Challenges and opportunities in Lattice QCD simulations and related fields
R-CCS workshop@Kobe (Feb. 15-17, 2023)

Nucleon structure from lattice QCD on $(10\ \mathrm{fm})^4$ lattices at the physical point

Shoichi Sasaki for PACS Collaboration

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In collaboration with: Y. Aoki, K.-I. Ishikawa, Y. Kuramashi, E. Shintani, R. Tsuji and T. Yamazaki

PACS Collaboration Members

PACS＝**P**rocessor **A**rray for **C**ontinuum **S**imulation

N. Ishizuka, Y. Kuramashi, E. Shintani, N. Ukita, T. Yamazaki, T. Yoshie — Tsukuba Univ.

Y. Aoki, Y. Nakamura, — RIKEN-CCS

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Nucleon Structure Project

PACS Collaboration Members

PACS = **P**rocessor **A**rray for **C**ontinuum **S**imulation

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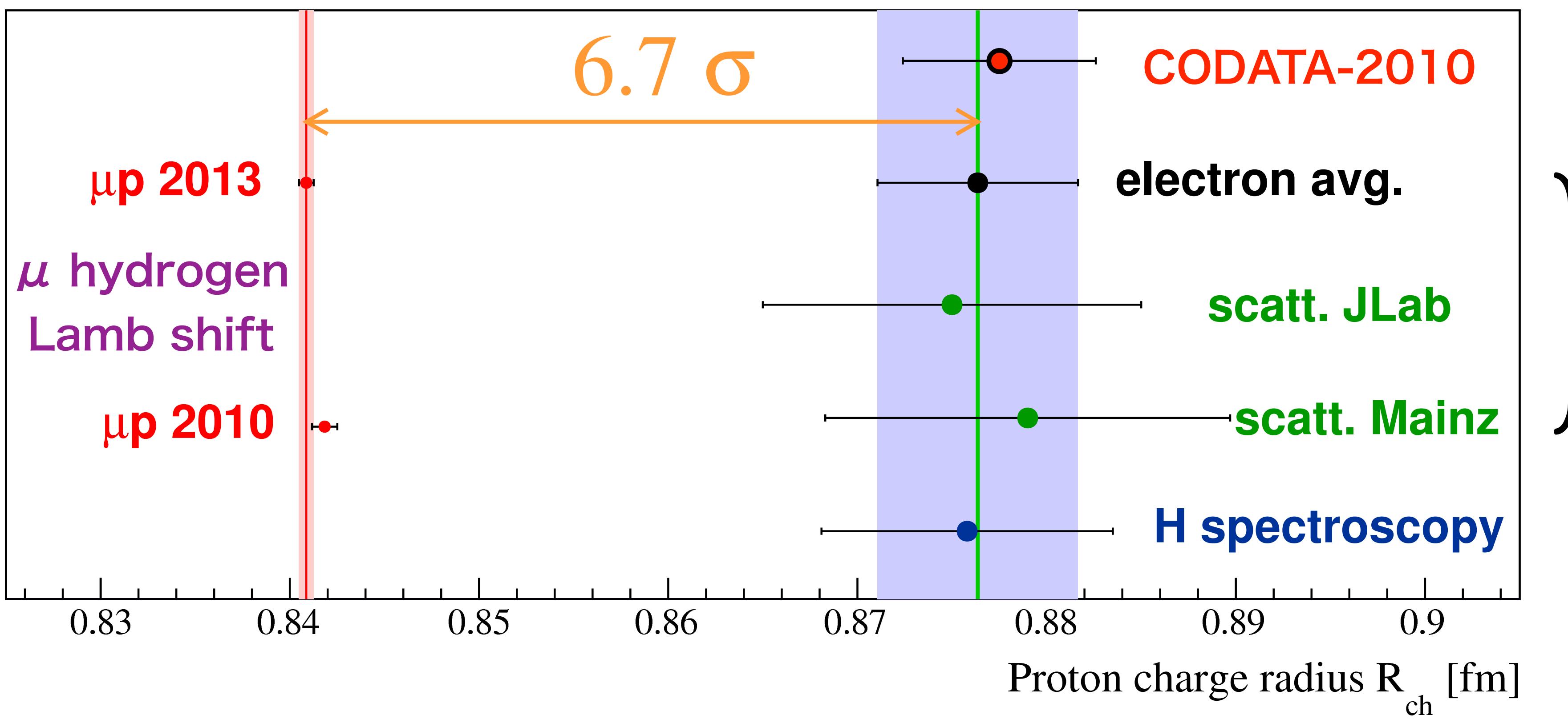
Poster session (today)

Nucleon Structure Project

Proton-size puzzle

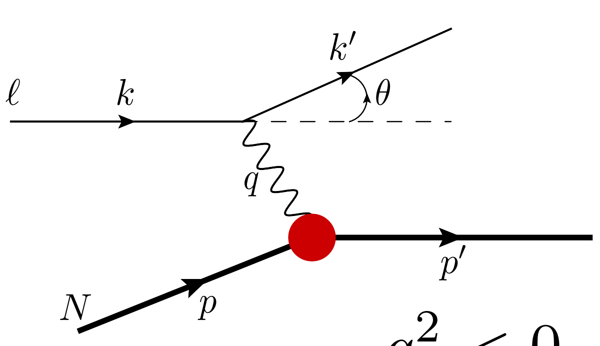
Proton charge radius : $G_E(q^2) = 1 - \frac{q^2}{6}\langle r^2\rangle_E + \mathcal{O}(q^4)$



ep scattering

Hydrongen Lamb shift

[Arrington, arXiv:1506.00873]



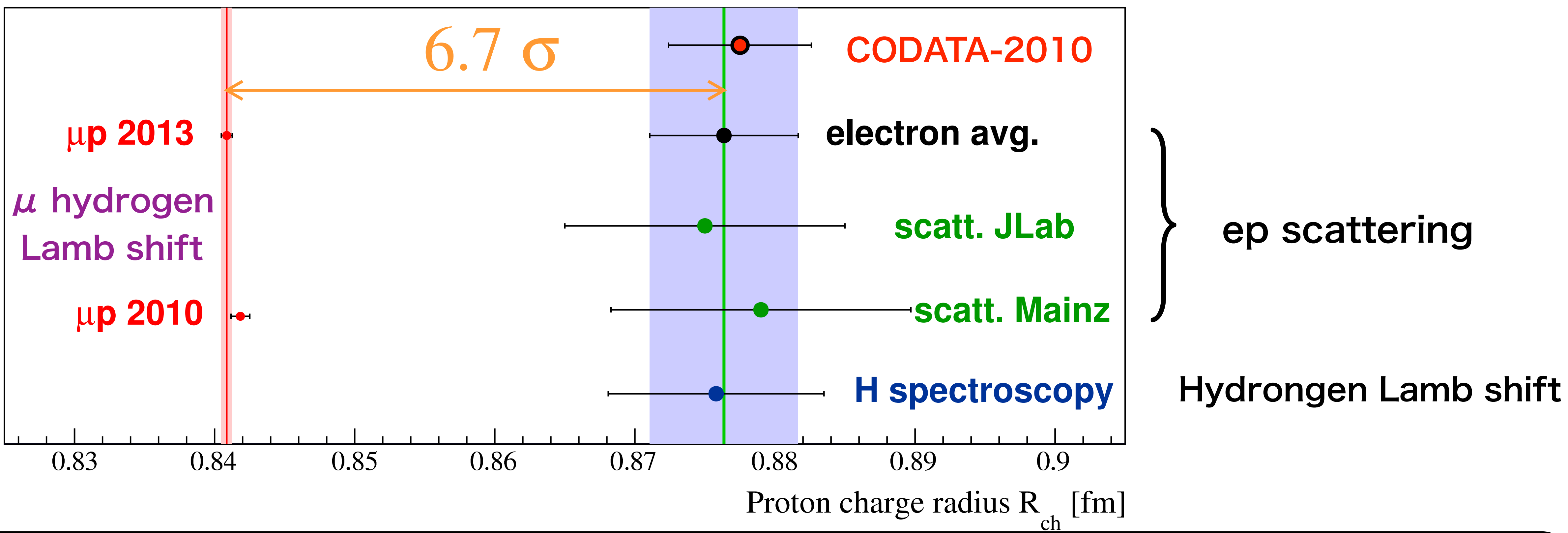
$q^2 < 0$

$$\langle p'|V^\mu(q)|p\rangle = \bar{u}(p')\left[\gamma^\mu F_1(q^2) + i\sigma^{\mu\nu}\frac{q_\nu}{2M}F_2(q^2)\right]u(p)$$

$$= \bar{u}(p')\left[\frac{(p'+p)^\mu}{2M}\frac{G_E(q^2) - \frac{q^2}{4M^2}G_M(q^2)}{1-\frac{q^2}{4M^2}} + i\sigma^{\mu\nu}\frac{q_\nu}{2M}G_M(q^2)\right]u(p)$$

Proton-size puzzle

Proton charge radius : $$G_E(q^2) = 1 - \frac{q^2}{6}\langle r^2\rangle_E + \mathcal{O}(q^4)$$



An important opportunity to develop our understanding of nucleon structure using lattice QCD simulations

Our strategy

✓ Use **PACS10** gauge configurations **(T. Yamazaki's talk on the last day)**

- **Physical point** → No chiral extrapolation
- **Very large spatial volume** → No finite size effect & Low q^2 physics
- **3 different lattice cut-offs** → Continuum limit (currently not available)

✓ **All-mode averaging technique** → High precision measurements

✓ **Highly tuned smearing** → Suppression of excited-state contributions

Status of PACS10 projects

T. Yamazaki' talk (tomorrow)

Configuration	PACS10			HPCI
Resource	Oakforest-PACS → Fugaku			K-computer
N_f	2+1			2+1
m_π [MeV]	135			146
L [fm]	10 fm			8.1 fm
L^3 x T	$128^4(64^4)$	160^4	256^4	96^4
a [fm]	0.085	0.063	~0.04	0.085
Status	done	done	running	done
Nucleon FF	done	continuing	planning	done
SF, NPR	done	planning	N/A	done

