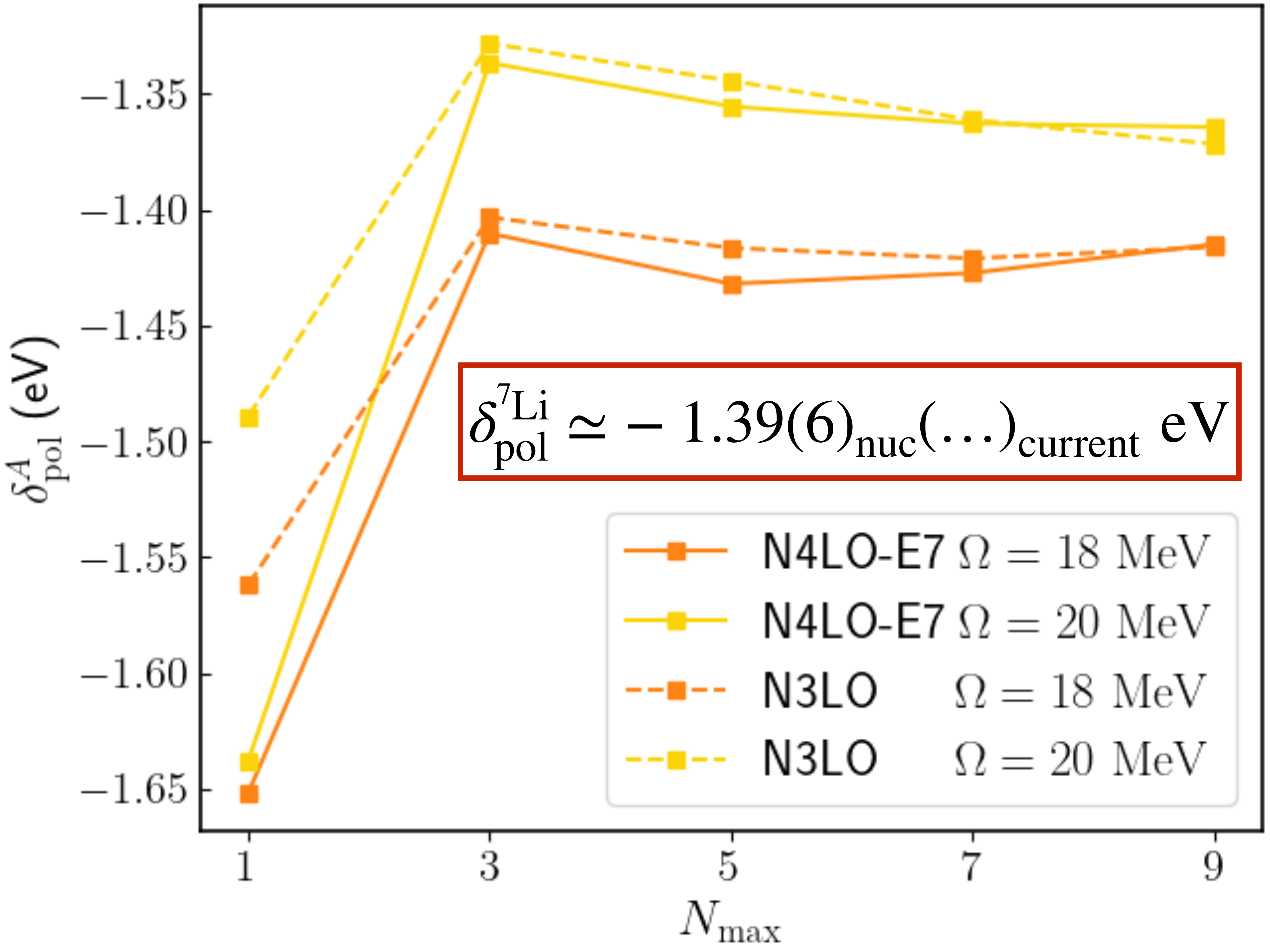
Dependence on (Ω, N_{max}) and the interaction



Numerical results

- Model-space dependence
  - Optimal frequency around 20 MeV
  - Run calculations for $\Omega = 18, 20$ MeV
  - Truncations for $N_{max} = 1 - 9$
  - ➡ (Ω, N_{max}) dependence: $\epsilon_{(\Omega, N_{max})} \simeq 0.05$ eV
- Interaction dependence
  - N3LO ≡ 2N-N3LO(500) + 3N-lnl
  - N4LO-E7 ≡ 2N-N4LO(500) + 3N-lnl-E7
  - ➡ interaction dependence: $\epsilon_{int} \simeq 0.01 - 0.02$ eV
- Current dependence
  - ➡ **On-going estimation of higher-order currents**

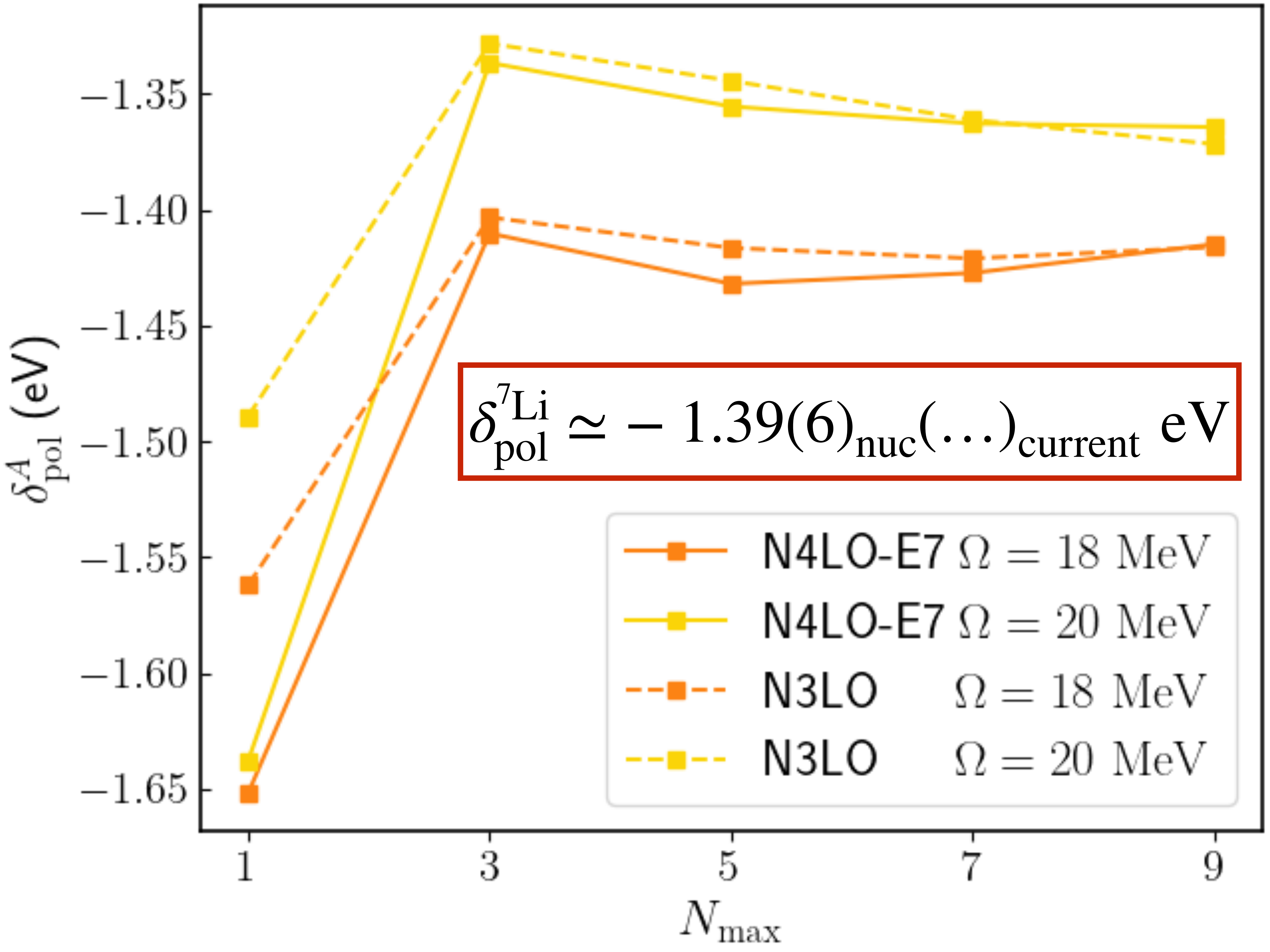
Dependence on $(\Omega, N_{\max})$ and the interaction



