TRIUMF

Canada's national laboratory
for particle and nuclear physics
and accelerator-based science

Ab initio calculation of dynamic observables and sum rules in light nuclei

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[5]The Hebrew University of Jerusalem

INT, Seattle — March 24 2017

Outline

- Summary
- Application
- Results
- Methods
- Motivation

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  Particularly, nuclear corrections are the bottleneck in μA spectroscopy.

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We use the **LSR method** to calculate the relevant sum-rules.
We proved its applicability using the LIT method.
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- Methods — We use the **LSR method** to calculate the relevant sum-rules.
  We proved its applicability using the LIT method.
  The LIT method has been successfully applied to calculate many EW-induced reactions. Some applications have yet to be demonstrated.
- Motivation — LIT & LSR were applied with Coupled-Cluster for calculations in: ^{4}He, ^{16,22}O, ^{40,48}Ca... (G. Hagen et al., PRC'14; PRC'16; Nature'16;...)


AND NOW FOR SOMETHING COMPLETELY
DIFFERENT
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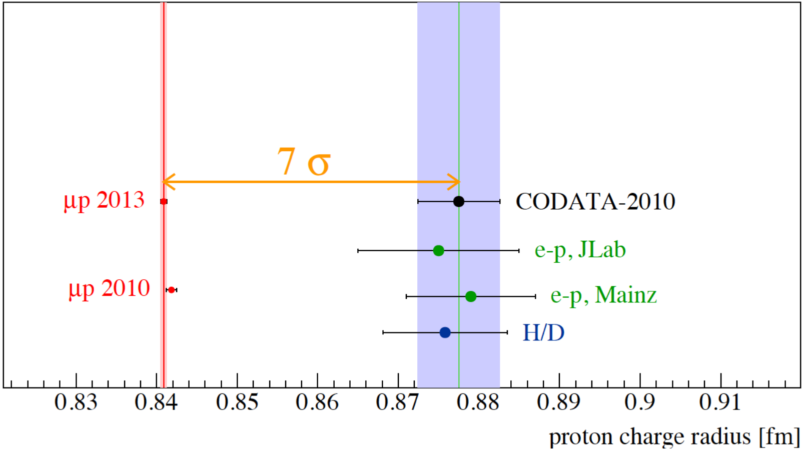
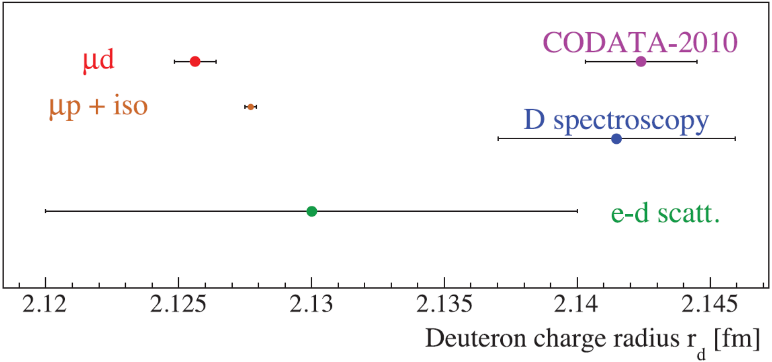
How big is the proton?



R. Pohl & J. Krauth @ CREMA

How big is the deuteron?



R. Pohl *et al.*, **Science 2016**

CREMA @ PSI

Extract precise **charge radii** $\boldsymbol{R_c}$ from Lamb shift (LS) in:

- μH (published 2010,2013: **proton radius puzzle)**
- μD (published 2016: **deuteron radius puzzle)**
- $\mu\,^4$He$^+$ (measured 2014, finalizing: **agreement with $e-^4$He ?!**)
- $\mu\,^3$He$^+$ (measured 2014, analyzing: **???)**

  $\Longrightarrow$ radius puzzle(s), QED tests, He isotope shift, nuclear *ab initio*, ...
- $\mu\,^3$H, $\mu\,^6$He$^+$, $\mu\,^{6,7}$Li^{+2} ... (possible?)