Iso-vector quantities

electromagnetic current

$$J_\mu^{\rm em} = \frac{2}{3}\bar{u}\gamma_\mu u - \frac{1}{3}\bar{d}\gamma_\mu d + \cdots$$

$$= \frac{1}{2}\boxed{(\bar{u}\gamma_\mu u - \bar{d}\gamma_\mu d)} + \frac{1}{6}\boxed{(\bar{u}\gamma_\mu u + \bar{d}\gamma_\mu d)} = J_\mu^V + \frac{1}{3}J_\mu^S$$

iso-vector — iso-scalar

matrix element (ME)

proton $\langle p|J_\mu^{\rm em}|p\rangle = \langle p|J_\mu^V|p\rangle + \frac{1}{3}\langle p|J_\mu^S|p\rangle$

neutron $\langle n|J_\mu^{\rm em}|n\rangle = \langle n|J_\mu^V|n\rangle + \frac{1}{3}\langle n|J_\mu^S|n\rangle$

iso-spin symmetry

$$\langle p|J_\mu^S|p\rangle = \langle n|J_\mu^S|n\rangle$$

$$\langle p|J_\mu^V|p\rangle = -\langle n|J_\mu^V|n\rangle$$

$$\langle p|J_\mu^{\rm em}|p\rangle - \langle n|J_\mu^{\rm em}|n\rangle = \boxed{\langle p|\bar{u}\gamma_\mu u - \bar{d}\gamma_\mu d|p\rangle} = \boxed{\langle p|\bar{u}\gamma_\mu d|n\rangle}$$

proton ME — **neutron ME** — **iso-vector** — Weak process

Iso-vector part receives NO disconnected contribution in 2+1 flavor QCD

Our published results on coarse lattice (a=0.085 fm)

- Our **old** HPCI results (PRD98 (2018) 074510)
  - (**8.1 fm**)^3 spatial volume with m_π = **146 MeV**

	iso-vector obs.	HPCI(96^4)	Expt.
Vector	$\sqrt{\langle r_E^2 \rangle}$	0.92(10) fm	0.939(6) fm (e-p) 0.907(1) fm (μH)
Vector	$\mu_v = G_M(0)$	4.81(79)	4.70589
Vector	$\sqrt{\langle r_M^2 \rangle}$	1.44(41) fm	0.862(14) fm
Axial	$g_A = F_A(0)$	1.16(8)	1.2724(23)
Axial	$\sqrt{\langle r_A^2 \rangle}$	0.46(11) fm	0.67(1) fm

Five basic quantities are barely consistent with experimental values,

Our published results on coarse lattice (a=0.085 fm)

- Our **old** HPCI results (PRD98 (2018) 074510)
  - (**8.1 fm**)^3 spatial volume with m_π = **146 MeV**

	iso-vector obs.	HPCI(96^4)	error	Expt.
Vector	$\sqrt{\langle r_E^2 \rangle}$	0.92(10) fm	~11%	0.939(6) fm (e-p) 0.907(1) fm (μH)
	$\mu_v = G_M(0)$	4.81(79)	~16%	4.70589
	$\sqrt{\langle r_M^2 \rangle}$	1.44(41) fm	~28%	0.862(14) fm
Axial	$g_A = F_A(0)$	1.16(8)	~7%	1.2724(23)
	$\sqrt{\langle r_A^2 \rangle}$	0.46(11) fm	~24%	0.67(1) fm

Five basic quantities are barely consistent with experimental values, but their statistical uncertainties are very large.

Our published results on coarse lattice (a=0.085 fm)

- Our **old** HPCI results (PRD98 (2018) 074510)
  - (**8.1 fm**)^3 spatial volume with m_π = **146 MeV**
- Our **previous** PACS10 results (PRD99 (2019) 014510)
  - (**10.8 fm**)^3 spatial volume with m_π = **135** MeV
  - **All-mode-averaging technique** (E. Shintani et al., PRD91 (2015) 114511)

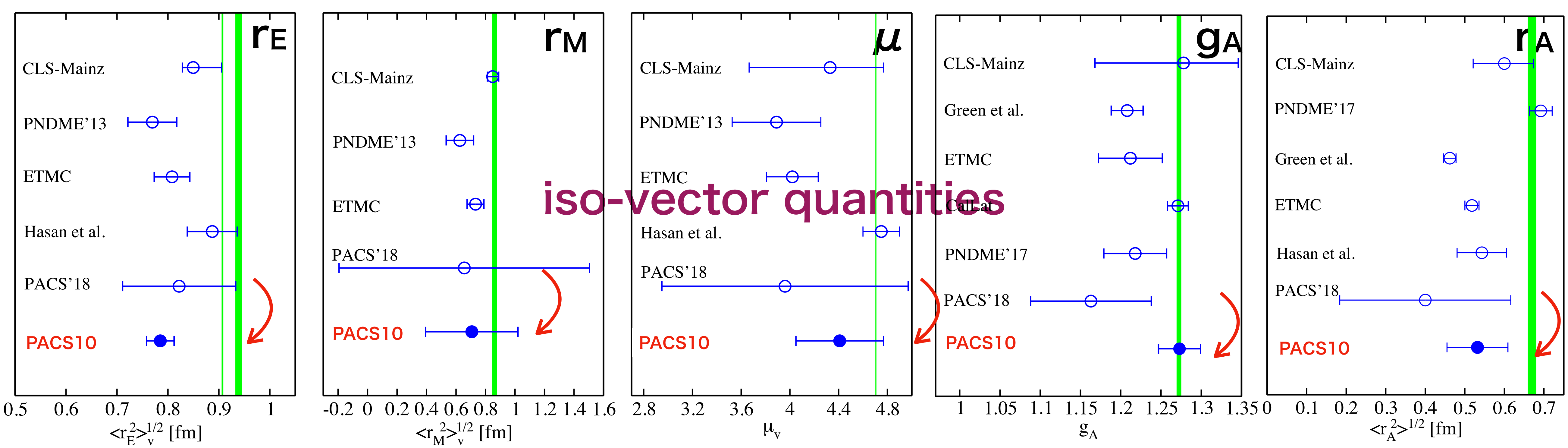
➡ gain **high statistical precision (a few % level)**

▶ **Five basic (isovector) quantities (r_E, r_M, μ, g_A, r_A)**

Our published results on coarse lattice (a=0.085 fm)

- Our **previous** PACS 10 results (PRD99 (2019) 014510)
  - (**10.8 fm**)^3 spatial volume with $m_\pi = \mathbf{135}$ MeV
  - **All-mode-averaging technique**

largely underestimated highly consistent underestimated



error

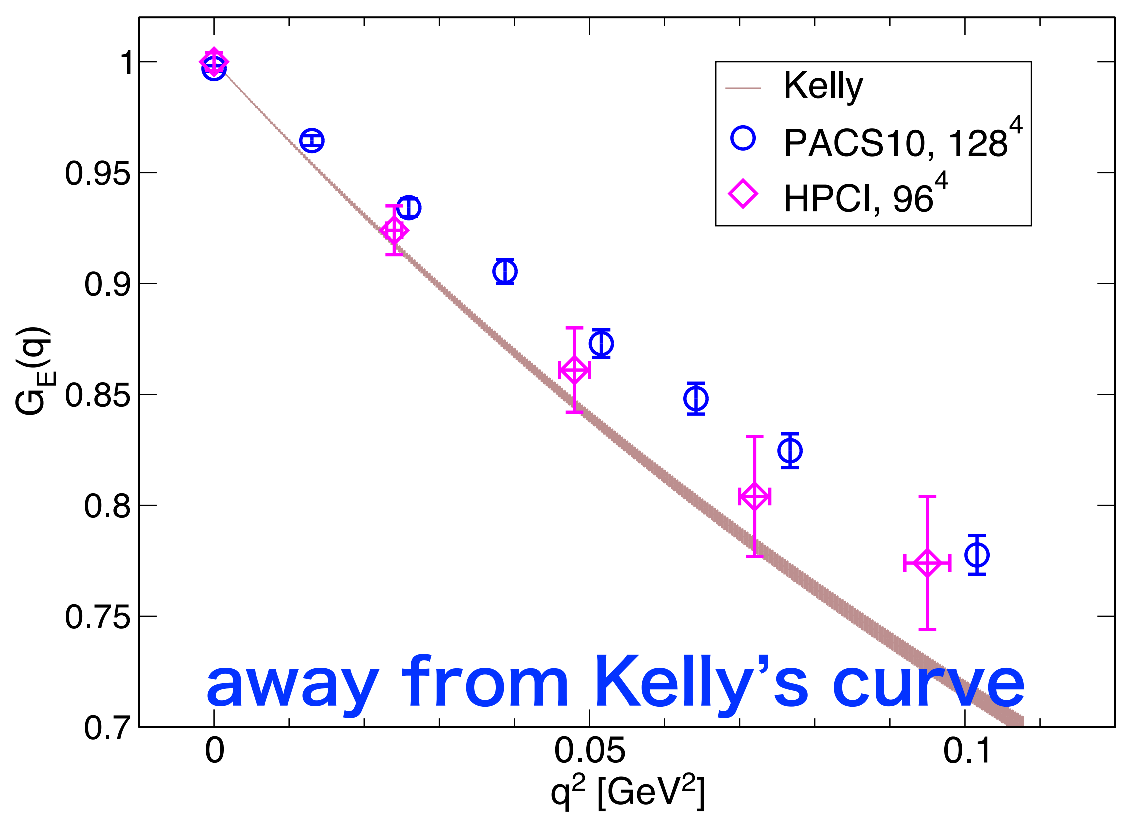
11% → 2% 28% →5% 16% →3% 7% →2% 24% →5%

Statistical uncertainties are significantly reduced thanks to all-mode averaging

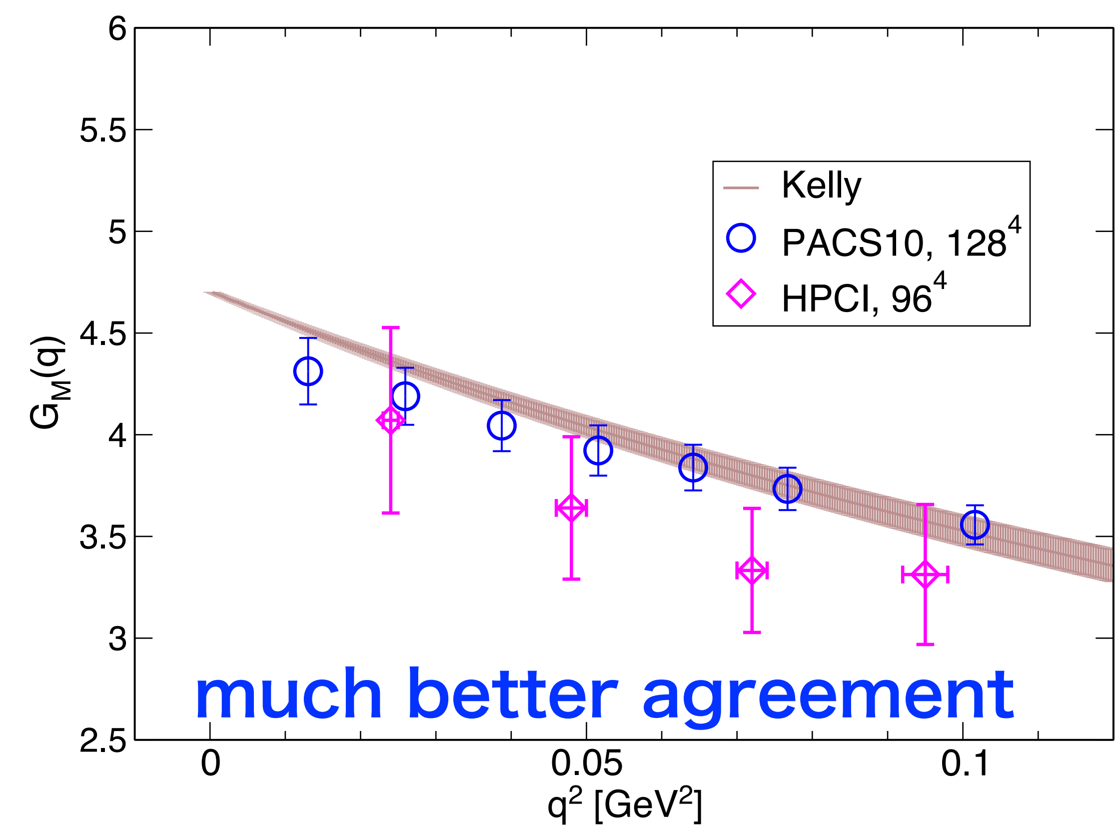
Our published results on coarse lattice (a=0.085 fm)