Numerical results

- Model-space dependence
  - Optimal frequency around 20 MeV
  - Run calculations for $\Omega = 18,\ 20$ MeV
  - Truncations for $N_{\max} = 1 - 9$
  - ➡ $(\Omega, N_{\max})$ dependence: $\epsilon_{(\Omega, N_{\max})} \simeq 0.05$ eV
- Interaction dependence
  - N3LO ≡ 2N-N3LO(500) + 3N-lnl
  - N4LO-E7 ≡ 2N-N4LO(500) + 3N-lnl-E7
  - ➡ interaction dependence: $\epsilon_{\mathrm{int}} \simeq 0.01 - 0.02$ eV
- Current dependence
  - ➡ **On-going estimation of higher-order currents**

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



$\delta^{^7\rm Li}_{\rm pol} \simeq -1.39(6)_{\rm nuc}(\ldots)_{\rm current}$ eV

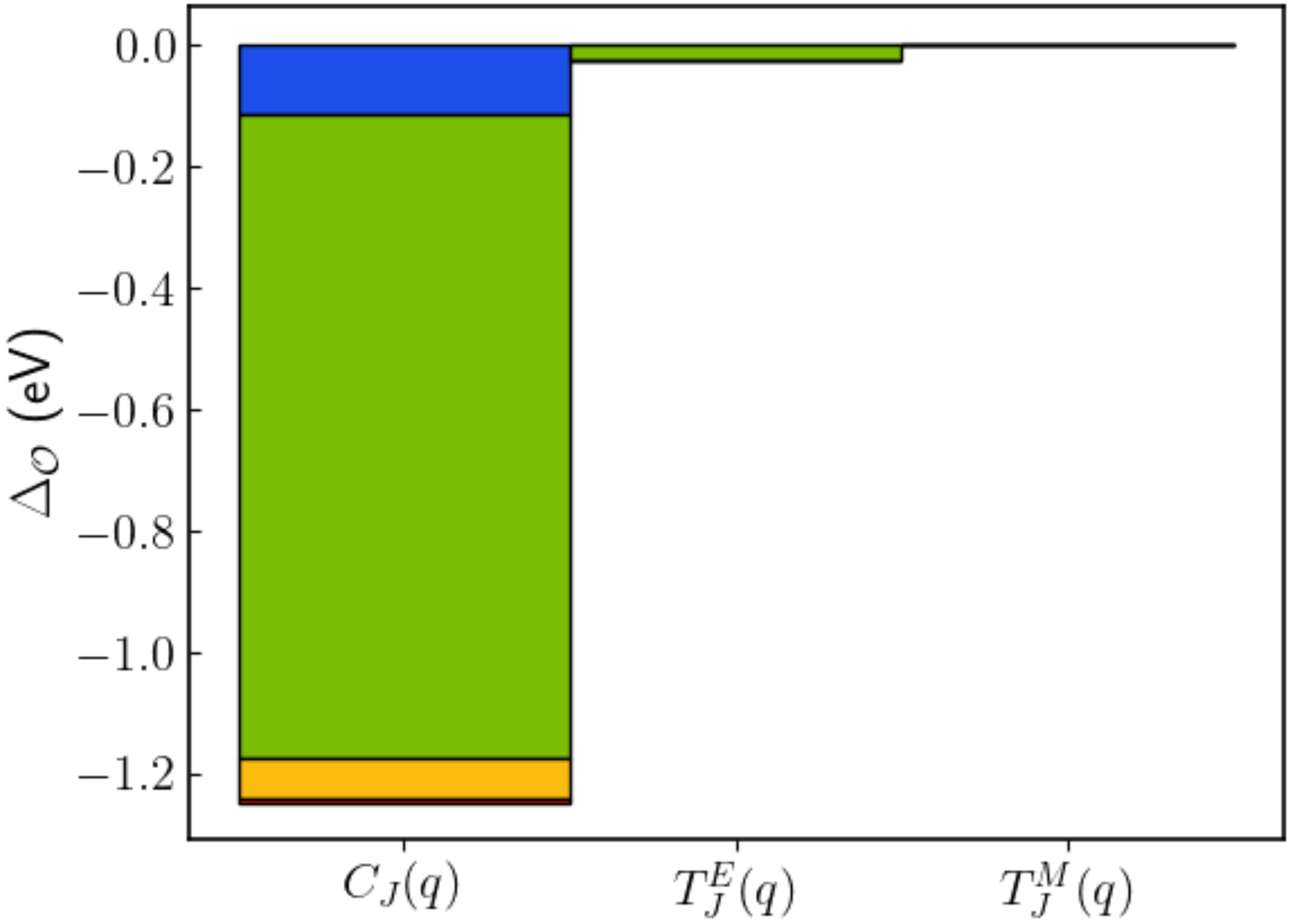
Numerical results

- Model-space dependence
  - Optimal frequency around 20 MeV
  - Run calculations for $\Omega = 18$, 20 MeV
  - Truncations for $N_{\max} = 1 - 9$
  - ➡ $(\Omega, N_{\max})$ dependence: $\epsilon_{(\Omega, N_{\max})} \simeq 0.05$ eV
- Interaction dependence
  - N3LO ≡ 2N-N3LO(500) + 3N-lnl
  - N4LO-E7 ≡ 2N-N4LO(500) + 3N-lnl-E7
  - ➡ interaction dependence: $\epsilon_{\rm int} \simeq 0.01 - 0.02$ eV
- Current dependence
  - ➡ **On-going estimation of higher-order currents**

0.1 - 0.2 eV precision expected for nuclear structure corrections!

