TRIUMF

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

Applicability of Lanczos sum rules

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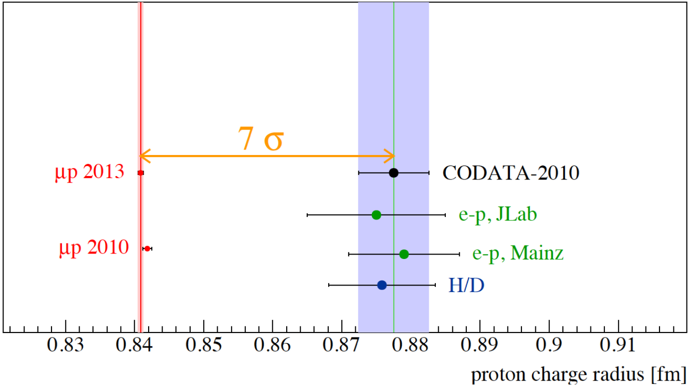
[6]Louisiana State Univ.

TRIUMF, Vancouver — Feb. 28 2018


AND NOW FOR SOMETHING COMPLETELY
DIFFERENT
memegenerator.net

How big is the proton?



R. Pohl & J. Krauth @ CREMA

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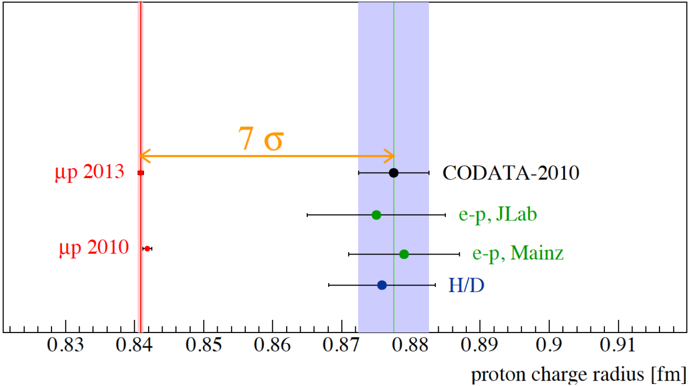
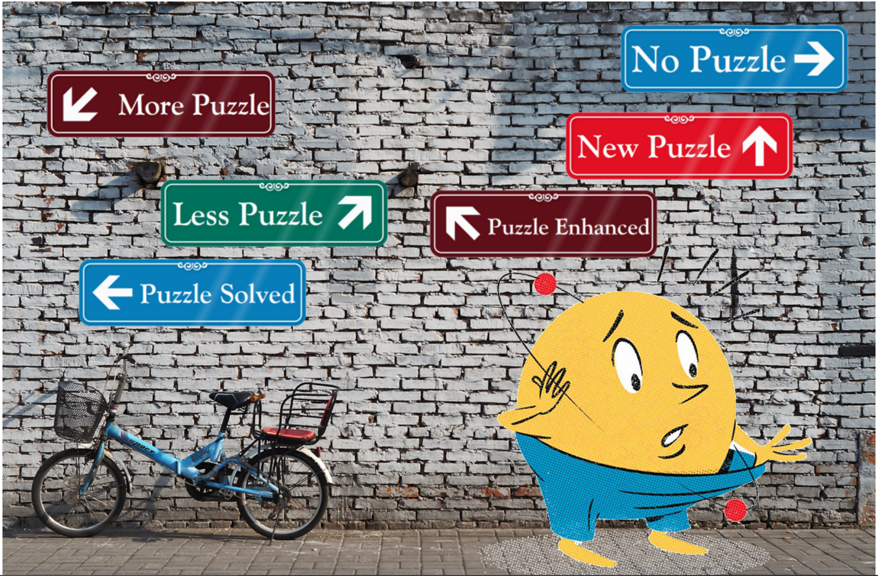


New H/D results:

