Subtraction contribution to the muonic-hydrogen Lamb shift from lattice QCD

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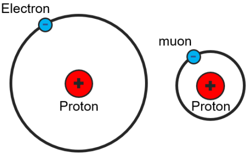
NREC 2024 @ Stony Brook University

Proton charge radius from atomic measurement

- μH Lamb shift: most precise way to measure proton charge radius



$$m_\mu \approx 200 m_e \quad \rightarrow \quad R_{\mu\mathrm{H}} \approx \frac{1}{200} R_\mathrm{H}$$

$\Rightarrow$ much more sensitive to proton structure (charge radius).

- Experiments done in 2010 and 2013, by CREMA at PSI

$$\sqrt{\langle r_p^2 \rangle} = 0.84087(26)_\mathrm{exp}(29)_\mathrm{theo}\ \mathrm{fm}$$

10 times more precise than hydrogen / scattering result.

(Nature 466 (2010) 213, Science 339 (2013) 417)

- Proton structure effects beyond charge radius also enhanced

$\Rightarrow$ Major source of theoretical uncertainty.

Muonic-hydrogen Lamb shift

- Theory for μH Lamb shift (Science 339 (2013) 417. Ann. of Phy. 331 (2013), 127)

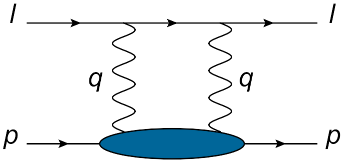
Exp. value Theory

$$\Delta E_{\text{2S-2P}} = \Delta E_{\text{structure indep.}} + \Delta E_{\text{proton size}} + \Delta E_{\text{TPE}}$$

$$202370.6(2.3) = 206033.6(1.5) - 5227.5(1.0)\langle r_p^2 \rangle + 33.2(2.0)$$

(Units in μeV and fm)

- Two-photon exchange (TPE): largest theoretical uncertainty



- Recent updates: (K. Pachucki et al., Rev. Mod. Phys. 2024, talk on Monday)

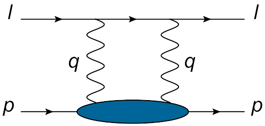
$$\Delta E_{\text{2S-2P}} = 206034.4(0.3) - 5225.9\langle r_p^2 \rangle + 28.9(2.5)$$

and exp. value will be improved by at least 5 times by PSI

- TPE will then dominate the total uncertainty

Two-photon Exchange

TPE correction:



- Bottom part: Compton tensor ($\nu = p \cdot q/M$)

$$T^{\mu\nu} = \frac{i}{8\pi M}\int \mathrm{d}^4 x e^{iqx} \langle p|\mathcal{T}[j^\mu(x) j^\nu(0)]|p\rangle$$

$$= \left(-g^{\mu\nu} + \frac{q^\mu q^\nu}{q^2}\right) T_1(\nu, Q^2) + \left(p^\mu - \frac{p\cdot q}{q^2} q^\mu\right)\left(p^\nu - \frac{p \cdot q}{q^2} q^\nu\right)\frac{T_2(\nu, Q^2)}{M^2}$$

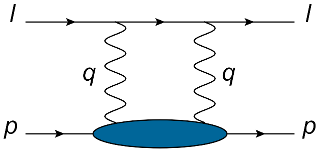
- TPE energy shift

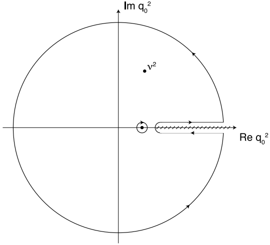
$$\Delta E = \frac{8\alpha^2 m}{\pi}|\phi_n(0)|^2 \int \mathrm{d}^4 Q \frac{(Q^2 + 2Q_0^2)\, T_1(iQ_0, Q^2) - (Q^2 - Q_0^2)\, T_2(iQ_0, Q^2)}{Q^4(Q^4 + 4m^2 Q_0^2)}$$

- This integral is IR divergent due to an exchange of soft photons

$\Rightarrow$ terms need to be subtracted: $\underbrace{\text{point-like proton + charge radius term}}_{\text{analytically known}}$

- After subtraction ΔE is IR finite, also avoid double-counting





- Dispersion relation: turn scattering data into amplitudes

$$T_{1,2}(q_0, Q^2) = \int_{\nu_{\text{el}}^2}^{\infty} \frac{\mathrm{d}\nu^2}{\pi} \frac{\text{Im } T_{1,2}(\nu, Q^2)}{\nu^2 - q_0^2}$$

requires sufficiently falling behavior at high energies to ensure convergence.

