Nuclear Structure Effects in Light Muonic Atoms

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Phys. Rev. Lett. **111**, 143402 (2013)
Phys. Rev. C **89**, 064317 (2014)
Few-Body Syst. **55**, 917 (2014)
Phys. Lett. B **736**, 344 (2014)

TRIUMF University of Manitoba האוניברסיטה העברית בירושלים The Hebrew University of Jerusalem

Outline

- **Introduction**
  - The proton radius puzzle
  - Lamb shift, charge radius & polarization
- **Methods**
  - *Ab-initio* calculation of nuclear polarization
  - The LSR method
- **Results**
  - $\boldsymbol{\mu^4\mathrm{He}^+}$
  - $\boldsymbol{\mu\mathrm{D}}$
  - $\boldsymbol{\mu^3\mathrm{He}^+}$ & $\boldsymbol{\mu\mathrm{T}}$ (preliminary)
- **Summary**
- **Outlook**

How large is the proton?

- **r_p from electron-proton interaction**
  1. e-p scattering: $r_p = 0.875(10)$ fm
  2. Hydrogen spectroscopy: $r_p = 0.8768(69)$ fm
  3. $\Longrightarrow$ CODATA-2010: $\boldsymbol{r_p = 0.8775(51)}$ fm

     Mohr *et al.*, Rev. Mod. Phys. (2012)

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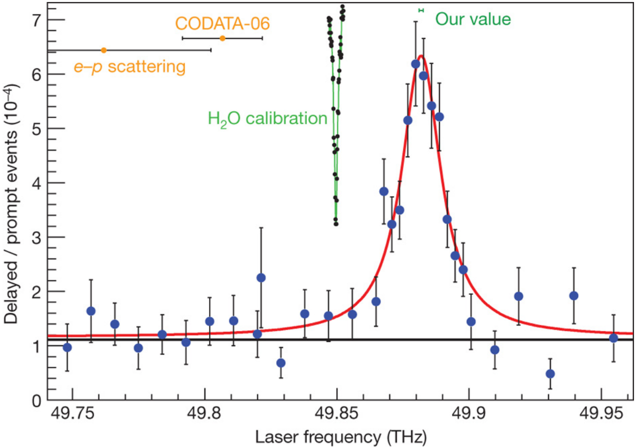
- **r_p from μH Lamb shift (2S-2P)**
  1. μH $2S_{1/2}^{F=1}$ - $2P_{3/2}^{F=2}$: $r_p = 0.84184(67)$ fm (5σ)

     Pohl *et al.*, Nature (2010)
  2. Combined with

     μH $2S_{1/2}^{F=0}$ - $2P_{3/2}^{F=1}$: $\boldsymbol{r_p = 0.84087(39)}$ fm (7σ)

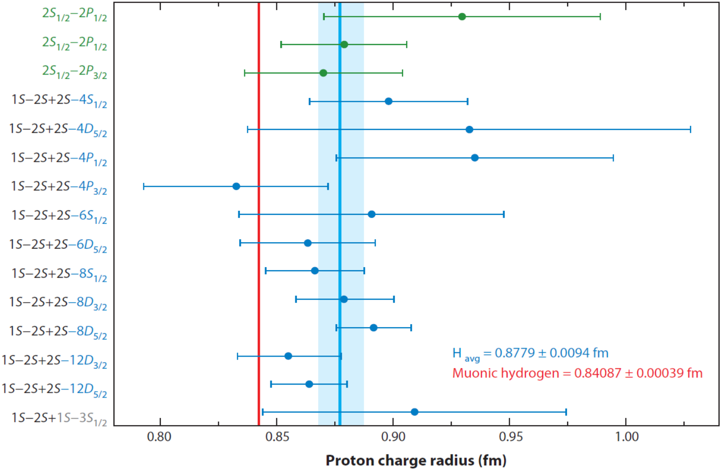
     Antognini *et al.*, Science (2013)

Proton radius puzzle



Origins of the discrepancy? — old data

Hydrogen spectroscopy



Pohl *et al.*, Annu. Rev. Nucl. Part. Sci. '13

Origins of the discrepancy? — old data

ep scattering measurements / fits?

(Q^2 not small enough / floating normalization)

$G_E^p(Q^2) = 1 - \frac{1}{6}\, \boldsymbol{r_p^2}\, Q^2 + \ldots$

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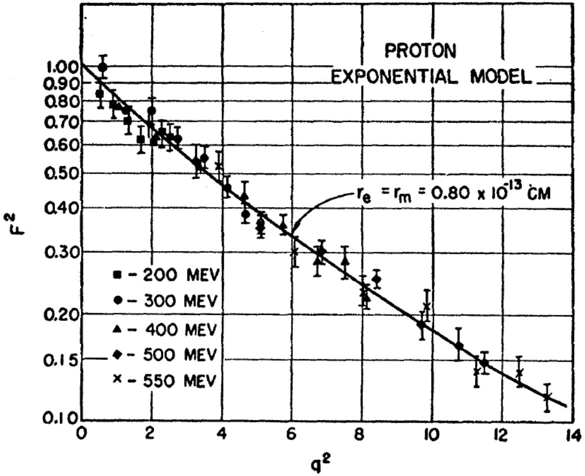

Chambers and Hofstadter, Phys. Rev. **103**, 1454 (1956)