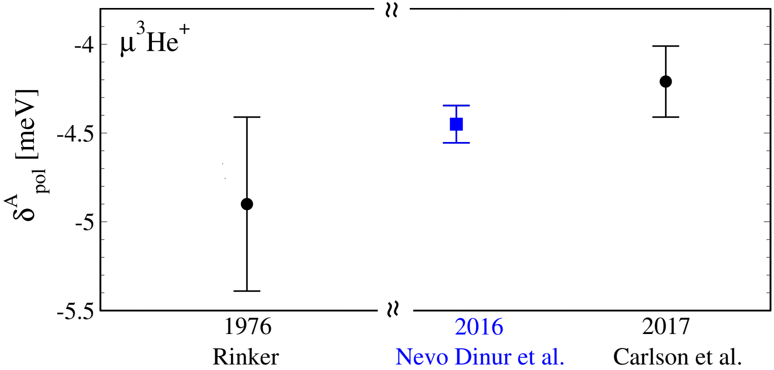
$r_p = 0.8335(95)$ fm (Garching, 2S-4P)

$r_p = 0.877(13)$ fm (Paris, 1S3S)

The proton radius puzzle



Summary of our results



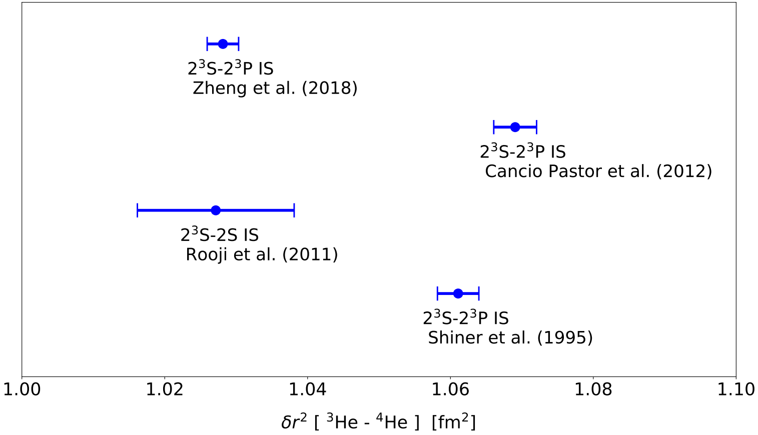
Chen Ji, NND *et al.*, **in prep.**

System	Our Ref.	Unc.	Experimental Status
$\mu\,^2$H	Phys. Lett. B '14, '18	1% $\rightarrow$ 1.3%	published *Science* '16
$\mu\,^4$He$^+$	Phys. Rev. Lett. '13	20% $\rightarrow$ 6%	measured, unpublished
$\mu\,^3$He$^+$	Phys. Lett. B '16	20% $\rightarrow$ 4%	measured, unpublished
$\mu\,^3$H	Phys. Lett. B '16	4%	measurable?

- Our results agree with other values and are more accurate

$\Rightarrow$ Unc. comparable with $\sim \mathbf{5\%}$ experimental needs
$\Rightarrow$ Will improve precision of $\boldsymbol{R_c}$ from Lamb shifts
$\Rightarrow$ May help shed light on the "proton (deuteron) radius puzzle"
$\Rightarrow$ ... and on the ^{3,4}He "isotope-shift puzzle"

He isotope shift puzzle



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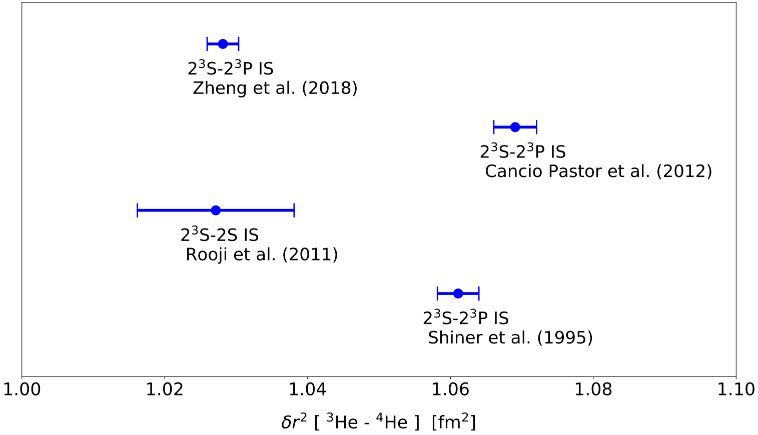
He isotope shift puzzle



