

Uncertainty Quantification in Nuclear Physics
MITP Workshop, Mainz June 2024

Bayesian uncertainty quantification to nuclear structure effects in atomic systems

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Short History of Atomic Physics

- Relativistic corrections $\sim Z\alpha$
- Radiative corrections $\sim \alpha$
- Recoil corrections $\sim m_e/m_N$
- Nuclear structure $\sim (r_N/r_e)^3$

Fine-structure
Relativistic Quantum
Mechanics

Lamb-shift
QED

Systems with different
expansion parameters

Muonic Atoms

Early 20th century

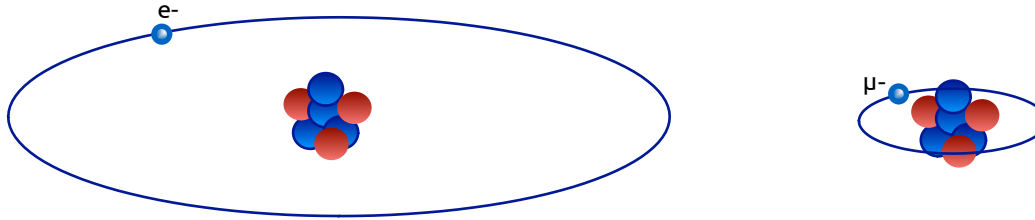
mid 20th century

late 20th century

Birth of Quantum
Mechanics

Recoil corrections
Nuclear structure effects

Muonic Atoms



Nuclear structure effects are enhanced in muonic atoms

Experimental campaign at
PSI by the **CREMA**
collaboration

Muonic Hydrogen

- Pohl et al., Nature (2010)
- Antognini et al., Science (2013)

Muonic Deuterium

- Pohl et al., Science (2016)

Muonic Helium isotopes

- Krauth et al., Nature (2021)
- Schuhmann et al., Arxiv (2023)

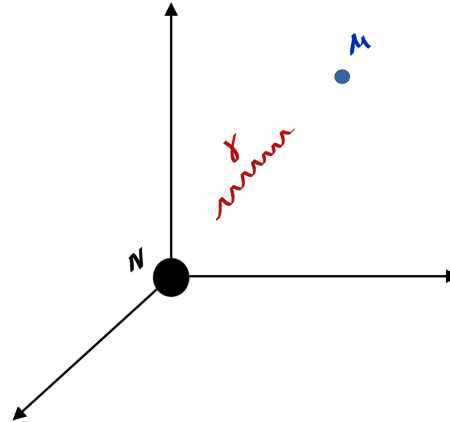
Lamb-shift and nuclear charge radii

$$E_{\text{LS}} = E_{\text{QED}} + Cr_c^2 + E_{\text{TPE}} + \dots$$

Lamb-shift and nuclear charge radii

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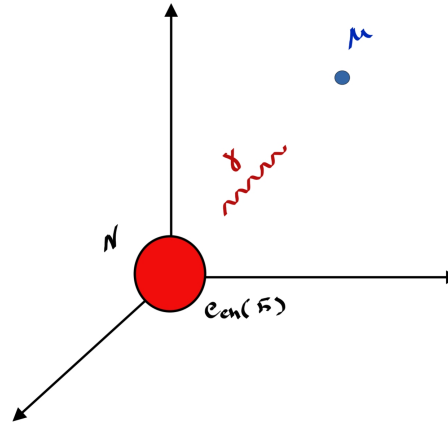
$$E_{\text{QED}} =$$



Lamb-shift and nuclear charge radii

$$E_{\text{LS}} = E_{\text{QED}} + Cr_c^2 + E_{\text{TPE}} + \dots$$

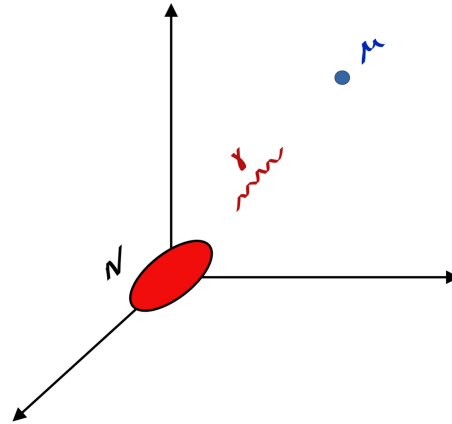
$$Cr_c^2 =$$



Lamb-shift and nuclear charge radii

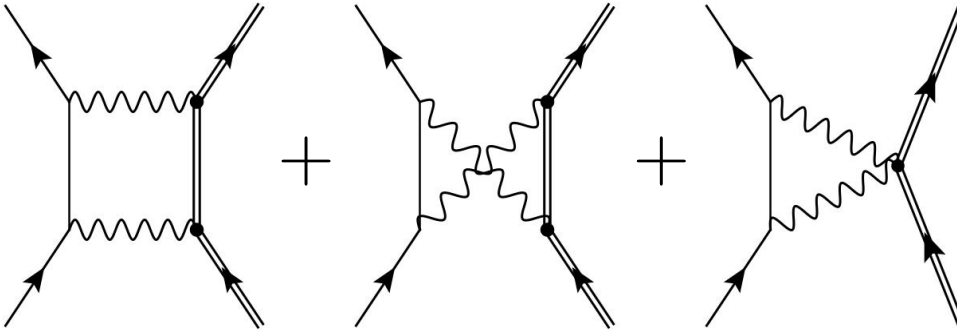
$$E_{\text{LS}} = E_{\text{QED}} + Cr_c^2 + E_{\text{TPE}} + \dots$$

$$E_{\text{TPE}} =$$



Lamb-shift and nuclear charge radii

$$E_{\text{LS}} = E_{\text{QED}} + Cr_c^2 + E_{\text{TPE}} + \dots$$

$$E_{\text{TPE}} =$$


The diagram shows three Feynman diagrams representing two-photon exchange (TPE) between two electrons. Each diagram consists of two electron lines (solid lines with arrows) and two photon lines (wavy lines). The first diagram shows a box-like exchange where two photons are exchanged between the two electrons. The second diagram shows a more complex exchange involving a virtual electron-positron pair. The third diagram shows a different topological arrangement of the two-photon exchange.

A matter of precision

$$E_{\text{LS}} = E_{\text{QED}} + Cr_c^2 + E_{\text{TPE}} + E_{\text{3PE}} + \dots$$

For muonic Helium-4 ion

$$E_{\text{QED}} = +1,644.348(8) \text{ meV}$$

$$C = -106.220(8) \text{ meV fm}^{-2}$$

$$E_{\text{TPE}} = +9.340(250) \text{ meV}$$

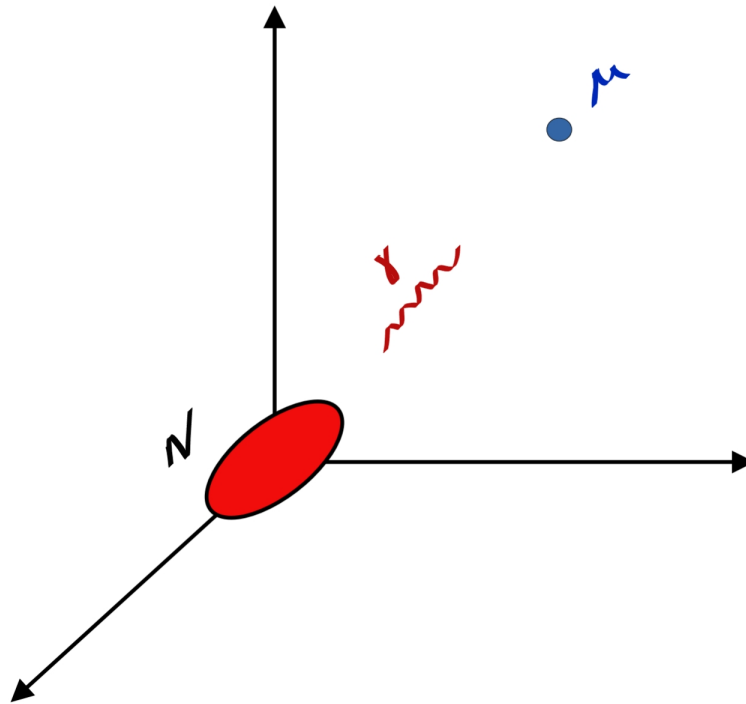
$$E_{\text{3PE}} = -0.150(150) \text{ meV}$$



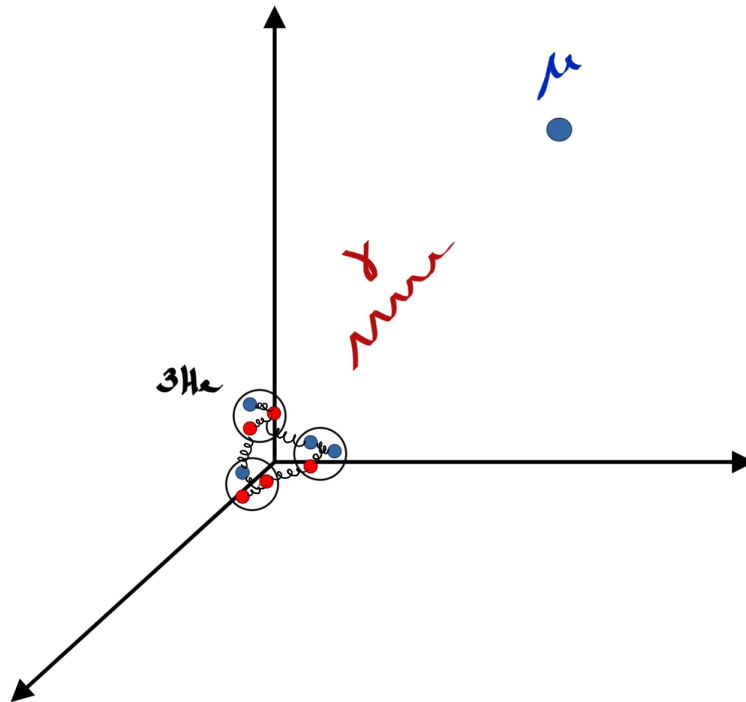
$$r_c = 1.67824(13)_{\text{ex}}(82)_{\text{th}} \text{ fm}$$