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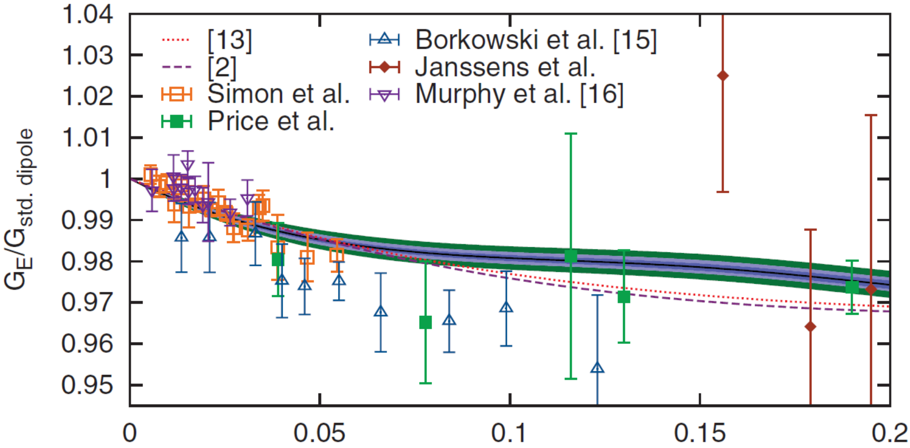

Bernauer *et al.*, Phys. Rev. Lett. **105**, 242001 (2010)

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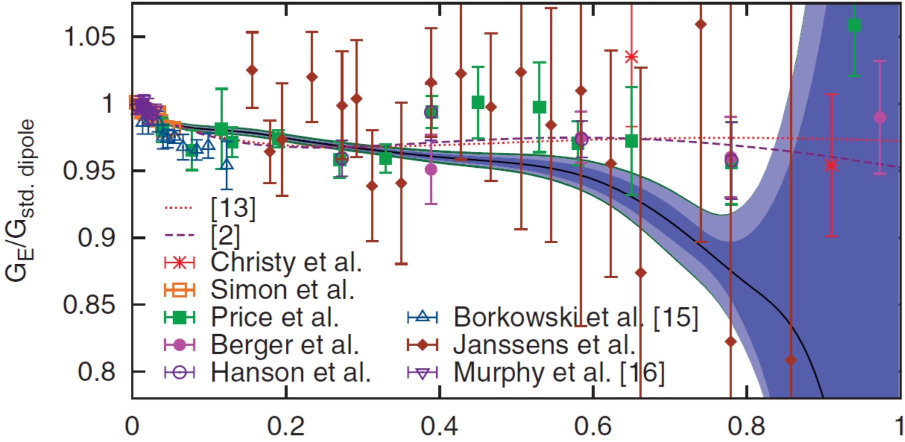

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- Problems with electronic measurements ?
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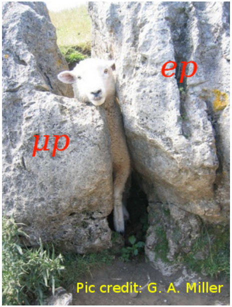

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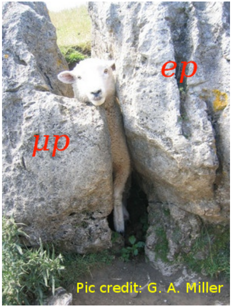
    - dispersion relations: $r_p = 0.84(1)$, $\chi^2_{\mathrm{r}} \approx 2.2$
      Lorenz *et al.*, EPJA '12



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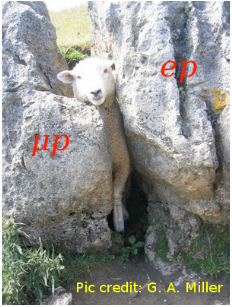

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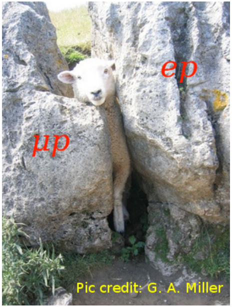

Parametrization	MAMI (1422 data points)	World data incl. MAMI (1922 data points)
Unconstrained z expansion	$r_E = 0.64, r_M = 1.97, (\chi_r^2 = 1.12)$	$r_E = 0.85, r_M = 0.98, (\chi_r^2 = 1.17)$
z expansion, $\lvert e_k \rvert < 10$	$r_E = 0.91, r_M = 0.79, (\chi_r^2 = 1.17)$	$r_E = 0.89, r_M = 0.77, (\chi_r^2 = 1.23)$
DR approach	$r_E = 0.84, r_M = 0.85, (\chi_r^2 = 1.41)$	$r_E = 0.84, r_M = 0.85, (\chi_r^2 = 1.32)$
Combination of the above	$r_E = 0.84, r_M = 0.85, (\chi_r^2 = 1.38)$	$r_E = 0.84, r_M = 0.85, (\chi_r^2 = 1.30)$

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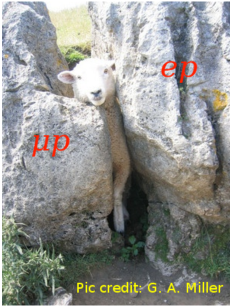

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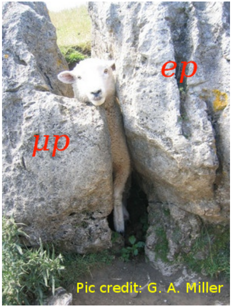
  Birse & McGovern, EPJA '12 *vs.* Miller, PLB '13
  Hill & Paz, PRD '10; PRL '11 & Jentschura PRA '13



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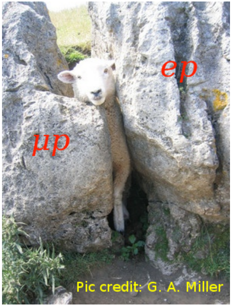