μHe precision: ~ 0.03 fm^2

PHYSICAL REVIEW A **94**, 062505 (2016)

Lamb shift in muonic ions of lithium, beryllium, and boron

A. A. Krutov, A. P. Martynenko, F. A. Martynenko, and O. S. Sukhorukova
Samara University, 443086, Moskovskoe shosse 34, Samara, Russia
(Received 1 October 2016; published 15 December 2016)

We present a precise calculation of the Lamb shift $(2P_{1/2} - 2S_{1/2})$ in muonic ions $(\mu_3^6\mathrm{Li})^{2+}$, $(\mu_3^7\mathrm{Li})^{2+}$, $(\mu_4^9\mathrm{Be})^{3+}$, $(\mu_4^{10}\mathrm{Be})^{3+}$, $(\mu_5^{10}\mathrm{B})^{4+}$, $(\mu_5^{11}\mathrm{B})^{4+}$. The contributions of orders $\alpha^3 \div \alpha^6$ to the vacuum polarization, nuclear structure and recoil, and relativistic effects are taken into account. Our numerical results are consistent with previous calculations and improved by additional corrections. The obtained results can be used for the comparison with future experimental data, and extraction more accurate values of nuclear charge radii.

TABLE I. Lamb shift $(2P_{1/2} - 2S_{1/2})$ in muonic ions $(\mu_3^7\mathrm{Li})^{2+}$ and $(\mu_3^6\mathrm{Li})^{2+}$. In parentheses are given the results obtained by other authors, with some references to their works, which discuss the calculation of corrections of this type.

	Contribution to the splitting	$(\mu_3^7\mathrm{Li})^{2+}$ (meV)	$(\mu_3^6\mathrm{Li})^{2+}$ (meV)
1	VP contribution of order $\alpha(Z\alpha)^2$ in 1γ interaction	4682.38 (4682.4 [7])	4664.95 (4665.0 [7])
2	Two-loop VP contribution of order $\alpha^2(Z\alpha)^2$ in 1γ interaction	32.54 (32.44 [7])	32.41(32.27 [7])
3	VP and MVP contribution in one-photon interaction	0.01	0.01
	⋮		
30	HVP contribution	1.17 [7,58–60]	1.16 [7,58–60]
31	Nuclear polarizability	21 ± 4 [7]	15 ± 4 [7]
32	Total contribution	1531.78	1161.85

Dynamical (polarization) contributions to δ_{TPE}

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

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- The leading polarization contribution relates to the dipole response

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

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

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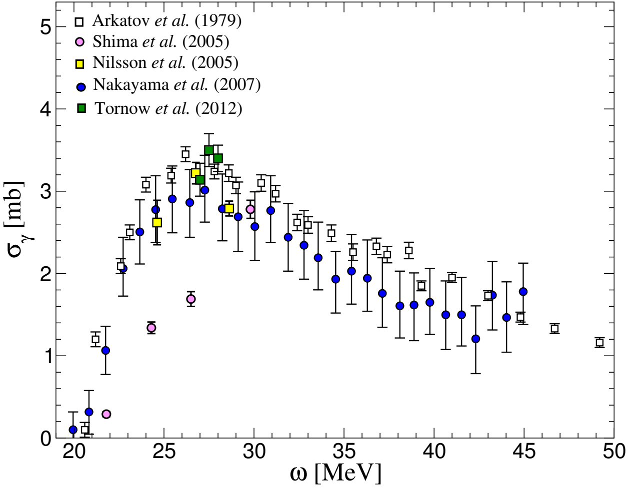
$\Rightarrow$ can be extracted from data (very imprecise)
$\Rightarrow$ or calculated (continuum few-body problem)

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

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



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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Schrödinger-like equation with a **local** source term
(and only the trivial solution to the homogeneous Eq.)

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

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

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

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2. Invert $\mathcal{L}_{\text{calc}}(\sigma) = \int d\omega \frac{S(\omega)}{(\omega-\sigma_r)^2+\sigma_i^2}$ using the common ansatz

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

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 $S(\omega) \Longrightarrow$ Harder to converge $\mathcal{L}_{\rm calc}(\sigma)$
- Larger σ_i improves the tail of $S(\omega)$ ...