- Our **previous** PACS 10 results (PRD99 (2019) 014510)
  - (**10.8 fm**)^3 spatial volume with $m_\pi = $ **135** MeV
  - **All-mode-averaging technique**

Kelly's form factor parameterization, PRC70 (04) 068202



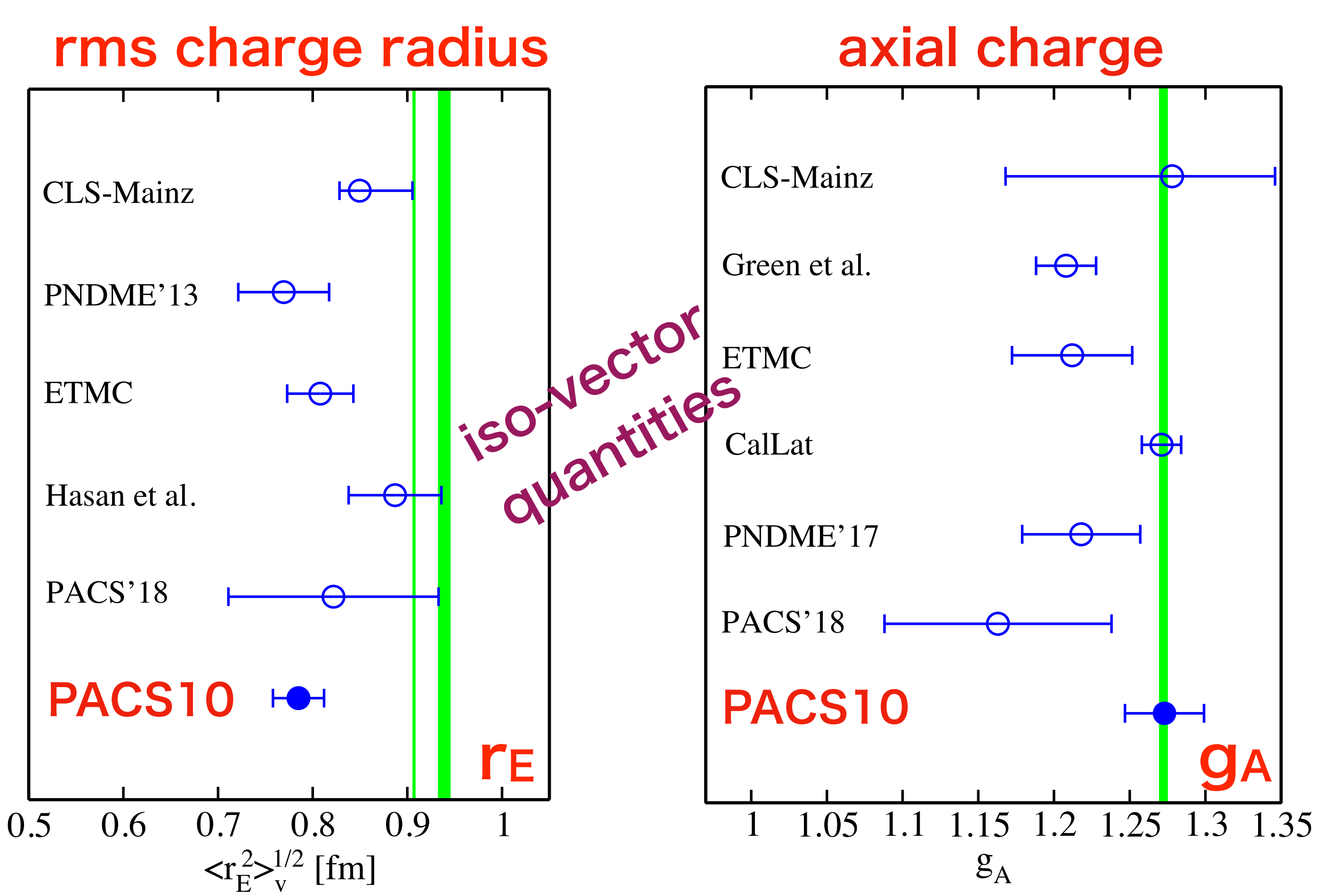
G_E form factor



G_M form factor

Topics covered in this talk

- Our **new PACS10** results at a=0.063 fm
  - $(\mathbf{10.1\ fm})^3$ spatial volume with $m_\pi = \mathbf{135}$ MeV
  - lattice discretization uncertainties on r_E and g_A

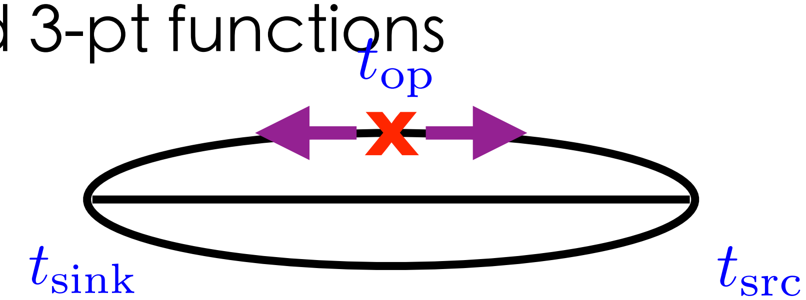


Current status of our nucleon project

	Previous results PRD99 (2019) 014510	Small Vol results PRD99 (2021) 074514	Preliminary results (Lattice 2022)
Volume	128^4 (10.9 fm)^4	64^4 (5.5 fm)^4	160^4 (10.1 fm)^4
lattice spacing	0.085 fm	0.085 fm	0.063 fm
m_π	135 MeV (physical)	138 MeV	135 MeV (physical)
$t_{sep}=\|t_{sink}-t_{src}\|$ dependence	t_{sep}/a=10, 12, 14, 16	t_{sep}/a=12, 14, 16	t_{sep}/a=13, 16, 19
observables	flavor diagonal (w/o disconnected contrib.)	iso-vector	flavor diagonal (w/o disconnected contrib.)

Measurement Details for $\mathbf{160^4}$

- Statistics: 19 configs (every 10 trajectories)
  - All-mode averaging technique (E. Shintani et al., PRD91 (2015) 114511)
    ➡ gain high statistical precision
  - O(100) measurements/config ⇒ O(10^3–10^4) measurements
- $L^3 \times T = 160^3 \times 160$ ⇒ (~10.1 fm)^3 spatial volume
- 7 choices for spatial momenta: $2\pi/L \times \vec{n}$
  - $\vec{n}$ = (1,0,0), (1,1,0), (1,1,1), (2,0,0), (2,1,0), (2,2,0)
  - minimum momentum=2π/L~122 MeV thanks to L~10.1 fm
  - allows to access FFs in the region of smaller Q^2
- Exponentially smeared src/sink operators for 2-pt and 3-pt functions
- 3 different src-sink separations: t_{sep}/a=13,16,19
  - fixed-sink in sequential source method



- Z_A and Z_V are not yet determined in SF scheme (in progress)

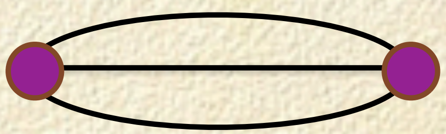
Nucleon correlation functions

- Compute **2-pt** and **3-pt** functions, using nucleon interpolator $\mathcal{H}$ and operator insertion $\mathcal{O}$

$\sum_i |i\rangle\langle i| = 1$

$$\langle \mathcal{H}(t)\mathcal{H}^\dagger(0)\rangle = \sum_i |\langle 0|\mathcal{H}(0)|i\rangle|^2 e^{-M_i t}$$

$$\rightarrow |\langle 0|\mathcal{H}|N\rangle|^2 e^{-M_N t}$$



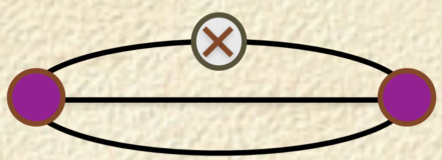
a sum of exponentials

$$\langle \mathcal{H}(t)\mathcal{O}(t')\mathcal{H}^\dagger(0)\rangle = \sum_{i,j} e^{-M_i(t-t')}\langle 0|\mathcal{H}|i\rangle\langle i|\mathcal{O}|j\rangle\langle j|\mathcal{H}^\dagger|0\rangle e^{-M_j t'}$$

$$\rightarrow |\langle 0|\mathcal{H}|N\rangle|^2 \langle N|\mathcal{O}|N\rangle e^{-M_N t}$$