J. J. Krauth et. al. Nature 589,527 (2021)

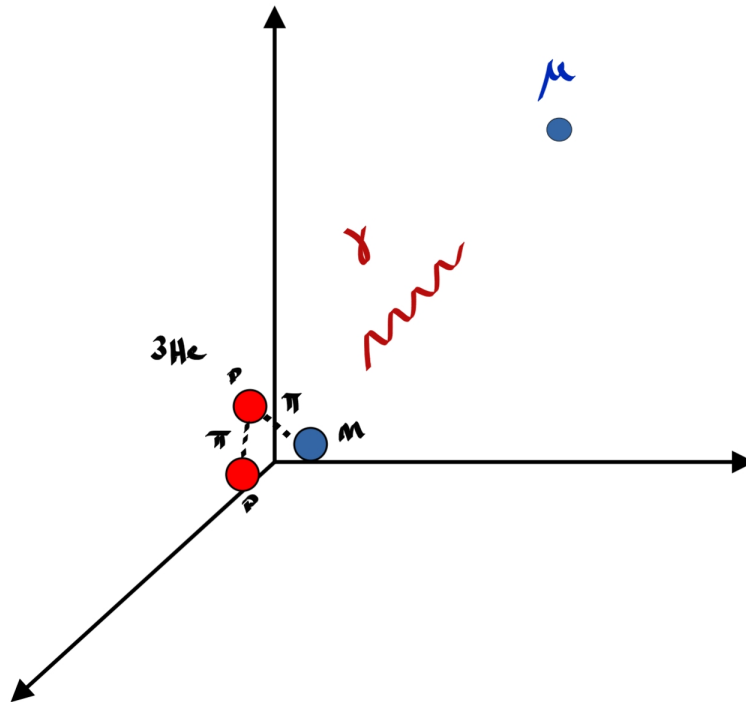
Ab-initio nuclear theory



Ab-initio nuclear theory



Ab-initio nuclear theory



Ab-initio nuclear theory

- Our strategy is to build models for the operators from first principles

$$\begin{array}{c} \text{H} \\ \{ \rho_{\text{ch}}, J_i, B_{ij} \} \end{array} \quad \text{from chiral effective field theory}$$

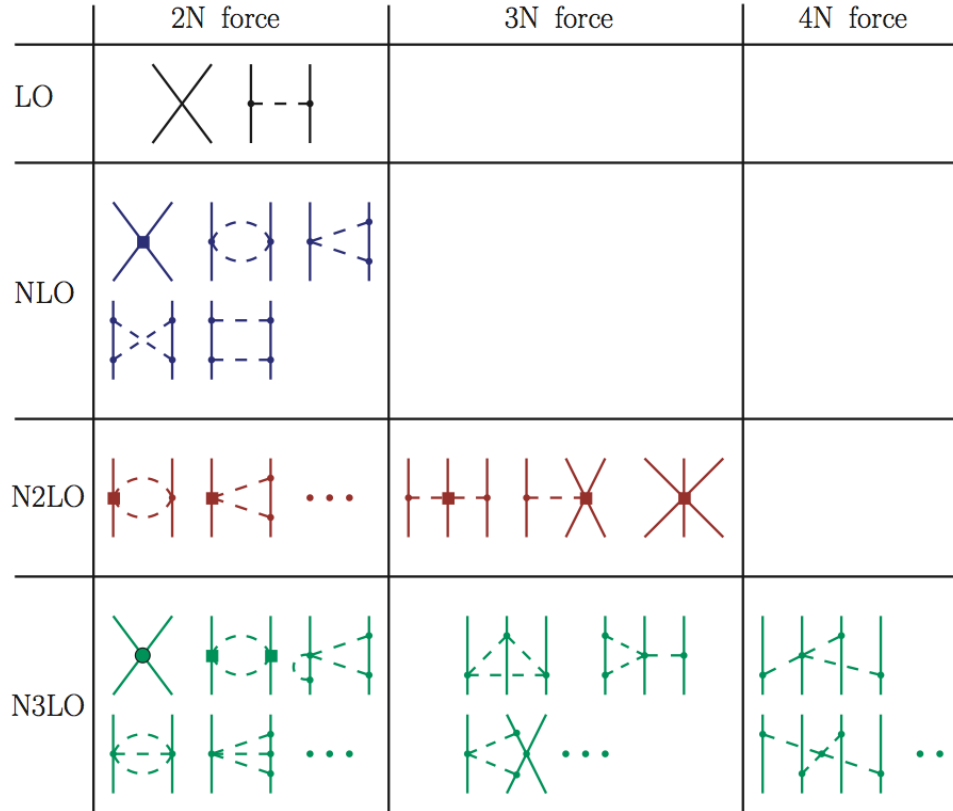
- Solve the many-body Schrödinger equation of the nucleus

$$\text{H} |N\rangle = E_N |N\rangle$$

- Calculate the relevant matrix elements with **controlled approximations**.

$$\langle N | \rho_{\text{ch}}(\mathbf{x}) | 0 \rangle$$

Nuclear Hamiltonians from ChEFT



Better precision

- Degrees of freedom
- Symmetries
- Power counting

Bayesian uncertainty quantification of ChEFT truncation errors

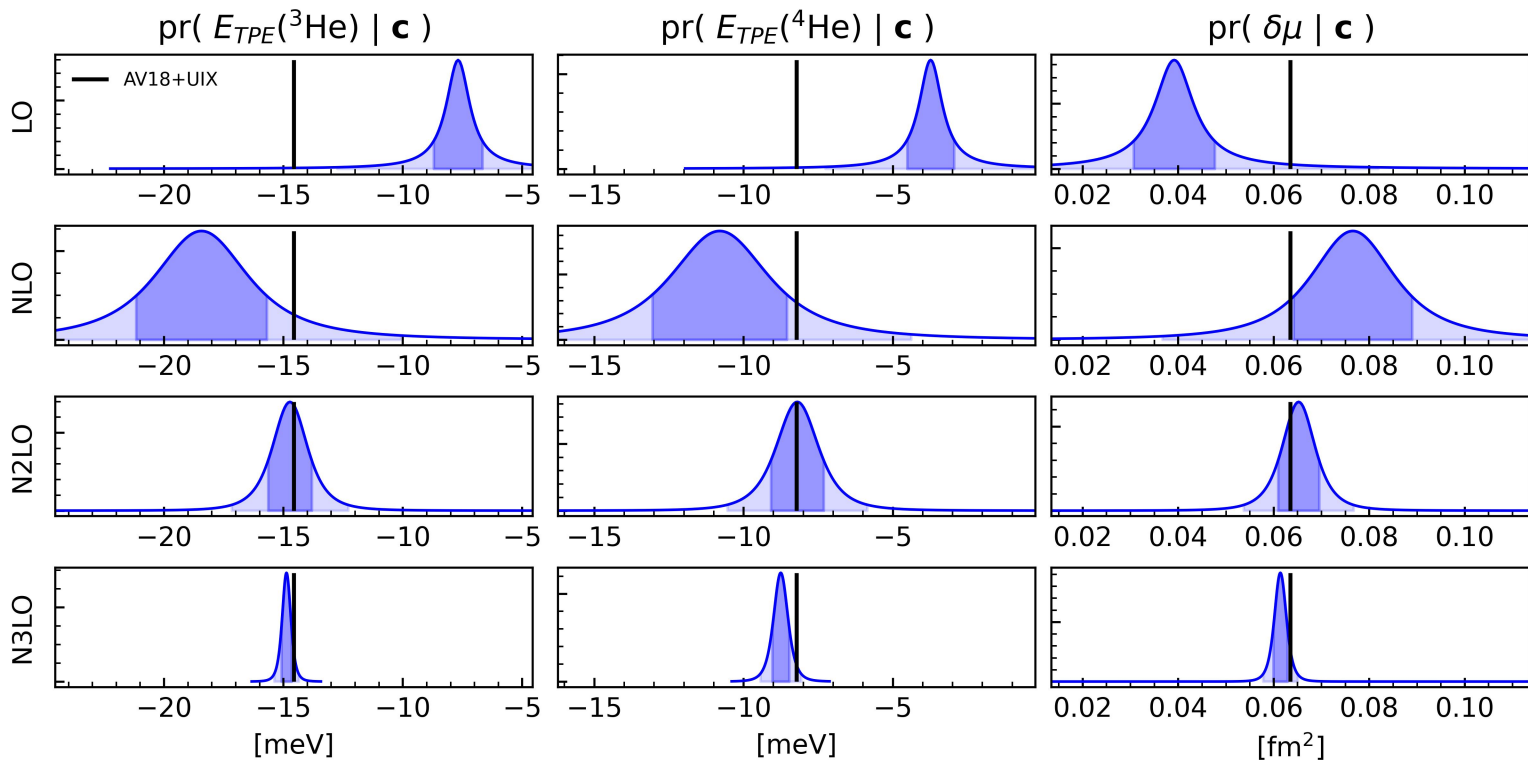
ChEFT is an expansion in powers of $Q = \frac{m_\pi}{\Lambda_\chi} \sim 0.3$