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Ongoing μ-Spectroscopy Experiments

CREMA @ PSI

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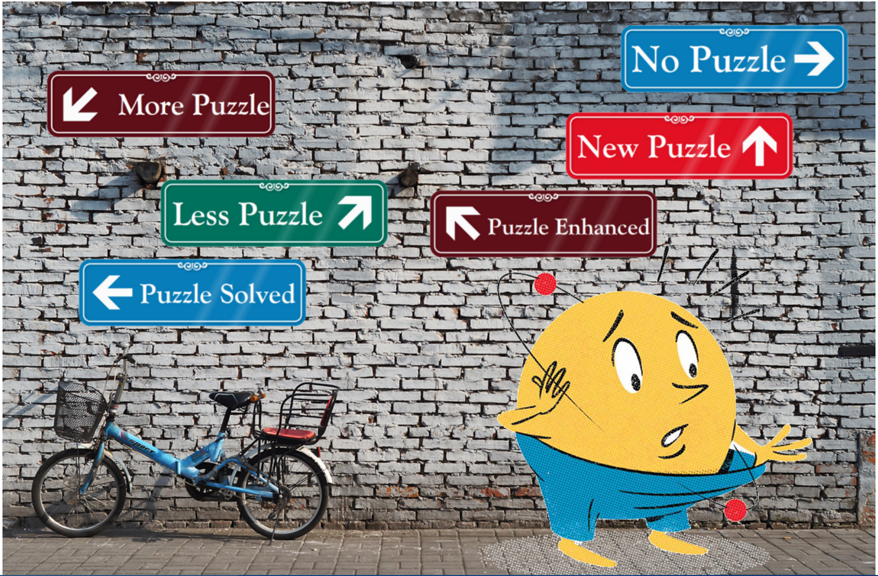
FAMU @ RIKEN-RAL / J-PARC

- HFS in μH in two new methods (planned)

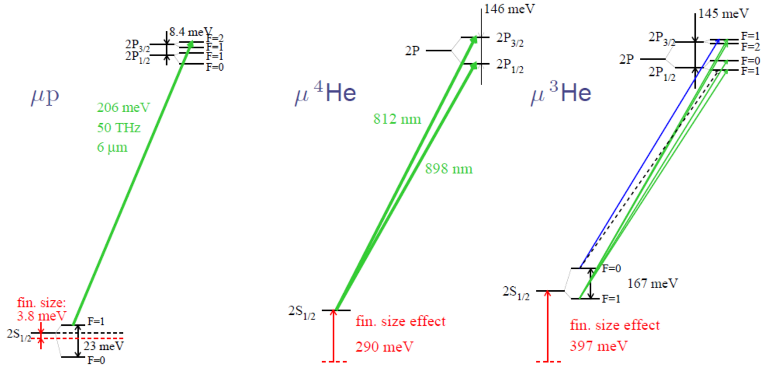
Precise R_c/R_m from μA LS/HFS

Require accurate theoretical inputs from QED, hadron and nuclear physics

The proton radius puzzle



Lamb shift, charge radius & nuclear corrections



R. Pohl (for CREMA), presentation at ECT*, Trento, Italy (2012)

Extract $R_c \equiv \sqrt{\langle r^2 \rangle}$ from Lamb shift measurement

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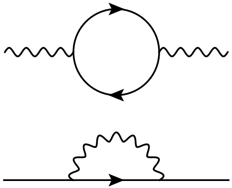
- QED corrections:
  - vacuum polarization
  - lepton self energy
  - relativistic recoil effects



- Theory of μ-p, D, ^{3,4}He$^+$ reexamined

  Martynenko *et al.* **'07**, Borie **'12**, Krutov *et al.* **'15**

  Karshenboim *et al.* **'15**, Krauth *et al.* **'15** ...