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

The LIT method (Lorentz Integral Transform)

The LIT method was applied to electroweak reactions, where the LIT equations were solved with:

- HH: Hyperspherical Harmonics (Jacobi coor., $A \leqslant 4$)
- EIHH (Jacobi coor., $A \leqslant 7$)
- NCSM (Jacobi coor., $A = 4$)

(Efros et al., JPG'07; Leidemann & Orlandini PPNP'13; Bacca & Pastore JPG'14)

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(Efros et al., JPG'07; Leidemann & Orlandini PPNP'13; Bacca & Pastore JPG'14)

It was recently used extensively also with the coupled-cluster method
(Bacca et al., PRL'13, ...)

Exclusive LIT and related applications

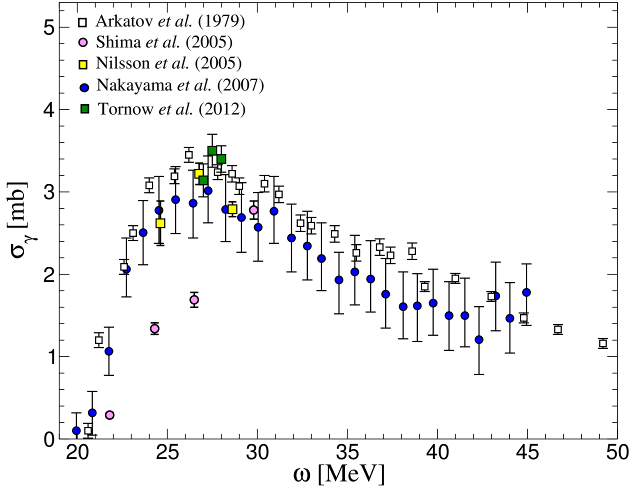
LIT can also be used for exclusive reactions.
The exclusive LIT equation is:

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

This allows many other applications:

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)

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



LIT calculations: ^{4}He Photoabsorption

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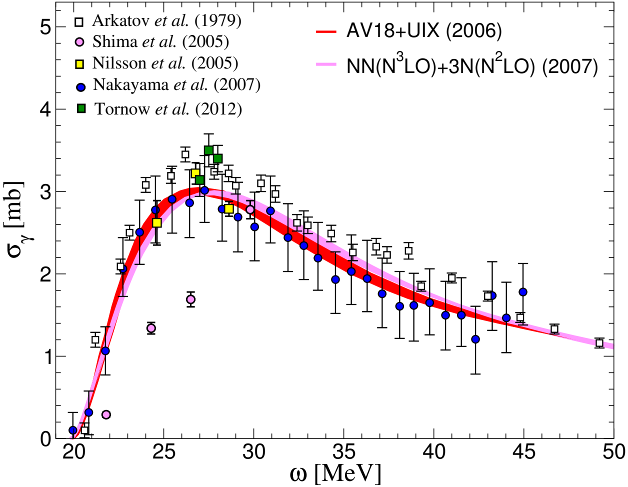


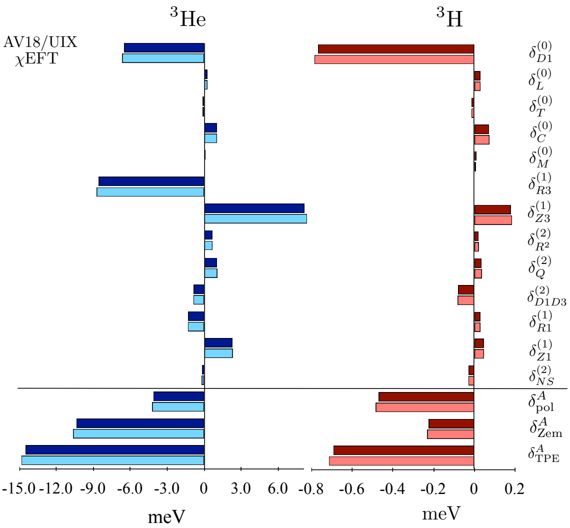
Gazit et al., PRL'06

Quaglioni & Navrátil PLB'07

Calculate sum rules

The work is not completed yet ...