Nuclear Polarizability of $^6\mathrm{Li}$ at $N_{\max} = 7$

Nuclear Polarizability of $^6\mathrm{Li}$ at $N_{\mathrm{max}} = 7$

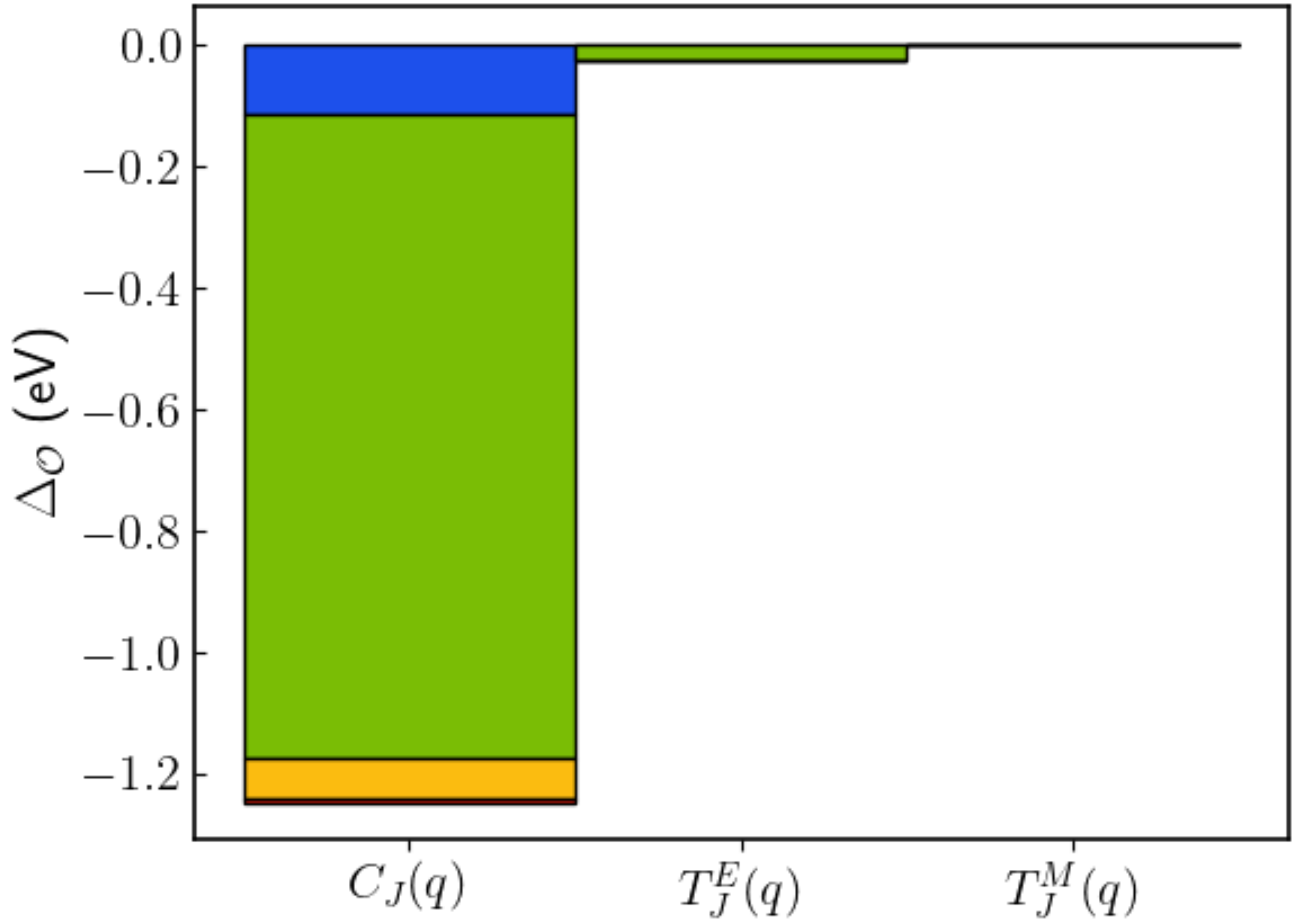


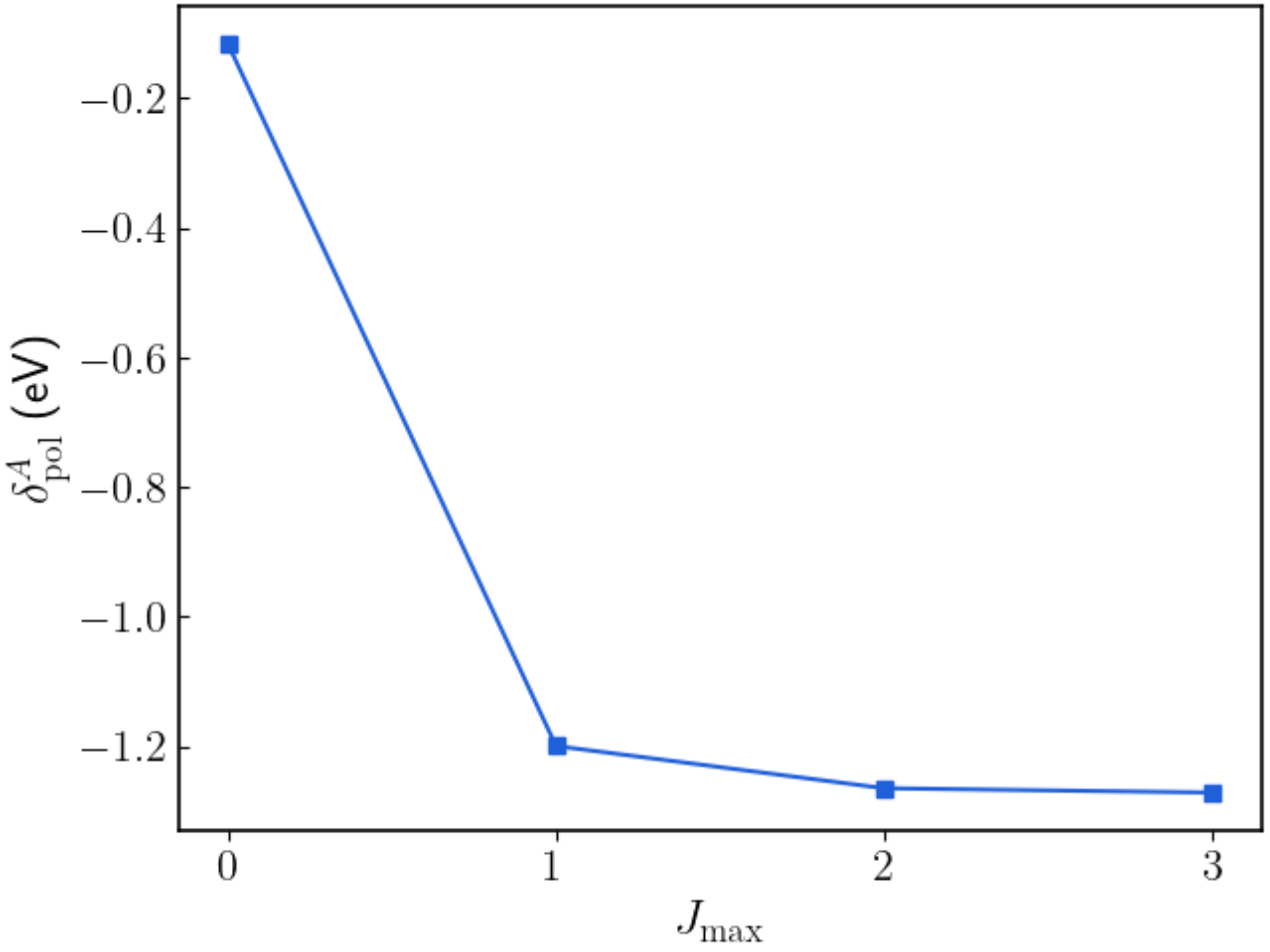
Numerical result

➡ Similar order of magnitude value as $^7\mathrm{Li}$

➡ Reasonable from similar $E_{\mathrm{ex}}^{E1} \sim 15 - 18$ MeV

Nuclear Polarizability of ^{6}Li at $N_{\max} = 7$





Numerical result

➡ Similar order of magnitude value as ^{7}Li

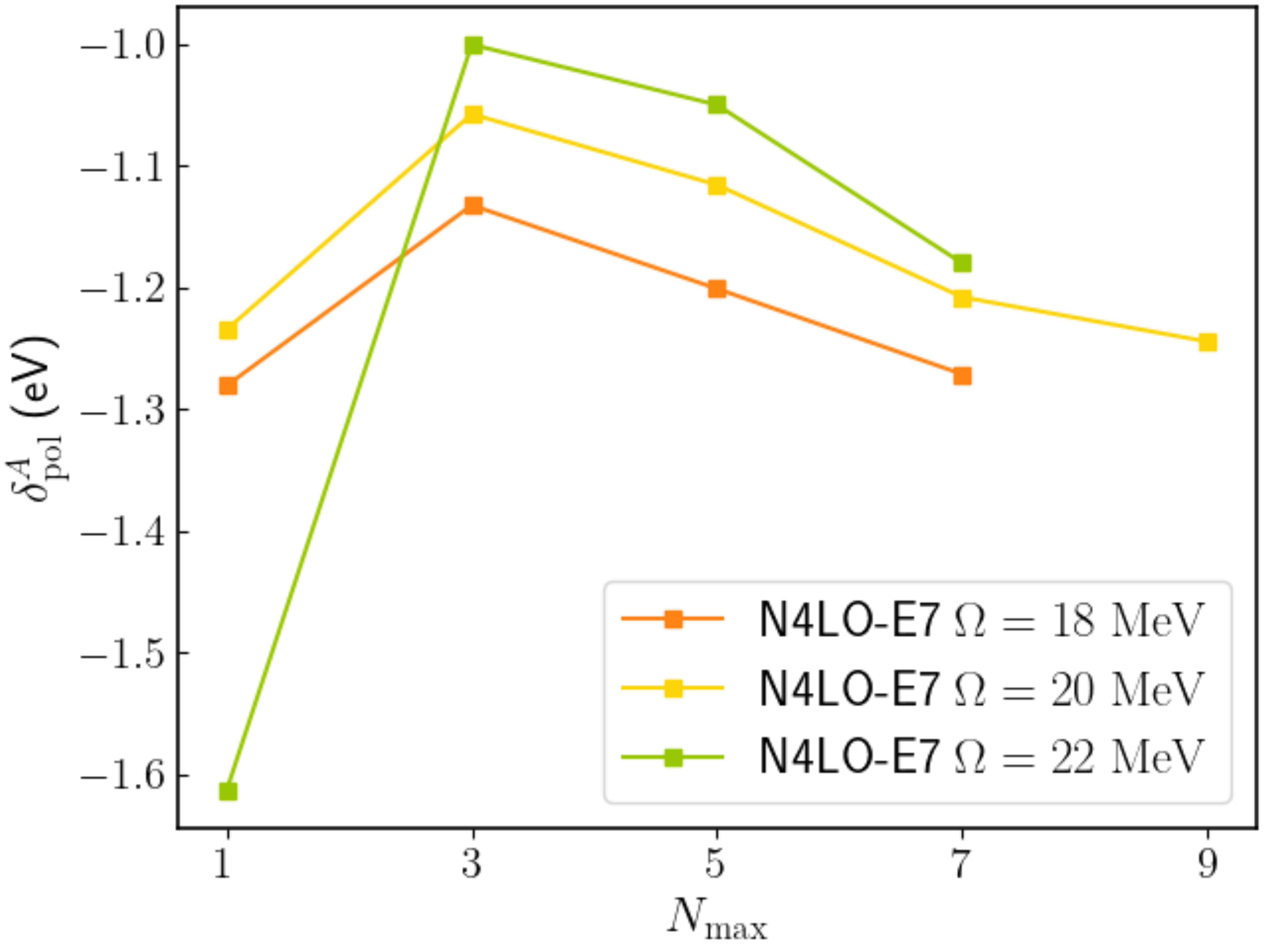
➡ Reasonable from similar $E_{\rm ex}^{E1} \sim 15 - 18$ MeV