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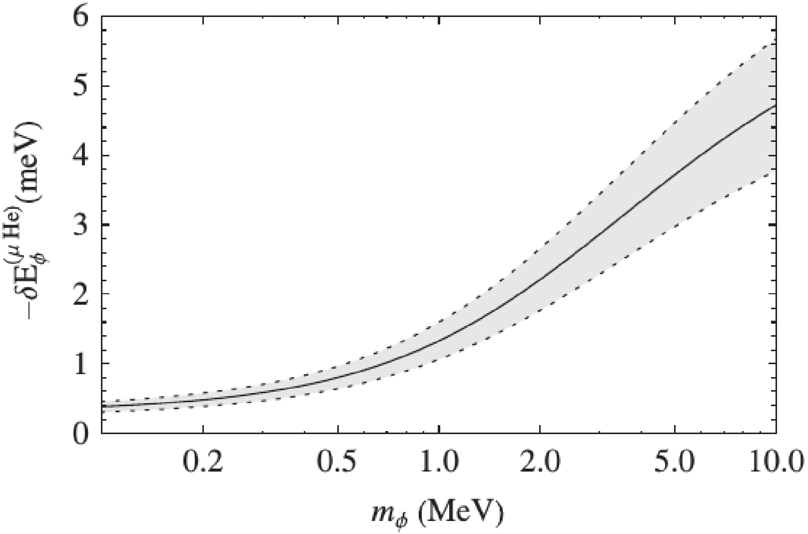
- beyond-standard-model physics?
  - new force carriers, e.g., dark photon: interact differently with e and μ
  - address both r_p puzzle & g_μ puzzle
    Tucker-Smith & Yavin, PRD '11; Batell, McKeen & Pospelov, PRL '11;
    Carlson & Rislow, PRD '12; PRD '14

Tucker-Smith & Yavin's prediction for $\mu^4\text{He}^+$



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New experiments to shed light on the puzzle

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  - and other electronic systems — Rydberg const. ...

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  - Lamb shift (2S-2P) & isotope shift (1S-2S) in μD (finishing)
  - Lamb shift in μ^4He$^+$ and μ^3He$^+$ (both measured in 2014)

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high-precision measurements $\Longleftrightarrow$ accurate theoretical inputs

Extract nuclear charge radius

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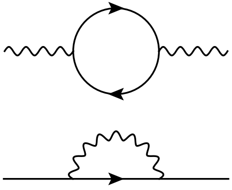
- QED corrections:
  - vacuum polarization
  - lepton self energy
  - relativistic recoil effects
- Calculations for $\mu^{3,4}\mathrm{He}^+$ reexamined



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$$\Delta E_{LS} = \delta_{QED} + \delta_{size}(r) + \delta_{\text{pol}}$$

- Nuclear finite-size corrections (elastic):
  - leading term: $\frac{m_r^3}{12}(Z\alpha)^4 \langle r^2 \rangle$
  - 3rd Zemach moment: $-\frac{m_r^4}{24}(Z\alpha)^5 \langle r^3 \rangle_{(2)} \quad \propto \langle r^2 \rangle^{3/2}$

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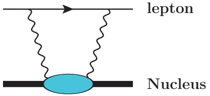
- Nuclear A polarization corrections (inelastic):
  - exchange of two virtual photons
  - dominant contribution $\sim (Z\alpha)^5$



- Nucleon p/n polarization corrections (inelastic)

Uncertainty in nuclear polarization

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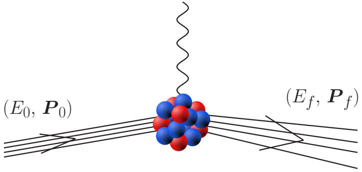
- Nuclear polarization $\Longrightarrow$ inputs from nuclear response functions

$$S_O(\omega) = \sum\!\!\!\!\!\!\int_f |\langle \psi_f | \hat{O} | \psi_0 \rangle|^2 \delta(E_f - E_0 - \omega)$$



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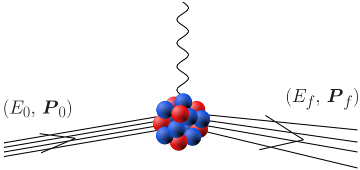

- Early calculations of δ_{pol} in muonic atoms:
  $\Rightarrow S_O(\omega)$ inputs were not accurate enough

Previous calculations of $S_O(\omega)$ & $\delta_{\rm pol}$

- μD
  - Modern forces: AV14 - Leidemann & Rosenfelder '95
  - State-of-the-art: AV18 - Pachucki '11
    - underestimates nuclear physics uncertainty
    - includes nucleon polarizability $\delta^p_{\rm pol}$ (incorrect?)
  - $\not\pi$EFT: zero-range expansion - Friar '13
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  - need to calculate $\delta_{\rm pol}$ using **modern potentials and *ab-initio* methods**

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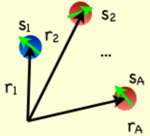
- **Our Goal**

  provide $\boldsymbol{\delta_{\rm pol}}$ with accuracy comparable to the $\mathbf{\pm 5\%}$ experimental needs

Nuclear potentials: two approaches



$$H_N|\psi_i\rangle = E_i|\psi_i\rangle$$

$$H_N = T + V_{NN} + V_{3N} + \ldots$$

High precision two-nucleon potentials:
well constraint on NN phase shifts

Three nucleon forces:
less known, constraint on A>2 observables

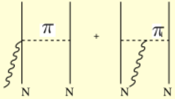
Traditional Nuclear Physics

AV18+UIX, ..., J2

Effective Field Theory

N²LO, N³LO ...

$$J^\mu = J^\mu_N + J^\mu_{NN} + \ldots$$



two-body currents (or MEC)

subnuclear d.o.f.

