Low
Nucleon Structure at Low Q
AVRA IMPERIAL HOTEL, CRETE, GREECE, 15 MAY – 21 MAY 2023

TPE contribution to the μH Lamb shift & proton polarizability from lattice QCD

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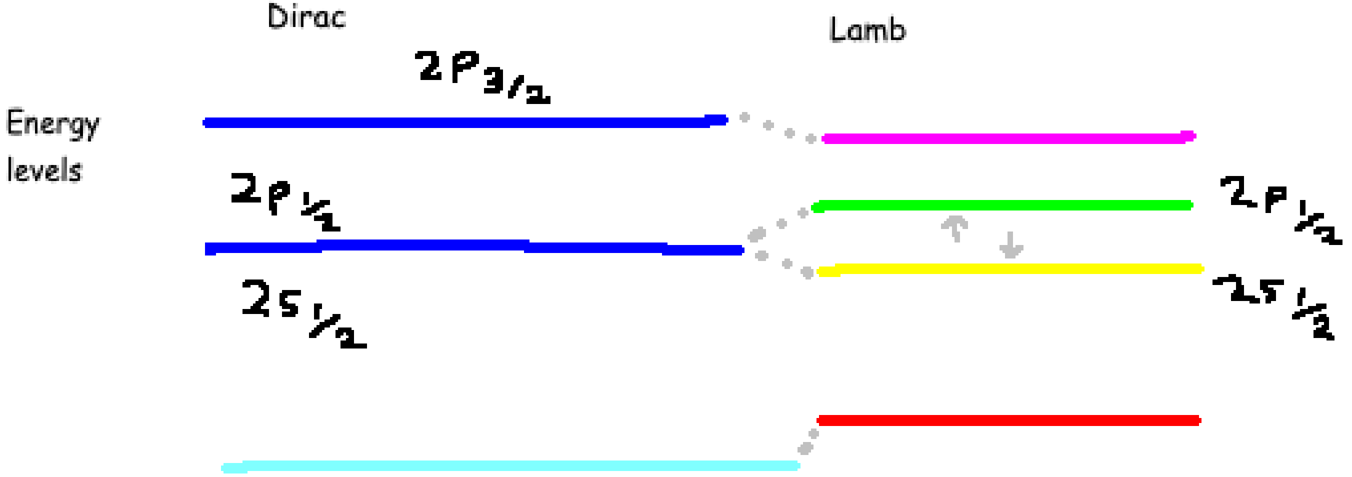
2023.05.17

Based on Y. Fu, XF, L. Jin, C. Lu, PRL 128 (2022) 17, 172002
+ new progress

Spectroscopy and quantum field theory

➢ Important observable – Lamb shift



1947, Lamb discovered the nondegeneracy

→ Lamb shift

1955

Dirac theory predicts that $2P_{1/2}$ and $2S_{1/2}$ states are degenerate

➢ QED - Lamb shift mainly originates from quantum fluctuation of EM fields (VP + electron self energy)

Theory： 1057832.3(3) kHz 【PRA 93 (2016) 022513】

Experiment： 1057829.8(3.2) kHz 【Science 365 (2019) 6457】

- Consistency between theory and experiment

  → Lay the foundation of QED

- High-precision measurement of spectroscopy

  → Provide information of proton’s structure

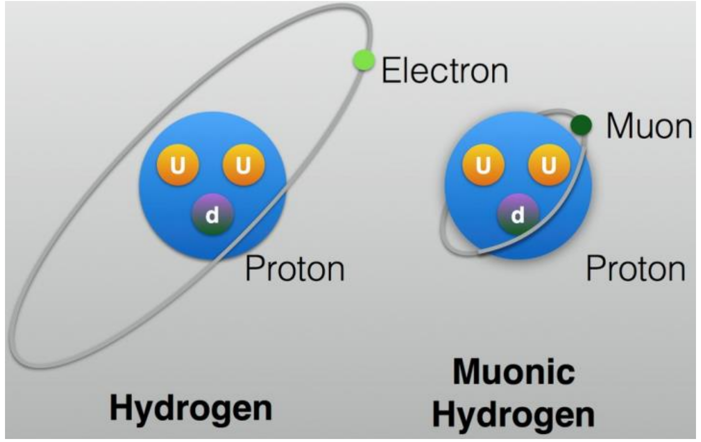
Tomonaga

Schwinger

Feynman

1965

Muonic hydrogen



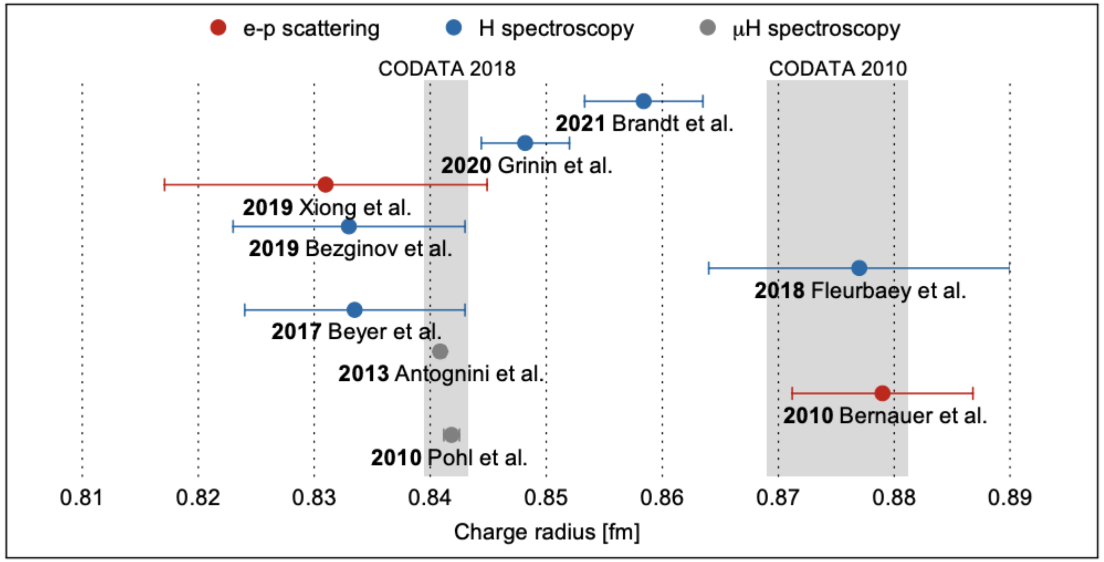
- Muon mass is about 200 times of electron
- Bohr radius for μH is 200 times smaller than H

➢ 2010, proton charge radius from μH

【Nature 466 (2010) 213】

- Precision 10 times better than before
- 4% smaller radius

5σ deviation → Proton size puzzle



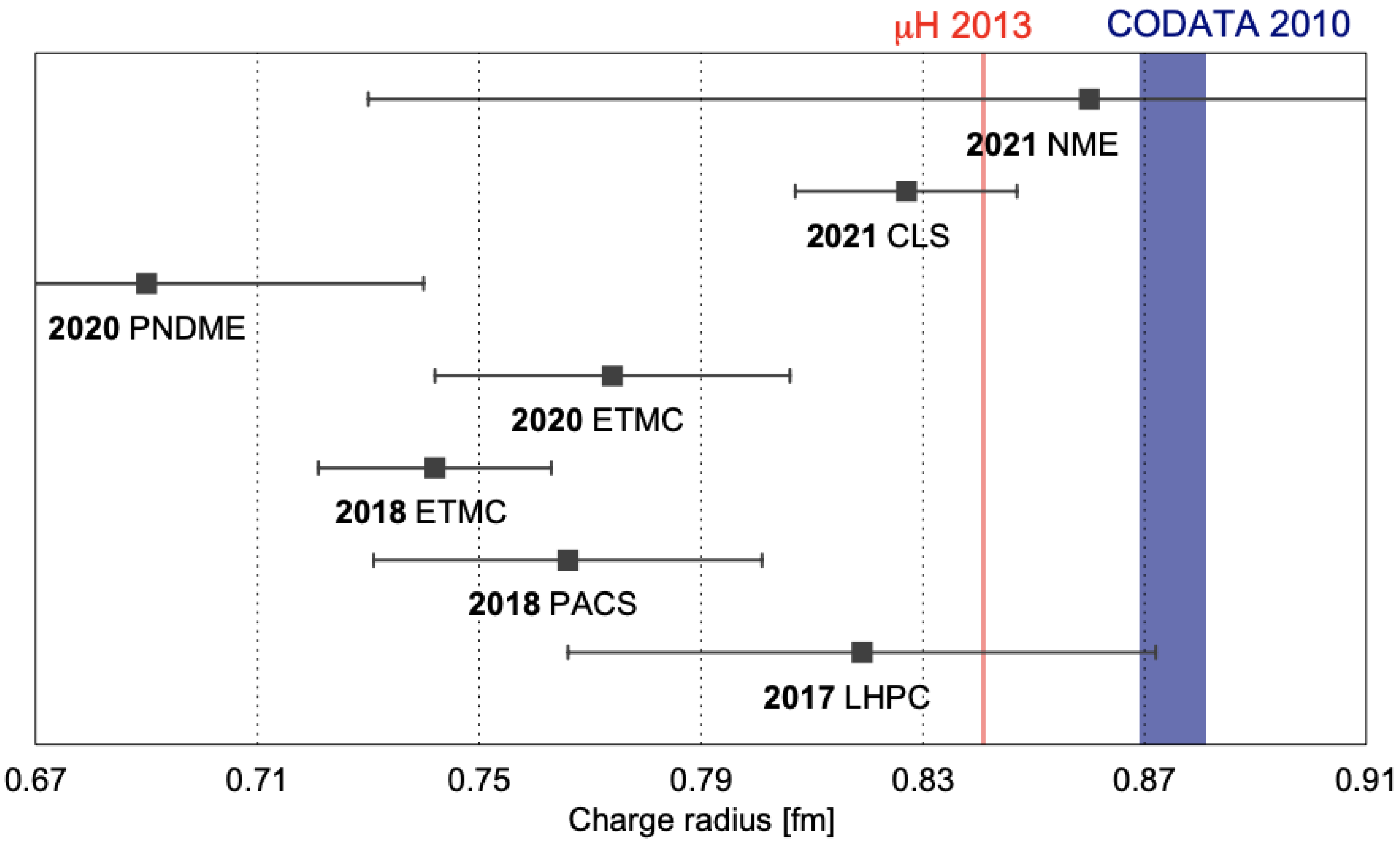
New experimental progress

➢ Still some discrepancies
➢ Consistently shrink the proton size

Puzzle possibly originates from experiments

However, as a fundamental quantity, the size of proton charge radius plays an important role in the theoretical prediction in spectroscopy

Direct lattice QCD calculation of charge radius



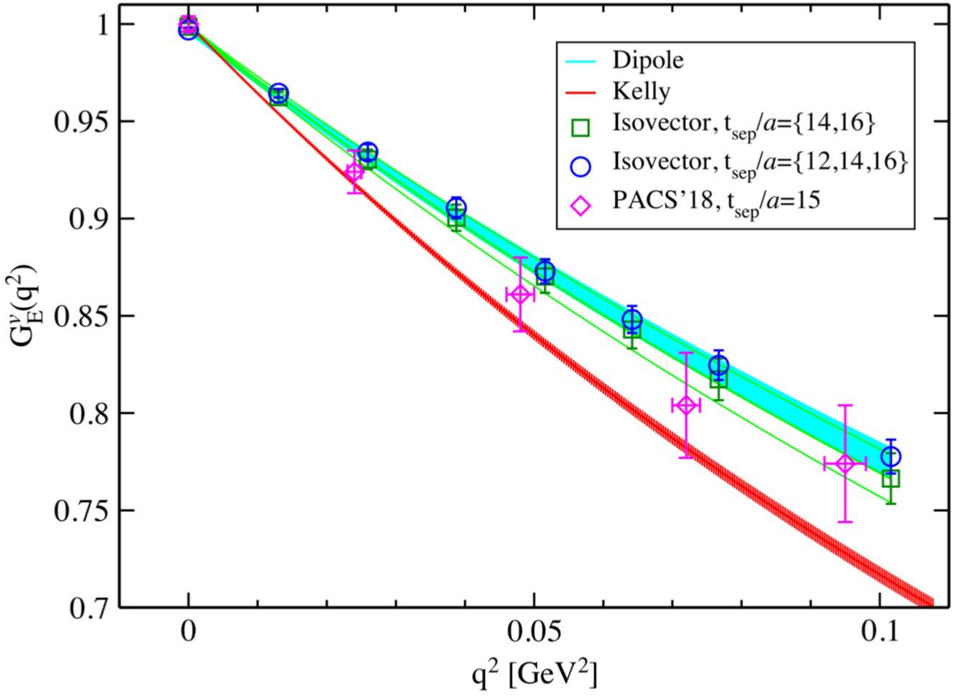
- Charge radius is the derivative of form factor ➡ still hard to achieve ~1% accuracy