Multipole dependence

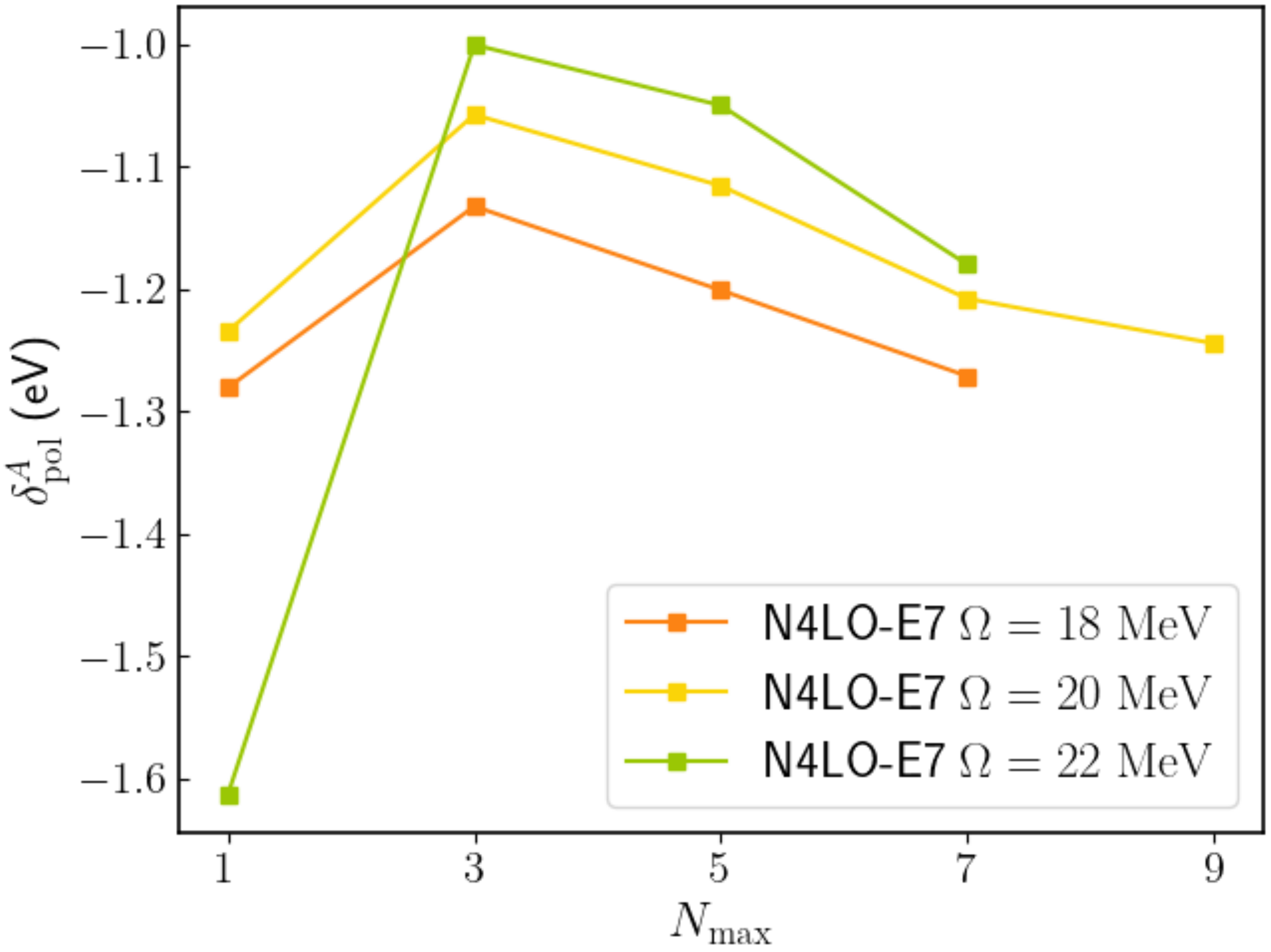
➡ Similar spreading among multipoles

➡ Again negligible uncertainty at $J_{\max} = 3$

Model-space dependence for $^{6}\mathrm{Li}$



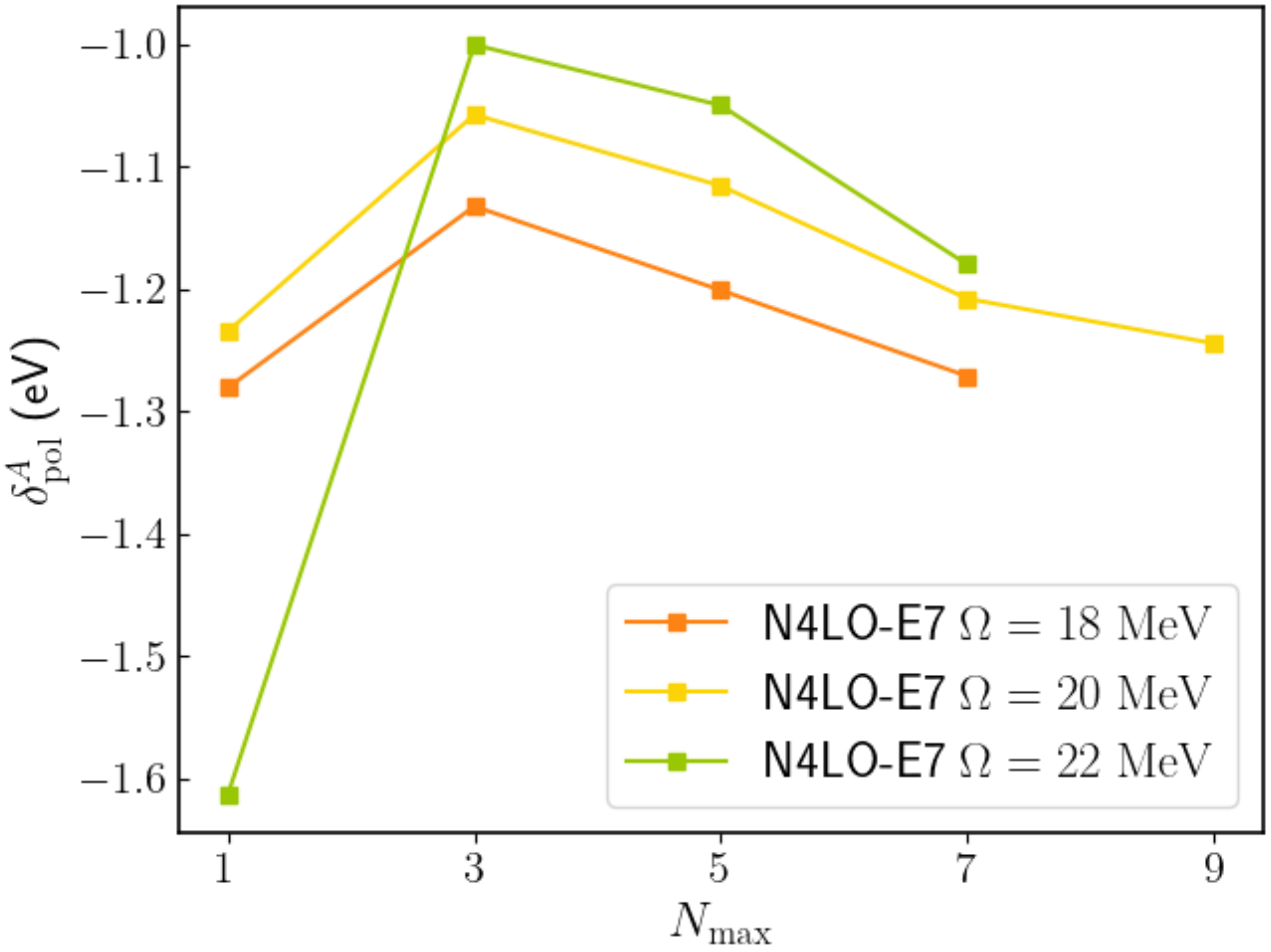
Model-space dependence for $^6\mathrm{Li}$



Preliminary numerical results

- Model-space dependence
  - Run calculations for $\Omega = 18,\ 20,\ 22$ MeV
  - Truncations for $N_{\mathrm{max}} = 1 - 9$
  - Encouraging convergence from first $N_{\mathrm{max}} = 9$ results
- ➡ **On-going calculations to finish soon**