Calculate many sum rules (and channels)



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

LSR: Lanczos sum rule method

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

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Problems:

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

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Sum rules are of general interest

1. Comparison with experiments
2. Checking analytic or assumed relations
3. Observables of interest ($\alpha_D \leftrightarrow R_{\rm ch} \leftrightarrow R_n - R_p \leftrightarrow L$ (SymmetryEnergy))

LSR: Lanczos sum rule method

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

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

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

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

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

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

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

LSR: Lanczos sum rule method

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$$g(\omega) = \frac{\sigma_i}{\pi}\int d\sigma_r \frac{\boldsymbol{h(\sigma)}}{(\omega-\sigma_r)^2+\sigma_i^2}$$

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\begin{aligned}
g\left(\omega\right) &= \frac{\sigma_i}{\pi}\int d\sigma_r \frac{\boldsymbol{h(\sigma)}}{\left(\omega-\sigma_r\right)^2+\sigma_i^2} \\
I &= \int d\omega \int d\sigma_r\, S\left(\omega\right)\frac{\sigma_i}{\pi}\frac{h(\sigma)}{\left(\omega-\sigma_r\right)^2+\sigma_i^2} \\
&= \int d\sigma_r\, \mathcal{L}(\sigma)h(\sigma) \\
\left|I-I_M\right| &\leq \varepsilon_M \int d\sigma_r \left|h(\sigma)\right|
\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)| \\
\text{Formally}: & \\
h(\sigma) &= \frac{1}{2\pi}\int dk\; e^{\sigma_i|k|}\tilde{\boldsymbol{g}}(\boldsymbol{k})e^{-ik\sigma_r}
\end{aligned}
$$

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

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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$\Rightarrow$ If $g(\omega)$ has narrow features, σ_i needs to be small $\Rightarrow$ harder to converge

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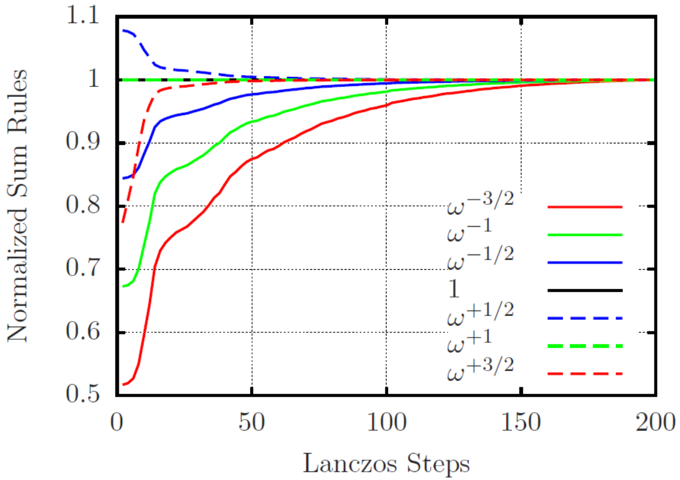
$\Rightarrow$ If $g(\omega)$ has narrow features, σ_i needs to be small $\Rightarrow$ harder to converge

- 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

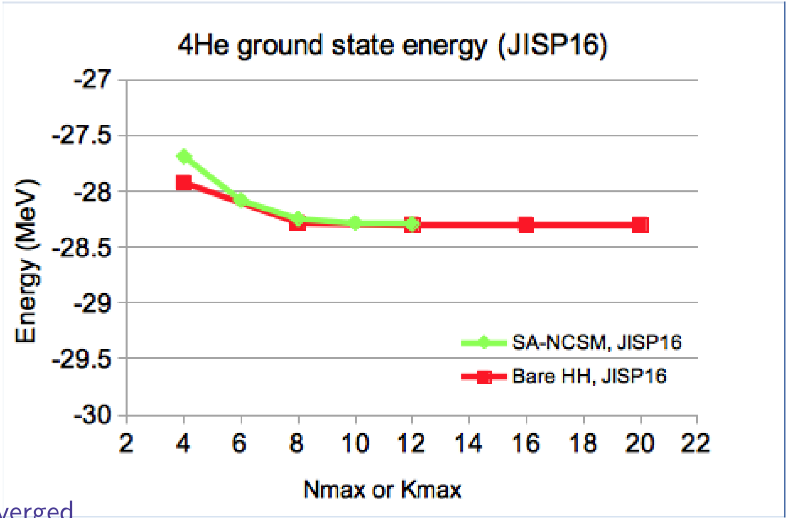


NND, Barnea, Ji, and Bacca, PRC (2014)