We assume that a similar expansion holds also for the calculated observables

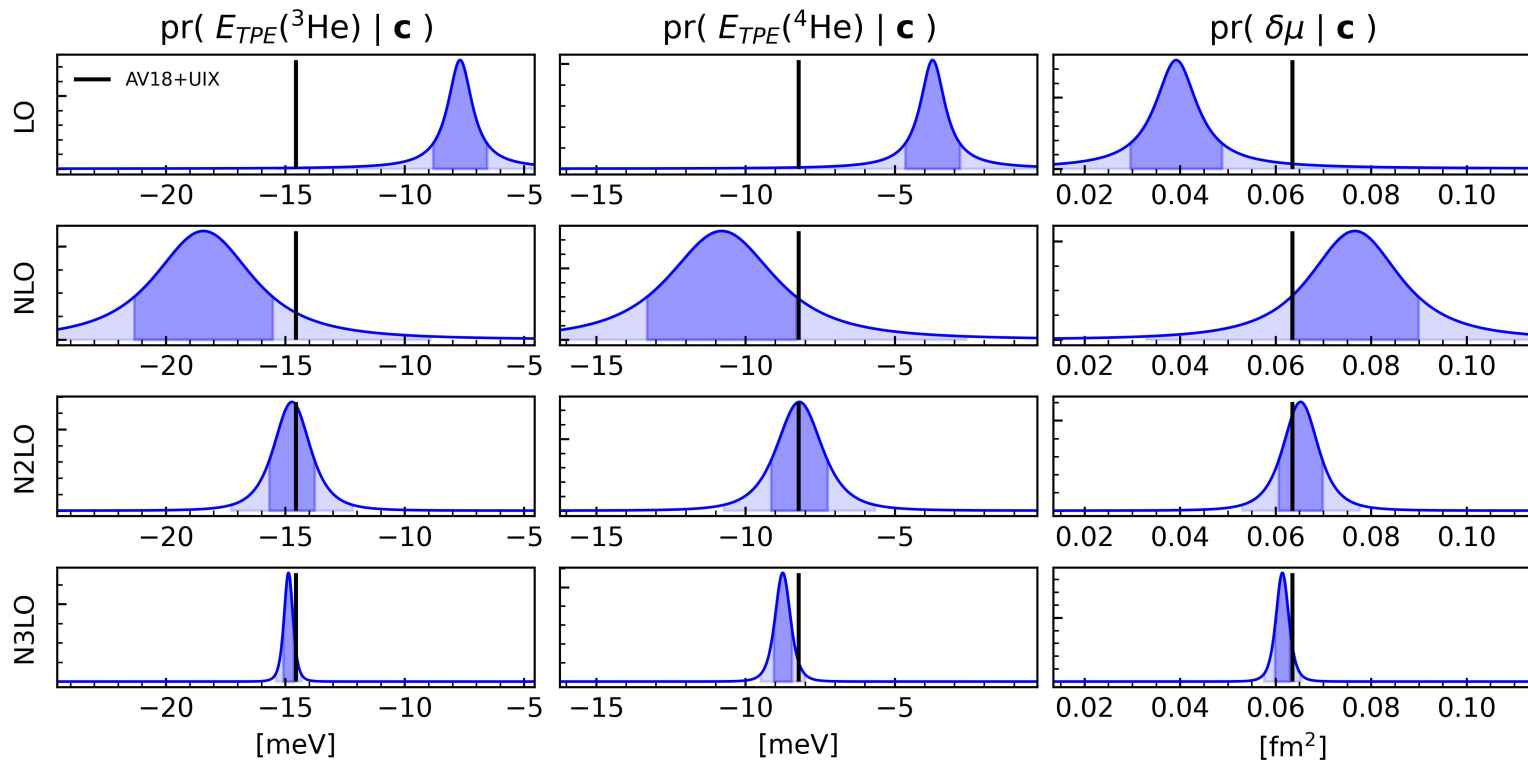
$$\begin{aligned} X &= \sum_{n=0}^k D_n + \sum_{n=k+1}^{\infty} D_n \\ &= X_{\text{ref}} \left[\sum_{n=0}^k c_n Q^n + \sum_{n=k+1}^{\infty} c_n Q^n \right] \end{aligned}$$

We assume that the expansion coefficients follow the same underlying distribution and use the calculated coefficients to learn about the distribution.

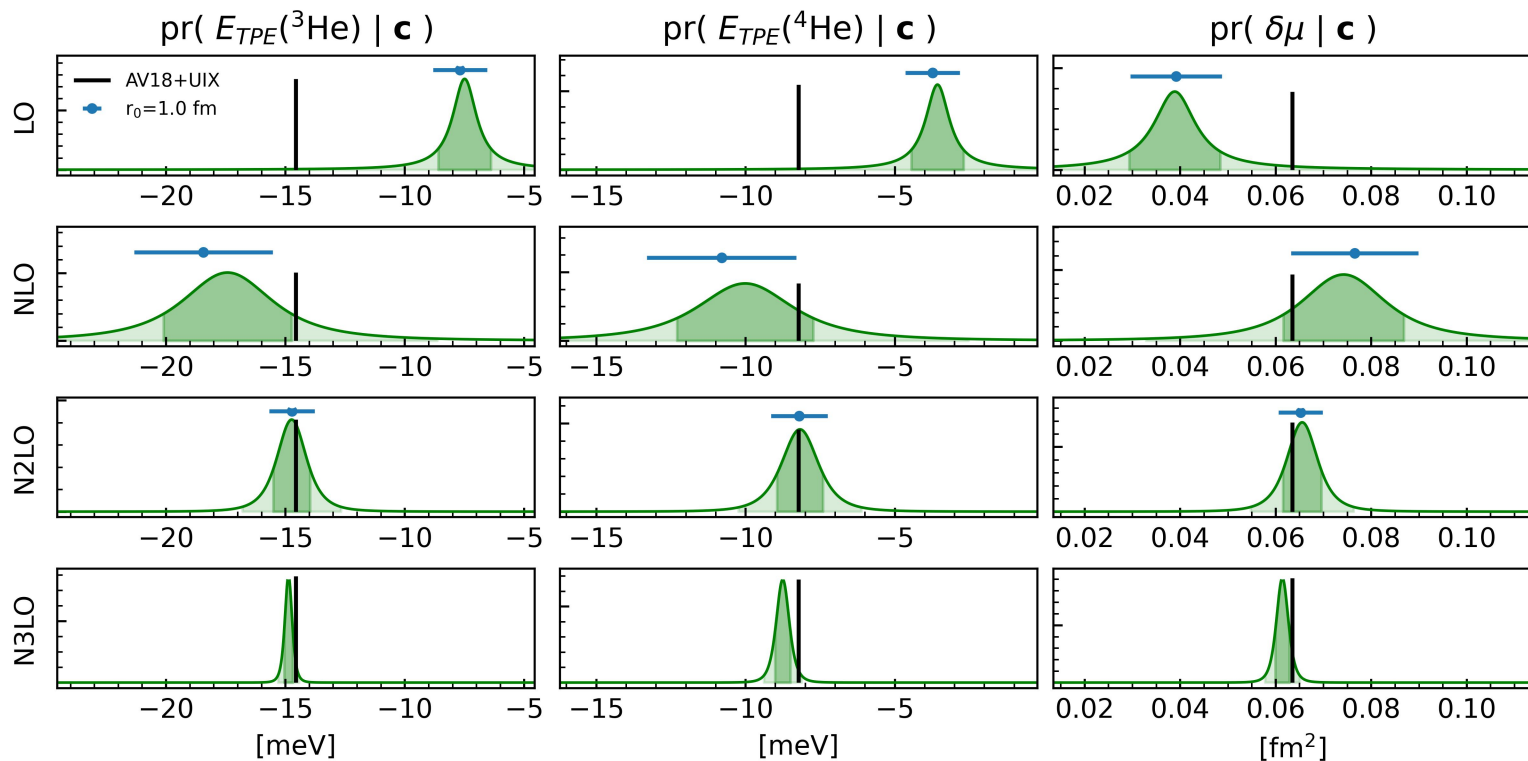
TPE corrections in muonic helium



TPE corrections in muonic helium: sub-leading truncation errors



TPE corrections in muonic helium: Regulator artifacts



TPE corrections in muonic helium: Total uncertainty

	$\mu^3\text{He}^+$ [%]	$\mu^4\text{He}^+$ [%]	
	Numerical	0.1	0.2
	Nuclear model	1.4	3.0
	η -expansion	1.4	0.2
	ISB	0.5	0.5
	Nucleon-size	0.9	1.2
	Relativistic	0.1	0.0
	Coulomb	0.9	0.1
	Total	2.4	3.5
Total uncertainty in the Two-photon nuclear structure effects			

– SSLM, Thomas R. Richardson, Sonia Bacca, Arxiv:2401.13424

– SSLM, et al. J. Phys. G: Nucl. Part. Phys. 49 105101 (2022)