- ➡ **Critical role of latest supercomputer generation**

Model-space dependence for $^{6}\mathrm{Li}$

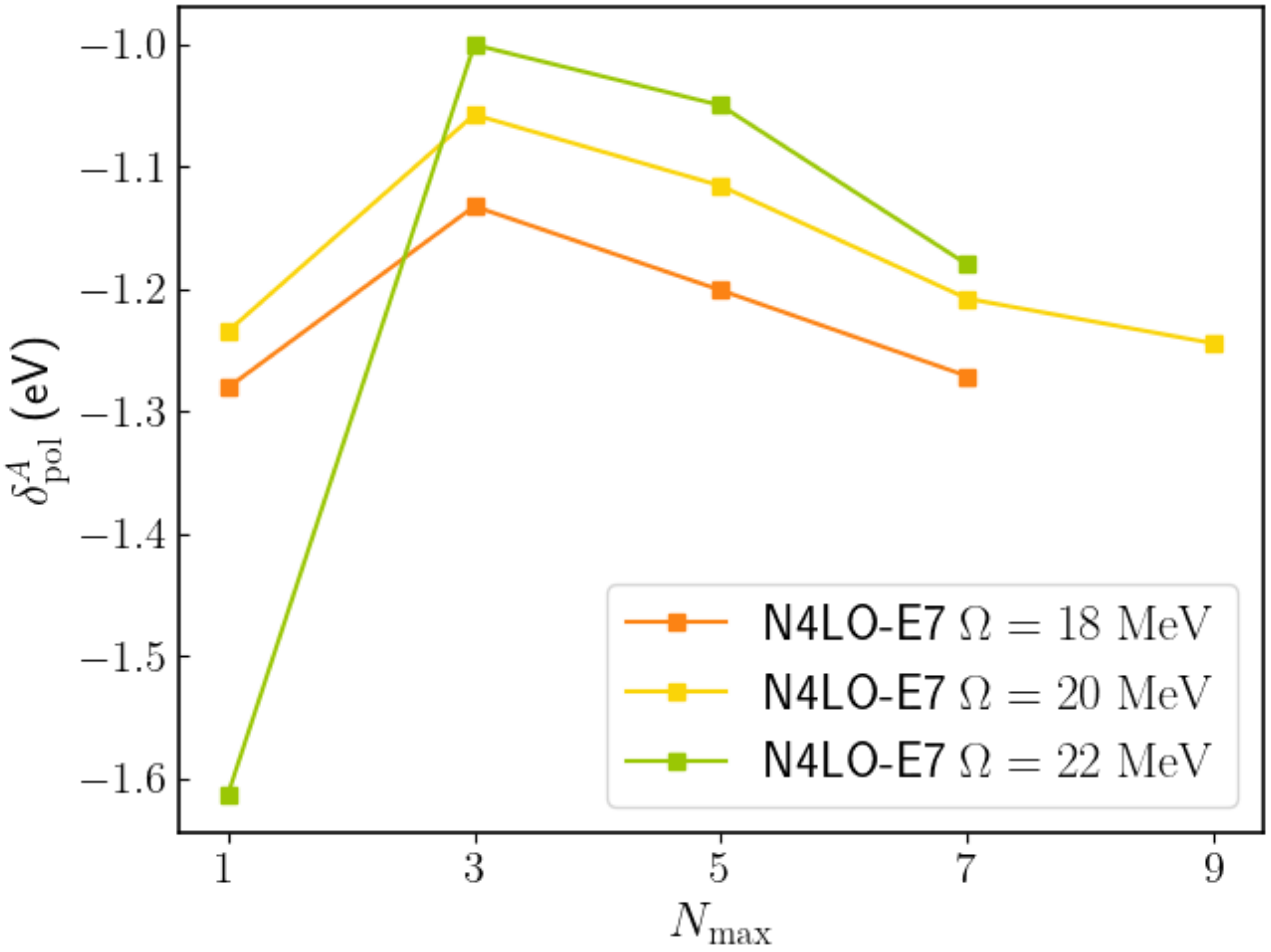


Preliminary numerical results

- Model-space dependence
  - Run calculations for $\Omega = 18,\ 20,\ 22$ MeV
  - Truncations for $N_{\mathrm{max}} = 1 - 9$
  - Encouraging convergence from first $N_{\mathrm{max}} = 9$ results
  - ➡ **On-going calculations to finish soon**
  - ➡ **Critical role of latest supercomputer generation**

- Uncertainty estimation
  - Model-space uncertainty: to be confirmed
  - Interaction uncertainty: to be tested if small again