Direct lattice QCD calculation of charge radius

- Various systematic effects, especially the model dependence

$$\langle H(p_f)|J_\mu|H(p_i)\rangle = \bar{u}(p_f)\left[\gamma_\mu F_1(q^2) + \frac{i\sigma^{\mu\nu}q_\nu}{2M}F_2(q^2)\right]u(p_i), \quad q^2 = (p_f - p_i)^2$$

- Momenta p_i and p_f on the lattice are always discrete: $\frac{2\pi}{L}n$ ➡ modeling of q^2-dependence to extract charge radius



Fit type	q^2_{cut} [GeV^2]	t_{sep}/a	Isovector $\sqrt{\langle r_E^2\rangle}$ [fm]	Isovector χ^2/dof
Linear	0.013	{12, 14, 16}	0.764(26)	⋯
		{14, 16}	0.806(35)	⋯
Dipole	0.102	{12, 14, 16}	0.785(17)	1.2(8)
		{14, 16}	0.806(26)	0.6(6)
Quadrature	0.102	{12, 14, 16}	0.785(19)	1.0(8)
		{14, 16}	0.783(30)	0.7(7)
z-exp ($k_{\text{max}} = 3$)	0.102	{12, 14, 16}	0.776(28)	1.2(9)
		{14, 16}	0.796(37)	0.8(8)

[PACS Collaboration used a (10.8 fm)^4 lattice, PRD 2020]

- Model dependence could cause a 3% shift in r_p, e.g. 0.806(26) → 0.783(30)
- Twisted boundary condition can help, but requires more computational resources and still a fit functional form
- Why not calculate the charge radius directly at q^2=0 ➡ A model-independent approach to extract charge radius

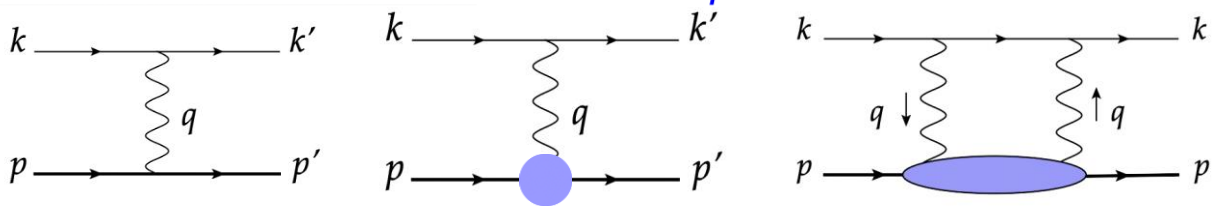
XF, Y. Fu, L. Jin, PRD 101 (2020) 051502

Various contributions to μH Lamb shift

Experiment | Theory | 【Science 339 (2013) 417】

$$E_{2P} - E_{2S} = \Delta E_{\mathrm{QED}} + \Delta E_{\text{proton size}} + \Delta E_{\mathrm{TPE}}$$

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



- Exp. vs Theory ➡ $r_p = 0.84087(39)$ fm ➡ Proton size puzzle
- Largest theoretical uncertainty from two-photon exchange (TPE)
- Uncertainty for structure independent contribution is further reduced

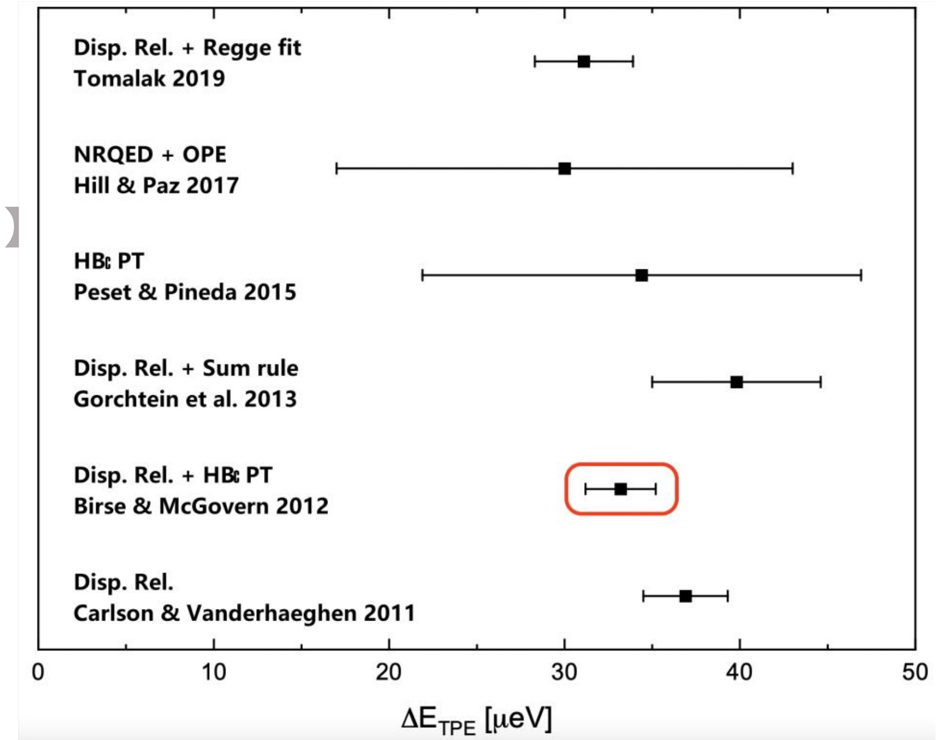
  $\Delta E_{\mathrm{QED}} = 206034.7(0.3)\quad \mu\mathrm{eV}$ 【Ann.Rev.Nucl.Part.Sci.72 (2022) 389】

  Upgrade of CREMA@PSI can reduce Exp. error by a factor of 5

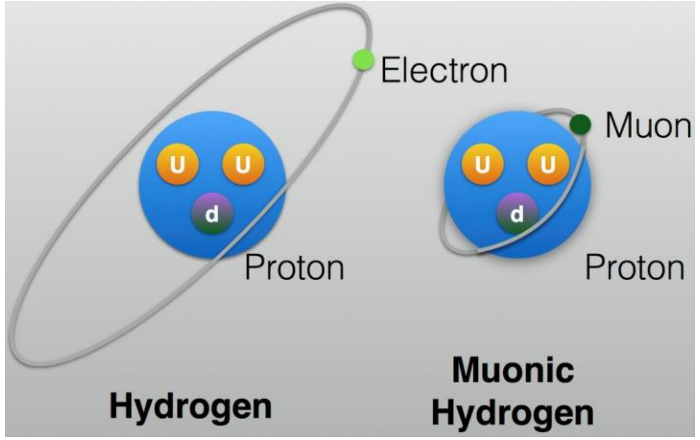
  Leaving TPE the important source for uncertainty!

- Theoretical prediction for TPE relies on data + models and ranges from 20 to 50 μeV

  Our target: obtain TPE from first principles ➡ Lattice QCD



Challenges from TPE (1): IR divergence

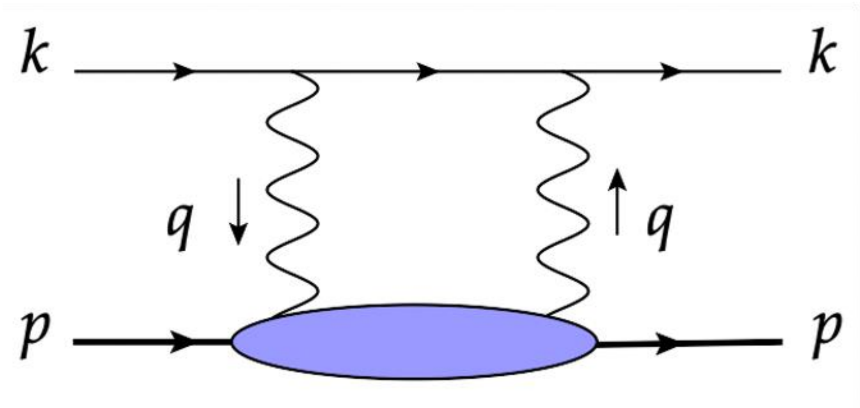


- Binding energy of μH serves as a natural IR cutoff

→ Bound-state QED

→ Proton treated as point-like particle + charge radius correction

No divergence, but rich structure information lost

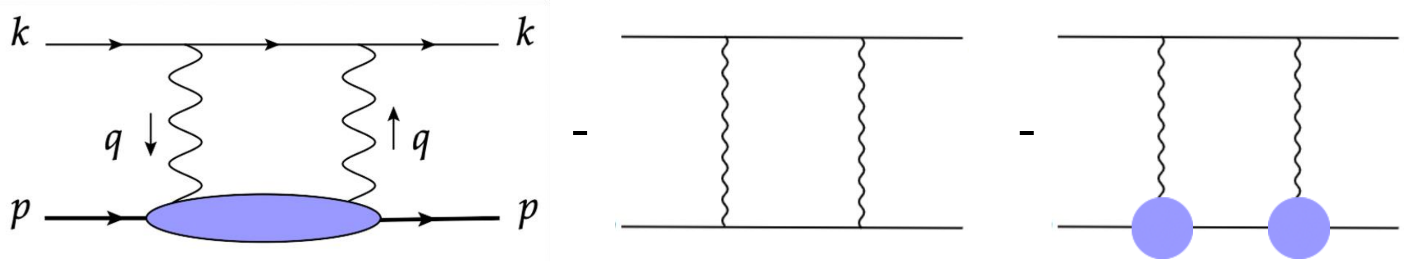


- QCD+QED: complete information of proton structure

→ Loop integral sensitive to hadronic scale → highly NP

→ Bound lepton → free lepton → IR divergence

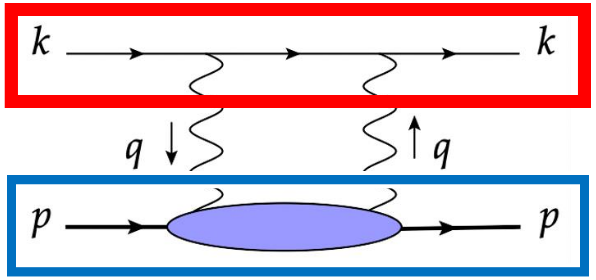
Solution: subtract the divergence



Point-like particle

Charge radius

Challenges from TPE (1): IR divergence



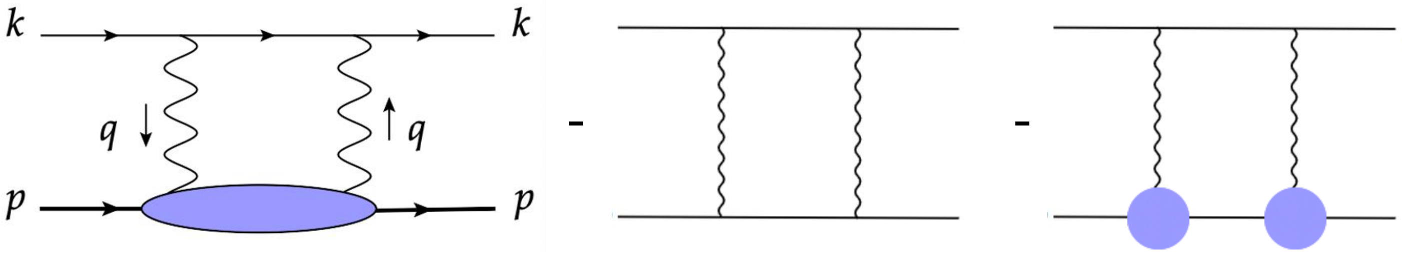
Leptonic part: $L_{\mu\nu}(q)$ $\rightarrow$ Analytically known

Hadronic part: $H_{\mu\nu}(q)$ $\rightarrow$ Provided by LQCD (statistical errors)

Loop integral

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

IR subtraction



divergence - divergence - divergence = finite

Key technical problem

Three diagrams contain diff. stat. errors ➡ How to maintain the error cancellation?