SA-NCSM-HH-LSR Benchmark

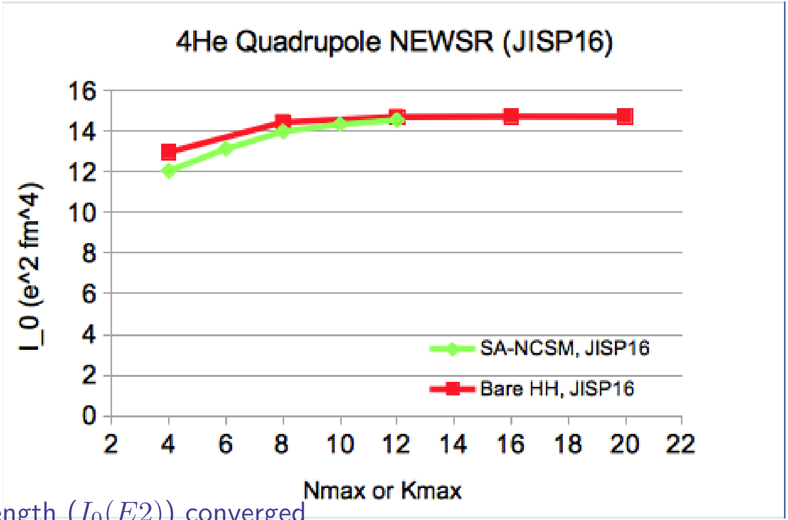
- ^{4}He: $J^\pi = 0^+$
- N3LO, JISP16
- Quadrupole (E2): IS+IV
  $\rightarrow$ Dipole (E1) & Isoscalar Monopole (E0)

Preliminary Results: ^{4}He



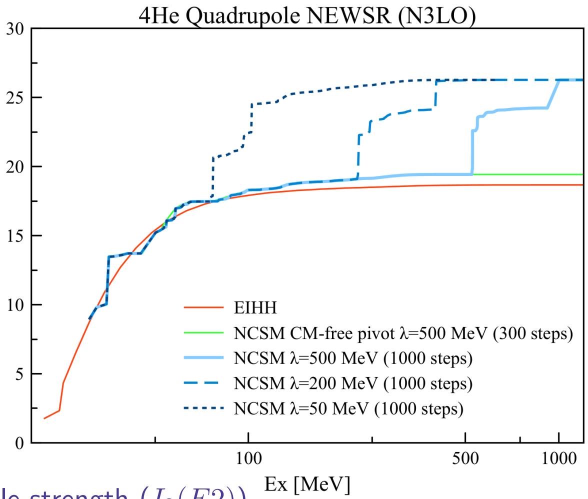
G.S. energy (E_i) converged

Preliminary Results: ^{4}He



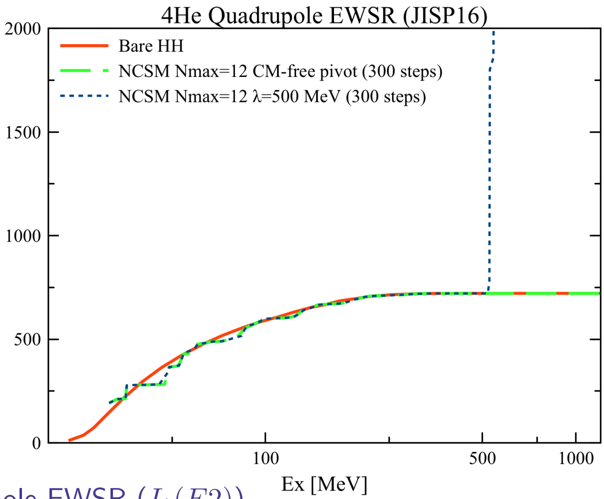
Total quadrupole strength $(I_0(E2))$ converged