Model-space dependence for $^6\mathrm{Li}$



Preliminary numerical results

- Model-space dependence
  - Run calculations for $\Omega = 18, 20, 22$ MeV
  - Truncations for $N_{\mathrm{max}} = 1 - 9$
  - Encouraging convergence from first $N_{\mathrm{max}} = 9$ results
  - ➡ **On-going calculations to finish soon**
  - ➡ **Critical role of latest supercomputer generation**
- Uncertainty estimation
  - Model-space uncertainty: to be confirmed
  - Interaction uncertainty: to be tested if small again

Results should be finalized by the end of the summer: $\delta^{^6\mathrm{Li}}_{\mathrm{pol}} \sim -1.3\ (\ldots)_{\mathrm{nuc}}(\ldots)_{\mathrm{current}}$ eV

Conclusion

Conclusion

Summary

- Muonic atoms: a precision probe for nuclear physics
  - Radii extraction: reference point + isotope-shift
  - Precise reference point: muonic atoms
  - ➡ **QUARTET**: 10x exp. improvement for $Z \lesssim 10$

Conclusion

Summary

- Muonic atoms: a precision probe for nuclear physics
  - Radii extraction: reference point + isotope-shift
  - Precise reference point: muonic atoms
  - ➡ **QUARTET**: 10x exp. improvement for $Z \lesssim 10$
- Nuclear polarization: reaching precision ab initio
  - Critical nuclear theory input for: $E_{1S} \to \langle r_c^2 \rangle$
  - **Theory Goal**: 0.1 eV precision on 1S δ_{TPE}

Conclusion

Summary

- <u>Muonic atoms: a precision probe for nuclear physics</u>
  - Radii extraction: reference point + isotope-shift
  - Precise reference point: muonic atoms
  - ➡ **QUARTET**: 10x exp. improvement for $Z \lesssim 10$

- <u>Nuclear polarization: reaching precision ab initio</u>
  - Critical nuclear theory input for: $E_{1S} \to \langle r_c^2 \rangle$
  - **Theory Goal**: 0.1 eV precision on 1S δ_{TPE}

- <u>Promising on going results for $^{6-7}$Li:</u>
  - Weak dependence between χEFT interactions
  - ➡ **NCSM**: **seems to converge within 0.1 - 0.2 eV**

Conclusion

Summary

- Muonic atoms: a precision probe for nuclear physics
  - Radii extraction: reference point + isotope-shift
  - Precise reference point: muonic atoms
  - ➡ **QUARTET**: 10x exp. improvement for $Z \lesssim 10$
- Nuclear polarization: reaching precision ab initio
  - Critical nuclear theory input for: $E_{1S} \to \langle r_c^2 \rangle$
  - **Theory Goal**: 0.1 eV precision on 1S δ_{TPE}
- Promising on going results for ^{6-7}Li:
  - Weak dependence between χEFT interactions
  - ➡ **NCSM**: **seems to converge within 0.1 - 0.2 eV**

Outlook

- Completing on-going ab initio calculation
  - Add current uncertainty quantification
  - Elastic component: δ^A_{el} with NCSMC
  - Extension to $^9\text{Be} \Rightarrow$ **ref for a new isotopic chain**

Conclusion

Summary

- Muonic atoms: a precision probe for nuclear physics
  - Radii extraction: reference point + isotope-shift
  - Precise reference point: muonic atoms
  - ➡ **QUARTET**: 10x exp. improvement for $Z \lesssim 10$
- Nuclear polarization: reaching precision ab initio
  - Critical nuclear theory input for: $E_{1S} \to \langle r_c^2 \rangle$
  - **Theory Goal**: 0.1 eV precision on 1S δ_{TPE}
- Promising on going results for $^{6-7}$Li:
  - Weak dependence between χEFT interactions
  - ➡ **NCSM**: **seems to converge within 0.1 - 0.2 eV**

Outlook

- Completing on-going ab initio calculation
  - Add current uncertainty quantification
  - Elastic component: δ^A_{el} with NCSMC
  - Extension to ^{9}Be $\Rightarrow$ **ref for a new isotopic chain**
- Future modelling improvements
  - Nuclear physics: **higher-order currents**
  - Atomic physics: three-photon exchange
  - Hadronic physics: more realistic model

Conclusion

Summary

- Muonic atoms: a precision probe for nuclear physics
  - Radii extraction: reference point + isotope-shift
  - Precise reference point: muonic atoms
  - ➡ **QUARTET**: 10x exp. improvement for $Z \lesssim 10$
- Nuclear polarization: reaching precision ab initio
  - Critical nuclear theory input for: $E_{1S} \rightarrow \langle r_c^2 \rangle$
  - **Theory Goal**: 0.1 eV precision on 1S δ_{TPE}
- Promising on going results for $^{6-7}$Li:
  - Weak dependence between χEFT interactions
  - ➡ **NCSM**: **seems to converge within 0.1 - 0.2 eV**

Outlook

- Completing on-going ab initio calculation
  - Add current uncertainty quantification
  - Elastic component: δ^A_{el} with NCSMC
  - Extension to ^{9}Be $\Rightarrow$ **ref for a new isotopic chain**
- Future modelling improvements
  - Nuclear physics: **higher-order currents**
  - Atomic physics: three-photon exchange
  - Hadronic physics: more realistic model
- Towards better controlling theoretical uncertainty
  - Shifting from pheno towards EFT approach
  - EFT based on **potential-NRQED** for $Z > 1$

[Peset et al., EPJA (2015)]

Backup slides

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)]

$$\Delta E(\mu\mathrm{H}) = 206.0336(15) - 5.2275(10) \times r_p^2 + 0.0332(20)$$
$$\Delta E(\mu\mathrm{D}) = 228.7767(10) - 6.1103(3) \times r_\mathrm{D}^2 + 1.7449(200)$$
$$\Delta E(\mu^4\mathrm{He}) = 1668.489(14) - 106.220(8) \times r_\alpha^2 + 9.201(291)$$

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)]

$$\Delta E(\mu\mathrm{H}) = 206.0336(15) - 5.2275(10) \times r_p^2 + 0.0332(20)$$
$$\Delta E(\mu\mathrm{D}) = 228.7767(10) - 6.1103(3) \times r_\mathrm{D}^2 + 1.7449(200)$$
$$\Delta E(\mu^4\mathrm{He}) = 1668.489(14) - 106.220(8) \times r_\alpha^2 + 9.201(291)$$

General many-body problem

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

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)]

$$\Delta E(\mu\mathrm{H}) = 206.0336(15) - 5.2275(10) \times r_p^2 + 0.0332(20)$$
$$\Delta E(\mu\mathrm{D}) = 228.7767(10) - 6.1103(3) \times r_\mathrm{D}^2 + 1.7449(200)$$
$$\Delta E(\mu^4\mathrm{He}) = 1668.489(14) - 106.220(8) \times r_\alpha^2 + 9.201(291)$$

General many-body problem

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

- Hamiltonian

  [Friar, Rosen, Annals of Physics (1974)]
  - For simplicity assume non-relativistic nucleons of equal mass

$$H = H_{Nucl} + e \int \mathrm{d}^3x \; J_\mu(x) A^\mu(x) + \frac{e^2}{2m} \int \mathrm{d}^3x \mathrm{d}^3y \; f_{SG}(x,y) \; \vec{A}(x).\vec{A}(y) + H_{QED}$$

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)]

$$\Delta E(\mu \mathrm{H}) = 206.0336(15) - 5.2275(10) \times r_p^2 + 0.0332(20)$$
$$\Delta E(\mu \mathrm{D}) = 228.7767(10) - 6.1103(3) \times r_\mathrm{D}^2 + 1.7449(200)$$
$$\Delta E(\mu^4\mathrm{He}) = 1668.489(14) - 106.220(8) \times r_\alpha^2 + 9.201(291)$$