$t - t' \gg 0$
and
$t' \gg 0$

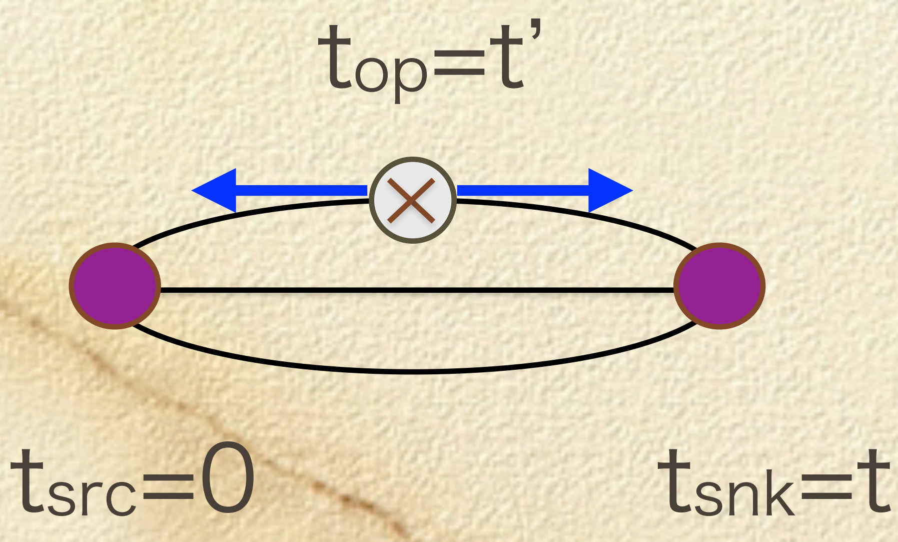
no t'-dependence

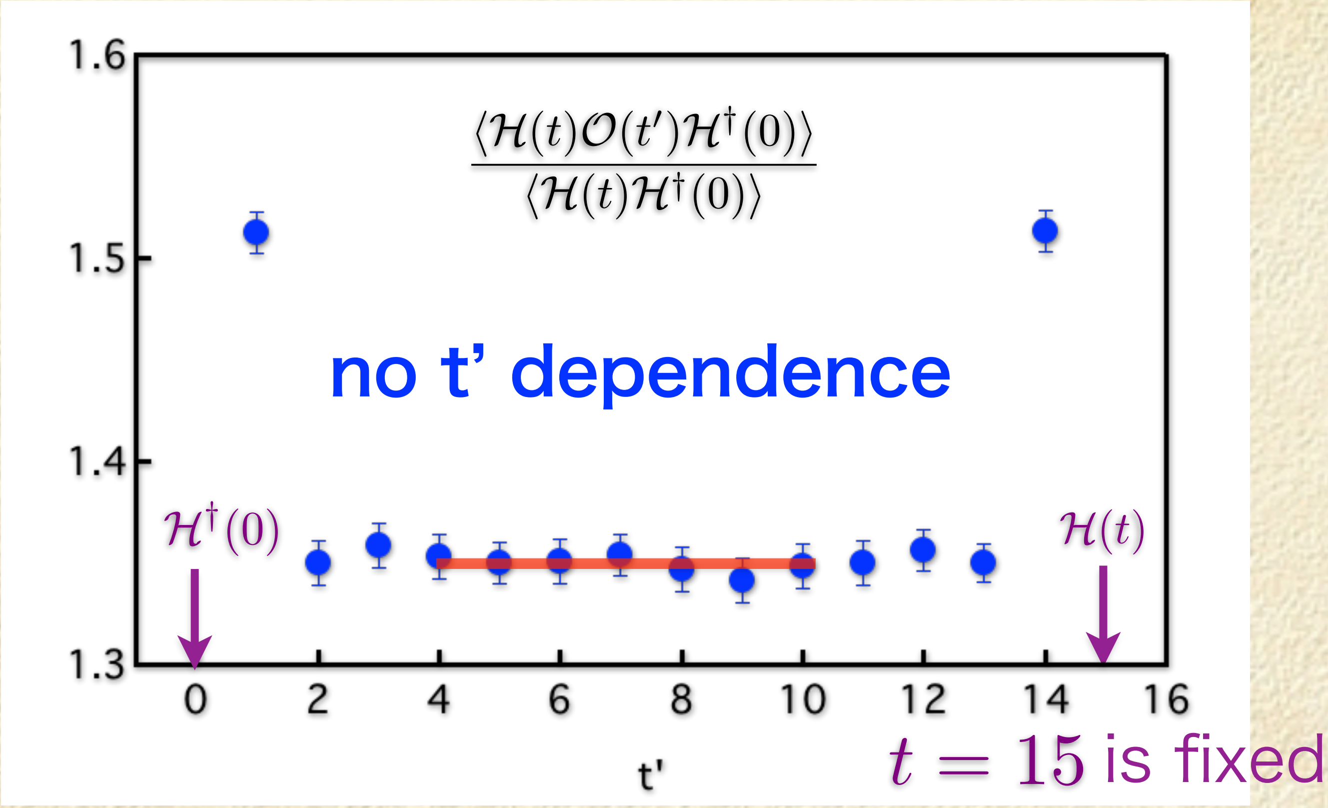


Ratio of 2-pt and 3-pt functions

✓matrix elements (form factors) can be determined from ratios of the 3-pt and 2-pt functions

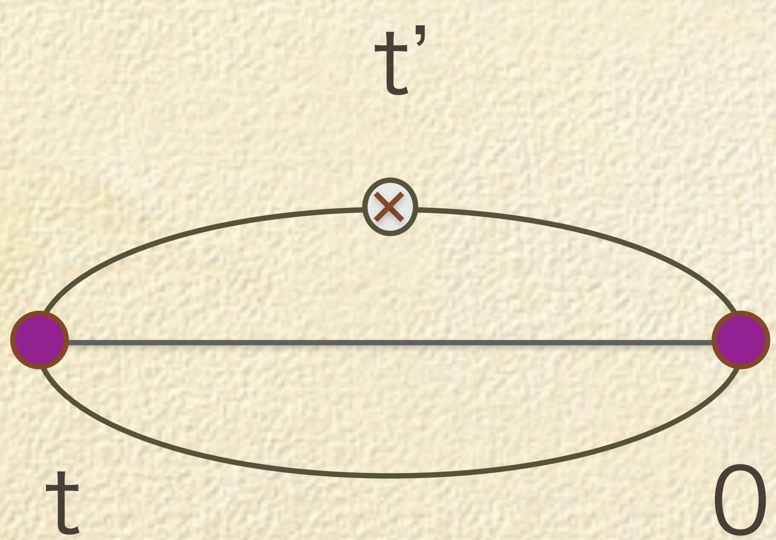
$$\frac{\langle \mathcal{H}(t)\mathcal{O}(t')\mathcal{H}^\dagger(0)\rangle}{\langle \mathcal{H}(t)\mathcal{H}^\dagger(0)\rangle} \to \langle N|\mathcal{O}|N\rangle$$



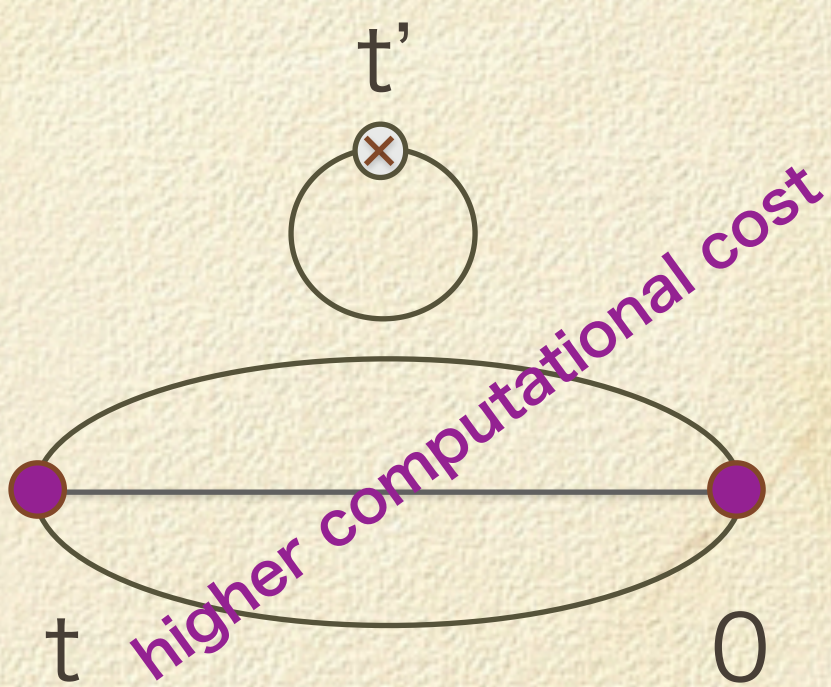


Connected/disconnected diagrams

$\langle \mathcal{H}(t)\mathcal{O}(t')\mathcal{H}^\dagger(0)\rangle$ has **two** types of quark contraction diagrams (Wick contractions)



connected contribution



disconnected contribution

✓ **iso-vector** quantities

✓ β-decay (weak matrix elements)

✓ **flavor diagonal** quantities

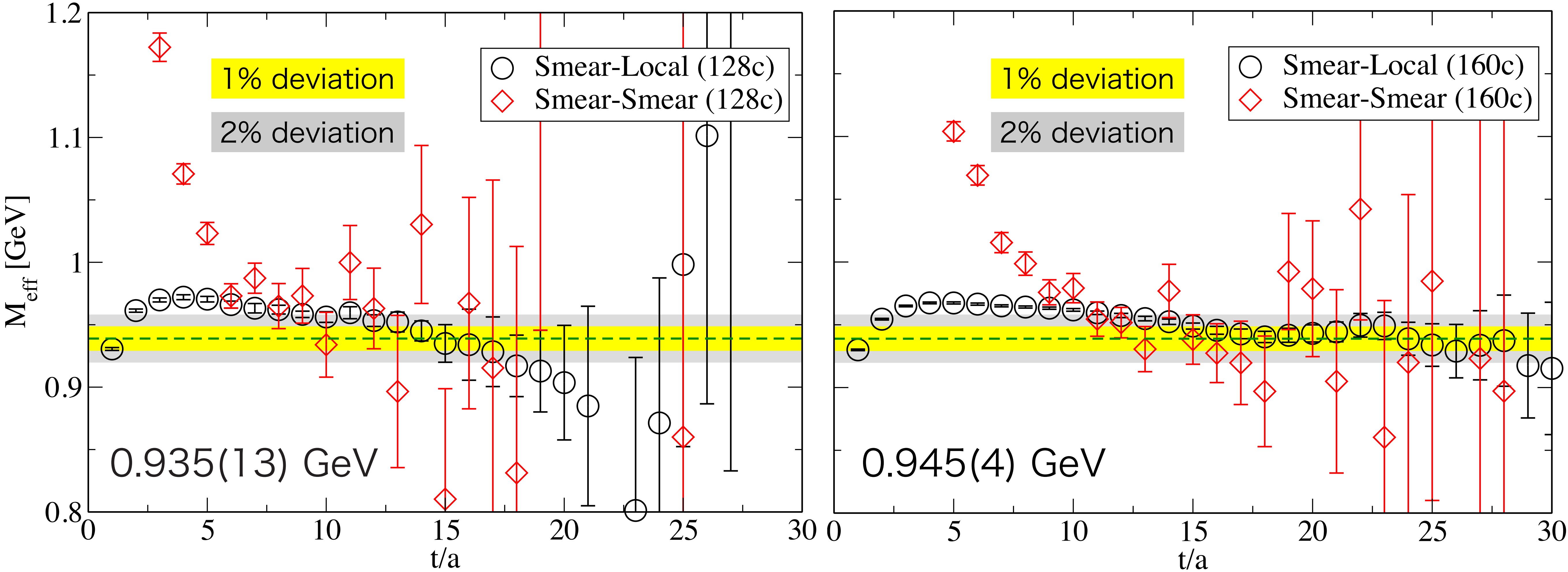
✓ electro-magnetic matrix elements

Nucleon mass

M_N

Effective mass plot for M_N

Smearing parameters are **highly tuned to maximize the ground-state dominance**.