Preliminary Results: ^{4}He

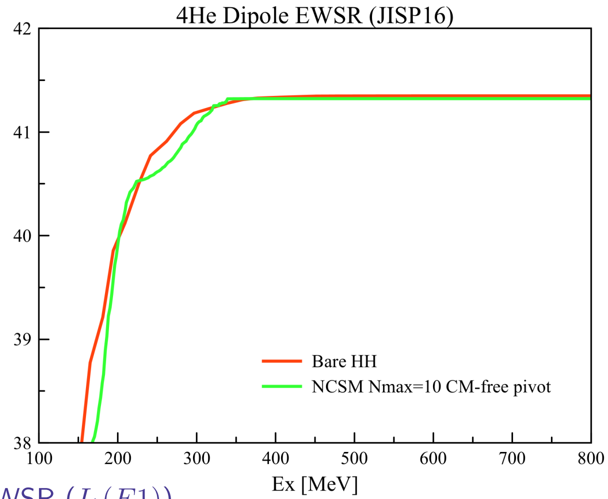


Removal of CM from quadrupole strength ($I_0(E2)$)

Preliminary Results: ^{4}He

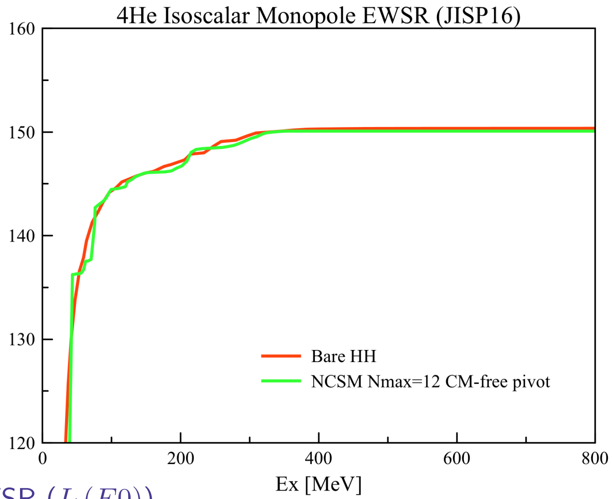


Removal of CM from quadrupole EWSR ($I_1(E2)$)



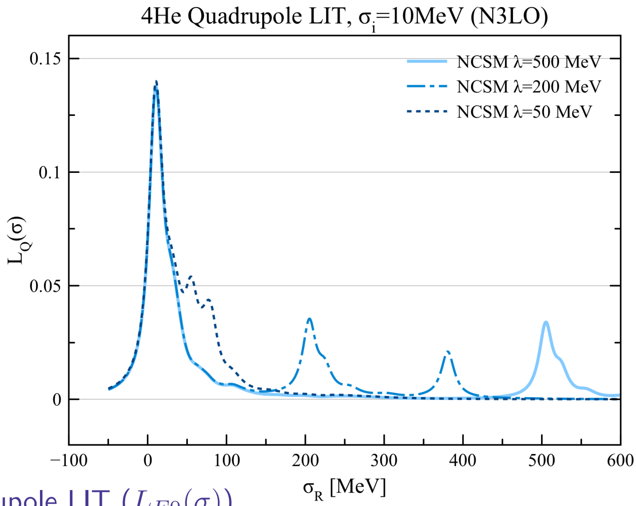
Removal of CM from dipole EWSR ($I_1(E1)$)

Preliminary Results: ^{4}He



Removal of CM from ISM EWSR ($I_1(E0)$)

Preliminary Results: ^{4}He



Removal of CM from quadrupole LIT ($L_{E0}(\sigma)$)