General many-body problem

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

- Hamiltonian

  [Friar, Rosen, Annals of Physics (1974)]
  - For simplicity assume non-relativistic nucleons of equal mass

$$H = H_{Nucl} + e \int \mathrm{d}^3x \; J_\mu(x) A^\mu(x) + \frac{e^2}{2m} \int \mathrm{d}^3x \mathrm{d}^3y \; f_{SG}(x,y) \; \vec{A}(x).\vec{A}(y) + H_{QED}$$

- 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

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)]

$$\Delta E(\mu \mathrm{H}) = 206.0336(15) - 5.2275(10) \times r_p^2 + 0.0332(20)$$
$$\Delta E(\mu \mathrm{D}) = 228.7767(10) - 6.1103(3) \times r_\mathrm{D}^2 + 1.7449(200)$$
$$\Delta E(\mu^4\mathrm{He}) = 1668.489(14) - 106.220(8) \times r_\alpha^2 + 9.201(291)$$

Radius extraction master formula

$$\delta_\mathrm{E} = \delta_\mathrm{QED} + \mathscr{C}\ r_c^2 + \delta_\mathrm{NS}$$

General many-body problem

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

- Hamiltonian

  [Friar, Rosen, Annals of Physics (1974)]
  - For simplicity assume non-relativistic nucleons of equal mass

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

- 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

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)]

$$\Delta E(\mu \mathrm{H}) = 206.0336(15) - 5.2275(10) \times r_p^2 + 0.0332(20)$$
$$\Delta E(\mu \mathrm{D}) = 228.7767(10) - 6.1103(3) \times r_\mathrm{D}^2 + 1.7449(200)$$
$$\Delta E(\mu^4\mathrm{He}) = 1668.489(14) - 106.220(8) \times r_\alpha^2 + 9.201(291)$$

Radius extraction master formula

$$\delta_\mathrm{E} = \delta_\mathrm{QED} + \mathscr{C}\, r_c^2 + \delta_\mathrm{NS}$$

Simple point-like nucleus → δ_QED

Finite nucleus size effect → $\mathscr{C}\, r_c^2$

Nuclear structure dependent → δ_NS

General many-body problem

- Main degrees of freedom
  - Nucleons → N ; photon → A ; Muon → ψ_μ

- Hamiltonian

  [Friar, Rosen, Annals of Physics (1974)]
  - For simplicity assume non-relativistic nucleons of equal mass

$$H = H_{Nucl} + e \int \mathrm{d}^3x \; J_\mu(x) A^\mu(x) + \frac{e^2}{2m} \int \mathrm{d}^3x \mathrm{d}^3y \; f_{SG}(x,y) \; \vec{A}(x).\vec{A}(y) + H_{QED}$$

- General approach to compute bound state of H
  - ✗ In principle use Bethe-Salpeter ⇒ bound states ≡ G_n poles
  - ✓ In practice use **effective external potential**
  - Corrections up to $(Z\alpha)^5$ to match exp accuracy

Bound states QED contributions

Bound states QED contributions

Bound muon within potential

- Zero-order: external Coulomb potential
  - Solve exactly for $H_0 = \frac{\vec{p}^2}{2m_r} - \frac{Z\alpha}{r}$
  - $E_{nl} = -\frac{(Z\alpha)^2 m_r}{2n^2} \equiv E^{(0)}$

Bound states QED contributions

Bound muon within potential

- Zero-order: external Coulomb potential
  - Solve exactly for $H_0 = \frac{\vec{p}^2}{2m_r} - \frac{Z\alpha}{r}$
  - $E_{nl} = -\frac{(Z\alpha)^2 m_r}{2n^2} \equiv E^{(0)}$

- 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 ⇒ **Distorted Wave Born approximation**

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

Bound states QED contributions

Bound muon within potential

- Zero-order: external Coulomb potential
  - Solve exactly for $H_0 = \frac{\vec{p}^2}{2m_r} - \frac{Z\alpha}{r}$
  - $E_{nl} = -\frac{(Z\alpha)^2 m_r}{2n^2} \equiv E^{(0)}$

- 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 ⇒ **Distorted Wave Born approximation**

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

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

Bound states QED contributions

Bound muon within potential

- Zero-order: external Coulomb potential
  - Solve exactly for $H_0 = \frac{\vec{p}^2}{2m_r} - \frac{Z\alpha}{r}$
  - $E_{nl} = -\frac{(Z\alpha)^2 m_r}{2n^2} \equiv E^{(0)}$

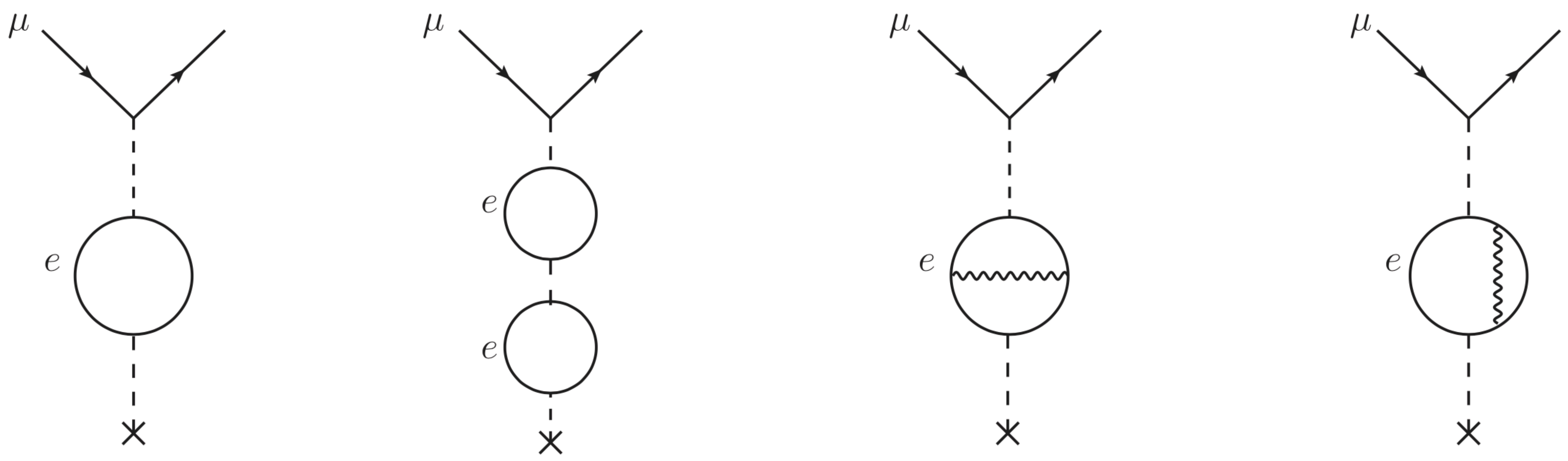
- What effective potential to apply on muon ?
  - **Effective potential** as perturbation away from Coulomb
  - Defined to **match QED** scattering at a given order
  - Bound-state ⇒ **Distorted Wave Born approximation**