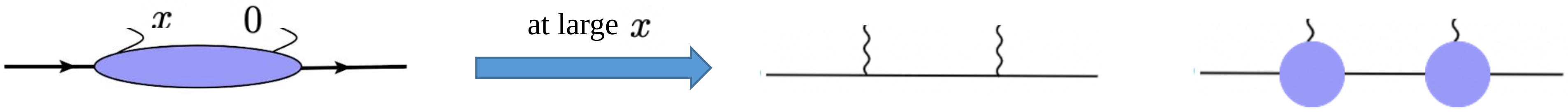
If signal cancels and error does not, then signal is completely hidden by error

Challenges from TPE (1): IR divergence

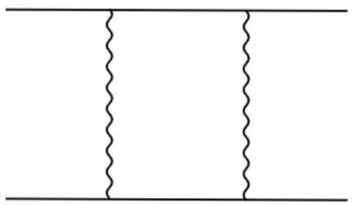
To solve IR divergence: infinite-volume reconstruction method 【X. Feng, L. Jin, PRD 100 (2019) 094509】

Basic idea: low-energy structure information is contained in the long-distance part of hadronic function

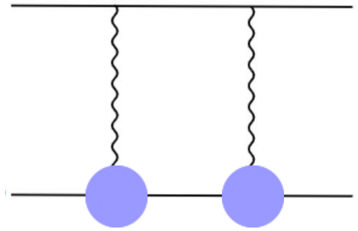
Use $H_{\mu\nu}(x)$ to reconstruct the quantities such as charge radius



- Find the appropriate weight functions $L_{\mu\nu}^{\text{pt-like}}$ and $L_{\mu\nu}^{\text{radius}}$ for the subtraction terms, yielding

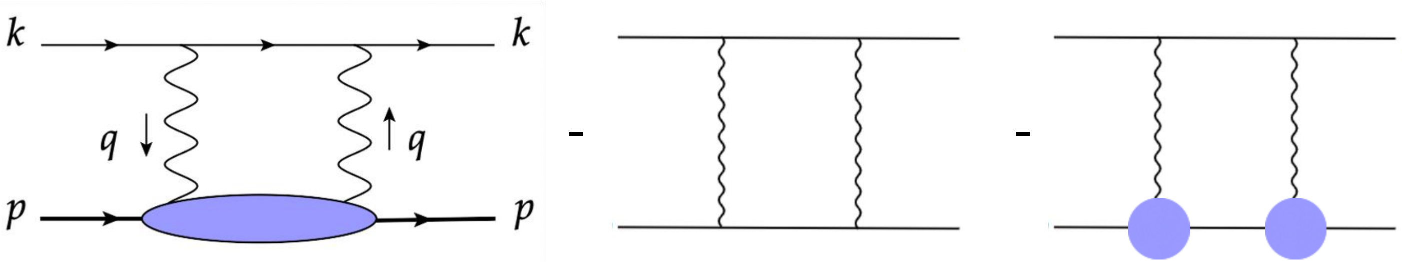


$$= \int d^4x\, L_{\mu\nu}^{\text{pt-like}}(x) H_{\mu\nu}(x)$$



$$= \int d^4x\, L_{\mu\nu}^{\text{radius}}(x) H_{\mu\nu}(x)$$

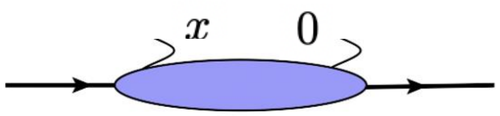
- Cancellation of IR divergence is rigorously fulfilled via the subtraction of weight functions



$$\Rightarrow L_{\mu\nu}^{\text{sub}} = L_{\mu\nu} - L_{\mu\nu}^{\text{pt-like}} - L_{\mu\nu}^{\text{radius}}$$

$$\Delta E^{\text{IR-finite}} = \int d^4x\, L_{\mu\nu}^{sub}(x) H_{\mu\nu}(x)$$ $\Rightarrow$ Error decreases coherently as signal. IR divergence is solved cleanly!

Challenges from TPE (2): Signal-to-noise problem

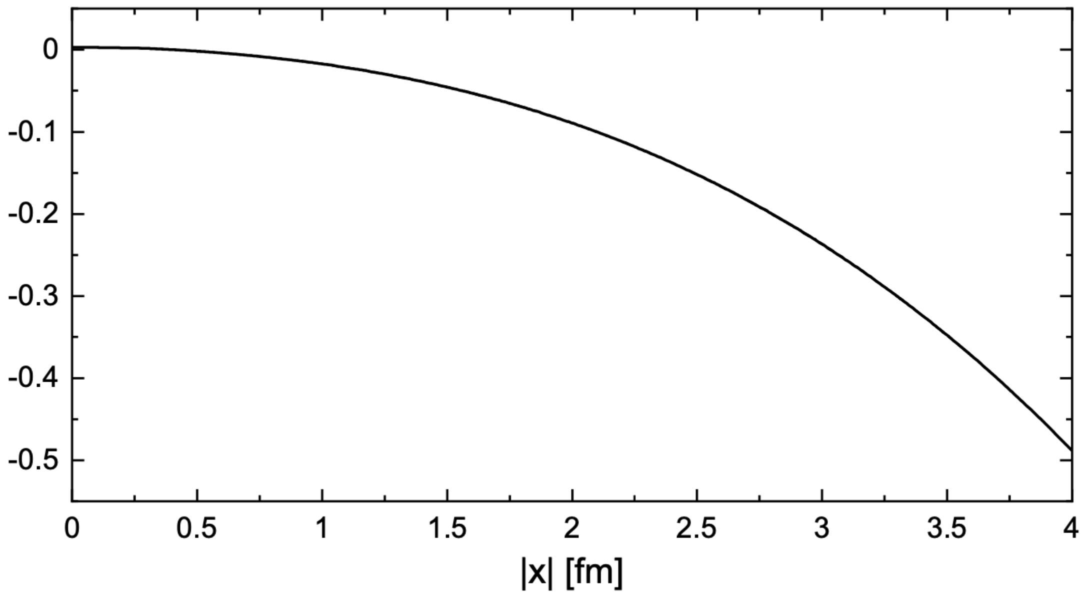


$H_{\mu\nu}(x)$

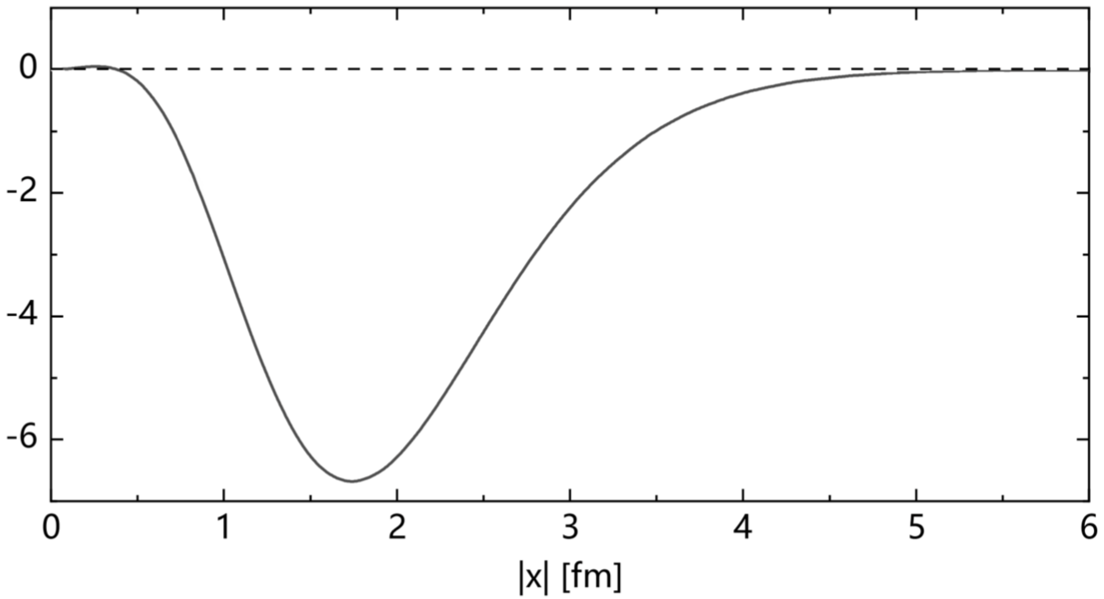
Property of lattice data:

As x increases, proton matrix element $H_{\mu\nu}(x)$ decreases as $e^{-M_p|x|}$

However, error decreases as $e^{-\frac{3}{2}M_\pi|x|}$



Weight function $L_{\mu\nu}^{sub}(x)$ increases fast, as x increases



Model estimate: Combine leptonic and hadronic part

Conclusion: take x as large as 5 fm to guarantee no information lost → Require a 10 fm lattice for simulation

Decrease of S/N ratio seems an inevitable problem

Challenges from TPE (2): Signal-to-noise problem

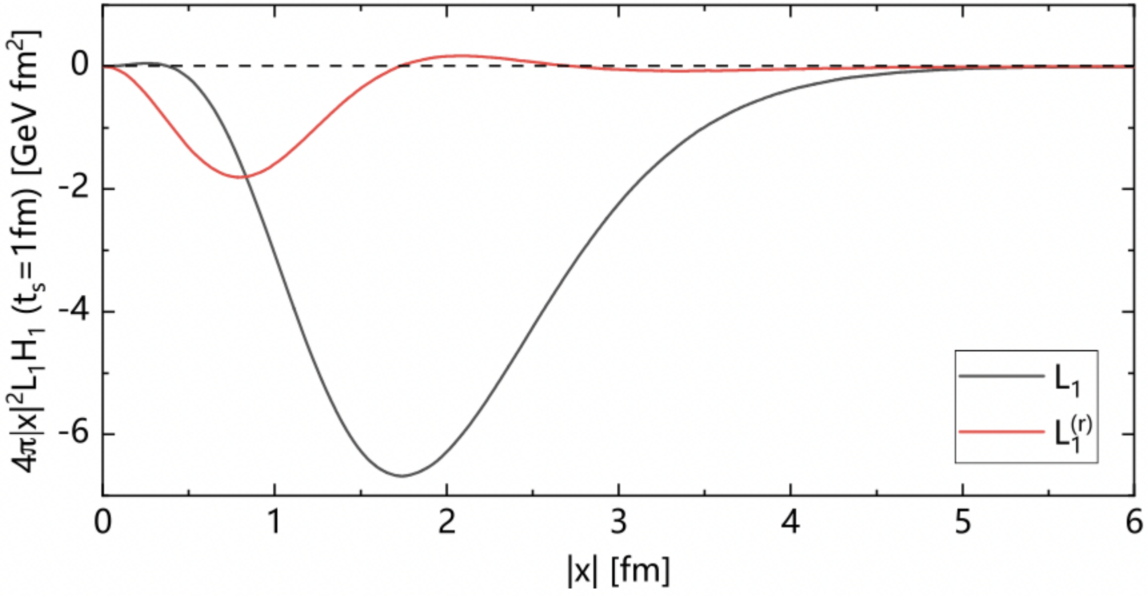
To solve S/N problem: optimized subtraction scheme 【Y. Fu, X. Feng, L. Jin, C. Lu, PRL 128 (2022) 172002】

Trick: A = (A – B) + B

Define the reduced weight function

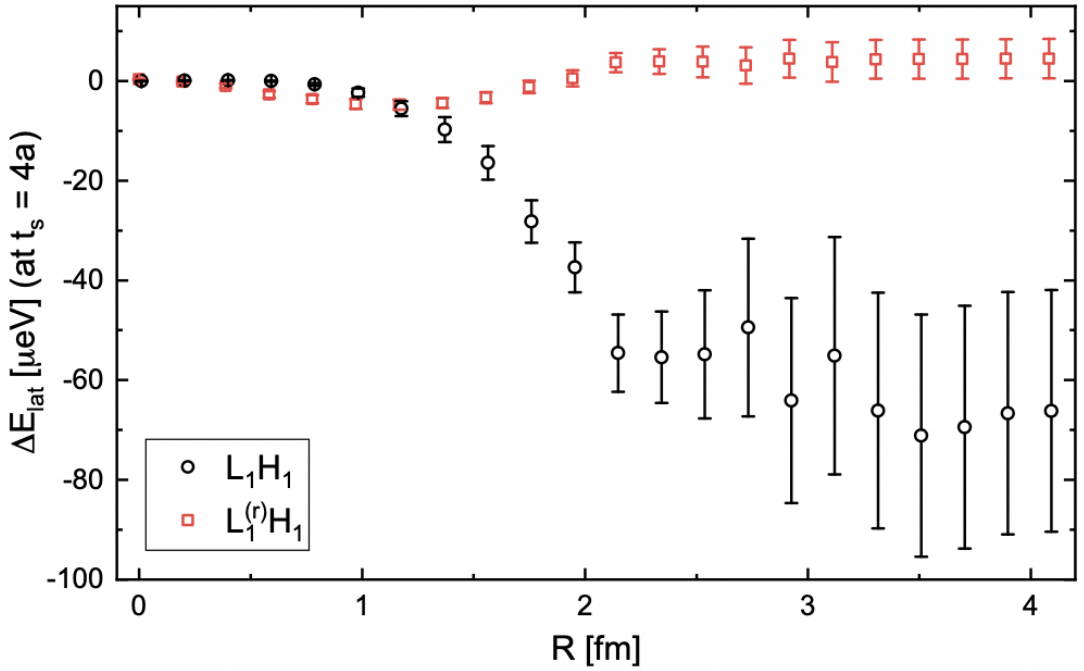
$$L^{(r)}(x) = L^{\text{sub}}(x) - c_0\, L^{\text{pt-like}}(x) - c_r\, L^{\text{radius}}(x)$$

- Choose c_0, c_r to minimize $L^{(r)}(x)$ in the region of 1-3 fm
- Using $L^{(r)}(x)$, (A-B) part is illustrated by the red curve



- Total contribution is $\Delta E = \Delta E^{(r)} + c_0 + c_r \cdot \langle r_p^2 \rangle$

Use optimized subtraction scheme in realistic calculation



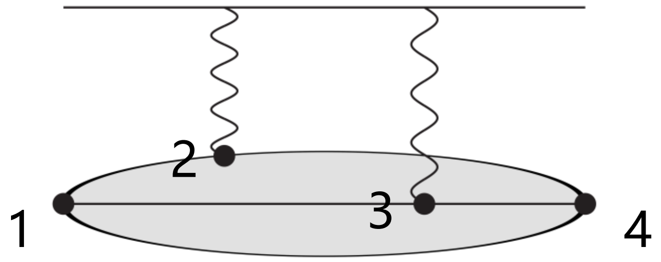
Integral within the range R:

using $L^{(r)}(x)$, error reduced by a factor of 6!