J^μ consistent with V

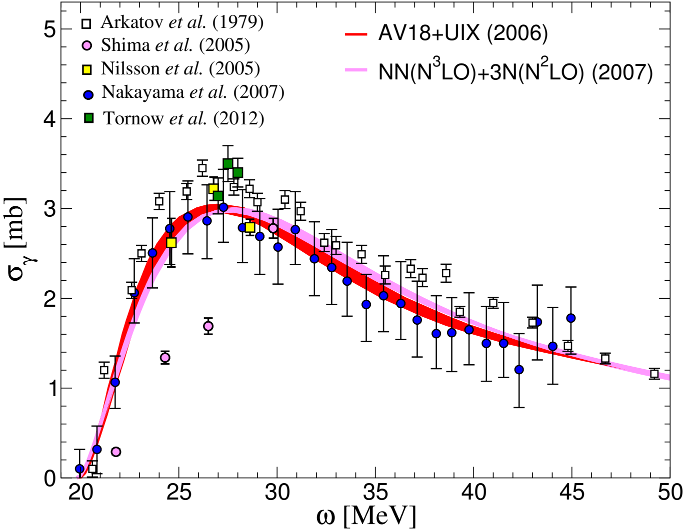
$$\nabla \cdot J = -i[V, \rho]$$

$$S(\omega) \propto |\langle\psi_f|J^\mu|\psi_0\rangle|^2$$

Exact Initial state &
Final state in the continuum at
different energies and for different A

Nuclear potentials: ^{4}He Photoabsorption

electric dipole photoabsorption cross section $\sigma_\gamma(\omega) = 4\pi^2\alpha\omega S_{D1}(\omega)$

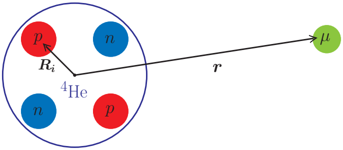


Nuclear polarization: basic idea

- Hamiltonian for muonic atoms

$$H = H_{nucl} + H_\mu + \Delta H$$

$$H_\mu = \frac{p^2}{2m_r} - \frac{Z\alpha}{r}$$



- Corrections to the point Coulomb from protons

$$\Delta H = \alpha \sum_i^Z \Delta V(\boldsymbol{r}, \boldsymbol{R}_i) \equiv \alpha \sum_i^Z \left(\frac{1}{r} - \frac{1}{|\boldsymbol{r} - \boldsymbol{R}_i|} \right)$$

- Evaluate inelastic effects of ΔH on muonic spectrum in 2^{nd}-order perturbation theory

$$\delta_{\rm pol} = \sum_{N \neq N_0, \mu} \langle N_0 \mu_0 | \Delta H | N \mu \rangle \frac{1}{E_{N_0} - E_N + \epsilon_{\mu_0} - \epsilon_\mu} \langle N \mu | \Delta H | \mu_0 N_0 \rangle$$

$|\mu_0\rangle$: muon wave function for $2S/2P$ state

Nuclear polarization: contributions

Systematic contributions to nuclear polarization

δ_{NR} **Non-Relativistic** limit

$\delta_L + \delta_T$ Longitudinal and Transverse **relativistic** corrections

δ_C **Coulomb** distortions

δ_{NS} Corrections from **finite Nucleon Size**

LSR: Lanczos sum rule method

- Nuclear polarization $\Longrightarrow$ energy-dependent sum rules of the response functions

$$\delta_{\text{pol}} \propto I_O = \int_0^{\infty} d\omega \, S_O(\omega) \, g(\omega)$$

LSR: Lanczos sum rule method

- Nuclear polarization $\Longrightarrow$ energy-dependent sum rules of the response functions

$$\delta_{\rm pol} \propto I_O = \int_0^\infty d\omega \, S_O\left(\omega\right) g\left(\omega\right)$$

- The Lanczos algorithm is an efficient method calculate the LIT of S_O.
  It can be extended to calculate the sum rules.

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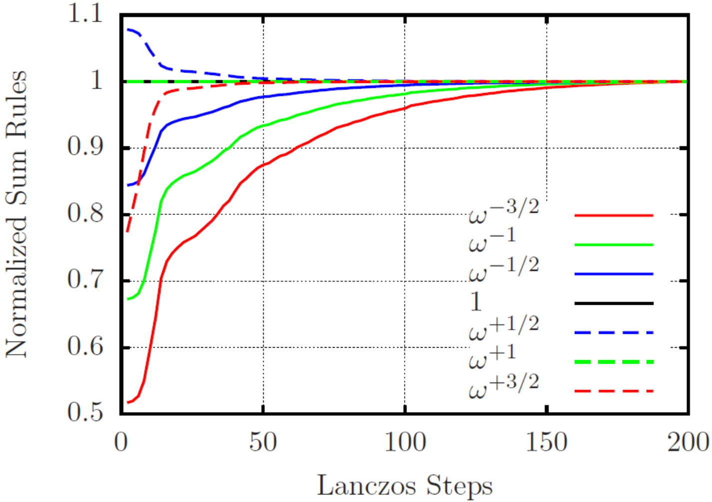
- With the Lanczos sum rule (LSR) method, we directly calculate I_O, without explicitly solving S_O.

- The calculated I_O converges as the LIT of S_O, if $g(\omega)$ is smooth.

NND, Ji, Bacca, Barnea, Phys. Rev. C **89**, 064317 (2014)

LSR: Example — ^{4}He dipole response integrals



(Model space size $M \sim 10^5$)

NND, Barnea, Ji, and Bacca, PRC (2014)

Nuclear polarization in $\mu^4\mathrm{He}^+$

[meV]		AV18+UIX	χEFT★
$\delta^{(0)}$	$\delta^{(0)}_{D1}$	-4.418	-4.701
	$\delta^{(0)}_{L}$	0.289	0.308
	$\delta^{(0)}_{T}$	-0.126	-0.134
	$\delta^{(0)}_{C}$	0.512	0.546

★ NN: N^{3}LO-EM
$3N$: N^{2}LO (c_D=1, c_E=-0.029)

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	$\delta^{(1)}_{Z1}$	1.753	1.811
	$\delta^{(2)}_{NS}$	-0.200	-0.210

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Nuclear polarization in $\mu^4\mathrm{He}^+$

[meV]	AV18+UIX	χEFT★
$\delta^{(0)}$	-3.743	-3.981
$\delta^{(1)}$	0.741	0.809
$\delta^{(2)}$	0.077	0.101
δ_{NS}	0.517	0.530
δ_{pol}	-2.408	-2.542