- Unfortunately for T_1 we need once-subtracted DR

$$T_1(q_0, Q^2) - T_1(0, Q^2) = \int_{\nu_{\text{el}}^2}^{\infty} \frac{\mathrm{d}\nu^2}{\pi} \left[\frac{1}{\nu^2 - q_0^2} - \frac{1}{\nu^2} \right] \text{Im } T_1(\nu, Q^2)$$

"Subtraction function" can not be fully extracted from exp. data

Subtraction function

- How well do we know about the subtraction function?

Small Q^2: Low-energy expansion, polarizabilities

$$\lim_{\nu, Q^2 \to 0} T_1(\nu, Q^2) = T_1^{\text{Born}}(\nu, Q^2) + \frac{\nu^2}{e^2}(\alpha_E + \beta_M) + \frac{Q^2}{e^2}\beta_M + \cdots$$

Large Q^2: operator product expansion   Hill & Paz, 2017

$$\lim_{Q^2 \to \infty} T_1(0, Q^2) \propto \frac{1}{Q^2}$$

- Besides that is not very well constrained

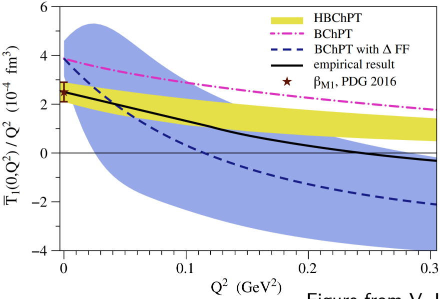


Figure from V. Lensky et al., PRD 2018

Two-photon exchange

Reference	$E_{2S}^{(\mathrm{subt})}$	$E_{2S}^{(\mathrm{inel})}$	$E_{2S}^{(\mathrm{pol})}$	$E_{2S}^{(\mathrm{el})}$	$E_{2S}^{\langle 2\gamma\rangle}$
DATA-DRIVEN DISPERSIVE EVALUATION					
(75) Pachucki '99	1.9	−13.9	−12(2)	−23.2(1.0)	−35.2(2.2)
(76) Martynenko '06	2.3	−16.1	−13.8(2.9)		
(77) Carlson *et al.* '11	5.3(1.9)	−12.7(5)	−7.4(2.0)		
(78) Birse and McGovern '12	4.2(1.0)	−12.7(5)	−8.5(1.1)	−24.7(1.6)	−33(2)
(79) Gorchtein *et al.*'13 [a]	−2.3(4.6)	−13.0(6)	−15.3(4.6)	−24.5(1.2)	−39.8(4.8)
(80) Hill and Paz '16					−30(13)
(81) Tomalak'18	2.3(1.3)		−10.3(1.4)	−18.6(1.6)	−29.0(2.1)
LEADING-ORDER BχPT					
(82) Alarcòn *et al.* '14			$-9.6^{+1.4}_{-2.9}$		
(83) Lensky *et al.* '17 [b]	$3.5^{+0.5}_{-1.9}$	−12.1(1.8)	$-8.6^{+1.3}_{-5.2}$		

Table from Ann. Rev. Nucl. Part. Sci. 72 (2022) 389

- Individual contributions:

- Subtraction part: poorly constrained

- Elastic part: still tension on $e-p$ scattering experiments

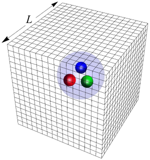
- Can be obtained from first principle $\rightarrow$ lattice QCD

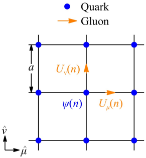
Lattice QCD

- Lattice QCD: path integral formalism of QCD in Euclidean space

$$\langle O \rangle = \frac{1}{Z} \int [DU]\, \hat{O} \exp\Big\{ \underbrace{-S_g[U]}_{\text{gluon}} + \underbrace{\mathrm{Tr}\ln(M[U])}_{\text{quark}} \Big\}$$

$$\Rightarrow \frac{1}{N} \sum_i O_i$$





- Dimension of the integral $\propto$ number of points $\sim 10^7 - 10^8$

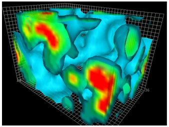
Monte Carlo method needed, average over configurations