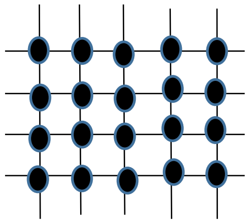
S/N problem is solved

Challenges from TPE (3): Computation of 4-point function

- TPE - hadronic part from a typical 4-point function

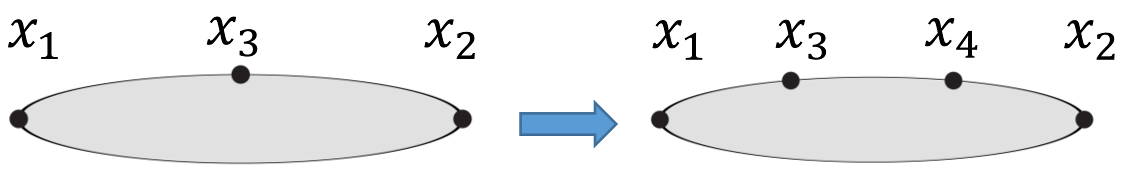


- Perform the volume summation for each point



$$\sum_{x\in L^3}$$

- From 3-point to 4-point function



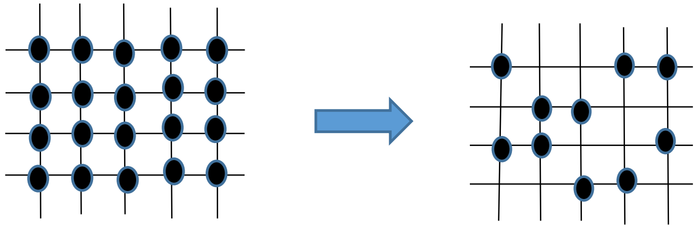
3-point: L^6 summation   4-point: L^9 summation

Increasing each point, computational cost increases by 10^4-10^5 times!
Cannot be solved by increasing resources …

Solution： Field sparsening method

【Y. Li, S. Xia, X. Feng, L. Jin, C. Liu, PRD 103 (2021) 014514】

【W. Detmold, D. Murphy, et. al. PRD 104 (2021) 034502】



- Less summation points may lead to lower precision
- It is not the case because of high correlation in lattice data

→ 10^2-10^3 times less points yields similar precision

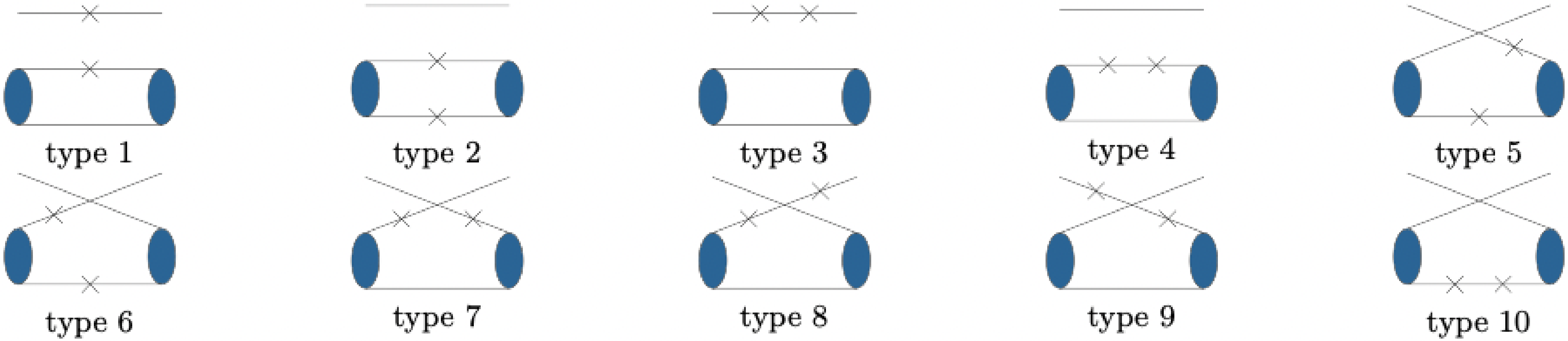
- Used for diff. physical system to confirm the universality

Utilize field sparsening method

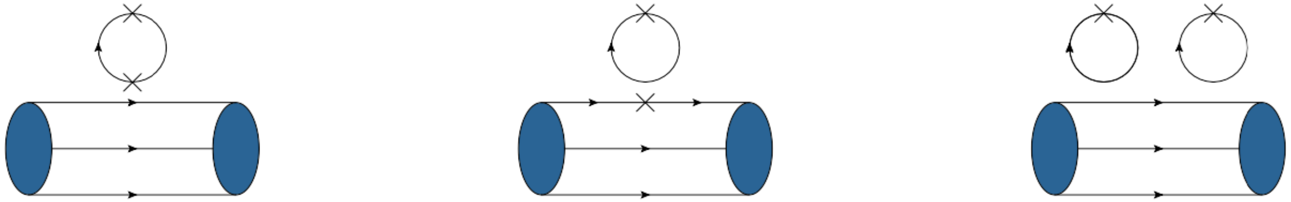
- Reduce the computational cost by a factor of 10^2-10^3 with almost no loss of precision!

Challenges from TPE (3): Computation of 4-point function

- Complicated quark field contraction for nucleon 4-point function – 10 types of connected diagrams

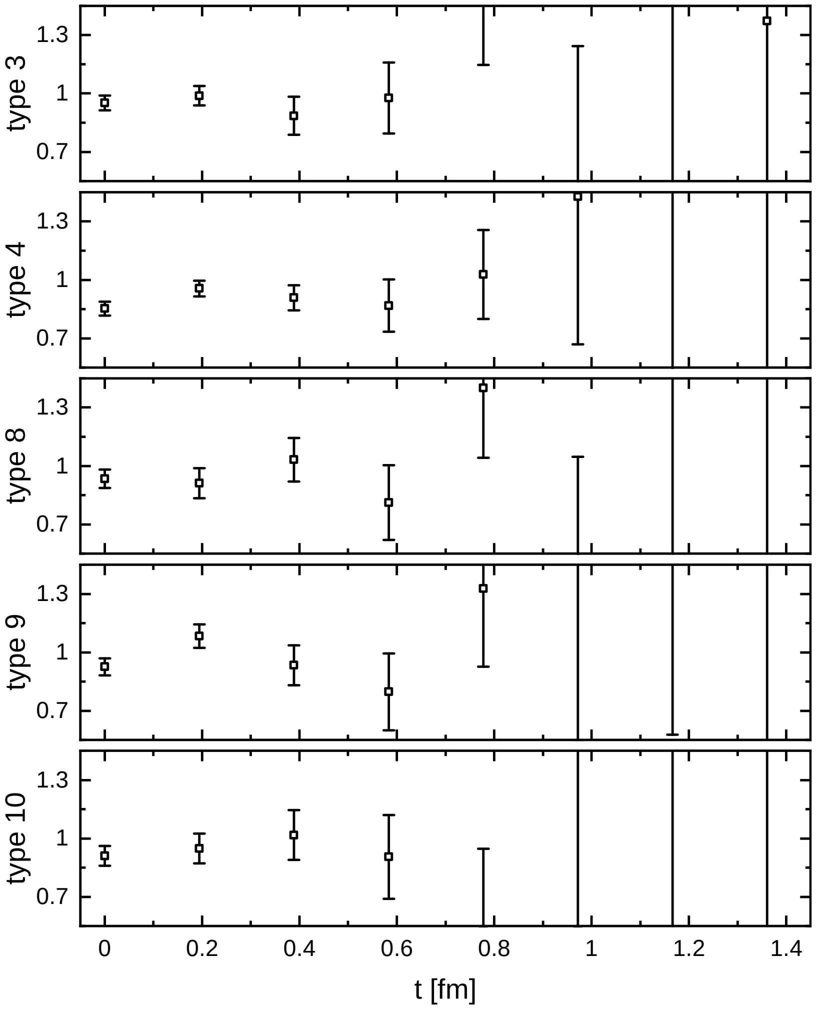


- There are also disconnected diagrams – notorious for high cost and bad S/N ratio

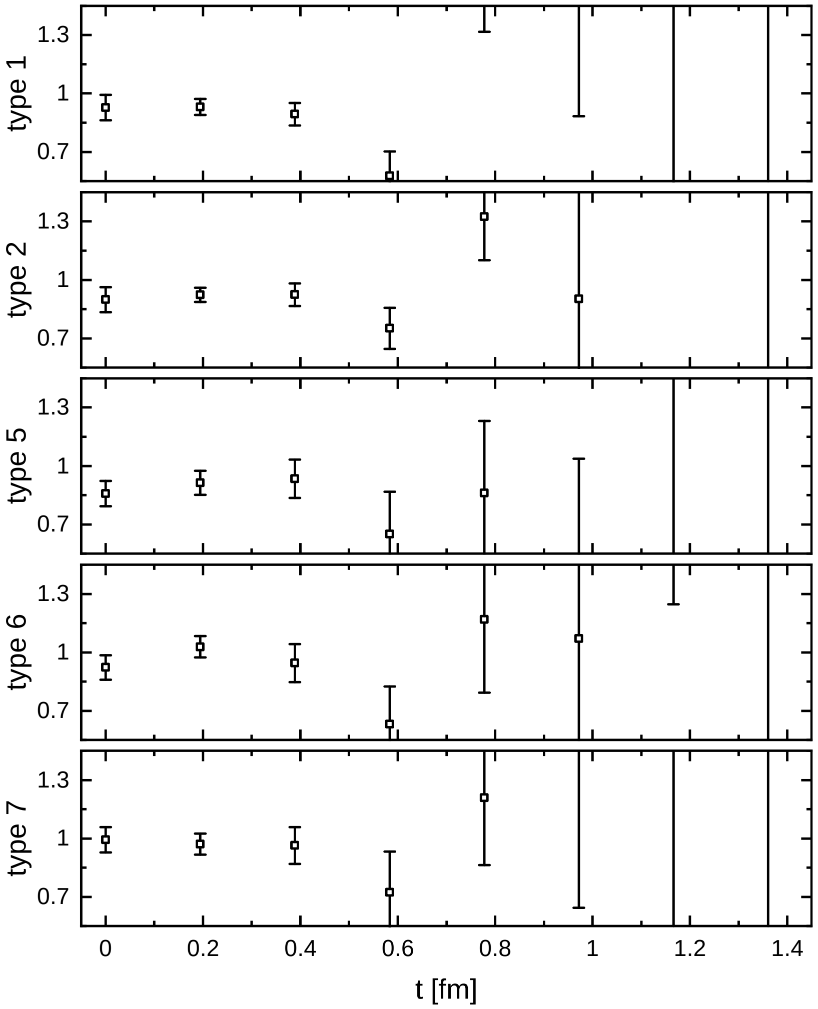


Our calculation contains both connected and the main disconnected diagrams

Challenges from TPE (3): Computation of 4-point function



Two currents inserted in one quark line



Two currents inserted in two quark lines

Using the conditions such as charge conservation to verify the contraction code

Lattice results

- Gauge ensemble used – nearly physical pion mass

Ensemble	m_π [MeV]	L/a	T/a	a [fm]	$N_{\rm conf}$
24D	142	24	64	0.1943(8)	131

$$\Delta E_{\rm lat} = \begin{cases} 27.6(4.5)\ \mu\text{eV}, & \text{connected part,} \\ 2.1(2.1)\ \mu\text{eV}, & \text{disconnected part,} \\ 29.7(4.9)\ \mu\text{eV}, & \text{total contribution.} \end{cases}$$

- The total TPE contribution is given by

$$\Delta E_{\rm TPE} = 0.77 + 93.72 \cdot \langle r_p^2 \rangle - \Delta E_{\rm lat}$$