L^4=128^4, a=0.085 fm L^4=160^4, a=0.063 fm

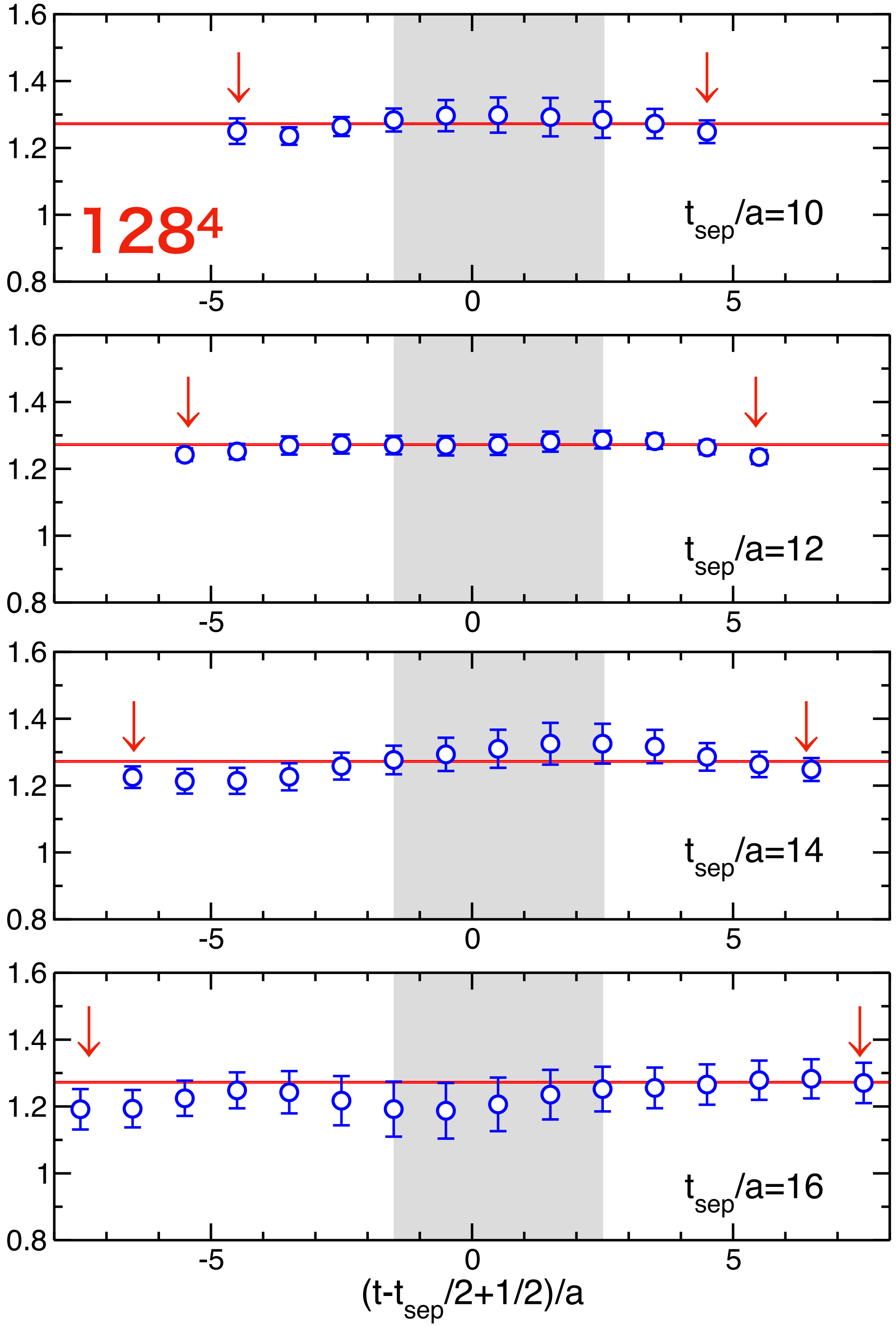
Achieving a percent level precision on the nucleon mass

Axial charge

g_A

Ratio for $F_A(0)=g_A$

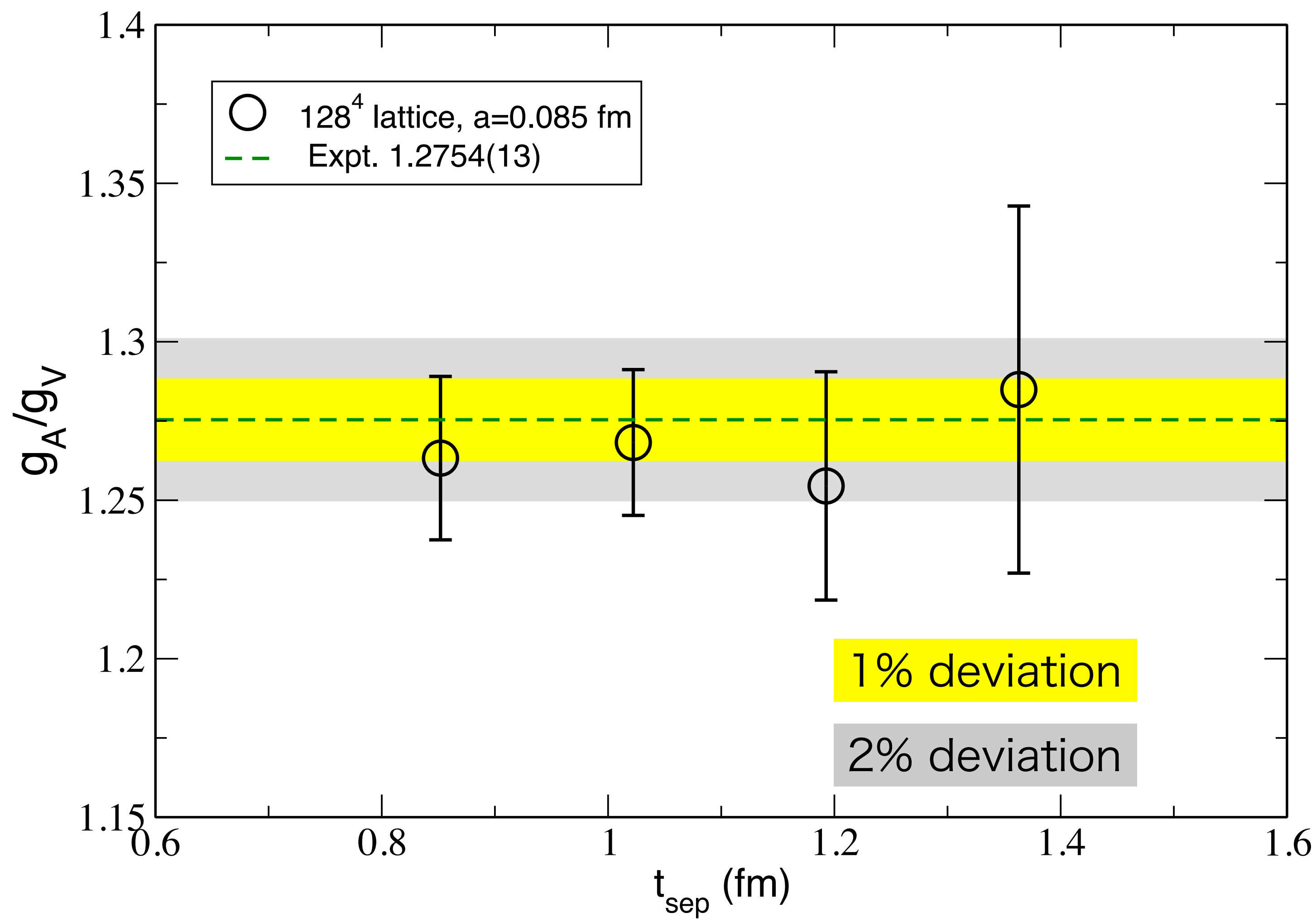
$$\mathcal{O} = \bar{u}\gamma_5\gamma_3 u - \bar{d}\gamma_5\gamma_3 d$$



E. Shintani et al. (PACS collaboration)
PRD99 (2019) 014510

$$\langle p'|A^\mu(q)|p\rangle$$

$$= \overline{u}(p')\left[\gamma^\mu\gamma_5 F_P(q^2) + iq^\mu\gamma_5 F_P(q^2)\right] u(p)$$