- Three limits for LQCD calculation to reach the physical point:

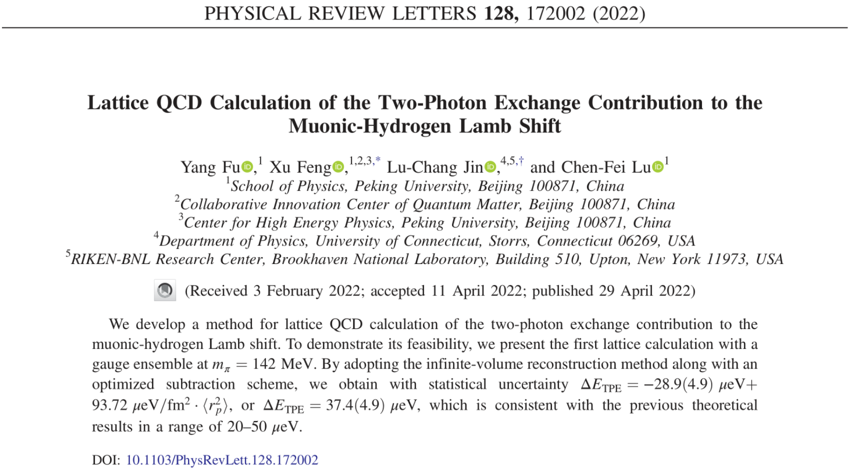
- lattice size $L \to \infty$

- lattice spacing $a \to 0$

- quark mass $m_q \to m_{q,\mathrm{phy}}$
(or pion mass $m_\pi \to m_{\pi,\mathrm{phy}}$)



TPE from lattice QCD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Lattice QCD Calculation of the Two-Photon Exchange Contribution to the Muonic-Hydrogen Lamb Shift

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We develop a method for lattice QCD calculation of the two-photon exchange contribution to the muonic-hydrogen Lamb shift. To demonstrate its feasibility, we present the first lattice calculation with a gauge ensemble at $m_\pi = 142$ MeV. By adopting the infinite-volume reconstruction method along with an optimized subtraction scheme, we obtain with statistical uncertainty $\Delta E_{\rm TPE} = -28.9(4.9)\ \mu{\rm eV} + 93.72\ \mu{\rm eV/fm}^2 \cdot \langle r_p^2 \rangle$, or $\Delta E_{\rm TPE} = 37.4(4.9)\ \mu{\rm eV}$, which is consistent with the previous theoretical results in a range of 20–50 μeV.

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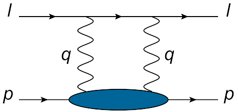
- First lattice calculation of TPE
- Some ideas can also be applied in the calculation of subtraction contribution

Two-photon exchange on lattice

- TPE is a QCD + QED correction with IR divergence

After subtraction is IR finite

ΔE =



− (point-like proton + charge radius term)

point-like and charge radius terms are analytically known

- Problems for LQCD calculation:

- QCD + QED: massless photon meets finite volume

⇒ How to deal with finite-volume effects?

- IR subtraction: large number cancellation, signal hidden by error

⇒ How to cancel IR divergence analytically? (as it always does in PT calculations)

- Infinite volume propagator $\Rightarrow$ finite-volume propagator

$$S^{\gamma}_{\mu\nu}(x) = \int \frac{\mathrm{d}^4 q}{(2\pi)^4} \frac{\delta_{\mu\nu}}{q^2} e^{iq\cdot x} \quad \Rightarrow \quad S^{\gamma}_{\mu\nu}(x) \overset{?}{=} \frac{1}{L^3 T} \sum_q \frac{\delta_{\mu\nu}}{q^2} e^{iq\cdot x}$$

There is a singularity when $q = 0$!