- Convergence from $\delta^{(0)}$ to $\delta^{(2)}$
  in a systematic expansion of
  $\sqrt{2m_r\omega}|\boldsymbol{R}-\boldsymbol{R}'| \sim \sqrt{m_r/M_N} \approx 0.3$

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  in a systematic expansion of
  $\sqrt{2m_r\omega}|\boldsymbol{R}-\boldsymbol{R}'| \sim \sqrt{m_r/M_N} \approx 0.3$
- AV18+UIX & χEFT differ:
  $\sim 5.5\%$ (0.134 meV)

★ NN: N^{3}LO-EM
$3N$: N^{2}LO (c_D=1, c_E=-0.029)

Nuclear physics uncertainty

^{4}He obesrvable		AV18+UIX	χEFT	Difference
binding energy	B_0 [MeV]	28.422	28.343	0.28%
point-proton nuclear radius	R_{pp} [fm]	1.432	1.475	3.0%
electric-dipole polarizability	α_E [fm^3]	0.0651	0.0694	6.4%
$\boldsymbol{\mu}^4\mathbf{He}^+$ nuclear polarization	δ_{pol} [meV]	-2.408	-2.542	5.5%

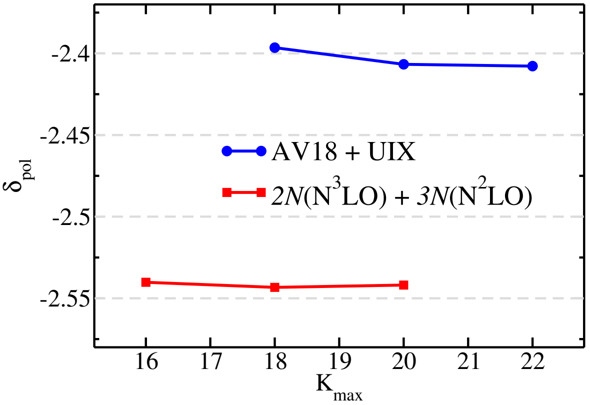
- B_0, R_{pp} & α_E in good agreement with previous calculations
  Kievsky *et al.* '08, Gazit *et al.* '06 & Stetcu *et al.* '09
- systematic uncertainty in δ_{pol} from nuclear physics:
  $\frac{5.5\%}{\sqrt{2}} \implies \pm 4\% \; (1\sigma)$

Numerical accuracy

- **Convergence with model space size**

  Compare $\delta_{\text{pol}}^{(K_{max})}$ with $\delta_{\text{pol}}^{(K_{max}-4)}$

  - AV18+UIX $\sim 0.4\%$
  - χEFT $\sim 0.2\%$



Error budget — $\mu^4\mathrm{He}^+$

- **Nuclear physics**
  4% from two potentials
- **Numerical accuracy**
  0.4% from convergence
- **Additional corrections**
  - $(Z\alpha)^6$ terms (beyond 2nd-order perturbation theory)
  - Rel. & Coulomb corrections (other than dipole)
  - higher-order nucleon-size corrections

  $\Rightarrow$ $\sim 4\%$ estimated from additional corrections
- **Final result (quadratic sum)**
  our prediction: $\delta_{\mathrm{pol}} = -2.47$ meV $\pm 6\%$
  previous estimates: $\delta_{\mathrm{pol}} = -3.1$ meV $\pm 20\%$
  experimental needs: δ_{pol} uncertainty $\sim 5\%$

Reflections on $\mu^4\mathrm{He}^+$

- The accuracy of δ_{pol} in $\mu^4\mathrm{He}^+$ is limited by the nuclear physics (AV18+UIX vs. χEFT-EM)
- To study this we can further vary the nuclear potentials
  - Use χEFT at different orders to track the convergence
  - At each order vary the cutoff to estimate the theoretical error (χEFT-EGM: Epelbaum, Glöckle, Meißner, NPA '05)

Reflections on μD — See Javier Hernandez

- Pachucki only used AV18
  - $\Rightarrow$ No nuclear physics uncertainty
  - $\Rightarrow$ We can add χEFT-EM & χEFT-EGM
- 2-body problem
  - $\Rightarrow$ only NN interaction
  - $\Rightarrow$ simple numerics
- Other issues
  - Pachucki did not include nucleon-size corrections
  - Pachucki did not treat nucleon-polarization correctly
  - We already reproduced Pachucki's leading term as a check for $\mu^4\mathrm{He}^+$
  - There is also a Magnetic contribution
  - It is beneficial to calculate $\delta^\star \equiv |\delta_{\mathrm{pol}} + \delta_{\mathrm{Zem}}|$

Work in progress

The work is not completed yet ...

Preliminary: $\delta_{\rm pol}$ in $\mu^3\rm He^+$

[meV]	AV18+UIX	χEFT★
$\delta^{(0)}$	-5.361	-5.469
$\delta^{(1)}$	-0.460	-0.396
$\delta^{(2)}$	0.841	0.930
δ_{NS}	0.797	0.805
δ_{Mag}	0.078	0.047
$\delta_{\rm pol}$	-4.104	-4.084

- Convergence from $\delta^{(0)}$ to $\delta^{(2)}$?
- AV18+UIX & χEFT agree:
  $< 1\%$ (~ 0.02 meV)

  c.f. $\mu^4\rm He^+$:
  5.5% (0.134 meV)

★ NN: N^{3}LO-EM
$3N$: N^{2}LO (c_D=1, c_E=-0.029)

Preliminary: $\delta_{\rm pol}$ in μT

[meV]	AV18+UIX	χEFT★
$\delta^{(0)}$	-0.680	-0.695
$\delta^{(1)}$	0.178	0.184
$\delta^{(2)}$	-0.025	-0.029
δ_{NS}	0.053	0.054
δ_{Mag}	0.010	0.006
$\delta_{\rm pol}$	-0.465	-0.480