Summary

- Precise nuclear calculations are crucial in many high-profile efforts, e.g. ν-less $\beta\beta$ decay; searches for EDMs; etc. Particularly, they are the bottleneck in μA spectroscopy.
- The LIT & LSR methods are crucial for *ab-initio* calculations needed for such efforts.
- They can be used with any bound-state method to obtain dynamical nuclear observables.
- However, the applicability is not guaranteed.
- They were used successfully with HH and NCSM in intrinsic Jacobi coordinates, and with Coupled-Cluster, for calculations of ^{3,4}He, ^{16,22}O, ^{40,48}Ca...
  Many applications have yet to be exhausted (Sonia and Gaute's talks).
- We used the LSR method to calculate the corrections for μA spectroscopy,
  and proved its applicability using LIT.
- Here we use the LIT & LSR with (SA)NCSM in the lab frame,
  demonstrate how the CM can be easily removed,
  and benchmark with HH.
- The use of SA-NCSM will allow high-N_{max} calculations of dynamical nuclear observables in open-shell nuclei, including for μA where $6 \leqslant A$.

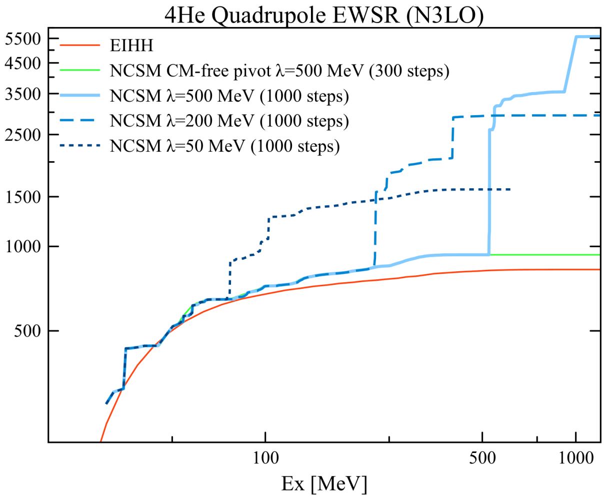
TRIUMF

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

Thank you!
Merci!

BACK UP

Preliminary Results: ^{4}He

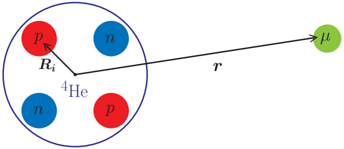


Removal of CM from quadrupole EWSR ($I_1(E2)$)

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

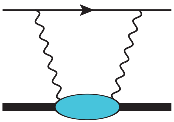
δ_{NR} **Non-Relativistic** limit

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

δ_C **Coulomb** distortions

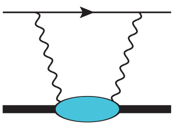
δ_{NS} Corrections from **finite Nucleon Size**

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

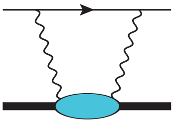


Non-relativistic limit

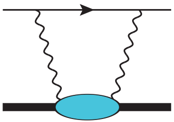
- **Neglect Coulomb interactions in the intermediate state**
- **Expand muon matrix element in powers of**
  $\eta \equiv \sqrt{2m_r\omega}|\boldsymbol{R} - \boldsymbol{R}'|$



Non-relativistic limit



- **Neglect Coulomb interactions in the intermediate state**
- **Expand muon matrix element in powers of** $\eta \equiv \sqrt{2m_r\omega}|\boldsymbol{R} - \boldsymbol{R}'|$
  - $|\boldsymbol{R} - \boldsymbol{R}'| \implies$ “virtual” distance the proton travels in 2γ exchange
  - uncertainty principal $|\boldsymbol{R} - \boldsymbol{R}'| \sim 1/\sqrt{2m_N\omega}$
  - $\eta \sim \sqrt{\frac{m_r}{m_N}} \approx 0.3$



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

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

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

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

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

- $S_{D_1}(\omega) \Longrightarrow$ 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

NR limit at NLO: $\boldsymbol{\delta^{(1)}_{NR}}$

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

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

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

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

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

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

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

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

NR limit at N^{2}LO: $\boldsymbol{\delta^{(2)}_{NR}}$

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

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

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

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

Uncertainty estimates

Error type	$\mu\,^3\mathrm{He}^+$ δ^A_{pol}	δ^A_{Zem}	δ^A_{TPE}	$\mu\,^3\mathrm{H}$ δ^A_{pol}	δ^A_{Zem}	δ^A_{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%