- Minimal treatment: remove the zero mode $\rightarrow$ QED$_L$

$\Rightarrow \mathcal{O}\left(\frac{1}{L^n}\right)$ power-law finite volume effects

Duncan, Eichten, and Thacker (1996). Hayakawa and Uno (2008)

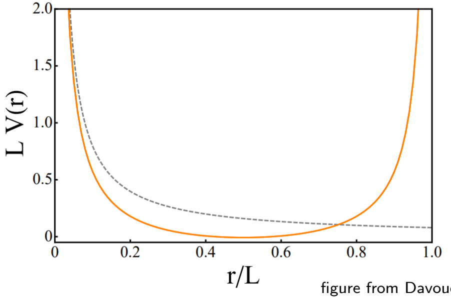
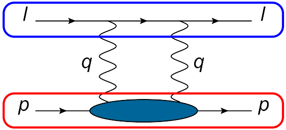


figure from Davoudi and Savagi, PRD (2014)

QED$_\infty$

- QED$_\infty$ — use infinite volume photon propagator in finite volume
- E.g., for two-photon exchange



Leptonic part $L_{\mu\nu}$
analytically known
Hadronic part $H_{\mu\nu}$
lattice QCD

$$\Delta E^{\text{box}} = \int \frac{d^4 q}{(2\pi)^4} L_{\mu\nu}(q) H_{\mu\nu}(q) = \int d^4 x \, L_{\mu\nu}(x) H_{\mu\nu}(x)$$

$$\Rightarrow \text{ Can we use } \quad \Delta E^{\text{box}} = \sum_{x \in \mathbb{L}} L_{\mu\nu}(x) H_{\mu\nu}(x) \ ?$$

- FV effects are exponentially suppressed if hadronic part falls exponentially

in long distance region.

But not the case here. For large $t \gg |\vec{x}|$

$$H_{\mu\nu}(x) \sim e^{-M(\sqrt{\vec{x}^2+t^2}-t)} \sim e^{-M|\vec{x}|^2/(2t)} \sim \mathcal{O}(1)$$

it still leads to power-law finite volume effects.

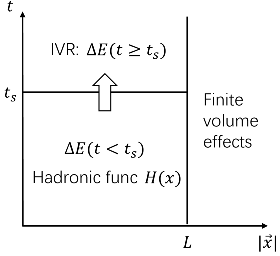
Infinite-volume reconstruction

- Infinite-volume reconstruction (IVR) method
- Idea: split the integral into two parts

- $|t| < t_s$: directly calculated

- $|t| \geq t_s$: different treatment required

X. Feng, L. Jin, PRD (2019)



Infinite-volume reconstruction

- Infinite-volume reconstruction (IVR) method
- Idea: split the integral into two parts

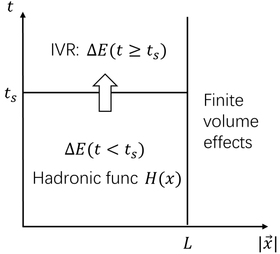
- $|t| < t_s$: directly calculated

- $|t| \geq t_s$: different treatment required

- At large $t(t > t_s)$, intermediate states are

dominated by the single proton state

X. Feng, L. Jin, PRD (2019)



$$H_{\mu\nu}(x) \approx \int \frac{\mathrm{d}^3\vec{q}}{(2\pi)^3} \left[\frac{1}{2E_{\vec{q}}} \langle p|j_\mu|p(\vec{q})\rangle\langle p(\vec{q})|j_\nu|p\rangle \right] e^{i\vec{q}\cdot\vec{x}-(E_{\vec{q}}-M)t}$$

we only need to calculate the matrix elements $\langle p|j_\mu|p(\vec{q})\rangle\langle p(\vec{q})|j_\nu|p\rangle$

- Inverse Fourier transformation at modest t_s gives values for all $\vec{Q}$

$$\int \mathrm{d}^3\vec{x}\; H_{\mu\nu}(\vec{x}, t_s) e^{-i\vec{q}\cdot\vec{x}+(E_{\vec{q}}-M)t_s} \approx \left[\frac{1}{2E_{\vec{q}}} \langle p|j_\mu|p(\vec{q})\rangle\langle p(\vec{q})|j_\nu|p\rangle \right]$$

Reconstruct $|t| > t_s$ from t_s $\rightarrow$ power-law FV effects eliminated with $t_s \lesssim L$

IR subtraction

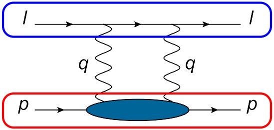
- Matrix elements $\langle p|j_\mu|p(\vec{q})\rangle\langle p(\vec{q})|j_\nu|p\rangle$ can be reconstructed

$\Rightarrow$ reconstruct point-like proton + charge radius

$\rightarrow G_E(0) = 1 \qquad \rightarrow G_E'(0)$

- We find the appropriate weight functions L^{pt}, L^{rad}

$\Delta E =$



$-$ (point-like proton + charge radius term)

$$= \int \mathrm{d}^4x \; L(x)H(x) - (\text{point-like proton} + \text{charge radius term})$$

$$= \int \mathrm{d}^4x \; \underbrace{\left[L(x) - c^{\text{pt}}L^{\text{pt}}(x) - c^{\text{rad}}L^{\text{rad}}(x)\right]}_{\text{IR finite}} H(x)$$

$$= \int \mathrm{d}^4x \; L^{\text{sub}}(x)H(x)$$

Weight function $L^{\text{sub}}(x)$ is IR finite $\rightarrow$ maintain IR cancellation automatically.