Lamb shift, charge radius & nuclear corrections

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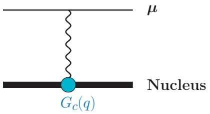
$$\Delta E_{2S-2P} = \delta_{QED} + \delta_{size}(R_c) + \delta_{\mathrm{TPE}}$$

- Nuclear structure corrections
  (One-Photon Exchange)
  - finite-size effect: $\delta_{size} = \frac{m_r^3}{12}(Z\alpha)^4 \times R_c^2$



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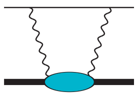
$\Rightarrow$ related to nuclear response functions:

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

$\Rightarrow$ can be extracted from data (very imprecise)

$\Rightarrow$ or calculated (continuum few-body problem)



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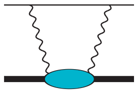
  - **Very small — is it important?**



The accuracy of R_c is limited by δ_{TPE}

Example — μD:

$$\begin{aligned}
\Delta E^{\text{LS}}_{\text{QED}} &= 228.77356(75)\,\text{meV} \\
\Delta E^{\text{LS}}_{\text{rad.-dep.}} &= -6.11025(28)\,r_{\text{d}}^2\,\text{meV/fm}^2 + 0.00300(60)\,\text{meV} \\
\Delta E^{\text{LS}}_{\text{TPE}} &= 1.70910(2000)\,\text{meV}
\end{aligned}$$

J. Krauth *et al.* (CREMA), **Ann. Phys. (2016)**; R. Pohl *et al.* (CREMA), **Science 2016**

Status — prior to $\mu^{3,4}$He^{+} measurements:

- Uncertainty in δ_{pol}: $\sim 20\%$
- Required: $\sim 5\%$
  (to determine R_c with $\sim 10^{-4}$ accuracy)

Dynamical (polarization) contributions to δ_{TPE}

$$\delta_{TPE} = \sum_a I_a = \sum_a \int d\omega \, S_a(\omega) \, g_a(\omega)$$

- The leading polarization contribution relates to the dipole response

$$I_{D1}^{(0)} \propto \int_{\omega_{\rm th}}^{\infty} d\omega \, S_{D_1}(\omega) \, \omega^{-1/2}$$

- $S_{D_1}(\omega) \Longrightarrow$ electric dipole response function $[\; \hat{D}_1 = R \, Y_1(\hat{R}) \;]$

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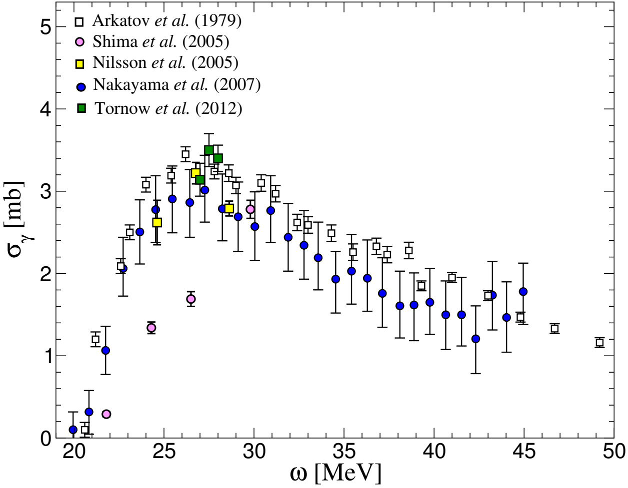
Extract δ_{TPE} from data: ^{4}He Photoabsorption

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



Summary of results: $2 \leqslant A \leqslant 4$

System	Our Ref.	Unc.	Experimental Status
$\mu\,^2$H	Phys. Lett. B '14	1% → 1.3%	published *Science* '16
$\mu\,^4\text{He}^+$	Phys. Rev. Lett. '13	20% → 6%	measured, unpublished
$\mu\,^3\text{He}^+$	Phys. Lett. B '16	20% → 4%	measured, unpublished
$\mu\,^3$H	Phys. Lett. B '16	4%	measurable?