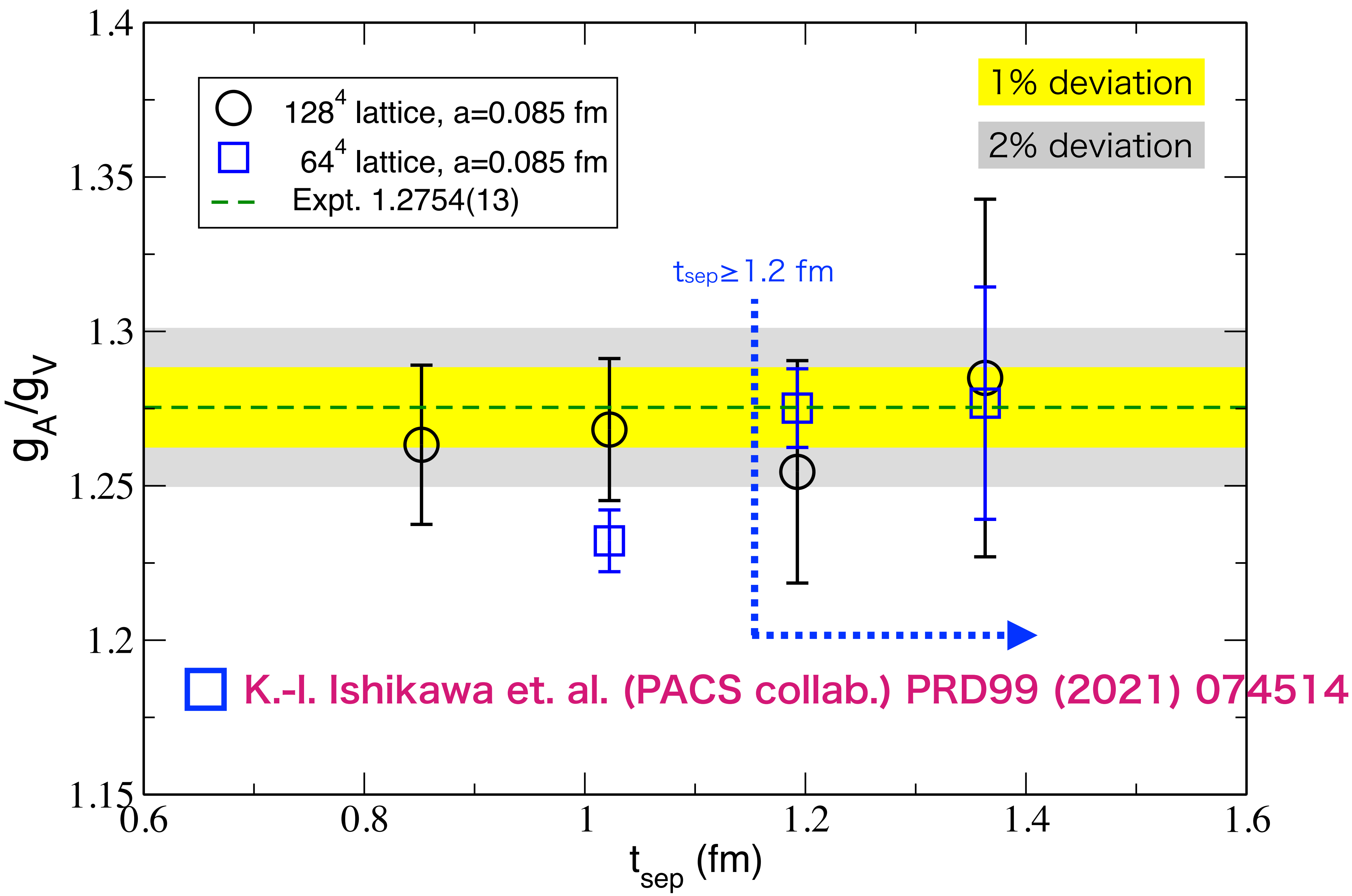


$$g_A = 1.273(24)$$

Good plateau for t_{sep}=10, 12, 14, 16

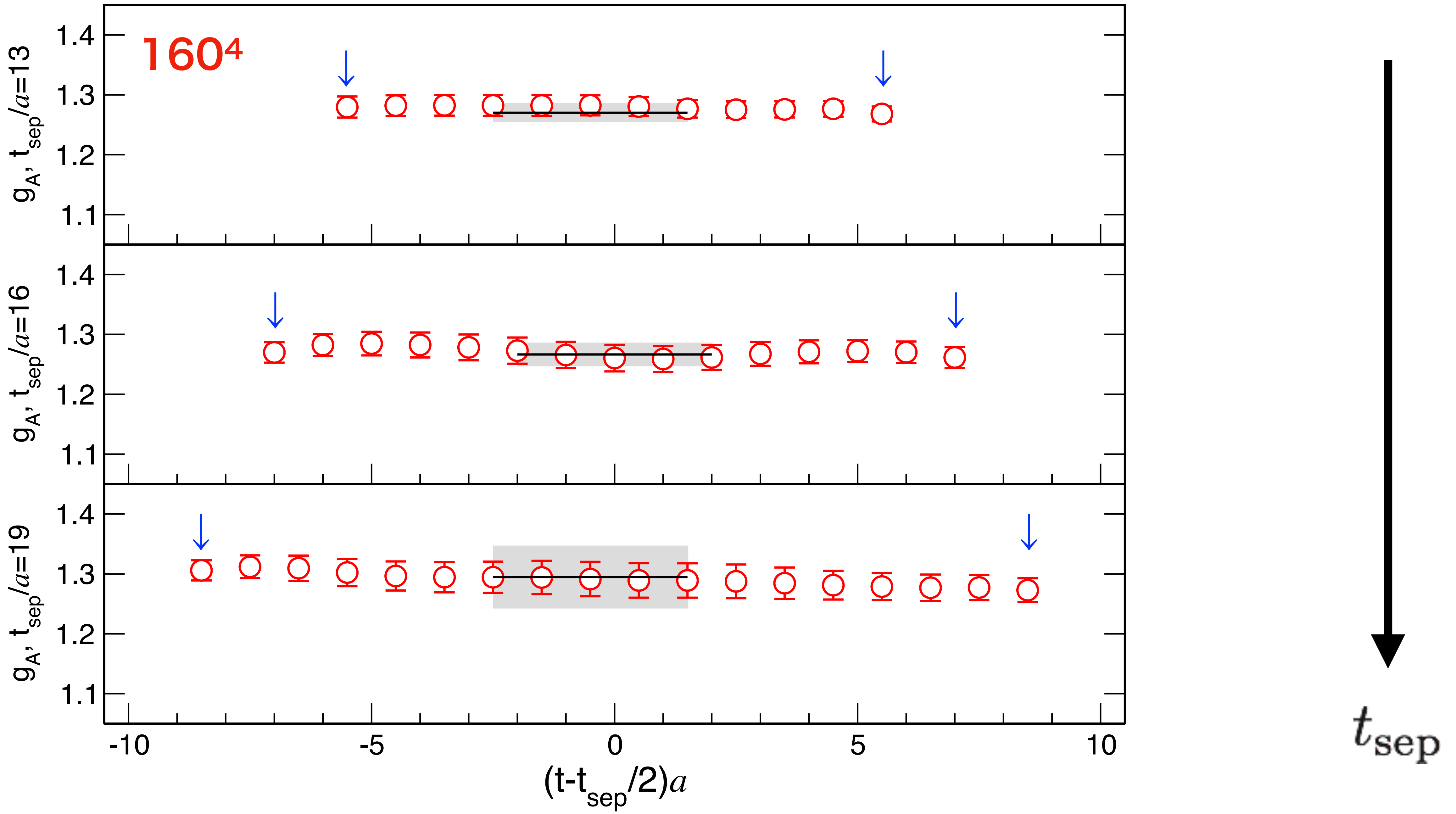
MC statistical uncertainty is less than 2%

A precent-level determination of g_A



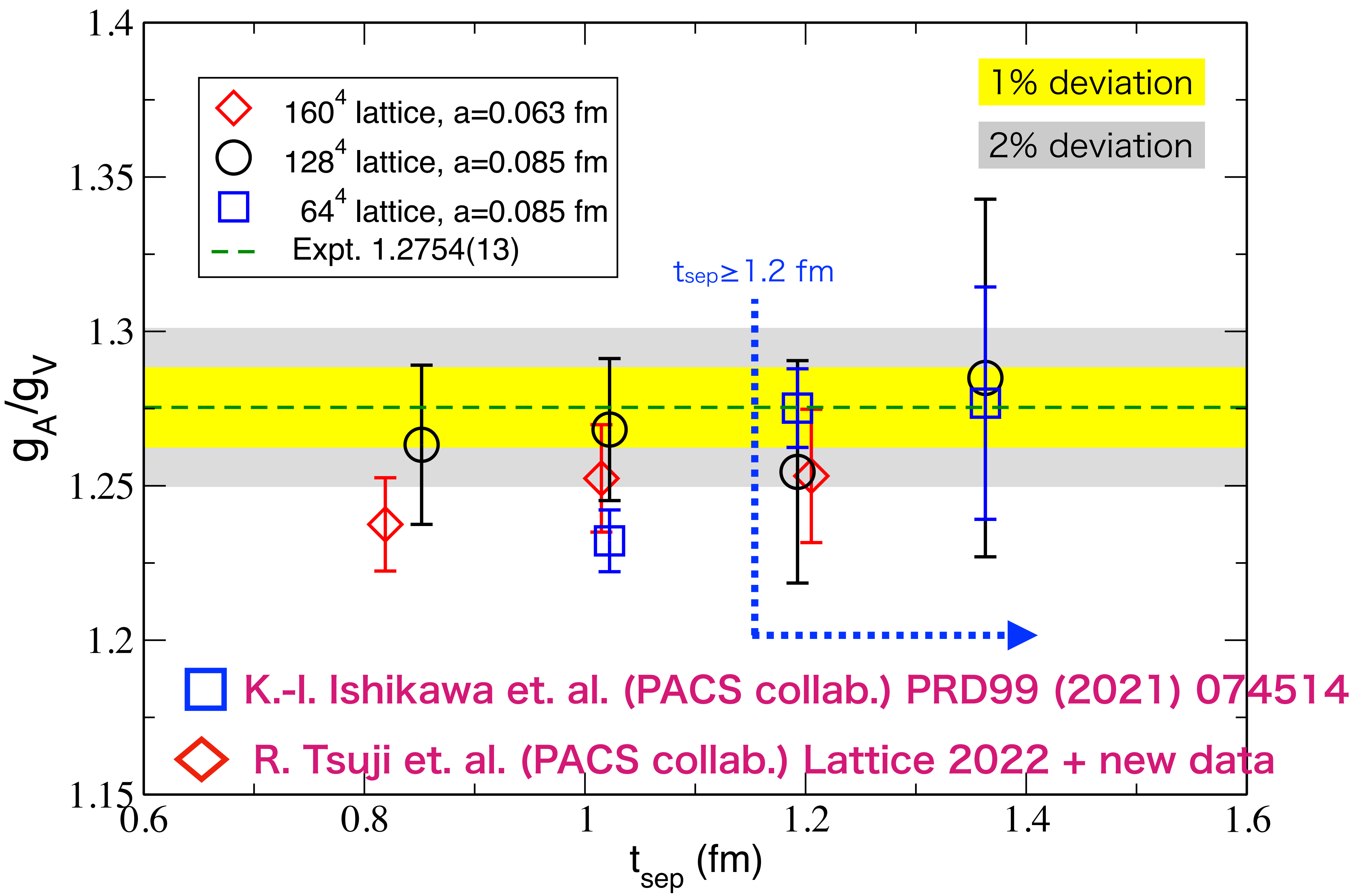
Effect of excited state contamination is negligible for $t_{sep} \geq 1.2$ fm.
Finite volume error is less than 1%.

Ratio for iso-vector g_A



Good plateau for t_{sep}=13, 16, 19

A precent-level determination of g_A



Effect of excited state contamination is negligible for $t_{sep} \geq 1.2$ fm.