Finite-volume effects

- Weight function $L^{\text{sub}}(x)$ increases rapidly as $|x|$ increases

$\Rightarrow$ Even $H(x)$ is exp. decaying, we still have significant finite-volume effects

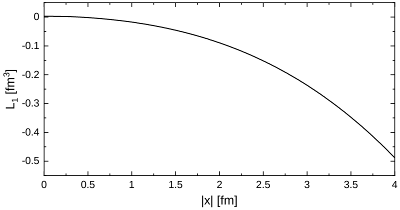


Figure: $L^{\text{sub}}(x)$ increases with $|x|$

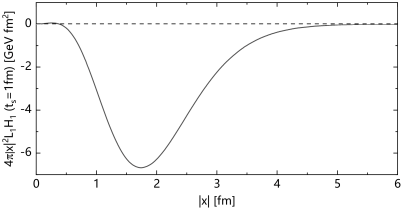
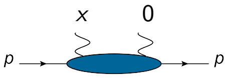


Figure: model estimate: $4\pi|x|^2 L(x)H(x)$

- Makes things worse: signal-to-noise ratio decays exponentially



$$H(x)/\delta H(x) \sim \exp\left\{-\left(M_p - \frac{3}{2}m_\pi\right)|x|\right\}$$

- $|x| \sim 5$ fm to guarantee no information lost.

$\Rightarrow$ $L \sim 10$ fm box required. Decrease of S/N seems to be an inevitable problem.

Optimized subtraction scheme

- Optimized subtraction scheme, idea: $A = (A - B) + B$

split the TPE correction into

$$\Delta E = \underbrace{\left(\Delta E - c_0 - c_r \cdot \langle r_p^2 \rangle\right)}_{\Delta E^{(r)}} + c_0 + c_r \cdot \langle r_p^2 \rangle$$

with $\Delta E^{(r)}$ calculated using reduced weight function

$$L^{(r)}(x) = L^{\rm sub}(x) - c_0 L^{\rm pt}(x) - c_r L^{\rm rad}(x)$$

- Optimize c_0, c_r to suppress weight function → suppressed FV effects

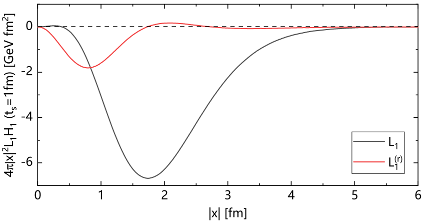


Figure: model estimate for $L(x)$ and $L^{(r)}(x)$

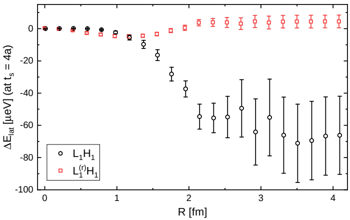
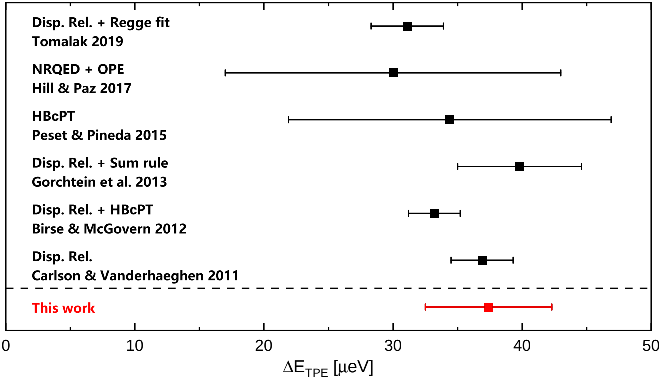


Figure: Numerical partial sum

⇒ Finite volume effect: $L \sim 10$ fm → 5 fm, with error reduced by ∼ 6 times.