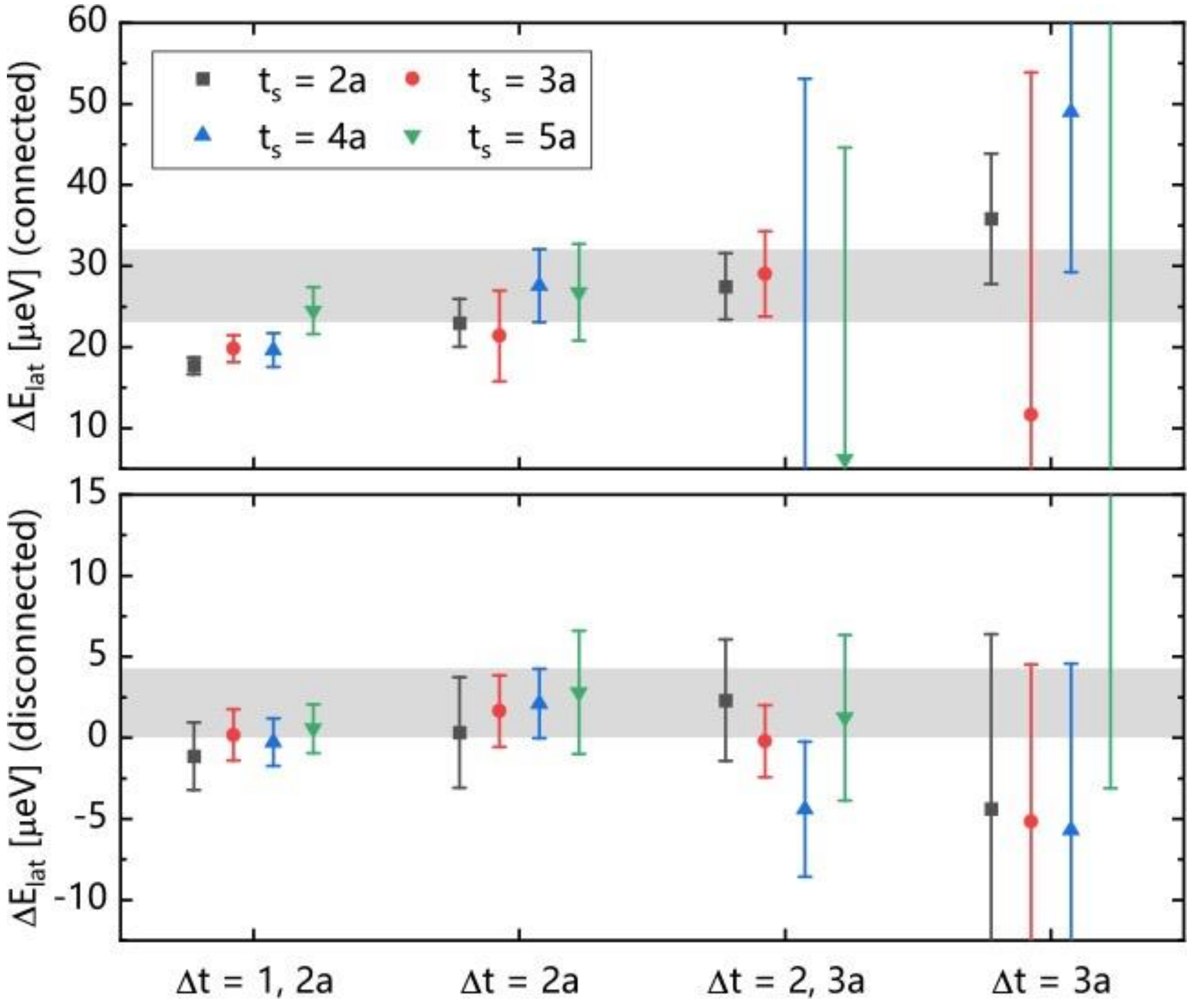
- Matching $\Delta E_{\rm TPE}$ with Exp. measurement, one gets

$$\sqrt{\langle r_p^2 \rangle} = 0.84136(65)\ \text{fm}$$

consistent with $0.84087(39)$ fm quoted by μH Exp

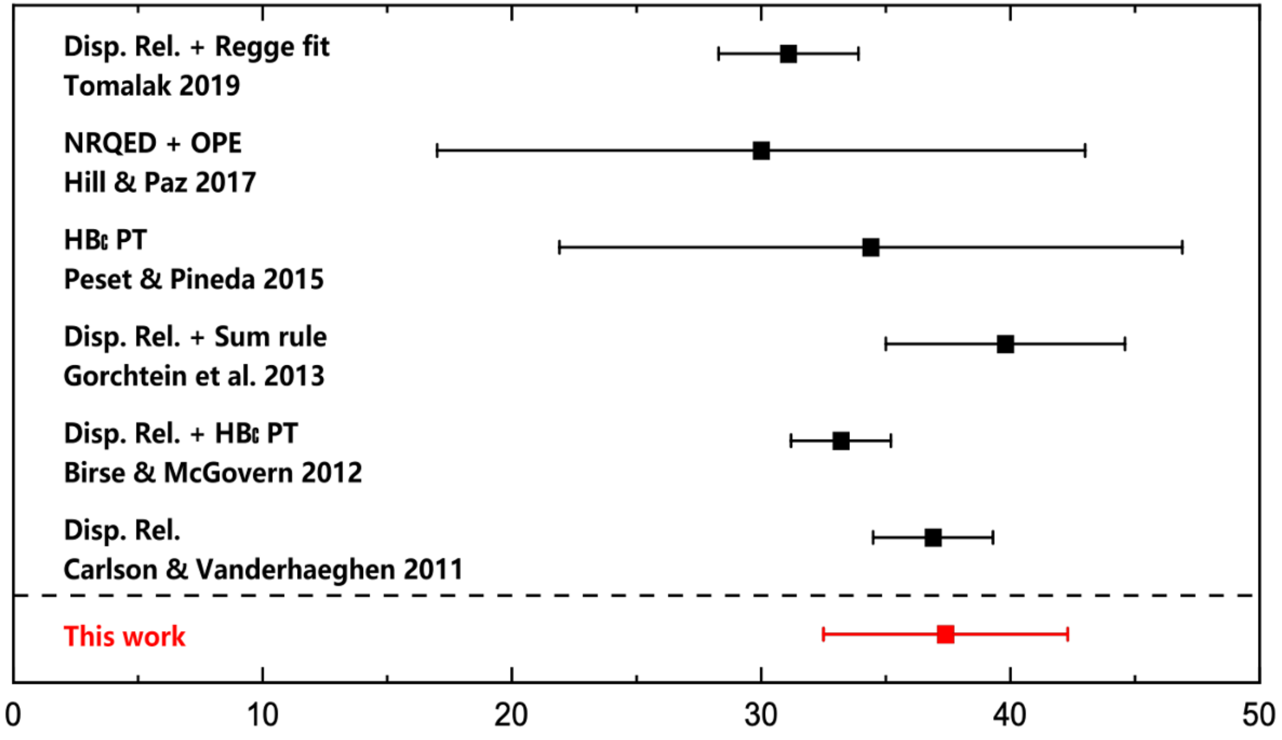
- Using μH value of charge radius as input, one gets

$$\Delta E_{\rm TPE} = 37.4(4.9)\ \mu\text{eV}$$



Lattice results

➢ Compared with other theoretical work



Y. Fu, XF, L. Jin, C. Lu, PRL 128 (2022) 17, 172002

Yang Fu (PhD, 5th year)
→ MIT postdoctor

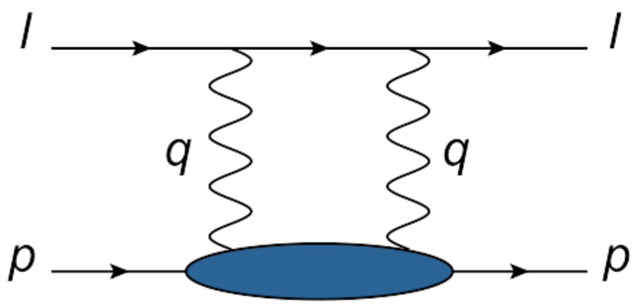
- First lattice result @ m_π=142 MeV

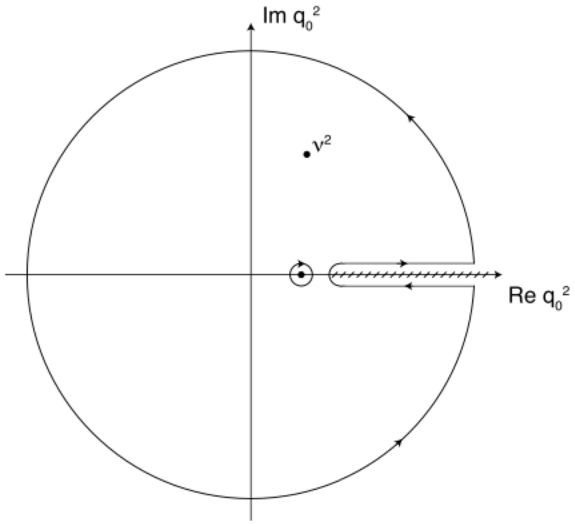
$$\Delta E_{\mathrm{TPE}} = 37.4(4.9) \quad \mu\mathrm{eV}$$

- Need to increase statistics and control systematic effects

Outlook: to help answer the question – what is the exact size of proton

Evaluate the subtraction function



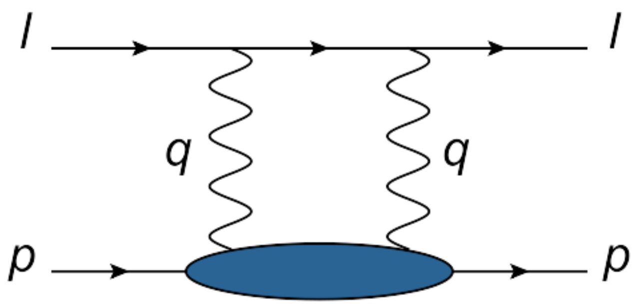


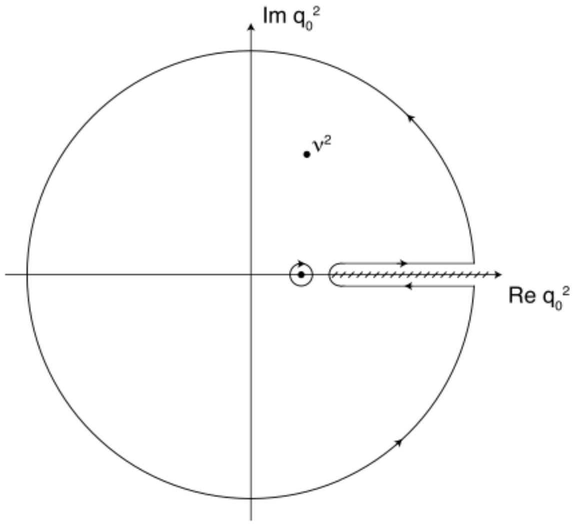
- Dispersion relation relate the scattering data to the TPE amplitude
- UV divergence requires the once-subtracted dispersion relation ➡ Subtraction function depends on model assumption
- F. Hagelstein & V. Pascalutsa propose a different subtraction point for lattice QCD calculation 【NPA 1016 (2021) 122323】

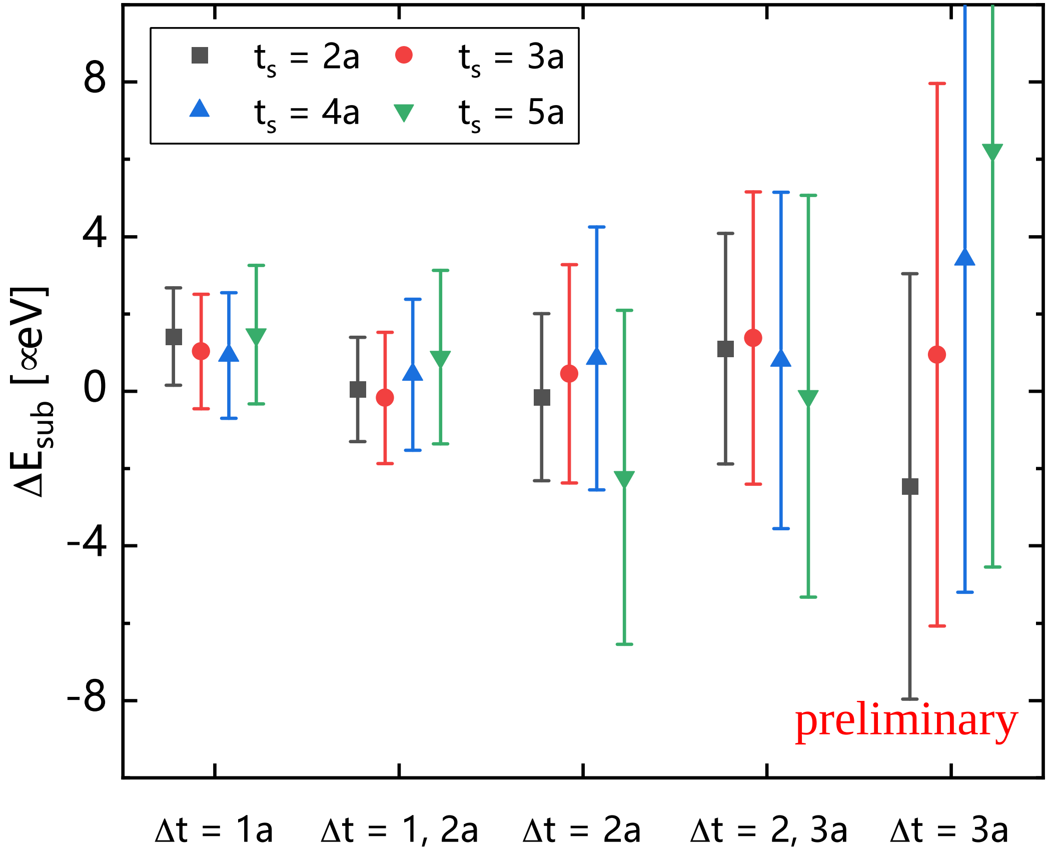
  Subtraction at (ν,Q^2)=(iQ,Q^2) rather than $(0,Q^2)$ ➡ Main non-Born contribution contained in the subtraction function