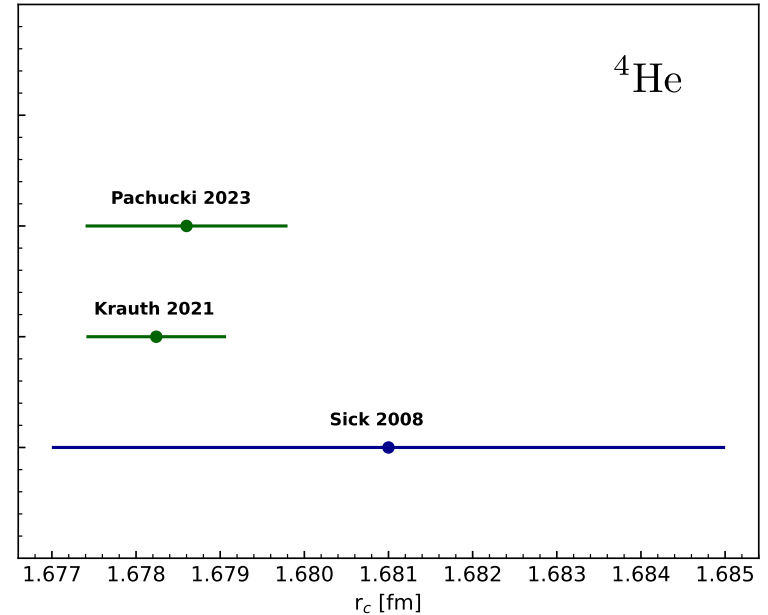
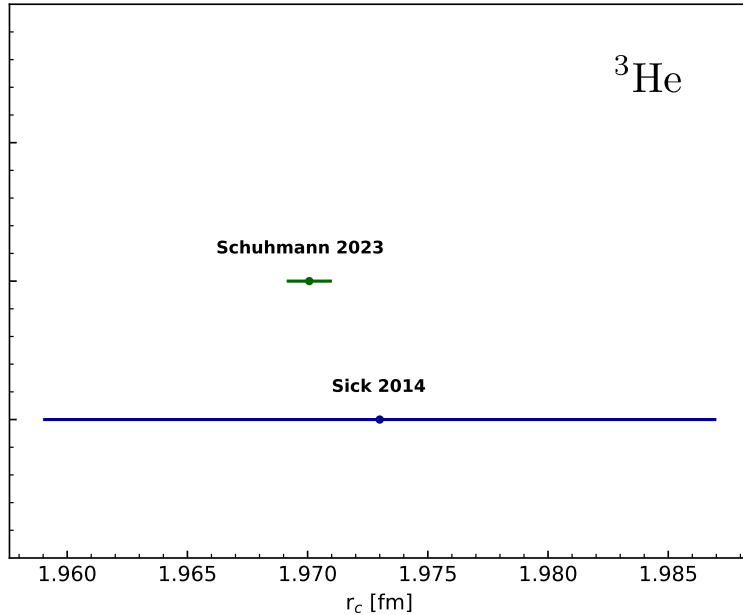
– C. Ji, et al. J. Phys. G: Nucl. Part. Phys. 45 (2018)

Nuclear structure in muonic helium: Total uncertainty

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
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	$\alpha(Z\alpha)^4$	$\mu\text{SE}^{(1)} + \mu\text{VP}^{(1)}$, 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)
IV.A	$(Z\alpha)^4$	r_C^2	-5.197 5 r_p^2	-6.073 2 r_d^2	-102.523 r_h^2	-105.322 r_a^2
IV.B	$\alpha(Z\alpha)^4$	eVP ⁽¹⁾ with r_C^2	-0.028 2 r_p^2	-0.034 0 r_d^2	-0.851 r_h^2	-0.878 r_a^2
IV.C	$\alpha^2(Z\alpha)^4$	eVP ⁽²⁾ with r_C^2	-0.000 2 r_p^2	-0.000 2 r_d^2	-0.009(1) r_h^2	-0.009(1) r_a^2
V.A	$(Z\alpha)^5$	TPE	0.029 2(25)	1.979(20)	16.38(31)	9.76(40)
V.B	$\alpha^2(Z\alpha)^4$	Coulomb distortion	0.0	-0.261	-1.010	-0.536
V.C	$(Z\alpha)^6$	3PE	-0.001 3(3)	0.002 2(9)	-0.214(214)	-0.165(165)
V.D	$\alpha(Z\alpha)^5$	eVP ⁽¹⁾ with TPE	0.000 6(1)	0.027 5(4)	0.266(24)	0.158(12)
V.E	$\alpha(Z\alpha)^5$	$\mu\text{SE}^{(1)} + \mu\text{VP}^{(1)}$ with TPE	0.000 4	0.002 6(3)	0.077(8)	0.059(6)
III	E_{QED}	Point nucleus	206.034 4(3)	228.774 0(3)	1644.348(8)	1668.491(7)
IV	$C r_C^2$	Finite size	-5.225 9 r_p^2	-6.107 4 r_d^2	-103.383 r_h^2	-106.209 r_a^2
V	E_{NS}	Nuclear structure	0.028 9(25)	1.750 3(200)	15.499(378)	9.276(433)
	E_L (exp)	Experiment ^a	202.370 6(23)	202.878 5(34)	1258.598(48)	1378.521(48)
	r_C	This review	0.840 60(39)	2.127 58(78)	1.970 07(94)	1.678 6(12)
	r_C	Previous work ^a	0.840 87(39)	2.125 62(78)	1.970 07(94)	1.678 24(83)

Helium isotopes charge radii

$$E_{LS} = E_{QED} + Cr_c^2 + E_{TPE} + E_{3PE} + \dots$$

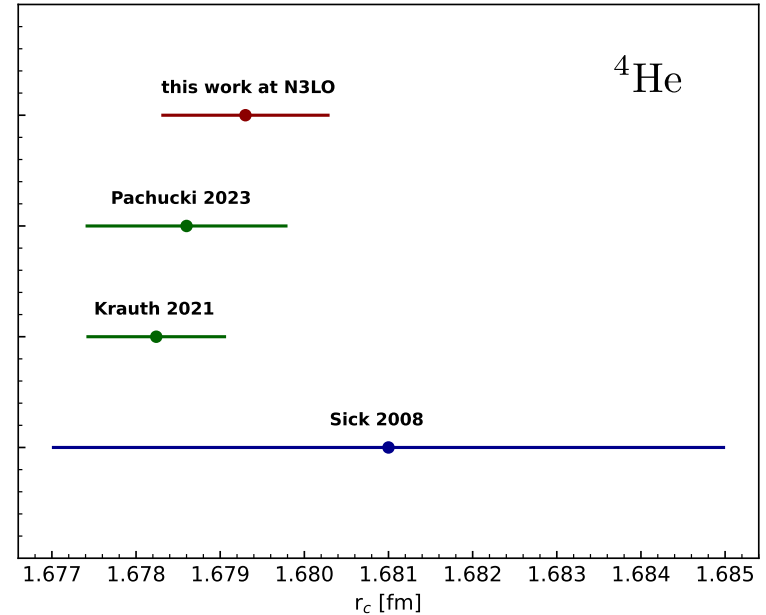
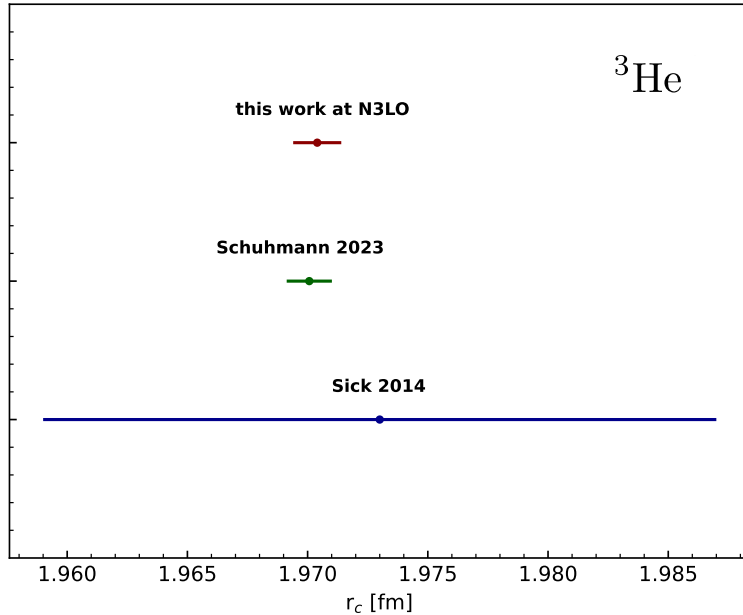


Helium isotopes charge radii

$$E_{LS} = E_{QED} + Cr_c^2 + E_{TPE} + E_{3PE} + \dots$$

Updating this

SSLM, Thomas R. Richardson, Sonia Bacca, Arxiv:2401.13424



Isotope shift of muonic helium

$$\delta r_c^2 = \left[\frac{E_{\text{LS}}(^3\text{He})}{C(^3\text{He})} - \frac{E_{\text{LS}}(^4\text{He})}{C(^4\text{He})} \right] + \left[\frac{E_{\text{TPE}}(^4\text{He})}{C(^4\text{He})} - \frac{E_{\text{TPE}}(^3\text{He})}{C(^3\text{He})} \right]$$

Define the nuclear structure part of this term as $\delta\mu$

$$+ \left[\frac{E_{3\text{PE}}(^4\text{He})}{C(^4\text{He})} - \frac{E_{3\text{PE}}(^3\text{He})}{C(^3\text{He})} \right] + \left[\frac{E_{\text{QED}}(^4\text{He})}{C(^4\text{He})} - \frac{E_{\text{QED}}(^3\text{He})}{C(^3\text{He})} \right] + \dots$$

Exploiting correlations

$$\frac{\Delta [X - Y]}{\text{Is obtained from the Bayesian analysis}} = \sqrt{\Delta X^2 + \Delta Y^2 - 2\rho \Delta X \Delta Y}$$