Full TPE contribution from lattice QCD

Ensemble	m_π [MeV]	L/a	T/a	a[fm]	N_{conf}
24D	142	24	64	0.194	131



- $\Delta E_{\text{TPE}} = -28.9(4.9)\ \mu\text{eV} + 93.72\ \mu\text{eV/fm}^2 \cdot \langle r_p^2 \rangle = 37.4(4.9)\ \mu\text{eV}$

Next step: increase statistics and better control lattice systematic effects

Back to dispersion relation

- Dispersion relation is powerful, we have good $e - p$ scattering data,

just the subtraction function is not good $\Rightarrow$ LQCD calculation

- A new "point" from F. Hagelstein & V. Pascalutsa:

Subtraction at Euclidean $(\nu_s, Q^2) = (iQ, Q^2)$ rather than $(0, Q^2)$.

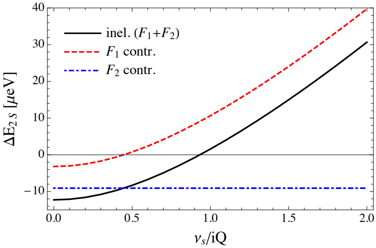
Nucl. Phys. A 1016 (2021) 122323. Talk on Tuesday

$\Delta E_{\text{TPE}}^{(\text{inel})}(\nu_s = iQ) = 1.6\ \mu\text{eV}$ vs

$\Delta E_{\text{TPE}}^{(\text{inel})}(\nu_s = 0) = -12.3\ \mu\text{eV}$

- inelastic part is suppressed

- this point can be directly accessed
  on lattice by setting $Q = (Q, \vec{0})$



- DR dominated by elastic part, can be very precise (if tension is solved)

improve the subtraction part $\rightarrow$ total uncertainty will be small

Subtraction contribution

- Subtleties:

EFTs usually calculate the non-Born subtraction function

LQCD can only simulate the full hadronic function $H(x)$, not $H^{\text{non-Born}}(x)$.

- The definition of subtraction contribution is different

here defined as contribution from $T_1(iQ, Q^2) - \lim_{Q\to 0} T_1(iQ, Q^2)$ (no IR divergence)

- The size of each part is estimated below

Subt. point	ΔE^{el}	ΔE^{inel}	ΔE^{subt} [μeV]	subt. from LQCD
$\nu_s = iQ$	~ 30	-1.6	$\lesssim 10$	OK
$\nu_s = 0$	~ -15	12.3	~ 30	not favored

Elastic: using dipole form factors with $\sqrt{r_E^2} = \sqrt{r_M^2} = 0.85$ fm
Inelastic: Christy-Bosted parameterization
Subtraction: assuming total $\Delta E_{\text{TPE}} \sim 30$ μeV

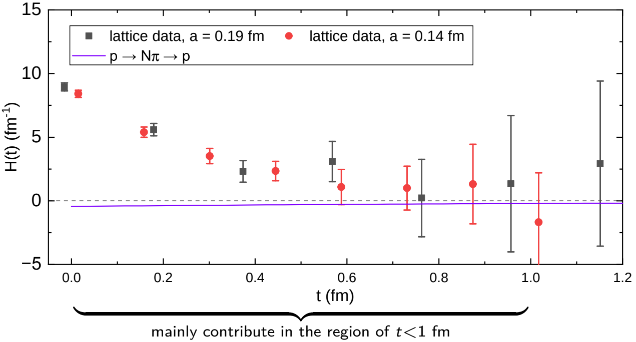
$\Rightarrow$ Conclusion: lattice calculation also favors $(q_0, Q^2) = (iQ, Q^2)$

LQCD calculation of subtraction function

- Subtraction function from correlator calculated on lattice

$$T_1(iQ, Q^2) = -\frac{1}{24\pi M}\int \mathrm{d}t\, e^{iQt} \underbrace{\langle p|\vec{J}(t)\cdot\vec{J}(0)|p\rangle}_{H(t)}$$

- $H(t) = \langle p|\vec{J}(t)\cdot\vec{J}(0)|p\rangle$ as a function of t



- lowest contributed state is $|N\pi\rangle$

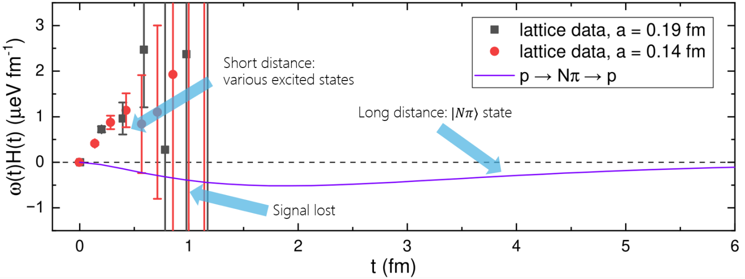
Seems negligible and is completely hidden by noise at long distance?