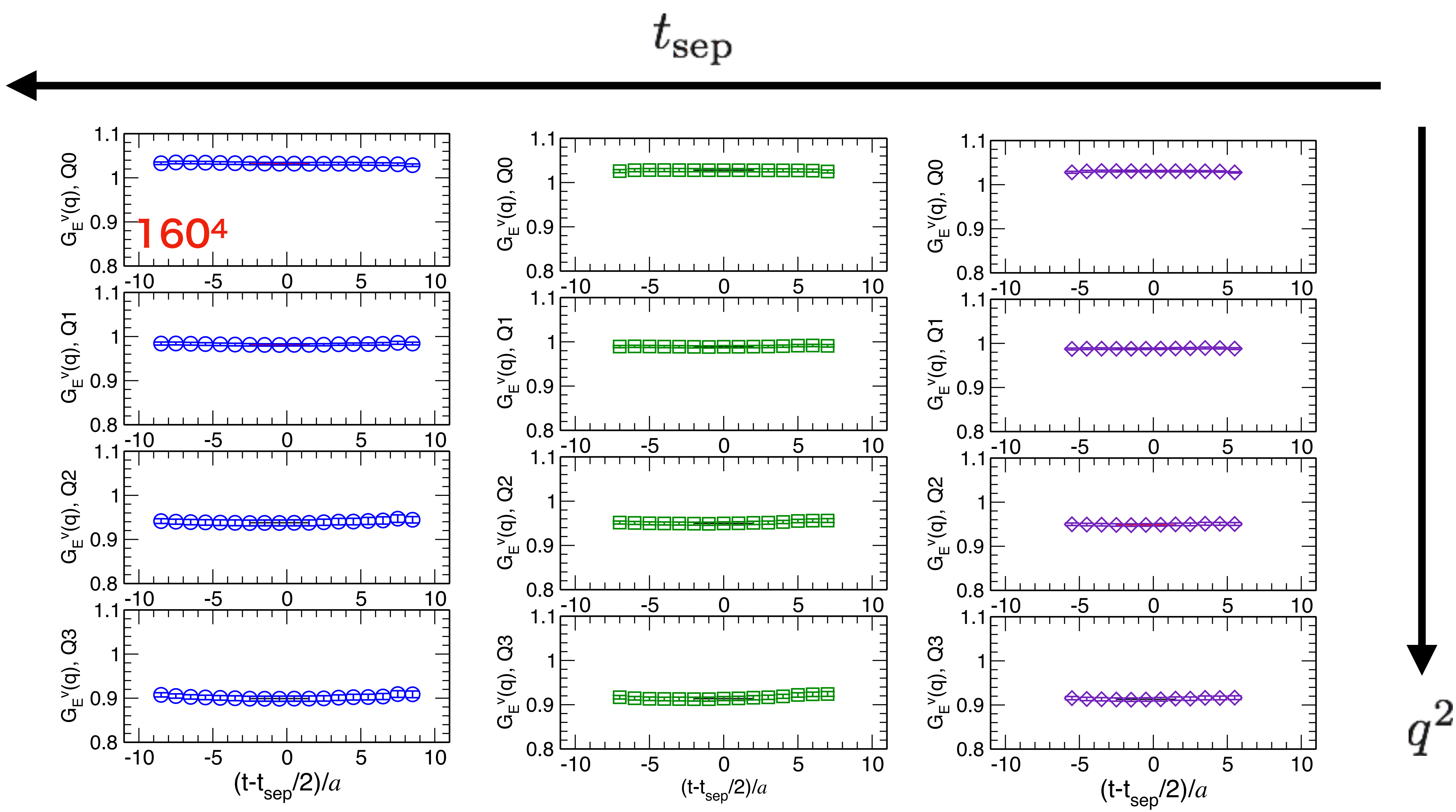
Finite volume error is less than 1%.

Discretization error is less than 1%.

Electric form factor

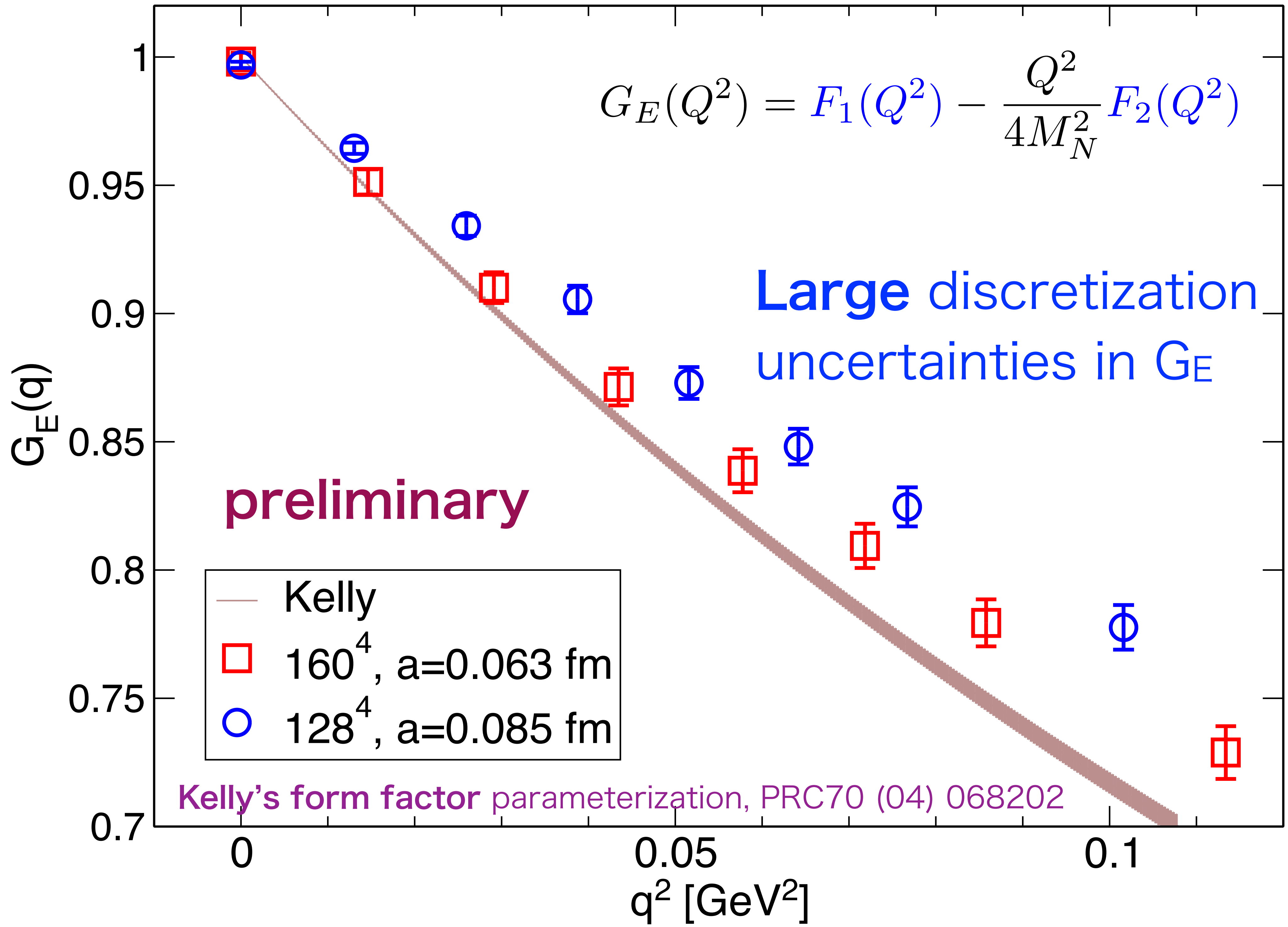
G_E

Ratio for iso-vector $G_E(q^2)$



Good plateau for t_{sep}=13, 16, 19

Iso-vector electric form factor G_E

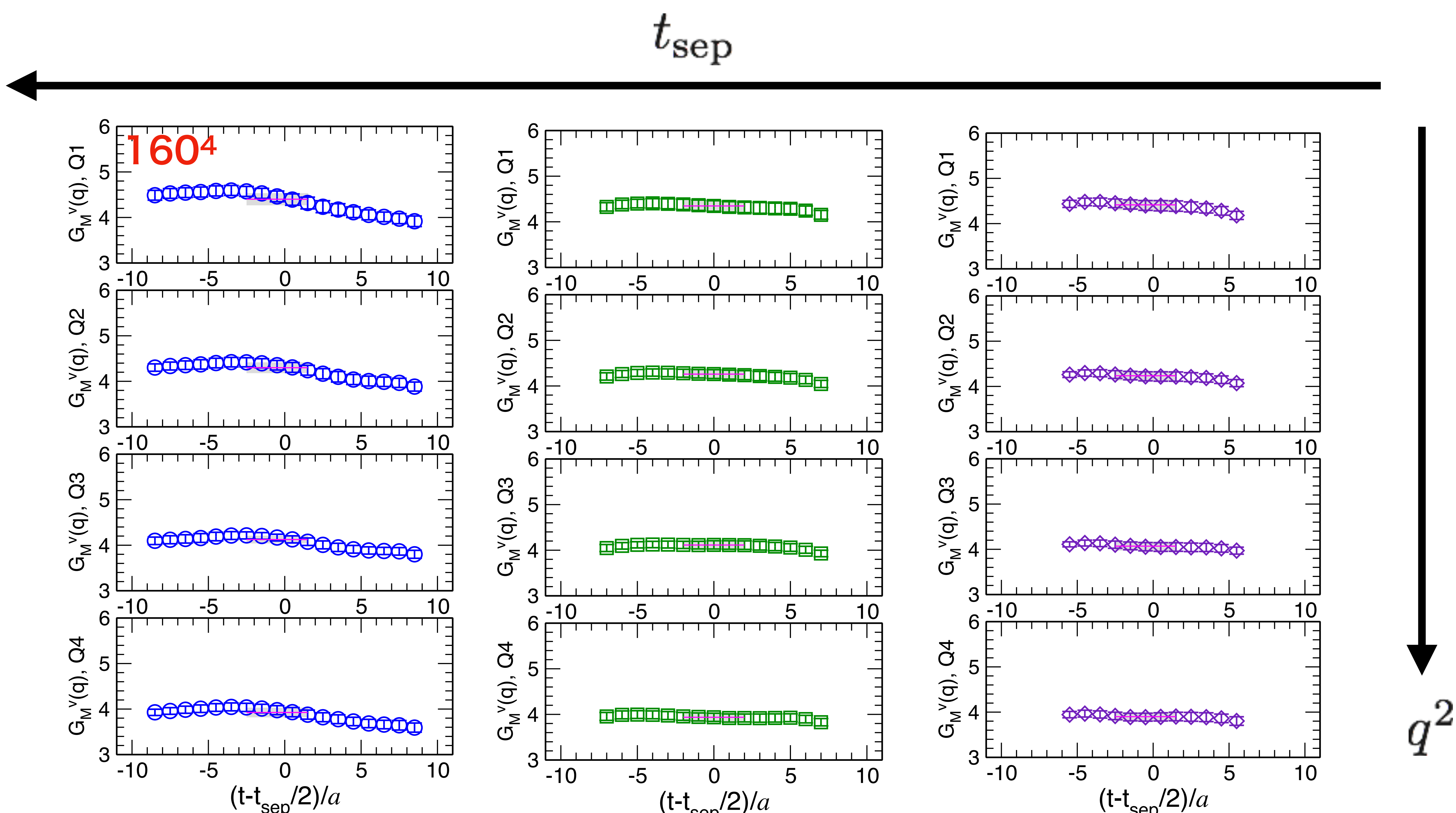


The results obtained with the fine lattice spacing (a≈0.06 fm) approaches to the Kelly's curve