Are obtained from the Bayesian analysis

with

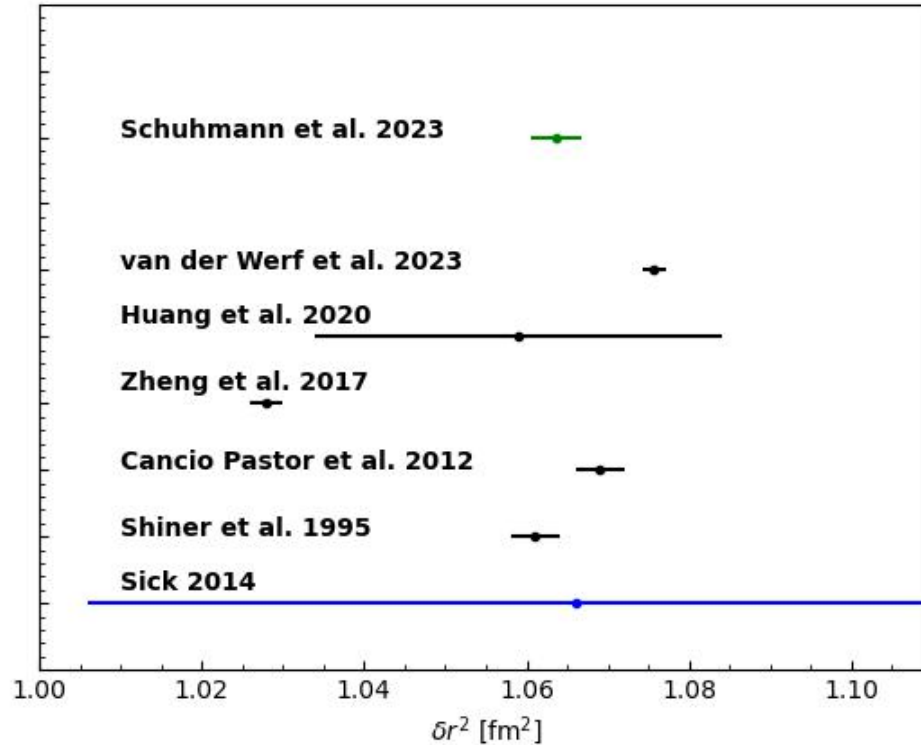
$$X = E_{\text{TPE}}(^4\text{He})/C(^4\text{He})$$

and

$$Y = E_{\text{TPE}}(^3\text{He})/C(^3\text{He})$$

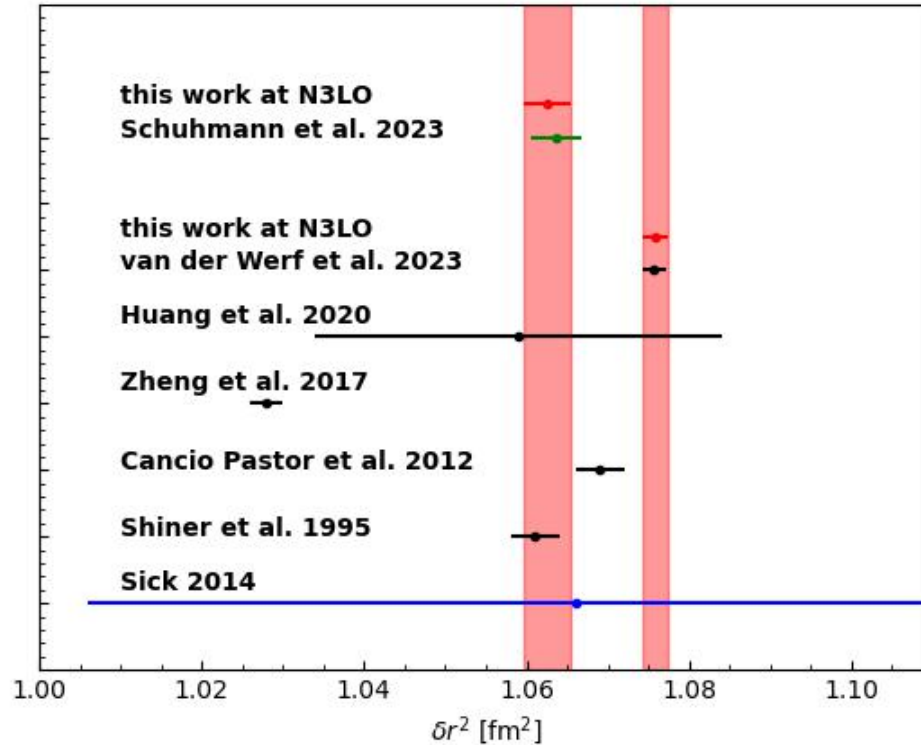
- We can extract the correlation coefficient
- $\rho \approx 0.8$
- Assume that remaining nuclear structure effects (3-photon-exchange, etc...) are correlated with the same correlation coefficient.

Isotope shift of muonic helium



Isotope shift of muonic helium

SSLM, Thomas R. Richardson, Sonia Bacca, Arxiv:2401.13424



Discussion points

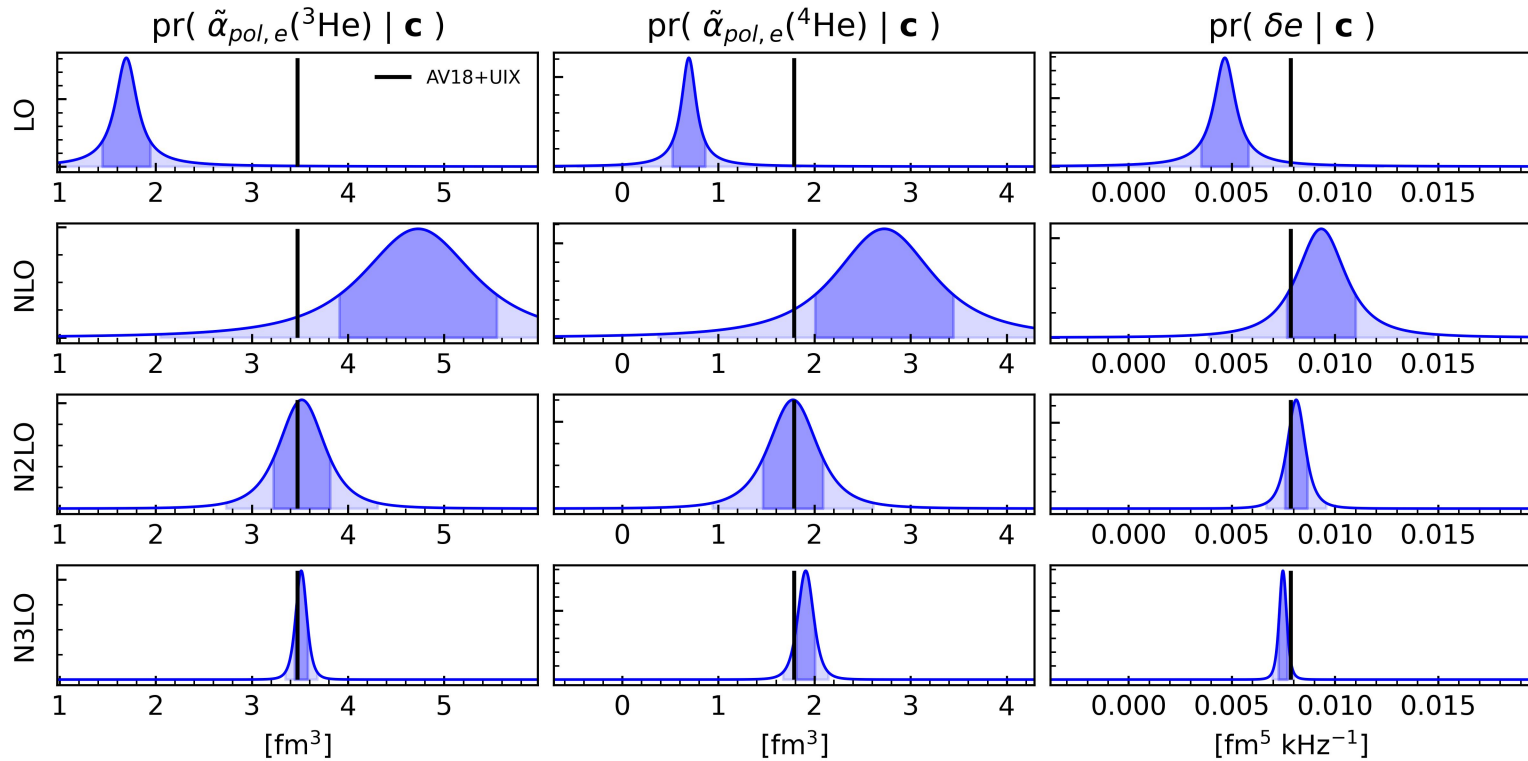
Uncertainty quantification is an excellent starting point to coordinate meaningful exchanges with experimental physics.

The LO ChEFT interaction is statistical worse than expected.

How to improve the predictive power of ChEFT by including information on correlations among observables in nuclei.