Hadronic part

- But we need energy shift $E^{(\mathrm{subt})} = \int \mathrm{d}t\ L(t)H(t)$

Leptonic weight function $L(t)$ increases rapidly as $|t|$ increases

- $L(t)H(t)$ as a function of t



- $N\pi$ contribution significantly enhanced by weight function $L(t)$
- Large temporal truncation error if only integrate to 1fm

$\Rightarrow$ Need to calculate $N\gamma^\star \to N\pi$ matrix element $\langle N\pi|J_i|p\rangle$

$N\gamma^\star \to N\pi$ matrix element

- Quark contraction: current $\to$ pion interpolating operator

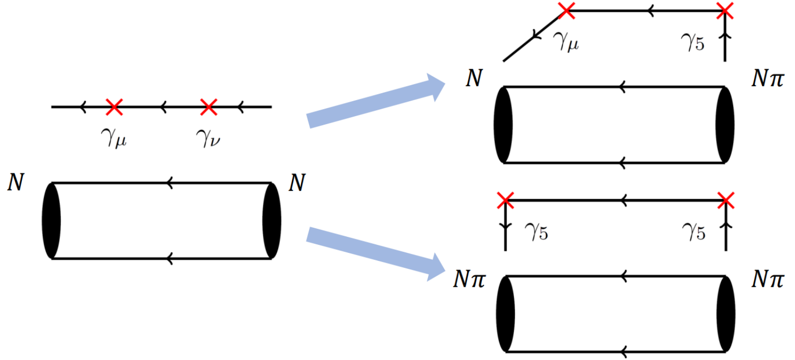


figure credit: Xuan-He Wang

$$I = 1/2:\ O_{N\pi}^{I_3=+\frac{1}{2}} = O_p O_{\pi^0} - \sqrt{2} O_n O_{\pi^+},\ O_{N\pi}^{I_3=-\frac{1}{2}} = \sqrt{2} O_n O_{\pi^0} - O_p O_{\pi^-}$$

$$I = 3/2:\ O_{N\pi}^{I_3=+\frac{1}{2}} = \sqrt{2} O_p O_{\pi^0} + O_n O_{\pi^+},\ O_{N\pi}^{I_3=-\frac{1}{2}} = O_n O_{\pi^0} + \sqrt{2} O_p O_{\pi^-}$$

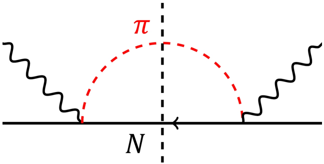
} Operators

More about $N\pi$ state and polarizability from LQCD: Xuan-He Wang et al., 2310.01168

Computational strategy

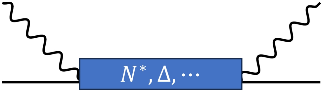
- Hadronic function decomposed into

Nucleon-pion contribution:



- constructed from $\langle N\pi|J_i|p\rangle$
- no temporal truncation error

all other excited states contribution:



- $H(\vec{x}, t)$ subtract Nπ state
- suppressed temporal truncation error

- (The idea of) optimized subtraction scheme can also be applied

Trick: $A = (A - B) + B$, calculate the reduced part $A - B$ with known B

$\rightarrow$ using well-known low-energy constants: radii, magnetic moment, polarizabilities

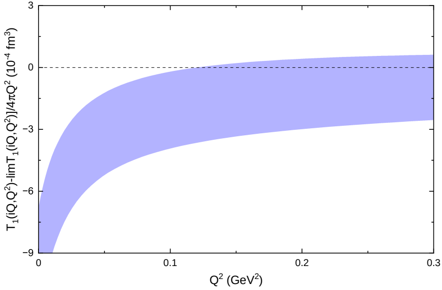
Subtraction function

- LQCD calculation on two ensembles with more stats:

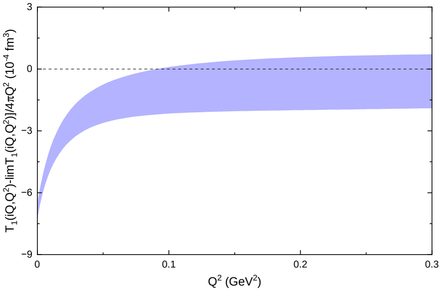
Ens.	m_π[MeV]	L/a	T/a	L	a[fm]	$N_{\rm conf}$
24D	142	24	64	4.6	0.194	207
32Df	142	32	64	4.6	0.143	69

- $\frac{1}{4\pi Q^2}[T_1(iQ,Q^2) - \lim_{Q\to 0} T_1(iQ,Q^2)]$ as a function of Q^2

- w/o optimized subtraction



- with optimized subtraction



Using low-energy constants essentially constrains the low-energy limit.

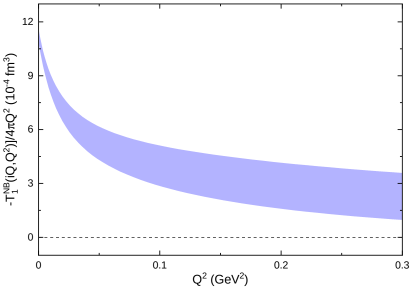
Subtraction function

- Compare with pheno. results:

Either we subtract the Born part, or pheno add the Born part

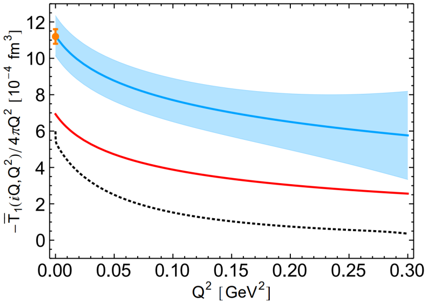
- $-\frac{1}{4\pi Q^2} T_1^{\text{non-Born}}(iQ, Q^2)$ as a function of Q^2

- LQCD subtract Born part



Born term with form factor parametrization from Kaushik et al., PRD 102, 074012

- pheno. Volodymyr et al., 2305.08814



NLO χPT
LO χPT
Sum rule with MAID model

Two-photon exchange

- Subtraction contribution to μH TPE is given by

$$\Delta E^{\text{subt}} = 5.1(1.3)_{\text{conn}}(1.6)_{\text{disc}}(0.4)_{\alpha_E}\ [\mu\text{eV}]$$
$$= 5.1(2.1)\ [\mu\text{eV}]$$

- Systematic error budget is relatively complete:

- physical pion mass, continuum extrapolation, temporal truncation effects

- spatial finite-volume effects not included yet but expected to be small
(no momentum in the spatial direction)

- Two-photon exchange

		ΔE [μeV]	Comment
DR	Elastic	$\sim 25 - 30$	error $\lesssim 2\%$ if no tension
	Inelastic	-1.6	suppressed
LQCD	Subt.	5.1(2.1)	Can be continuously improved with more stats. and ensembles

Thank you for your attention!

Backup Slides

Hadronic part at long distance

- Hadronic function not always fall exponentially in long distance region

$$H_{\mu\nu}(x) = \langle p | j_\mu(x) j_\nu(0) | p \rangle$$

Insert hadronic intermediate state

$$\int \frac{\mathrm{d}^3 \vec{q}}{(2\pi)^3} \underbrace{\langle p | j_\mu(x) | p(\vec{q}) \rangle} \frac{1}{2E_{\vec{q}}} \langle p(\vec{q}) | j_\nu(0) | p \rangle$$

$$\Downarrow$$

$$\sim \int \frac{\mathrm{d}^3 \vec{q}}{(2\pi)^3} \frac{e^{Mt} e^{-E_{\vec{q}} t} e^{i\vec{q}\cdot\vec{x}}}{2E_{\vec{q}}} \sim \int \frac{\mathrm{d}^4 q}{(2\pi)^4} \frac{e^{ipx}}{p^2 + M^2} e^{Mt} \to e^{-M(\sqrt{\vec{x}^2+t^2}-t)}$$

- For large $t \gg |\vec{x}|$

$$H_{\mu\nu}(x) \sim e^{-M(\sqrt{\vec{x}^2+t^2}-t)} \sim e^{-M|\vec{x}|^2/(2t)} \sim \mathcal{O}(1)$$

Essentially leads to power-law finite volume effects