- Our results agree with other values and are more accurate

⇒ Unc. comparable with $\sim 5\%$ experimental needs
⇒ Will improve precision of R_c from Lamb shifts
⇒ May help shed light on the "proton (deuteron) radius puzzle"

The LIT method (Lorentz Integral Transform)

Calculating $S_O(\omega) = \sum\!\!\!\!\!\!\int_f |\langle f|\hat{O}|i\rangle|^2 \delta(\omega_f - \omega)$ **using LIT**

V.D. Efros et al., PLB'94; JPG'07

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(and only the trivial solution to the homogeneous Eq.)

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$\Rightarrow$ Can be solved using **any bound-state method**

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$$S_N(\omega) = \sum_n^N c_n \phi_n(\alpha) \quad \Longrightarrow \quad ||\mathcal{L}_{\text{calc}}(\sigma) - \mathcal{L}_N(\sigma)|| < \epsilon$$

Efros et al., JPG'07; Barnea FBS'10; Orlandini et al., FBS'17

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- This method is not sensitive to a specific energy-range of $\mathcal{L}_{\rm calc}(\sigma) - \mathcal{L}_N(\sigma)$
- Small σ_i is needed to resolve fine details of $S(\omega) \implies$ Harder to converge $\mathcal{L}_{\rm calc}(\sigma)$
- Large σ_i captures better the tail of $S(\omega)$ ...

Efros et al., JPG'07; Barnea FBS'10; Orlandini et al., FBS'17

The LIT method (Lorentz Integral Transform)

Using few-body bound-state methods, the LIT was applied to electroweak reactions of $2 \leqslant A \leqslant 7$, such as: (Efros et al., JPG'07; Leidemann & Orlandini PPNP'13; Bacca & Pastore JPG'14)

1. Photoabsorption cross sections
2. Photon scattering
3. Electron scattering (longitudinal and transverse response)
4. Neutrino breakup of light nuclei in supernovae

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Including exclusive reactions

(LaPiana & Leidemann NPA'00; Quaglioni et al., PRC'04,'05; Andreasi et al., EPJA'06; NND et al., FBS'14)

which require solving the exclusive LIT equations:

$$(H - \sigma^*)|\tilde{\psi}_f\rangle = \hat{V}_f|\phi_f\rangle$$

Exclusive LIT and related applications

The solution of the exclusive LIT equation:

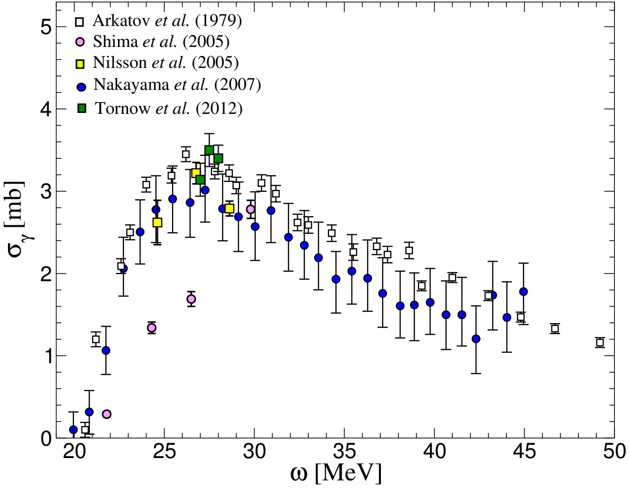
$$(H - \sigma^*)|\tilde{\psi}_f\rangle = \hat{V}_f|\phi_f\rangle$$

can also be used for:

1. Radiative capture (by exchanging $i \leftrightarrow f$ in exclusive photodisintegration)
2. Semi-inclusive $(e, e'N)$ using the "spectral function approximation " (demonstrated by Efros et al., PRC'98)
3. Astrophysical S-factors (demonstrated by S. Deflorian et al., FBS'17)
4. Hadron scattering (suggested by V.D. Efros, PAN'99, PIC'17)
5. Glauber approximation (suggested by V.D. Efros et al., JPG'07)