- Convergence from $\delta^{(0)}$ to $\delta^{(2)}$?
- AV18+UIX & χEFT agree:
  $\sim 3\%$ (~ 0.02 meV)
- $\delta^{N}_{\rm pol}$ of the nucleons ?
- Precise triton radius

★ NN: N^{3}LO-EM
$3N$: N^{2}LO (c_D=1, c_E=-0.029)

Summary

- **Lamb shifts in muonic atoms**
  - raise interesting questions about lepton universality
  - probe isospin dependence of the proton radius puzzle
  - allow high precision determination of the nuclear charge radius $\langle \boldsymbol{r^2} \rangle$
  - For $A > 1$ the precision of $\langle \boldsymbol{r^2} \rangle$ is bound by the nuclear polarization $\delta^A_{\rm pol}$

- **We perform the first *ab-initio* calculation of $\delta^\star = \left| \delta^A_{\rm pol} + \delta_{\rm Zem} \right|$ in $\mu^{3,4}\mathrm{He}^+$ & $\mu\mathrm{T}$, and improve the nuclear uncertainty in μ D**

μD	$\delta^\star = 1.66(2)$	meV	[PLB **736**, 344 (2014)]
μT	$\delta^\star = 0.70(2)$	meV	(preliminary)
μ^3He$^+$	$\delta^\star = 14.5(4)$	meV	(preliminary)
μ^4He$^+$	$\delta^\star = 8.6(3)$	meV	[PRL **111**, 143402 (2013)]

  - more accurate than previous calculations
  - will significantly improve the precision of $\langle \boldsymbol{r^2} \rangle$ extracted from ongoing $\boldsymbol{\mu^{3,4}\mathrm{He}^+}$ Lamb shift measurements

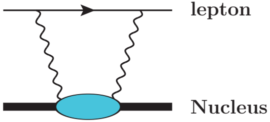
Outlook

- Study higher-order terms
- Reduce nuclear physics uncertainty
  - understand why various nuclear potentials differ
  - further explore the various parameterizations (3NF?)
  - include higher-order or otherwise improved χEFT forces
- Investigate nuclear polarization in *e.g.* $\boldsymbol{\mu^6\mathrm{Li}^{+2}}$, $\boldsymbol{\mu^6\mathrm{He}^{+}}$, $\cdots$
- Investigate nuclear polarization in HFS of electronic and muonic atoms

The muonic Lamb shift is still puzzling !!!

Non-relativistic limit

- **Neglect Coulomb interactions in the intermediate state**



Non-relativistic limit

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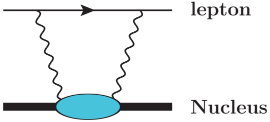
- **Expand muon matrix element in powers of** $\sqrt{2m_r\omega}|\boldsymbol{R}-\boldsymbol{R}'|$



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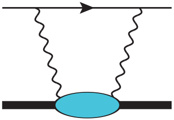

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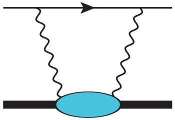
  - $|\boldsymbol{R}-\boldsymbol{R}'| \Longrightarrow$ "virtual" distance the proton travels in 2γ exchange
  - uncertainty principal $|\boldsymbol{R}-\boldsymbol{R}'| \sim 1/\sqrt{2m_N\omega}$
  - $\sqrt{2m_r\omega}|\boldsymbol{R}-\boldsymbol{R}'| \sim \sqrt{\frac{m_r}{m_N}} \approx 0.3$

Non-relativistic limit



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$$P \simeq \frac{m_r^3(Z\alpha)^5}{12}\sqrt{\frac{2m_r}{\omega}}\left[|\boldsymbol{R}-\boldsymbol{R}'|^2 - \frac{\sqrt{2m_r\omega}}{4}|\boldsymbol{R}-\boldsymbol{R}'|^3 + \frac{m_r\omega}{10}|\boldsymbol{R}-\boldsymbol{R}'|^4\right]$$

$\delta_{NR} = \delta_{NR}^{(0)} + \delta_{NR}^{(1)} + \delta_{NR}^{(2)} =$ LO $+$ NLO $+$ $\mathrm{N^2LO}$

NR limit at LO: $\delta_{NR}^{(0)}$

$$\delta_{NR} = \delta_{NR}^{(0)} + \delta_{NR}^{(1)} + \delta_{NR}^{(2)}$$

- $\delta_{NR}^{(0)} \propto |\boldsymbol{R} - \boldsymbol{R}'|^2$

$$\delta_{D1}^{(0)} = -\frac{2\pi m_r^3}{9}(Z\alpha)^5 \int_{\omega_{\rm th}}^{\infty} d\omega \sqrt{\frac{2m_r}{\omega}} S_{D_1}(\omega)$$

- $S_{D_1}(\omega) \Longrightarrow$ electric dipole response function $[\ \hat{D}_1 = R Y_1(\hat{R})\ ]$
- $\delta_{D1}^{(0)}$ is the dominant contribution to $\delta_{\rm pol}$

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- $\Longrightarrow$ Rel. and Coulomb corrections added at this order

NR limit at NLO: $\delta_{NR}^{(1)}$

$$\delta_{NR} = \delta_{NR}^{(0)} + \delta_{NR}^{(1)} + \delta_{NR}^{(2)}$$

- $\delta_{NR}^{(1)} \propto |\boldsymbol{R} - \boldsymbol{R}'|^3$

$$\boxed{\delta_{NR}^{(1)} = \delta_{R3pp}^{(1)} + \delta_{Z3}^{(1)}}$$

$$\delta_{R3pp}^{(1)} = -\frac{m_r^4}{24}(Z\alpha)^5 \iint d\boldsymbol{R}d\boldsymbol{R}'|\boldsymbol{R} - \boldsymbol{R}'|^3 \langle N_0|\hat{\rho}^\dagger(\boldsymbol{R})\hat{\rho}(\boldsymbol{R}')|N_0\rangle$$

$$\delta_{Z3}^{(1)} = \frac{m_r^4}{24}(Z\alpha)^5 \iint d\boldsymbol{R}d\boldsymbol{R}'|\boldsymbol{R} - \boldsymbol{R}'|^3 \rho_0(\boldsymbol{R})\rho_0(\boldsymbol{R}')$$