  See Franziska Hagelstein's talk this morning
- Our lattice calculation also favors this subtraction point
  - Statistical errors are reduced
  - Less requirement for the computation of hadronic function, only H_{ii}

Evaluate the subtraction function







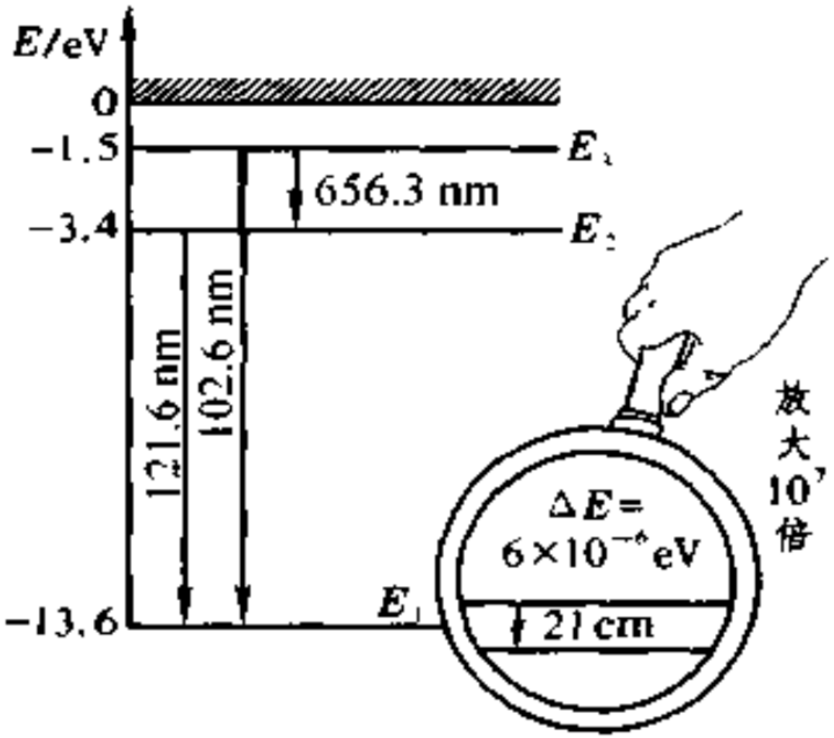
- Conventional subtraction function used in dispersion relation contains only the inelastic contribution
- Lattice results @m_π=142 MeV, with elastic and inelastic terms

  ➡ Separating elastic part requires the calculation of momentum dependence of form factors

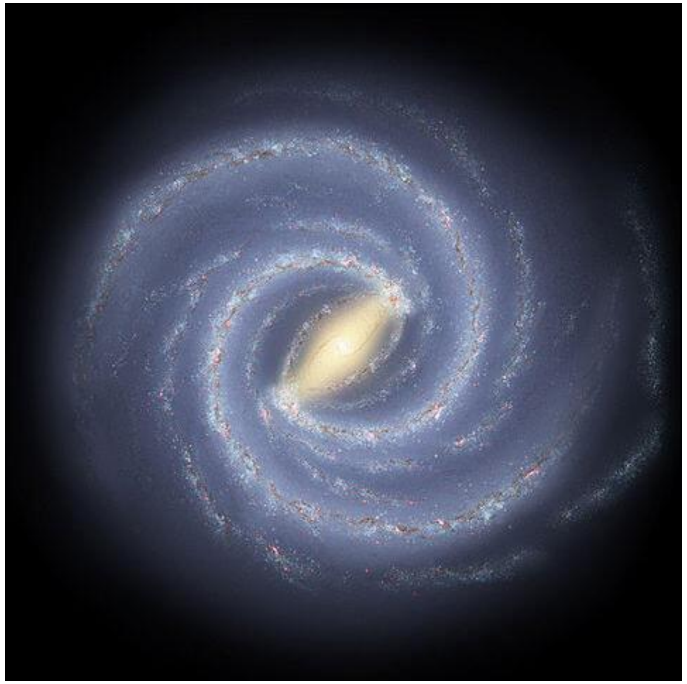
- Contribute <10% to the total TPE
- With disconnected diagrams, elastic + inelastic part consistent with 0

From Lamb shift to hyperfine splitting

- Hyperfine splitting arises from proton magnetic moment interacting with the magnetic field generated by the lepton



- Hydrogen 21cm line comes from hyperfine splitting



- It marked the birth of spectral-line radio astronomy
- In 1952 the first maps of hydrogen in the Galaxy were made and the spiral structure of the Milky Way was revealed

- Largest theoretical uncertainty to determine hyperfine splitting also originates from TPE

- Lamb shift is related to charge radius, while hyperfine splitting is related to proton magnetic moment. Thus in many aspects e.g. computational method and IR structure, they're quite different.

Another interesting theoretical research work!

From Lamb shift to hyperfine splitting

- Hydrogen hyperfine splitting

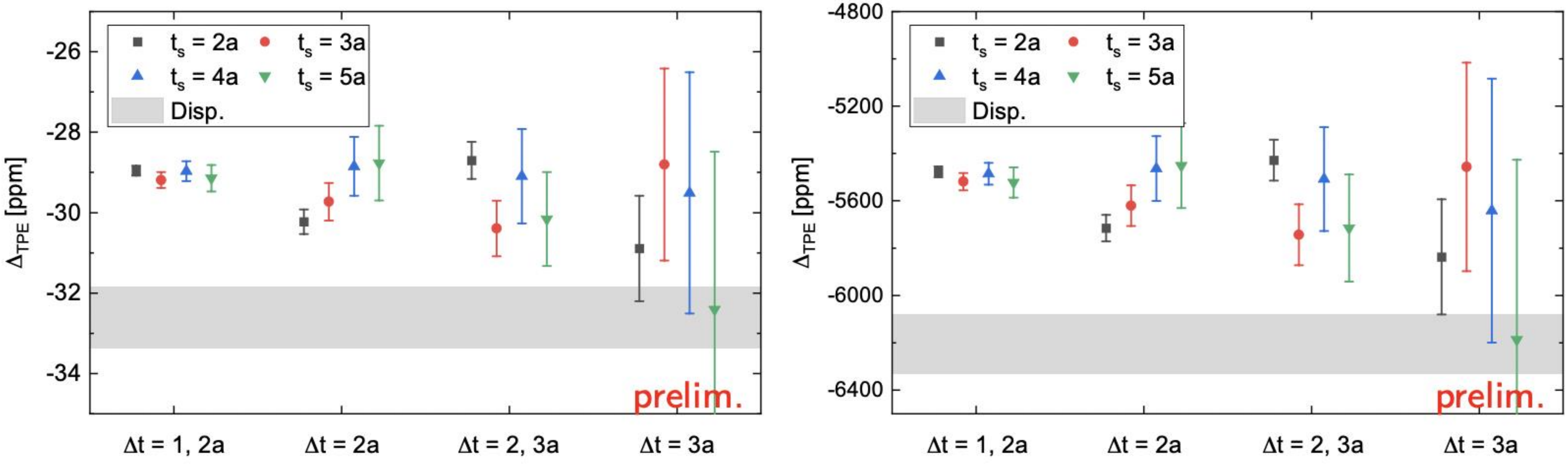
A. Antognini, F. Hagelstein, V. Pascalutsa, Ann. Rev. Nucl. Part. Sci. 72 (2022) 389

About E_{Fermi} see Carl Carlson's tak this morning

$$\Delta E_{\text{HFS}}(1S) = (1 + \Delta_{\text{structure-indep.}} + \Delta_{\text{TPE}}) \times E_{\text{Fermi}}(1S)$$
$$= (1 + 1136.861(2) \times 10^{-6} - 32.6(8) \times 10^{-6}) \times 1418840.1 \text{ kHz}$$

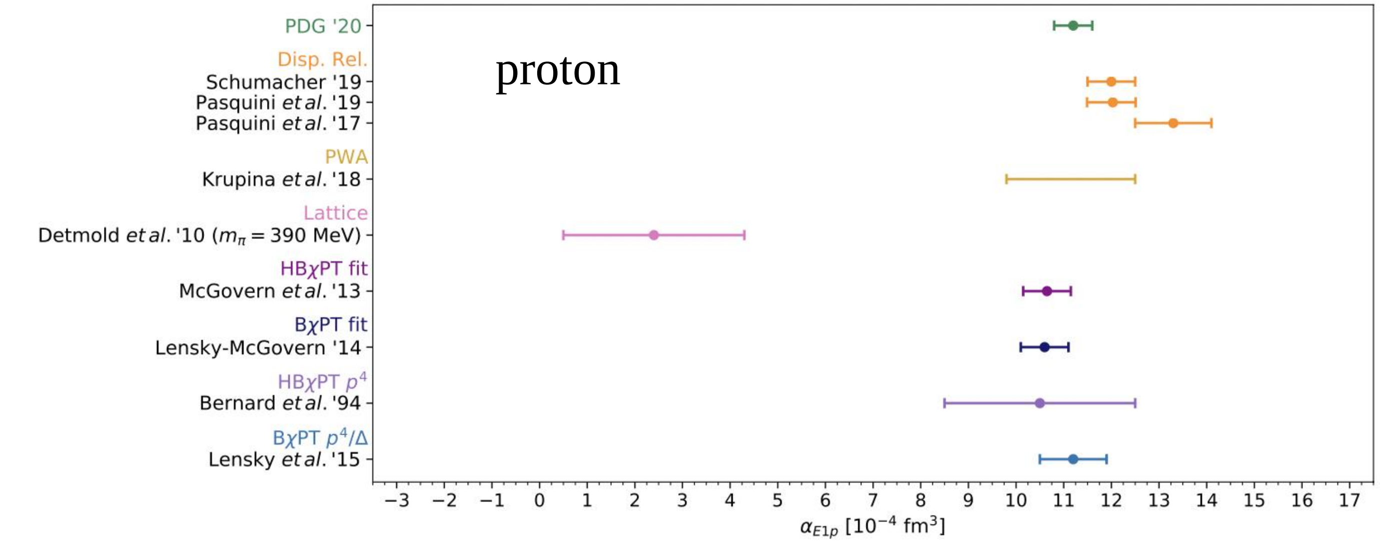
TPE contribution comes from dispersive analysis

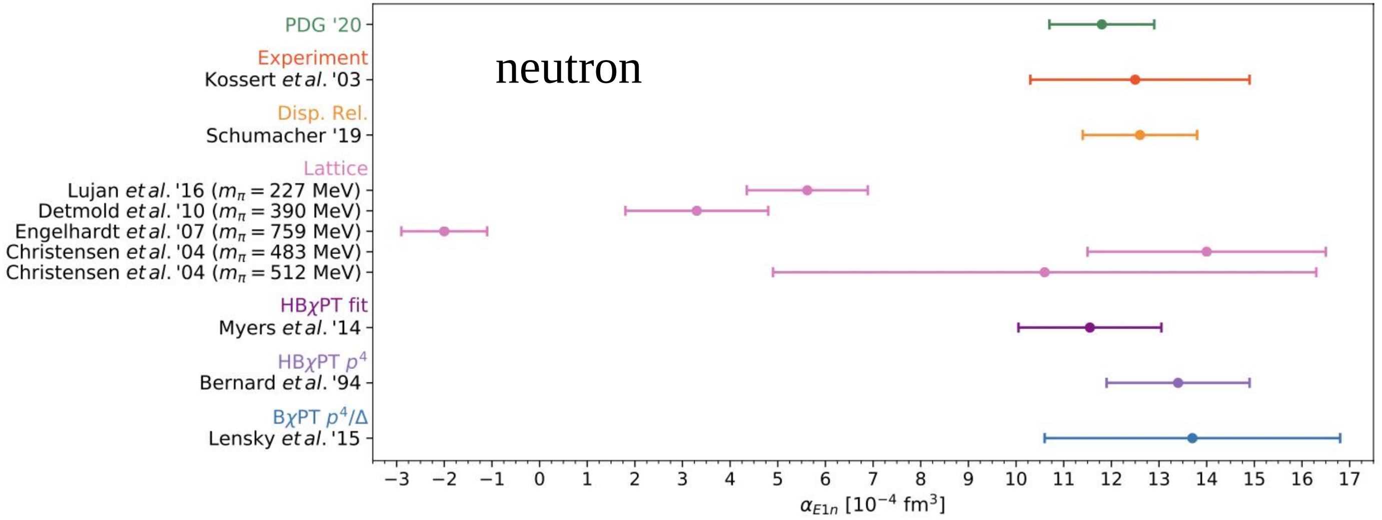
- Lattice results @ m_π=142 MeV, a=0.194 fm - hydrogen (left), muonic hydrogen (right)