LIT calculations: ^{4}He Photoabsorption

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



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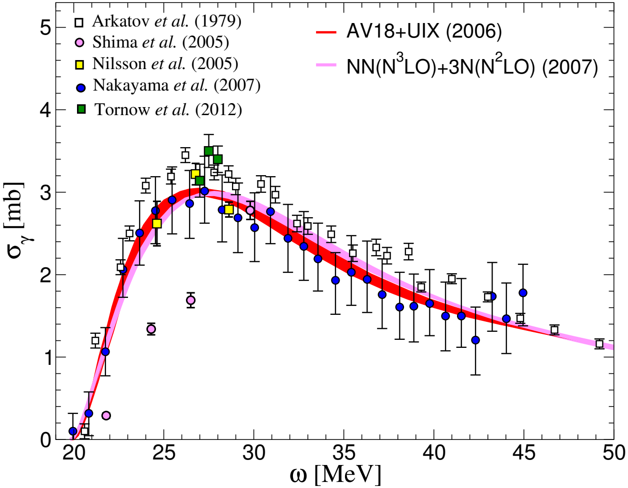
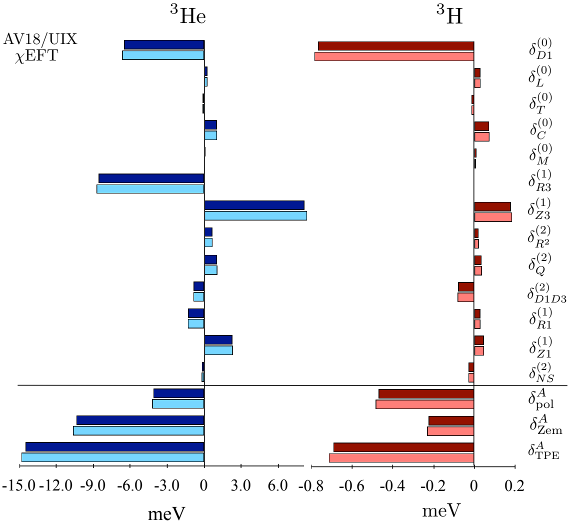


Gazit et al., PRL'06

Quaglioni & Navrátil PLB'07

The work is not completed yet ...

Results: $A = 3$



NND *et al.*, **Phys. Lett. B (2016)**

LSR: Lanczos sum rule method

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2. Checking analytic or assumed relations
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Problems:

1. (May) need to know $S(\omega)$ with good resolution over wide range of energies
2. Need to extrapolate $S(\omega)g(\omega)$ to $\omega \to \infty$, difficulty depends on $g(\omega)$ (and $\hat{O}$)

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A model-space of size M is used to calculate the LIT of $S\left(\omega\right)$

$$\mathcal{L}(\sigma) = \frac{\sigma_i}{\pi} \int d\omega \frac{S(\omega)}{(\omega - \sigma_r)^2 + \sigma_i^2}\ , \ \sigma_i \equiv Im(\sigma) > 0$$

$$\mathcal{L}_M(\sigma) = \frac{\sigma_i}{\pi} \sum_{\mu}^{M} \frac{|\langle \mu | \hat{O} | i \rangle|^2}{(\omega_\mu - \sigma_r)^2 + \sigma_i^2}$$

$$\Rightarrow \quad |\mathcal{L}(\sigma) - \mathcal{L}_M(\sigma)| \leq \varepsilon_M$$

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- smaller $\sigma_i \Rightarrow$ better resolution, slower convergence

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$$\begin{aligned} I &= \int d\omega \int d\sigma_r\, S(\omega)\, \frac{\sigma_i}{\pi}\frac{h(\sigma)}{(\omega-\sigma_r)^2+\sigma_i^2} \\ &= \int d\sigma_r\, \mathcal{L}(\sigma) h(\sigma) \end{aligned}$$