- $\delta_{R3pp}^{(1)} \Rightarrow$ 3rd-order proton charge correlation
- $\delta_{Z3}^{(1)} \Longrightarrow$ 3rd-order Zemach moment

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- $\delta_{R3pp}^{(1)} \Rightarrow$ 3rd-order proton charge correlation
- $\delta_{Z3}^{(1)} \Longrightarrow$ 3rd-order Zemach moment
  cancels Zemach moment in finite-size corrections
  c.f. Pachucki '11 & Friar '13 (μD)

NR limit at N^2LO: $\delta_{NR}^{(2)}$

$\delta_{NR} = \delta_{NR}^{(0)} + \delta_{NR}^{(1)} + \delta_{NR}^{(2)}$

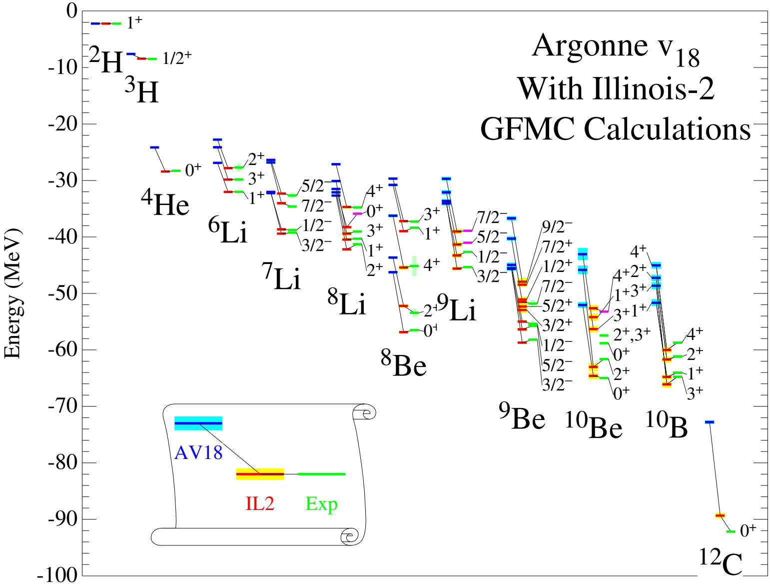
- $\delta_{NR}^{(2)} \propto |\boldsymbol{R} - \boldsymbol{R}'|^4$

$$\delta_{NR}^{(2)} = \frac{m_r^5}{18}(Z\alpha)^5 \int_{\omega_{\rm th}}^{\infty} d\omega \sqrt{\frac{\omega}{2m_r}} \left[S_{R^2}(\omega) + \frac{16\pi}{25} S_Q(\omega) + \frac{16\pi}{5} \mathcal{S}_{D_1 D_3}(\omega) \right]$$

- $S_{R^2}(\omega) \Longrightarrow$ monopole response function
- $S_Q(\omega) \Longrightarrow$ quadrupole response function
- $S_{D_1 D_3}(\omega) \Longrightarrow$ interference between D_1 and D_3 $[\ \hat{D}_3 = R^3 Y_1(\hat{R})\ ]$

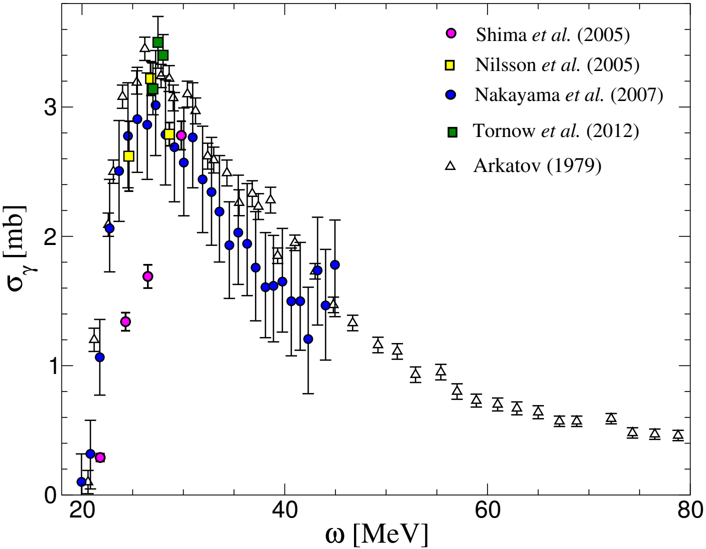
BACK UP

Phenomenological potentials



^{4}He photoabsorption cross sections

electric-dipole photoabsorption cross section $\sigma_\gamma(\omega) = 4\pi^2\alpha\omega S_{D1}(\omega)$



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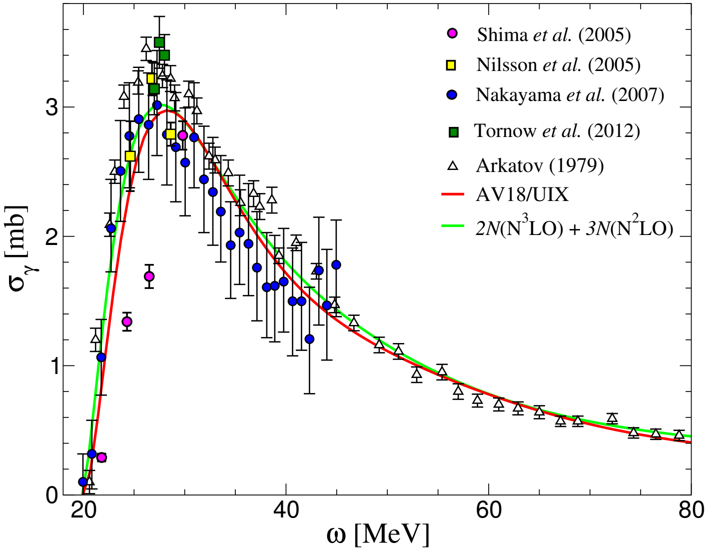