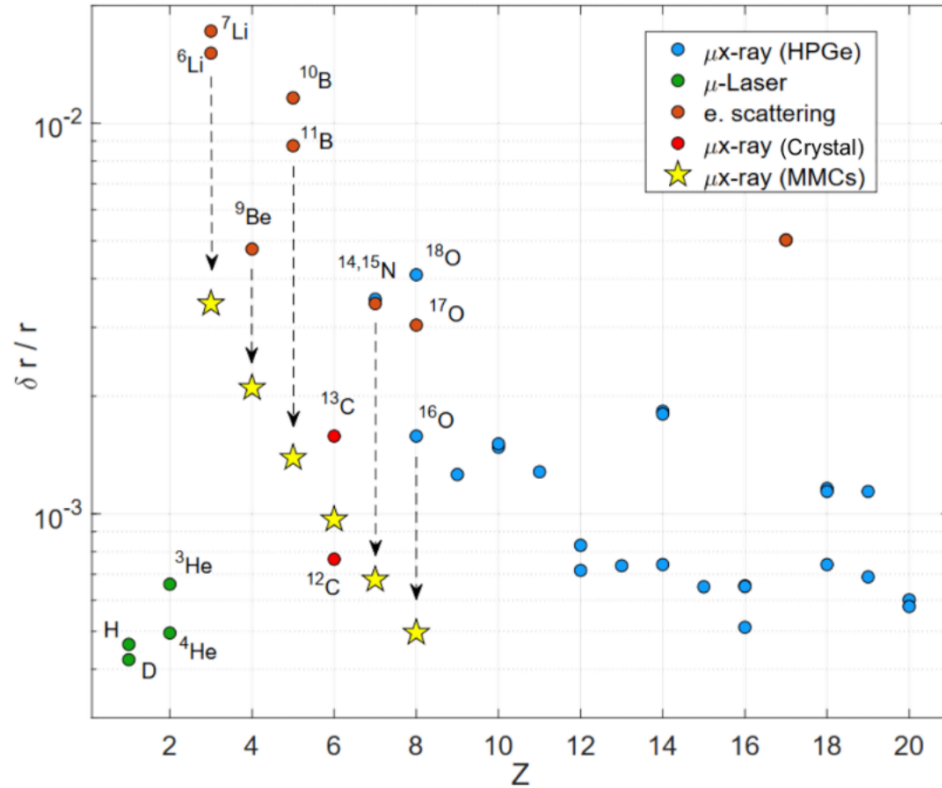
Backup

Two-photon nuclear structure effects in helium atoms

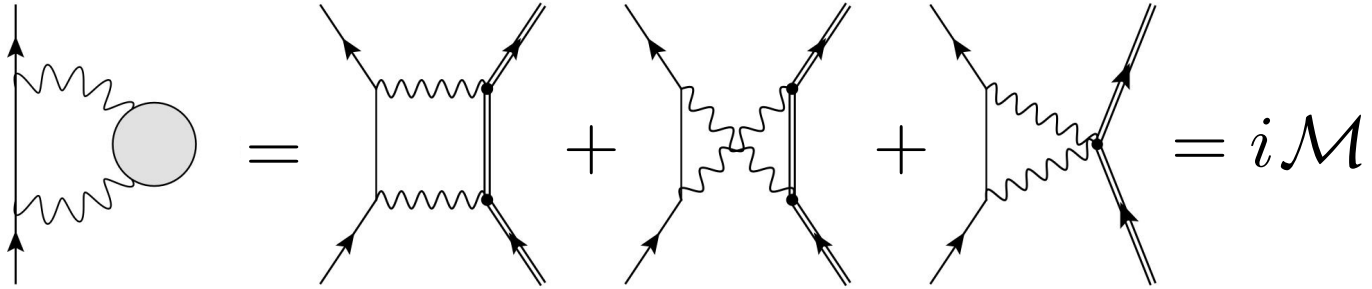


The future pipeline

A. Antognini et al, Arxiv:2210.16929



Evaluation of the TPE term



The amplitudes define a complex potential that shift the 2S-energy of the bound muon by

$$\Delta E_{2S} = \langle \phi_{2S} | \text{Re} [i\mathcal{M}] | \phi_{2S} \rangle$$

With $|\phi_{2S}\rangle$ being the 2S-state of the muon. At our level of precision there are no corrections to 2P-states.

Evaluation of the TPE term

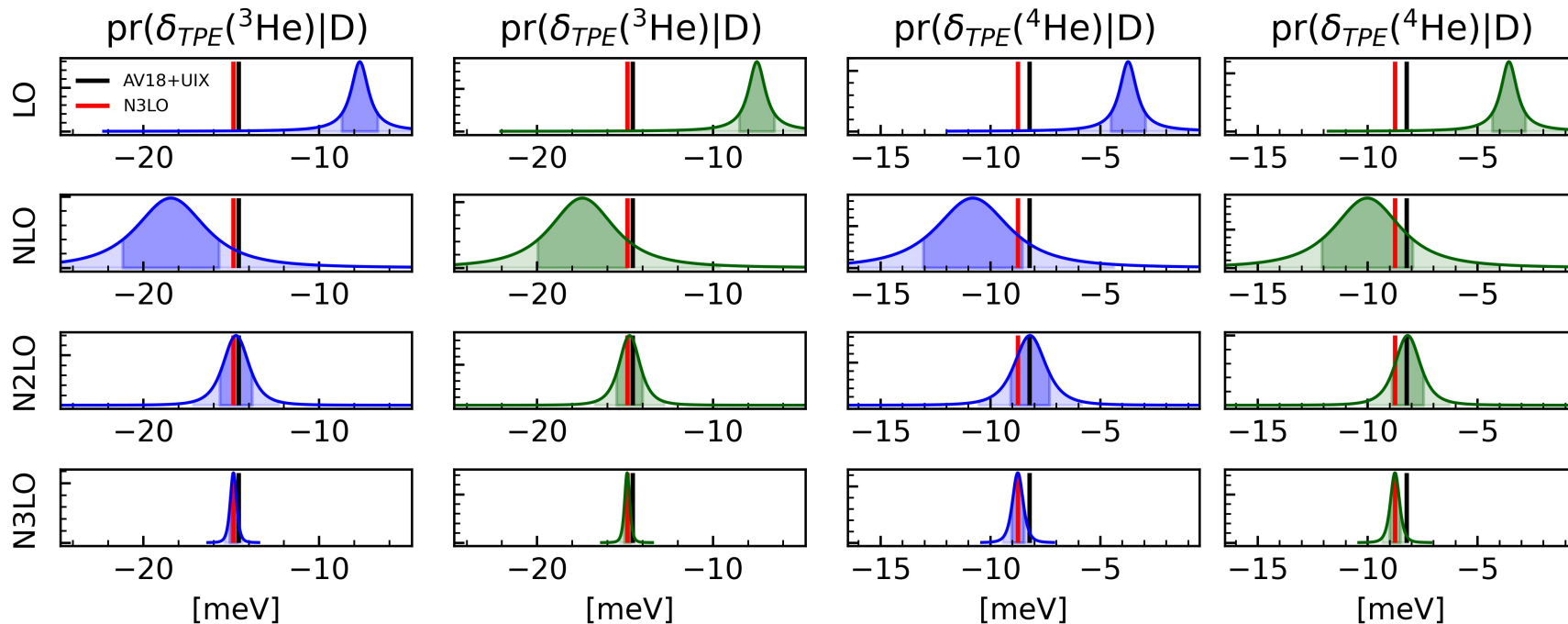
$$\begin{aligned} \Delta E_{2S} = & -8\alpha^2 m \phi_{2S}^2 \left\{ \sum_{N \neq 0} \int d^3x d^3y \langle 0 | \rho_{\text{ch}}^\dagger(\mathbf{y}) | N \rangle \langle N | \rho_{\text{ch}}(\mathbf{x}) | 0 \rangle I_N(z) \right. \\ & + \sum_{N \neq 0} \int d^3x d^3y \langle 0 | J_i^\dagger(\mathbf{y}) | N \rangle \langle N | J_j(\mathbf{x}) | 0 \rangle \left[\delta_{ij} J_N(z) + z^i z^j \bar{J}_N(z) \right] \\ & \left. + \int d^3x d^3y B^{ij}(\mathbf{x}, \mathbf{y}) \frac{1}{2} \left[\delta_{ij} K(z) + z_i z_j \bar{K}(z) \right] \right\}. \end{aligned}$$

With $z = |\mathbf{x} - \mathbf{y}|$.

- The **five structure functions** are known by calculating the leptonic part of the Feynman diagrams.
- The **nuclear matrix elements** must be calculated numerically from Nuclear Theory.

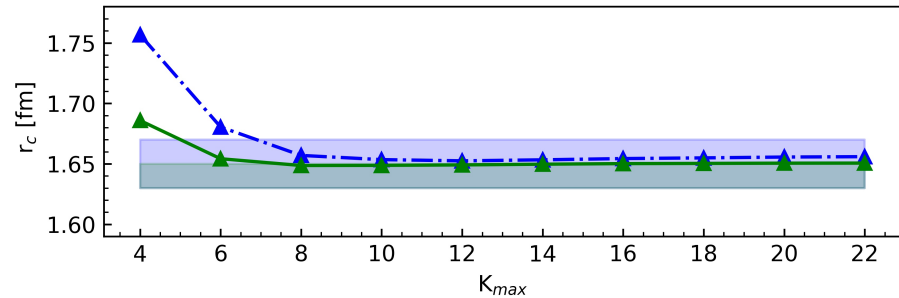
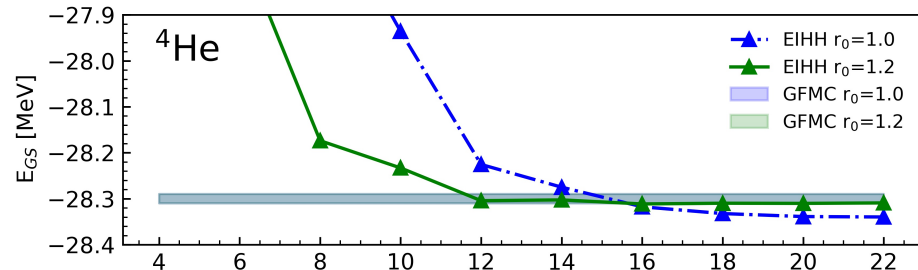
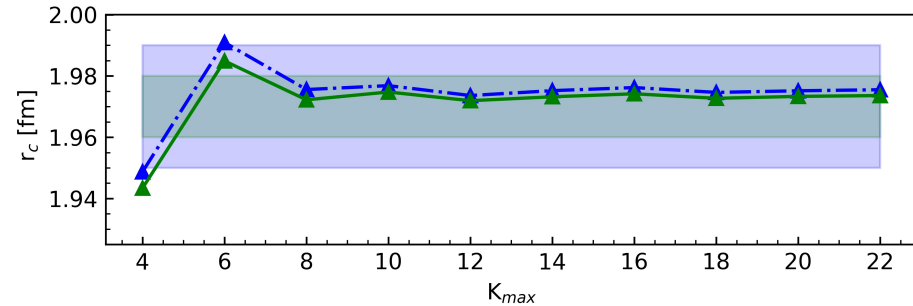
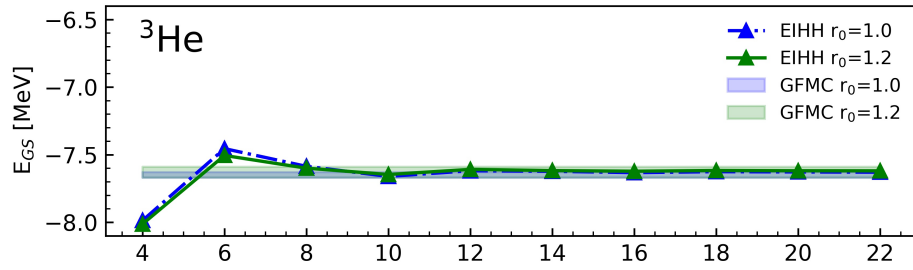
TPE corrections in muonic Helium