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$$= \int d\sigma_r\, \mathcal{L}(\sigma) h(\sigma)$$

$$|I - I_M| \leq \varepsilon_M \int d\sigma_r\, |h(\sigma)|$$

Formally :

$$h(\sigma) = \frac{1}{2\pi}\int dk\, e^{\sigma_i |k|} \tilde{\boldsymbol{g}}(\boldsymbol{k}) e^{-ik\sigma_r}$$

Efros, **Phys. At. Nucl. (1999)**

LSR: Lanczos sum rule method

The applicability depends on the form of $g(\omega)$. For example:

$$g(\omega) = \frac{\beta}{\pi}\frac{1}{(\omega-\omega_0)^2+\beta^2} \xrightarrow[\beta\to 0]{} \delta(\omega-\omega_0),$$

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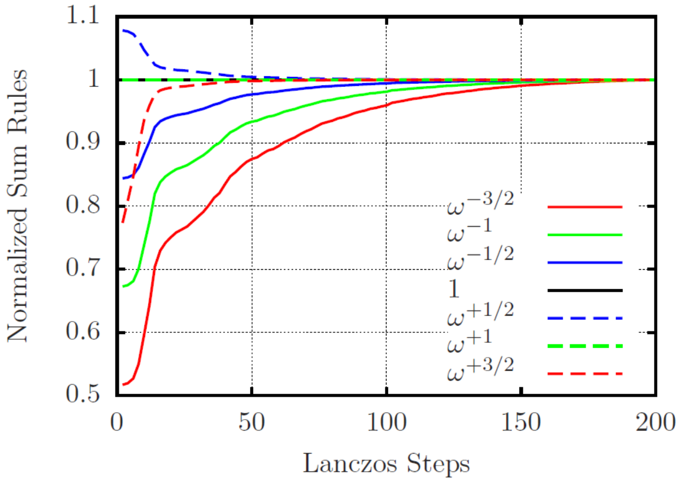
- The LSR method uses Lanczos to obtain I_M (NND et al., PRC'14)
  1. without solving $S(\omega)$
  2. efficiently and accurately
  3. with rapid convergence

  (generalizes similar methods as in:
  Haxton et al., PRC'05; Gazit et al., PRC'06; Stetcu et al., PLB'08, PRC'09)

- For example, for the dipole response, calculated with $M \sim 10^5$, we get



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

Outline

- Summary — The LIT & LSR Methods can be used with any bound-state method to obtain dynamic observables (e.g., in the nuclear continuum)
- Application — Precise nuclear calculations are crucial in many high-profile efforts, e.g. ν-less $\beta\beta$ decay; searches for EDMs; etc.
  Particularly, nuclear corrections are the bottleneck in μA spectroscopy.
- Results — For A =3,4 we reduced the uncertainties in these corrections from $\sim 20\%$ to 4–6% as required for ongoing experiments.
- Methods — We use the **LSR method** to calculate the relevant sum-rules.
  We proved its applicability using the LIT method.
  The LIT method has been successfully applied to calculate many EW-induced reactions. Some applications have yet to be demonstrated.
- Motivation — LIT & LSR were applied with Coupled-Cluster for calculations in:
  ^{4}He, ^{16,22}O, ^{40,48}Ca... (G. Hagen et al., PRC'14; PRC'16; Nature'16;...)

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Canada's national laboratory
for particle and nuclear physics
and accelerator-based science

Thank you!
Merci!

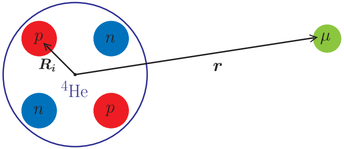
BACK UP

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

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

- 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

Systematic contributions to nuclear polarization

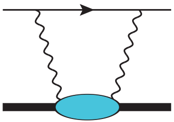
δ_{NR} **Non-Relativistic** limit

$\delta_L + \delta_T$ **L**ongitudinal and **T**ransverse **relativistic** corrections