Dispersive results from O. Tomalak, Eur. Phys. J. A 55 (2019) 64

Electric polarizability from lattice QCD





Summary by Franziska Hagelstein, Symmetry 12 (2020) 1407

- Previous calculations are performed at unphysical pion mass, ranging from 227 – 759 MeV
- External E&M field are incorporated as background
  - Only two-point correlation are required
  - Uniform E&M field distorted by finite volume
    - Quantized value for field → not so weak
    - Dirichlet boundary condition → tune the point to reduce the effects caused by the boundary
- Extract polarizability directly from Compton tensor

Also suggested by Frank Lee's talk on Tuesday

Electric polarizability from lattice QCD

- Unpolarized VVCS

$$T^{\mu\nu} = \int d^4x e^{i\mathbf{q}\cdot\mathbf{x}} \langle p|\mathcal{T}[J^\mu(t,\mathbf{x})J^\nu(0)]|p\rangle = T^{\mu\nu}_{Born} + \frac{2M}{\alpha_{em}}[-\beta_M \mathcal{K}_1^{\mu\nu} + (\alpha_E+\beta_M)\mathcal{K}_2^{\mu\nu}]$$

- Set up momentum for proton $P=(M,\mathbf{0})$ and photon $q=(0,\boldsymbol{\xi})$

$$\frac{2M}{\alpha_{em}}\alpha_E^N = \left(\frac{\partial T^{00}}{\partial \xi^2} - \frac{\partial T^{00}_{Born}}{\partial \xi^2}\right)\Bigg|_{\xi\to 0}$$

- For proton

$$\frac{2M}{\alpha_{em}}\alpha_E = \frac{1}{2M^2} + \frac{2}{3}\langle r_E^2\rangle + \frac{\kappa^2}{2M^2} + \left(\frac{t_s}{M} + t_s^2 + \frac{4}{3}M\langle r_E^2\rangle t_s\right) + \int_{|t|<t_s} d^4x \left(-\frac{|\mathbf{x}|^2}{6}\right) H(\mathbf{x},t)$$

Long-distance part   Short-distance part

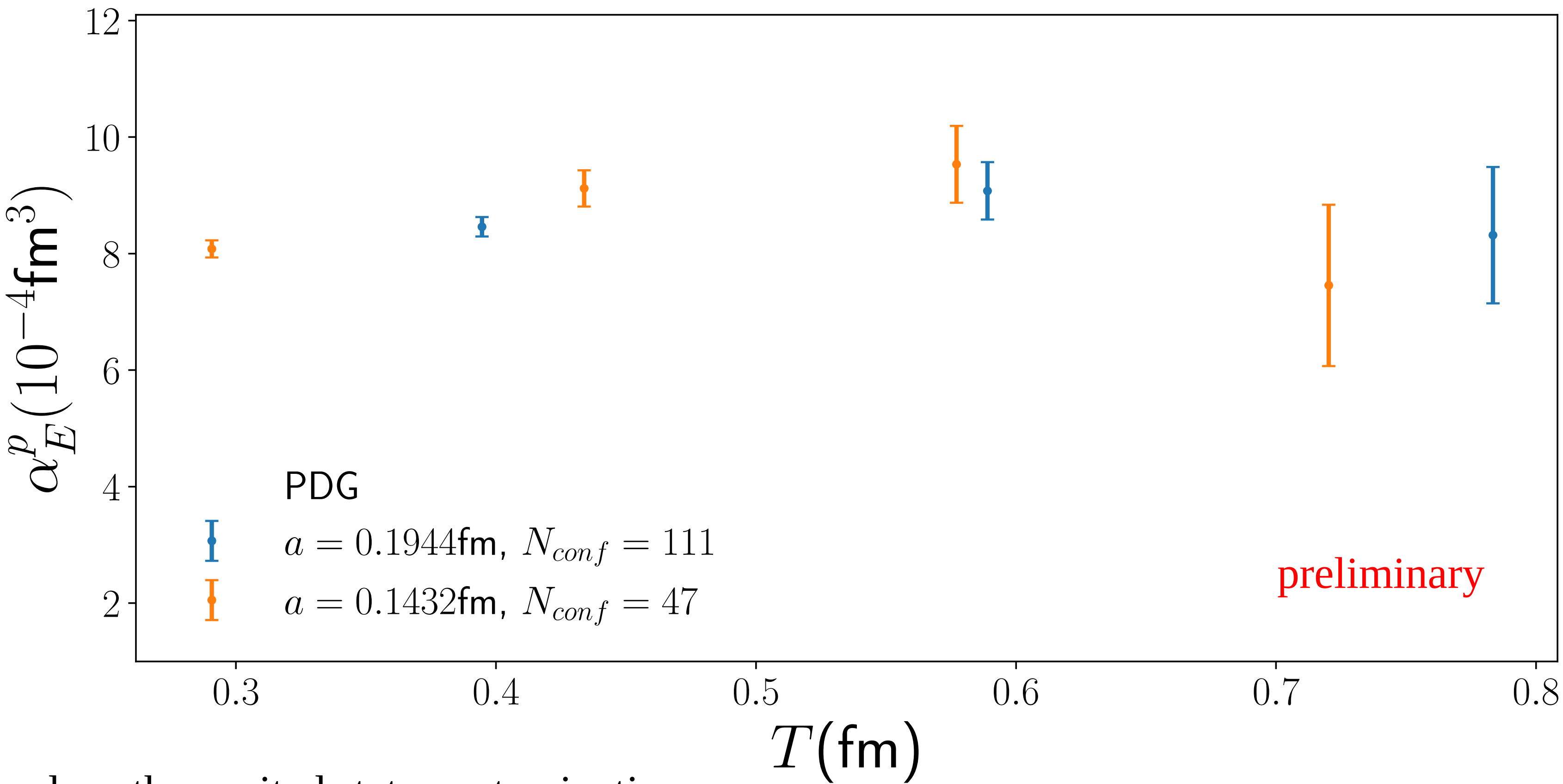
- For neutron

$$\frac{2M}{\alpha_{em}}\alpha_E^{(n)} = \frac{\kappa_{(n)}^2}{2M^2} + \int_{|t|<t_s} d^4x \left(-\frac{|\mathbf{x}|^2}{6}\right) H_{(n)}(\mathbf{x},t)$$

Lattice results for proton electric polarizability

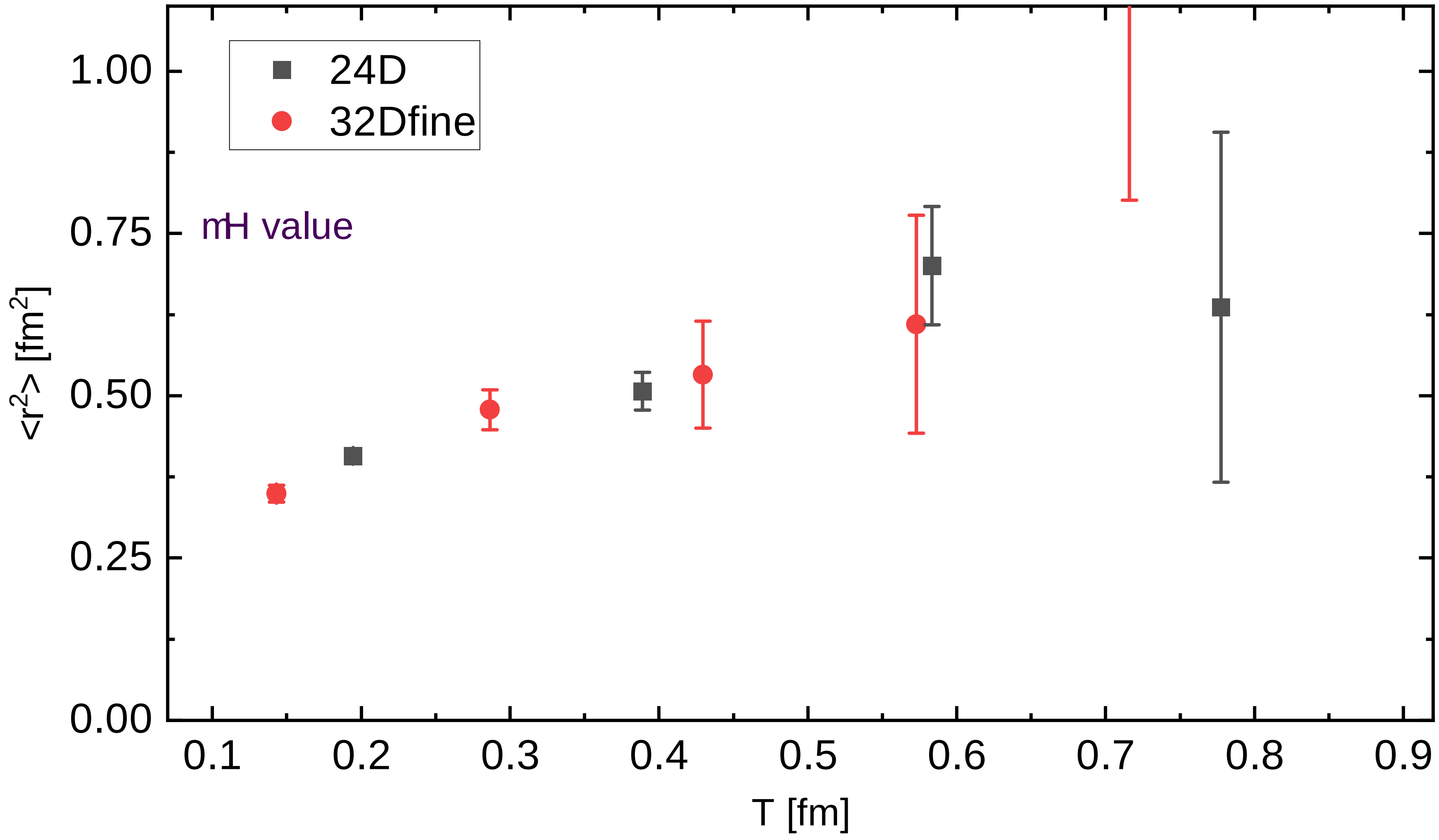
$$\frac{2M}{\alpha_{em}}\alpha_E = \frac{1}{2M^2} + \frac{2}{3}\langle r_E^2\rangle + \frac{\kappa^2}{2M^2} + \left(\frac{t_s}{M} + t_s^2 + \frac{4}{3}M\langle r_E^2\rangle t_s\right) + \int_{|t|<t_s} d^4x\left(-\frac{|\mathbf{x}|^2}{6}\right)H(\mathbf{x},t)$$

X.-H. Wang (PhD 3rd year)



- ➢ Using summation method to reduce the excited state contamination
- ➢ Maximal source-sink separation T+2a is 1.16 fm and 0.86 fm, respectively

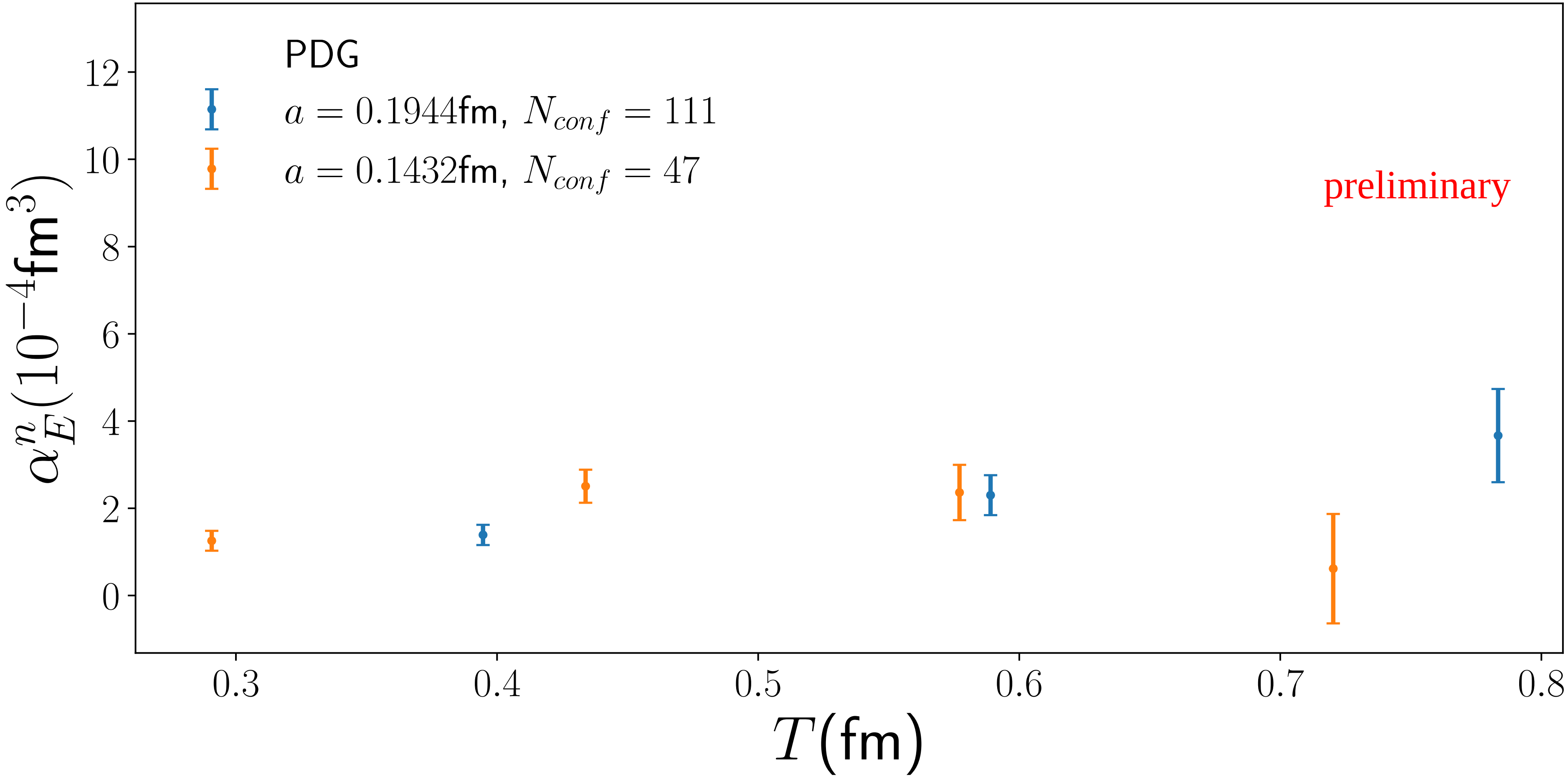
Long-distance contribution reproduces charge radius