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

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

Example: electron vacuum polarization corrections

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



$\Rightarrow$ $\delta_{\rm QED}$ term in $\delta_{\rm E}$

Bound states QED contributions

Bound muon within potential

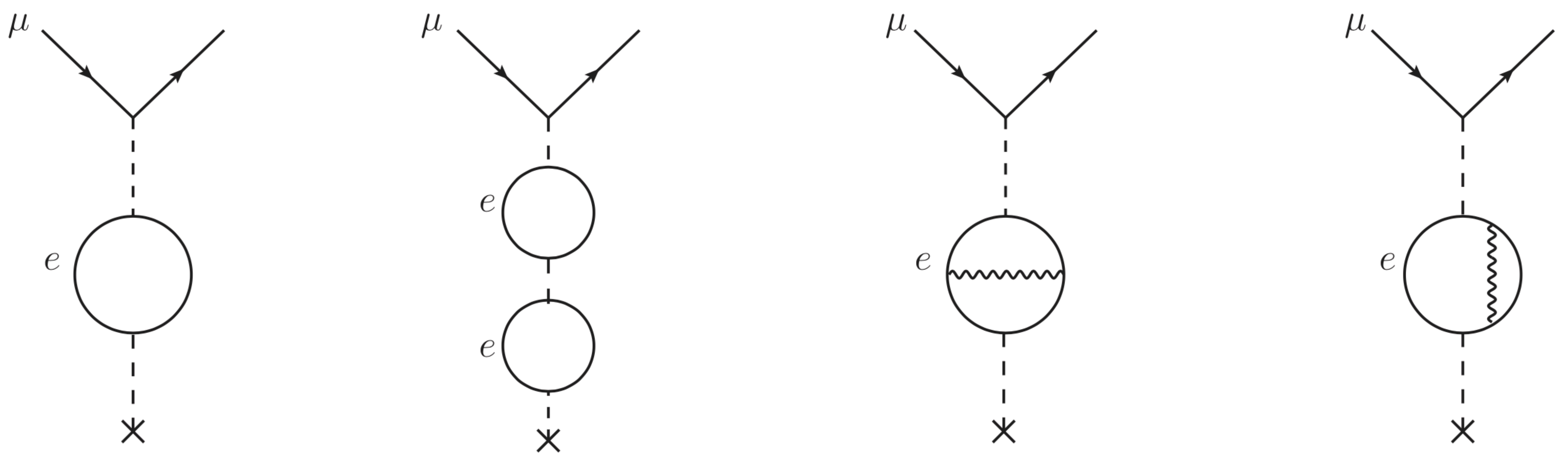
- Zero-order: external Coulomb potential
  - Solve exactly for $H_0 = \frac{\vec{p}^2}{2m_r} - \frac{Z\alpha}{r}$
  - $E_{nl} = -\frac{(Z\alpha)^2 m_r}{2n^2} \equiv E^{(0)}$
- What effective potential to apply on muon ?
  - **Effective potential** as perturbation away from Coulomb
  - Defined to **match QED** scattering at a given order
  - Bound-state ⇒ **Distorted Wave Born approximation**

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

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

Example: electron vacuum polarization corrections

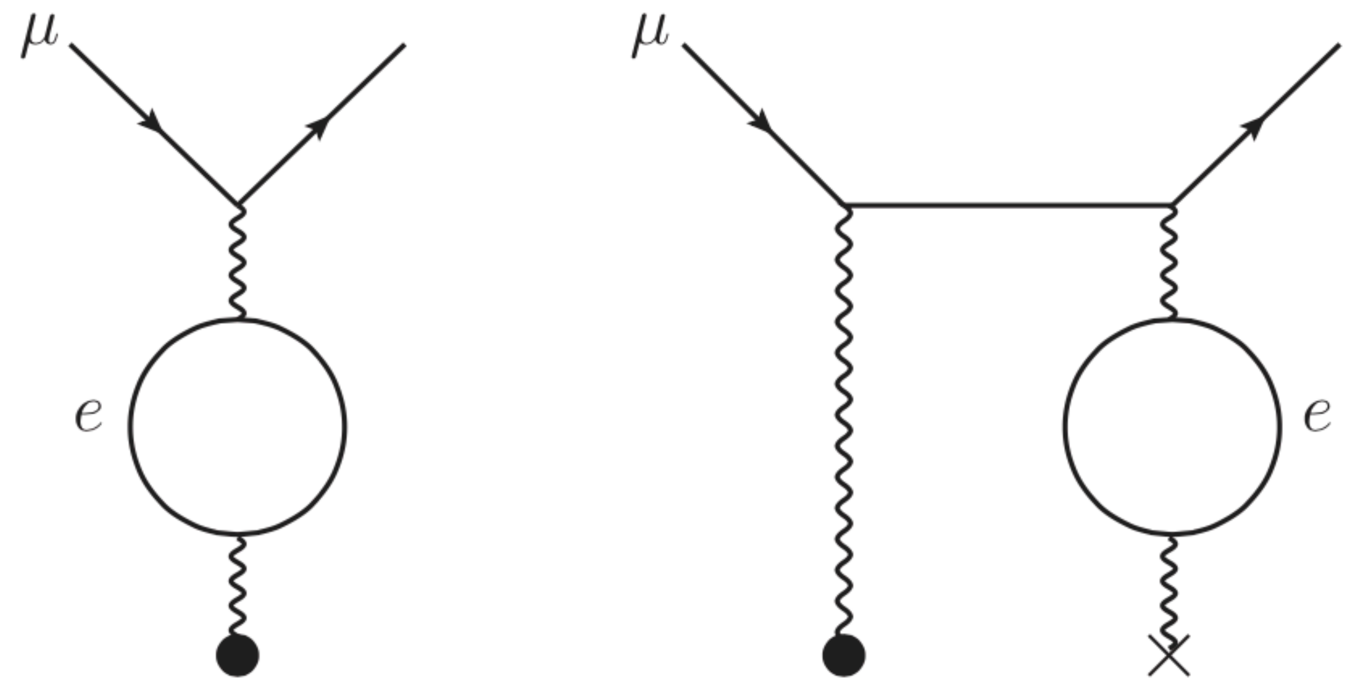
[Pachucki et al. Review of Modern Physics (2024)]



$\Rightarrow$ δ_{QED} term in δ_{E}

Example: finite-size corrections

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



$\Rightarrow$ $\mathscr{C} r_c^2$ term in δ_{E}

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)]

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

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

- Multipole decomposition of nuclear currents

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

  - $M_{JM_J;TM_T}(q) \equiv \int d^3x\ \mathbf{M}_J^{M_J}(qx) J_0(x)_{TM_T}$
  - $T^E_{JM_J;TM_T}(q) \equiv \int d^3x \left[\frac{1}{q}\nabla \times \vec{\mathbf{M}}_{JJ}^{M_J}(qx)\right] . \vec{J}(x)_{TM_T}$
  - $T^M_{JM_J;TM_T}(q) \equiv \int d^3x \vec{\mathbf{M}}_{JJ}^{M_J}(qx) . \vec{J}(x)_{TM_T}$

➡ **Truncation at $J = 3$**

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

- Multipole decomposition of nuclear currents

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

  - $M_{JM_J;TM_T}(q) \equiv \int d^3x\ \mathbf{M}_J^{M_J}(qx) J_0(x)_{TM_T}$
  - $T^E_{JM_J;TM_T}(q) \equiv \int d^3x \left[\frac{1}{q}\nabla \times \vec{\mathbf{M}}_{JJ}^{M_J}(qx)\right] . \vec{J}(x)_{TM_T}$
  - $T^M_{JM_J;TM_T}(q) \equiv \int d^3x \vec{\mathbf{M}}_{JJ}^{M_J}(qx) \,.\, \vec{J}(x)_{TM_T}$

➡ **Truncation at $J = 3$**

Model used for 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**

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

- Multipole decomposition of nuclear currents

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

  - $M_{JM_J;TM_T}(q) \equiv \int d^3x\, \mathbf{M}_J^{M_J}(qx) J_0(x)_{TM_T}$
  - $T^E_{JM_J;TM_T}(q) \equiv \int d^3x \left[\frac{1}{q}\nabla \times \vec{\mathbf{M}}^{M_J}_{JJ}(qx)\right] . \vec{J}(x)_{TM_T}$
  - $T^M_{JM_J;TM_T}(q) \equiv \int d^3x \vec{\mathbf{M}}^{M_J}_{JJ}(qx) \, . \, \vec{J}(x)_{TM_T}$

➡ **Truncation at $J = 3$**

Model used for 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 many-body basis: (Ω, N_{max})

  ➡ **Estimate model space truncation uncertainty**

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

- **Multipole decomposition of nuclear currents**

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

➡ **Truncation at $J = 3$**

Model used for 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 many-body basis: $(\Omega, N_{\max})$

  ➡ **Estimate model space truncation uncertainty**

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

  ➡ **Negligible many-body approximation uncertainty**

Nuclear spectrum for Li isotopes