S.S.LM, et al. In preparation for 2023



Benchmark tests

S.S. LM, S. Bacca , N. Barnea, *Front. Phys.* 9, 671869 (2021)



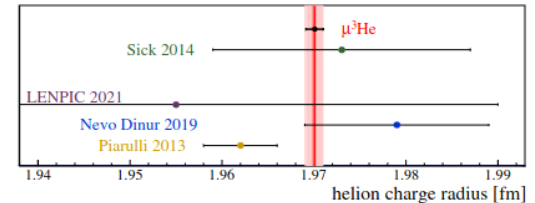
A matter of precision

$$\delta_{\text{LS}} = \delta_{\text{QED+NR}} + \delta_{\text{FS}}^{(4)} \times r_c^2 + \delta_{\text{TPE}}^{(5)} + \delta_{\text{3PE}}^{(6)} + \dots$$

For the muonic Helium-3 ion

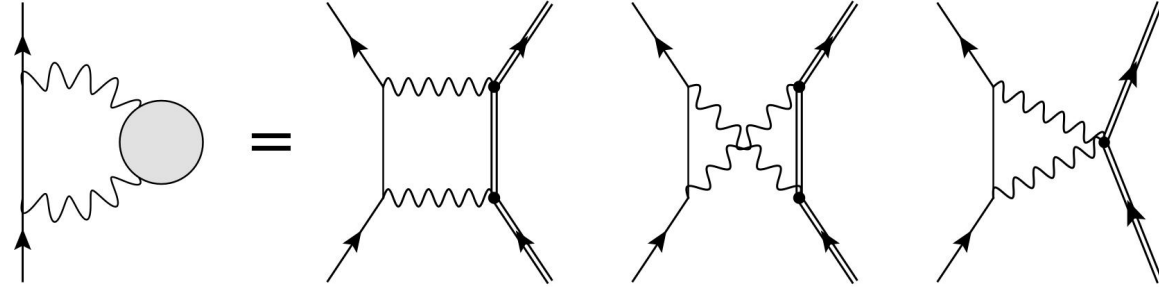
$$\begin{aligned}\delta_{\text{QED+NR}} &= +1,644.348(8) \text{ meV} \\ \delta_{\text{FS}}^{(4)} &= -103.383 \text{ meV fm}^{-2} \\ \delta_{\text{TPE}}^{(5)} &= +15.499(378) \text{ meV} \\ \delta_{\text{3PE}}^{(6)} &= -0.214(214) \text{ meV} \\ \delta_{\text{HO}}^{(5)} &= -0.667(25) \text{ meV}\end{aligned}$$

$$r_c = 1.97007(12)_{\text{ex}}(93)_{\text{th}} \text{ fm}$$



K. Schuhmann et. al. Arxiv 2305.11679 (2023)

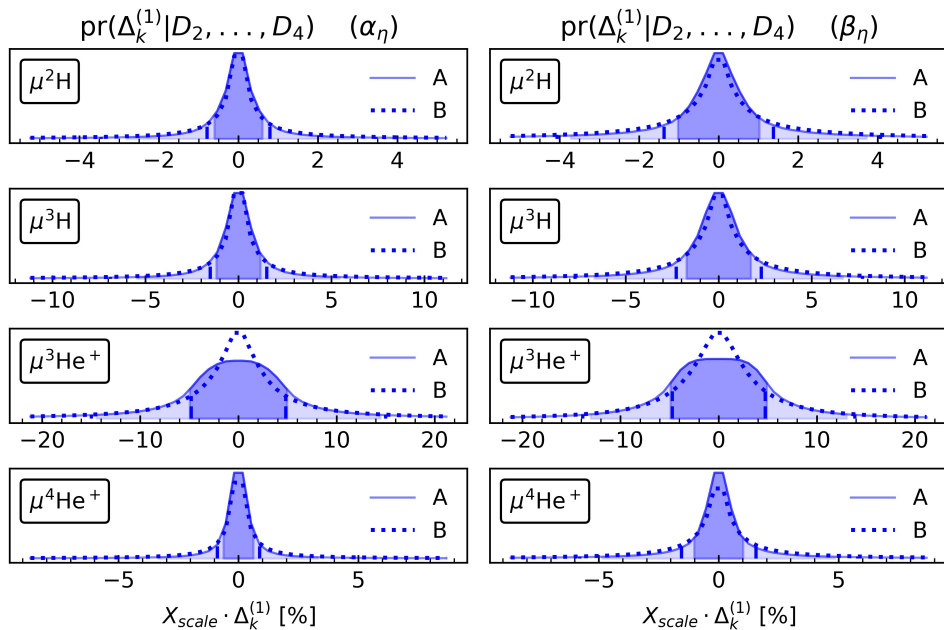
Evaluation of the NS effects



$$\begin{aligned}
 \Delta E_{nl} = & -8\alpha^2 m \phi_{nL}^2 \int \frac{d^3q}{4\pi} \left\{ \sum_{N \neq 0} |\langle N | \rho_{\text{ch}}(\mathbf{q}) | 0 \rangle|^2 \frac{(2E_q + \omega_N)}{q^4 E_q [(E_q + \omega_N)^2 - m^2]} \right. \\
 & + \sum_{N \neq 0} |\langle 0 | \mathbf{J}_\perp(\mathbf{q}) | N \rangle|^2 \left[\frac{q^2}{4m^2} \frac{(2E_q + \omega_N)}{q^4 E_q [(E_q + \omega_N)^2 - m^2]} - \frac{1}{4m^2 q^3} \frac{\omega_N + 2q}{(\omega_N + q)^2} \right] \\
 & \left. + B_\perp(\mathbf{q}) \frac{1}{8m^2 q^2} \left(\frac{1}{q} - \frac{1}{E_q} \right) \right\}
 \end{aligned}$$

eta-expansion uncertainty

$$\begin{aligned} \Delta E_{nl}^{\text{NR}} &= -8\alpha^2 \phi_{nl}^2 \sum_{N \neq 0} \int d^3x d^3y \langle 0 | \rho_{\text{ch}}^\dagger(\mathbf{y}) | N \rangle \langle N | \rho_{\text{ch}}(\mathbf{x}) | 0 \rangle I_{\text{NR}}(z) \\ &= -8\alpha^2 \phi_{nl}^2 \sum_{N \neq 0} \int d^3x d^3y \langle 0 | \rho_{\text{ch}}^\dagger(\mathbf{y}) | N \rangle \langle N | \rho_{\text{ch}}(\mathbf{x}) | 0 \rangle \left(I_{\text{NR}}^{(2)}(z) + I_{\text{NR}}^{(3)}(z) + I_{\text{NR}}^{(4)}(z) + \dots \right) \end{aligned}$$



S.S.LM, et al. 2022 J. Phys. G: Nucl. Part. Phys. 49 105101

	$\mu^2\text{H}$	$\mu^3\text{H}$	$\mu^3\text{He}^+$	$\mu^4\text{He}^+$
C. Ji, et al. (2018)	0.4%	1.3%	1.1%	0.8%
This work	0.8%	1.5%	4.8%	0.9%