- Charge radius from 4-point correlation function is noisy, but consistent with μH value

Lattice results for neutron electric polarizability

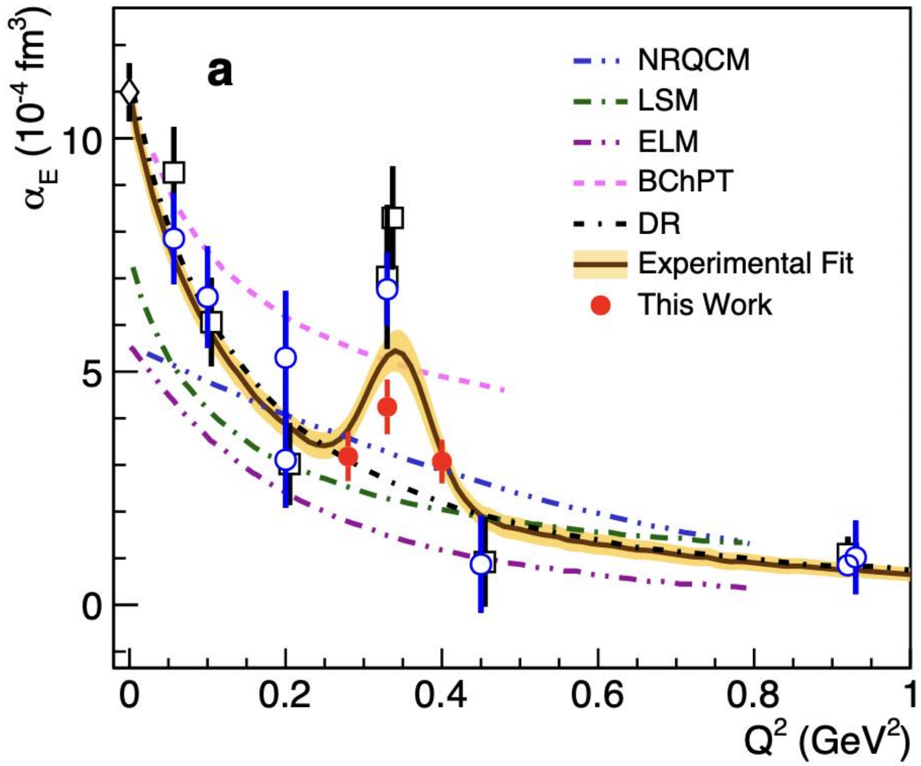
$$\frac{2M}{\alpha_{em}}\alpha_E^{(n)} = \frac{\kappa_{(n)}^2}{2M^2} + \int_{|t|<t_s} d^4x \left(-\frac{|\mathbf{x}|^2}{6}\right) H_{(n)}(\mathbf{x},t)$$



- Much smaller value for neutron electric polarizability
- Add disconnected diagram, increase statistics and further reduce systematics

Future directions to explore

- Q^2-dependence of E&M polarizability for VVCS
- Q^2-dependence of E&M polarizability for VCS



R. Li, N. Sparveris, et. al. Nature 611 (2022) 265

OR

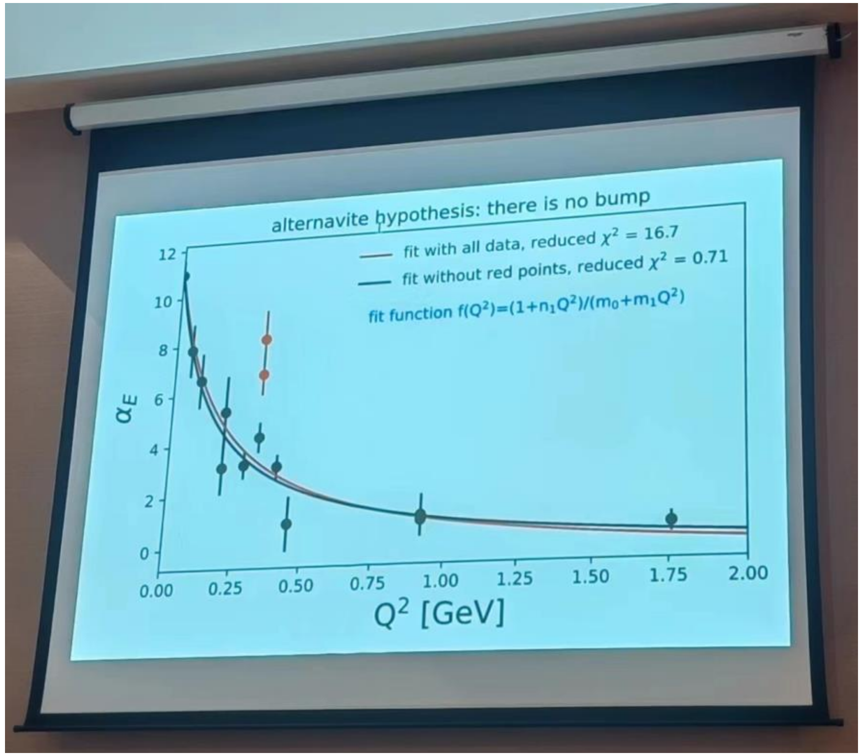
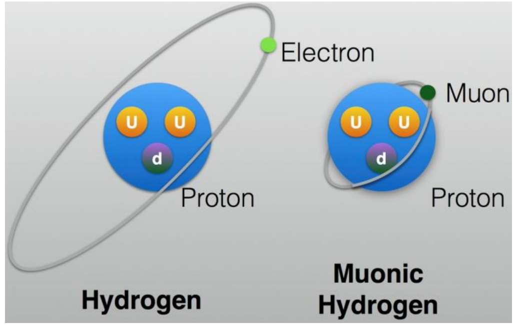


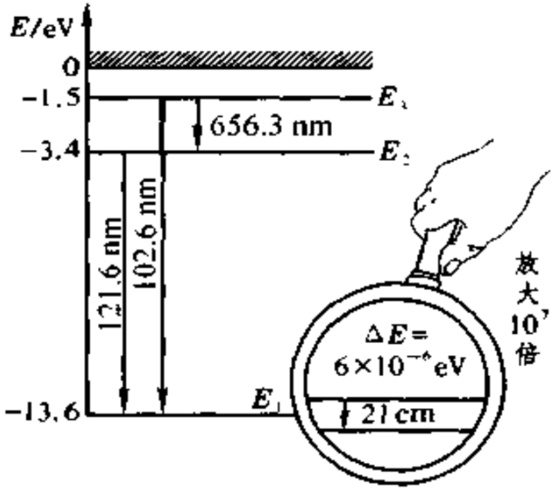
Figure shown by D. Higinbotham on Tuesday

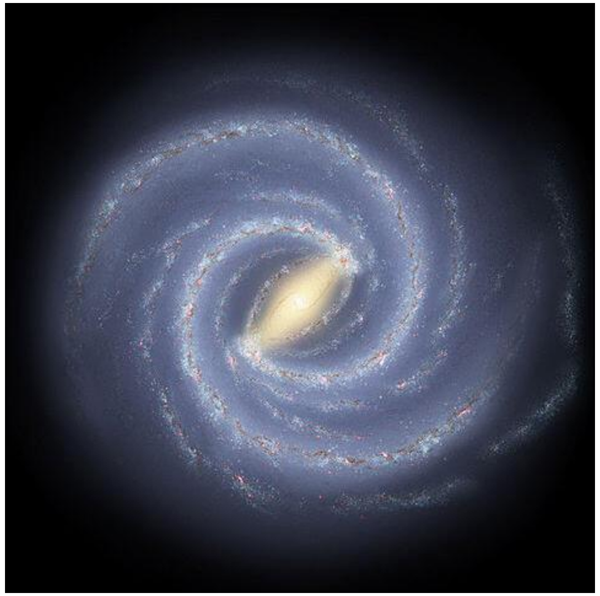
- Spin polarizability [Summary talk by M. Vanderhaeghen on Monday & talk by A. Deur on Tuesday]
- …

Conclusion

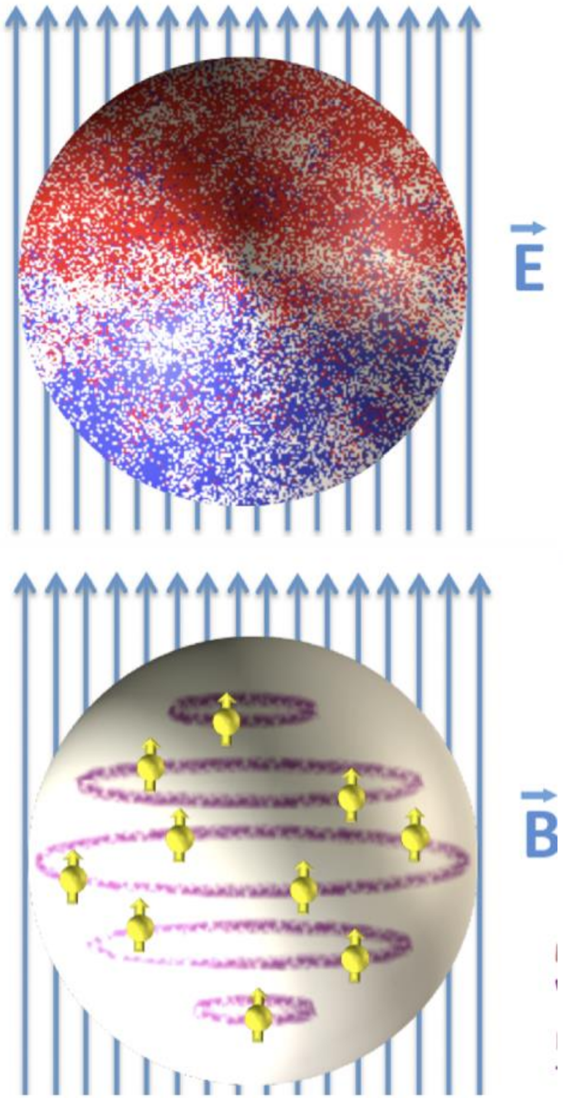


Lamb shift

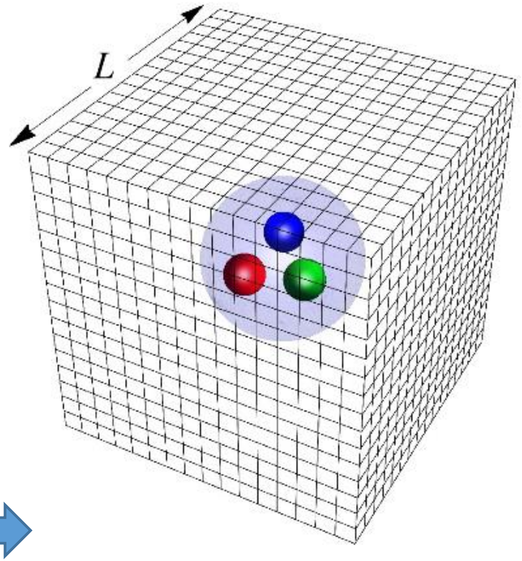


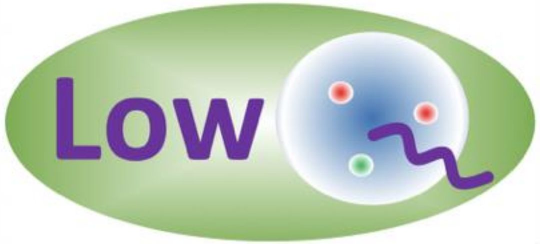


Hyperfine splitting



E&M polarizability





Nucleon structure at low Q is an exciting field for lattice QCD to explore!