δ_C **Coulomb** distortions

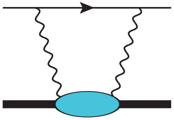
δ_{NS} Corrections from **finite Nucleon Size**

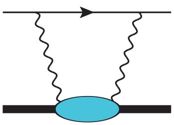
- **Neglect Coulomb interactions in the intermediate state**



Non-relativistic limit

- **Neglect Coulomb interactions in the intermediate state**
- **Expand muon matrix element in powers of**
  $\eta \equiv \sqrt{2m_r\omega}|\boldsymbol{R} - \boldsymbol{R}'|$





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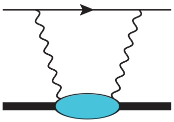
  - $|\boldsymbol{R} - \boldsymbol{R}'| \implies$ "virtual" distance the proton travels in 2γ exchange
  - uncertainty principal $|\boldsymbol{R} - \boldsymbol{R}'| \sim 1/\sqrt{2m_N\omega}$
  - $\eta \sim \sqrt{\frac{m_r}{m_N}} \approx 0.3$

Non-relativistic limit



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

$$\delta_{NR} = \delta_{NR}^{(0)} + \delta_{NR}^{(1)} + \delta_{NR}^{(2)} \quad \sim \quad \eta^2 \quad + \quad \eta^3 \quad + \quad \eta^4$$

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

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

- $\delta_{NR}^{(0)} \propto \eta^2$

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

- $S_{D_1}(\omega) \Longrightarrow$ electric dipole response function [$\hat{D}_1 = RY_1(\hat{R})$]
- $\delta_{D1}^{(0)}$ is the dominant contribution to $\delta_{\rm pol}$
- $\Longrightarrow$ Rel. and Coulomb corrections added at this order

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

- $\delta^{(1)}_{NR} \propto \eta^3$

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

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

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

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

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

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

- $\delta_{NR}^{(1)} \propto \eta^3$

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

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$$\delta_{Z3}^{(1)} = \frac{m_r^4}{24}(Z\alpha)^5 \iint d\boldsymbol{R}d\boldsymbol{R}'|\boldsymbol{R}-\boldsymbol{R}'|^3 \rho_0(\boldsymbol{R})\rho_0(\boldsymbol{R}') = \frac{m_r^4}{24}(Z\alpha)^5 \langle \boldsymbol{r^3}\rangle_{\boldsymbol{(2)}}$$

- $\delta_{R3pp}^{(1)} \Rightarrow$ 3rd-order proton-proton correlation
- $\delta_{Z3}^{(1)} \Longrightarrow$ 3rd Zemach moment
  cancels *elastic* Zemach moment of finite-size corrections
  c.f. Pachucki '11 & Friar '13 (μD) $\Longrightarrow \boldsymbol{\delta_{\mathrm{TPE}}} \equiv |\delta_{\mathrm{Zem}} + \delta_{\mathrm{pol}}|$

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

- $\delta_{NR}^{(2)} \propto \eta^4$

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

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

Error type	$\mu\,^3$He$^+$ $\delta^A_{\rm pol}$	$\delta^A_{\rm Zem}$	$\delta^A_{\rm TPE}$	$\mu\,^3$H $\delta^A_{\rm pol}$	$\delta^A_{\rm Zem}$	$\delta^A_{\rm TPE}$
Numerical	0.4	0.1	0.1	0.1	0.0	0.1
Nuclear model	1.5	1.8	1.7	2.2	2.3	2.2
ISB	2.0	0.2	0.5	0.9	0.2	0.6
Nucleon size	1.6	1.5	0.6	0.6	1.3	0.0
Relativistic	0.6	-	1.5	1.4	-	0.3
Coulomb	1.2	-	0.3	0.3	-	0.2
Multipole expansion	2.0	-	0.6	2.0	-	1.4
Higher $Z\alpha$	1.5	-	0.4	0.7	-	0.5
Magnetic MEC	0.4	-	0.1	0.3	-	0.2
Total	4.1%	2.3%	2.5%	3.6%	2.7%	2.7%