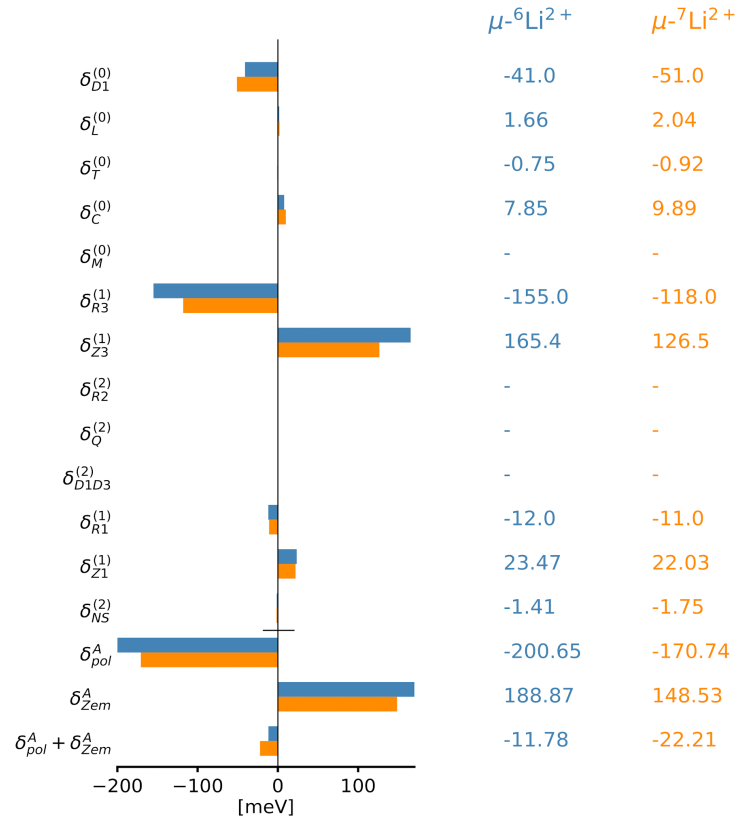
Preliminary works on Li atoms

$$\delta_{\text{TPE}} = \delta_{D1}^{(0)} + \delta_C^{(0)} + \delta_{Z1}^{(1)} + \delta_{Z3}^{(1)} + \delta_{NS}^{(2)} + \delta_Q^{(2)} + \dots$$

δ_{TPE}	Ref. (1) (meV)	Ref. (2) (meV)
$\mu\text{-}^6\text{Li}^{2+}$	-11.8(3)	-15(4)
$\mu\text{-}^7\text{Li}^{2+}$	-22.2(4)	-21(4)

(1) S.L., A.Poggialini, S.Bacca, SciPost Phys. Proc. 3, 028 (2020)

(2) Drake et al, Phys. Rev. A **32**, 713 (1985)



Priors

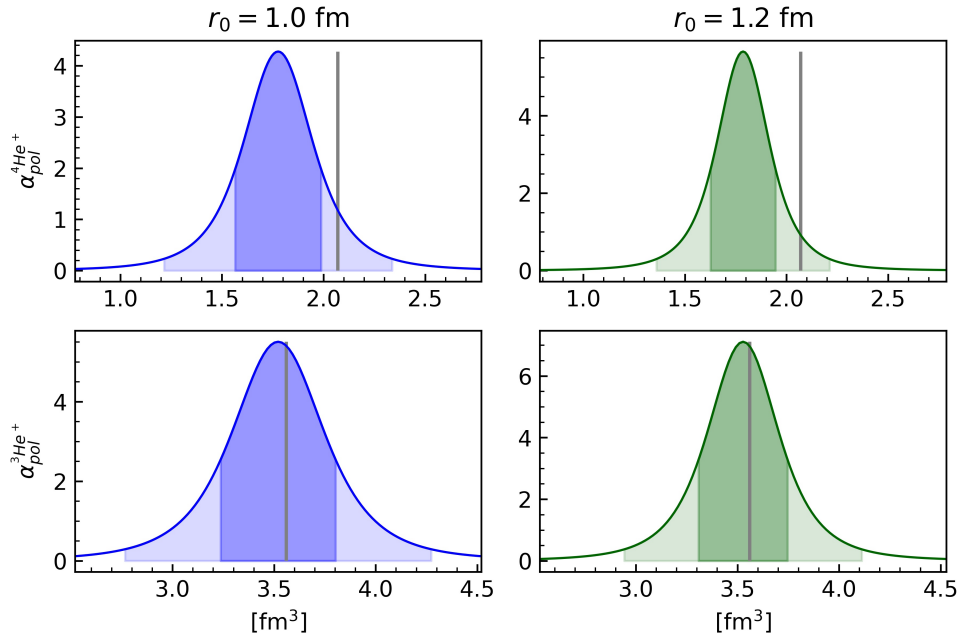
$$\begin{aligned}
 X &= \sum_{n=0}^k D_n + \sum_{n=k+1}^{\infty} D_n \\
 &= X_{\text{ref}} \left[\sum_{n=0}^k c_n Q^n + \sum_{n=k+1}^{\infty} c_n Q^n \right]
 \end{aligned}$$

Priors	$\text{pr}(\eta)$
α_η	$\frac{1}{\lambda} \exp\left(\frac{\eta}{\lambda}\right)$
β_η	$\beta(a, b)$

Priors	$\text{pr}(c_i \bar{c})$	$\text{pr}(\bar{c})$
A	$\frac{1}{2\bar{c}} \theta(\bar{c} - c_i)$	$\frac{1}{\ln(\bar{c}_>/\bar{c}_<)\bar{c}} \theta(\bar{c} - \bar{c}_<) \theta(\bar{c}_> - \bar{c})$
B	$\frac{1}{\sqrt{2\pi\bar{c}}} \exp\left(-\frac{c_i^2}{2\bar{c}^2}\right)$	$\frac{1}{\ln(\bar{c}_>/\bar{c}_<)\bar{c}} \theta(\bar{c} - \bar{c}_<) \theta(\bar{c}_> - \bar{c})$

NS effects in 3He^+ and 4He^+

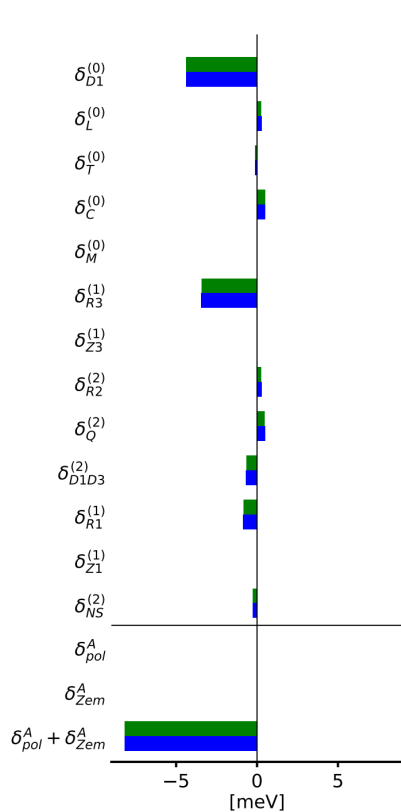
$$\delta_{\text{pol}}^{(5)} = -m\alpha^4 \left\langle \sum_a \delta^3(r_a) \right\rangle (m^3 \alpha_{\text{pol}})$$



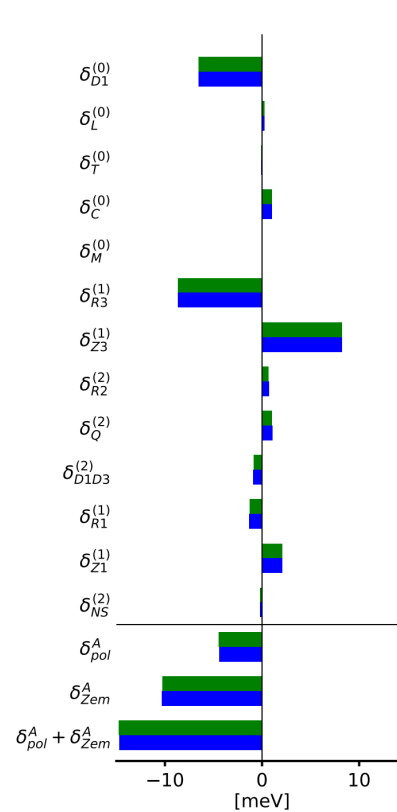
	3He^+	4He^+
1S-2S		
[1]	48(5)kHz	28(3)kHz
This work	48(6)kHz	24(4)kHz

— [1] K. Pachucki, A.M. Moro Phys.Rev.A 75,032521(2007)

NS corrections in $\mu^4\text{He}^+$



	$r_0 = 1.2$	$r_0 = 1.0$
$\delta_{D1}^{(0)}$	-4.386	-4.373
$\delta_L^{(0)}$	0.272	0.287
$\delta_T^{(0)}$	-0.124	-0.125
$\delta_C^{(0)}$	0.517	0.514
$\delta_M^{(0)}$	0.011	0.011
$\delta_{R3}^{(1)}$	-3.422	-3.477
$\delta_{Z3}^{(1)}$	-	-
$\delta_{R2}^{(2)}$	0.267	0.285
$\delta_Q^{(2)}$	0.484	0.505
$\delta_{D1D3}^{(2)}$	-0.668	-0.69
$\delta_{R1}^{(1)}$	-0.846	-0.856
$\delta_{Z1}^{(1)}$	-	-
$\delta_{NS}^{(2)}$	-0.272	-0.277
δ_{pol}^A	-	-
δ_{Zem}^A	-8.174	-8.196



	$r_0 = 1.2$	$r_0 = 1.0$
$\delta_{D1}^{(0)}$	-6.562	-6.552
$\delta_L^{(0)}$	0.232	0.232
$\delta_T^{(0)}$	-0.104	-0.104
$\delta_C^{(0)}$	1.018	1.015
$\delta_M^{(0)}$	0.008	0.008
$\delta_{R3}^{(1)}$	-8.674	-8.691
$\delta_{Z3}^{(1)}$	8.223	8.255
$\delta_{R2}^{(2)}$	0.67	0.696
$\delta_Q^{(2)}$	1.043	1.062
$\delta_{D1D3}^{(2)}$	-0.877	-0.899
$\delta_{R1}^{(1)}$	-1.297	-1.302
$\delta_{Z1}^{(1)}$	2.054	2.057
$\delta_{NS}^{(2)}$	-0.191	-0.193
δ_{pol}^A	-4.458	-4.411
δ_{Zem}^A	-10.277	-10.312
$\delta_{pol}^A + \delta_{Zem}^A$	-14.735	-14.723