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1. $\sim R^2$ **term:**

- $\Delta E_{NR}^{(2)}$ **is the dominant polarizability contribution**

$$\Delta E_{NR}^{(2)} = -\frac{2\pi m_r^3}{9}(Z\alpha)^5 \int_{\omega_{\mathrm{th}}}^{\infty} d\omega \sqrt{\frac{2m_r}{\omega}} S^{D_1}(\omega)$$

- $S^{D_1}(\omega) = \frac{1}{2J_0+1} \sum_{N\neq N_0, J} |\langle N_0 J_0 || \hat{D}_1 || N J\rangle|^2 \delta(\omega - E_N + E_{N_0})$
- $\hat{D}_1 = \frac{1}{Z}\sum_i^Z R_i Y_1(\hat{R}_i)$

Non-Relativistic Approximation

- Coulomb interactions in the (virtual) intermediate state are neglected
- Results are expressed in an expansion of $\sqrt{2m_r\omega}|\boldsymbol{R}-\boldsymbol{R}'|$

$$\Delta E_{NR} = \Delta E_{NR}^{(2)} + \Delta E_{NR}^{(3)} + \Delta E_{NR}^{(4)}$$

2. $\sim R^3$ **term:**

$$\Delta E_{NR}^{(3)} = -\frac{m_r^4}{24}(Z\alpha)^5 \left[\iint d^3R d^3R' |\boldsymbol{R}-\boldsymbol{R}'|^3 \langle N_0|\hat{\rho}^\dagger(\boldsymbol{R})\hat{\rho}(\boldsymbol{R}')|N_0\rangle - \langle r^3\rangle_{(2)}\right]$$

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  vanishes in point-nucleon limit

- 2nd term: Zemach moment
  $\langle r^3\rangle_{(2)} = \iint d^3R d^3R' |\boldsymbol{R}-\boldsymbol{R}'|^3 \rho_0(\boldsymbol{R})\,\rho_0(\boldsymbol{R}')$
  $\rho_0(\boldsymbol{R}) = \langle N_0|\hat{\rho}(\boldsymbol{R})|N_0\rangle$

  cancels exactly the **Zemach term** in (elastic) finite-size corrections
  c.f. Pachucki PRL 2011 (μD)

Non-Relativistic Approximation

3. $\sim R^4$ **term:**

- $\Delta E_{NR}^{(4)}$ **corresponds to higher-multipole corrections**

$$\Delta E_{NR}^{(4)} = \frac{m_r^5}{18}(Z\alpha)^5 \int_{\omega_{\rm th}}^{\infty} d\omega \sqrt{\frac{\omega}{2m_r}} \left[S^{Q_0}(\omega) + \frac{16\pi}{25} S^{Q_2}(\omega) + \frac{16\pi}{5} S^{D_{13}}(\omega) \right]$$

- $S^{R^2}(\omega) = \frac{1}{2J_0+1} \sum_{N \neq N_0, J} |\langle N_0 J_0 || \hat{R}^2 || N J \rangle|^2 \delta(\omega - E_N + E_{N_0})$

  $S^{Q_2}(\omega) = \frac{1}{2J_0+1} \sum_{N \neq N_0, J} |\langle N_0 J_0 || \hat{Q}_2 || N J \rangle|^2 \delta(\omega - E_N + E_{N_0})$

  $S^{D_{13}}(\omega) = \frac{1}{2J_0+1} \sum_{N \neq N_0, J} (-1)^{J_0 - J}$

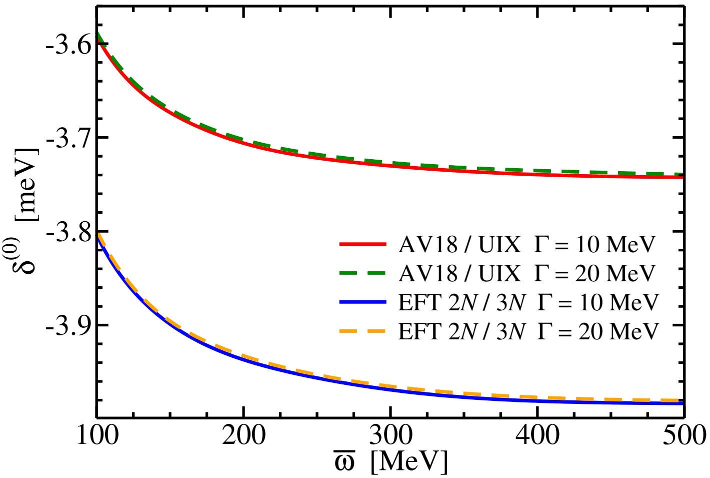
  $\times \mathrm{Re} \left(\langle N_0 J_0 || \hat{D}_3 || N J \rangle \langle N J || \hat{D}_1 || N_0 J_0 \rangle \right) \delta(\omega - E_N + E_{N_0})$

- $\hat{R}^2 = \frac{1}{Z} \sum_i^Z R_i^2$ $\qquad$ $\hat{D}_1 = \frac{1}{Z} \sum_i^Z R_i Y_1(\hat{R}_i)$

  $\hat{Q}_2 = \frac{1}{Z} \sum_i^Z R_i^2 Y_2(\hat{R}_i)$ $\qquad$ $\hat{D}_3 = \frac{1}{Z} \sum_i^Z R^3 Y_1(\hat{R}_i)$

Convergence of Ab-initio calculations

Convergence of $\bar{\omega}$



Convergence of Ab-initio calculations

$\delta^{(0)}$ convergence with the largest model space K_{max}