Magnetic form factor

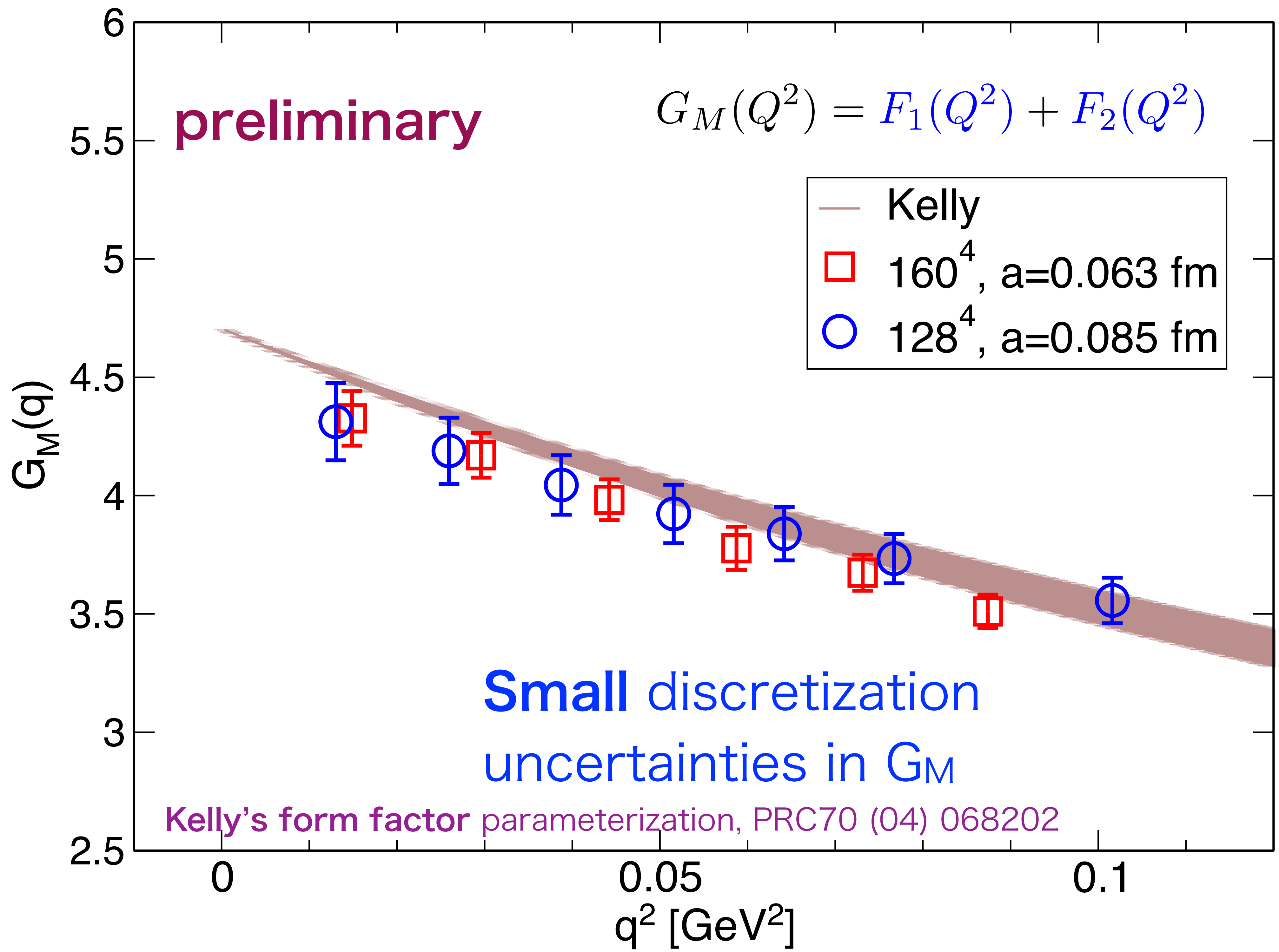
G_M

Ratio for iso-vector $G_M(q^2)$



Good plateau for t_{sep}=13, 16, 19

Iso-vector magnetic form factor G_M



The results obtained with the fine lattice spacing (a≈0.06 fm) remain barely consistent with the Kelly's curve.

Summary

- We have studied nucleon form factors (vector/axial-vector) calculated in 2+1 flavor QCD **at the physical point** on **(10 fm)^4** lattice at **two lattice spacings (a=0.085 and 0.063 fm)**

✓ Large spatial volume allows investigation in the **small momentum transfer region**, $q^2 < (2 m_\pi)^2$

✓ **High statistical precision** is achieved by all-mode averaging technique

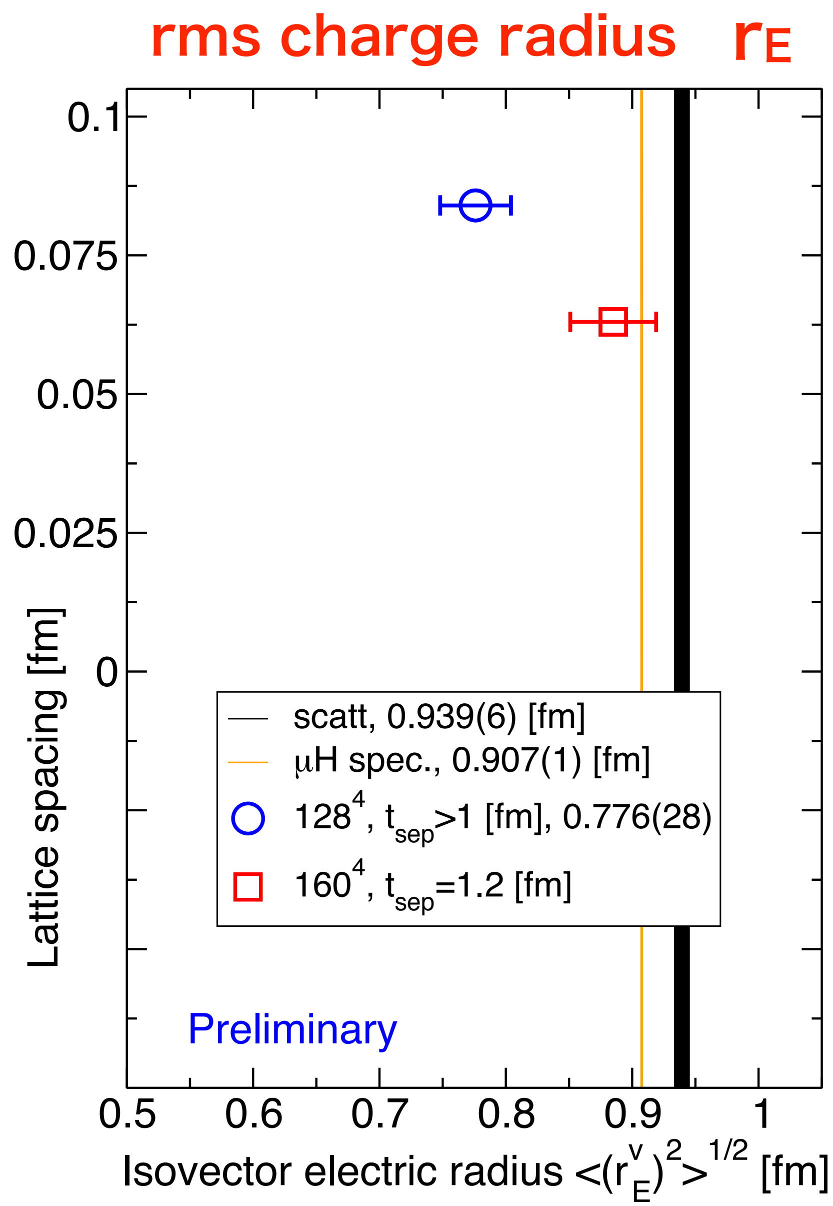
✓ t_{sep} dependence is systematically investigated

➡ g_A and G_E, G_M show **no t_{sep} dependence**

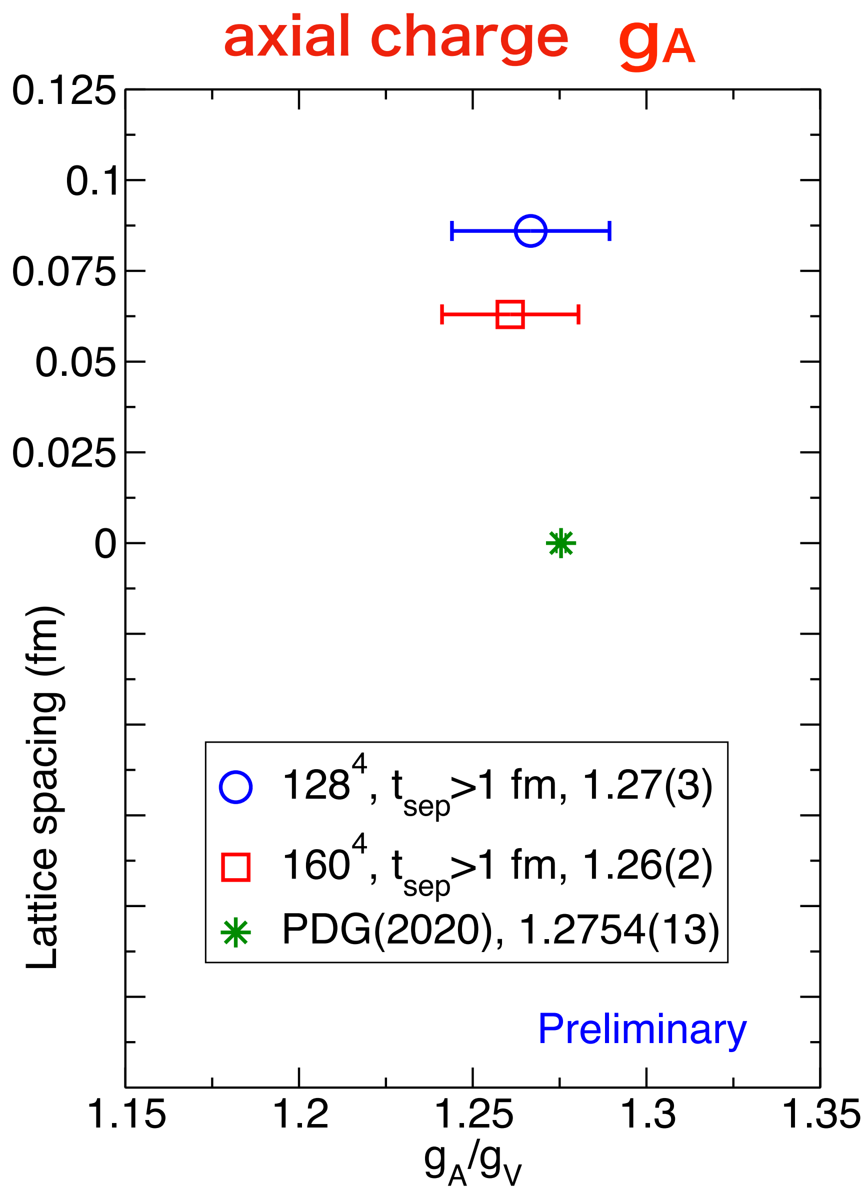
➡ excited-state contributions are negligible for $t_{sep} \geq 1.2$ fm

Summary (Cont.)

- **Lattice discretization uncertainties** on r_E and g_A



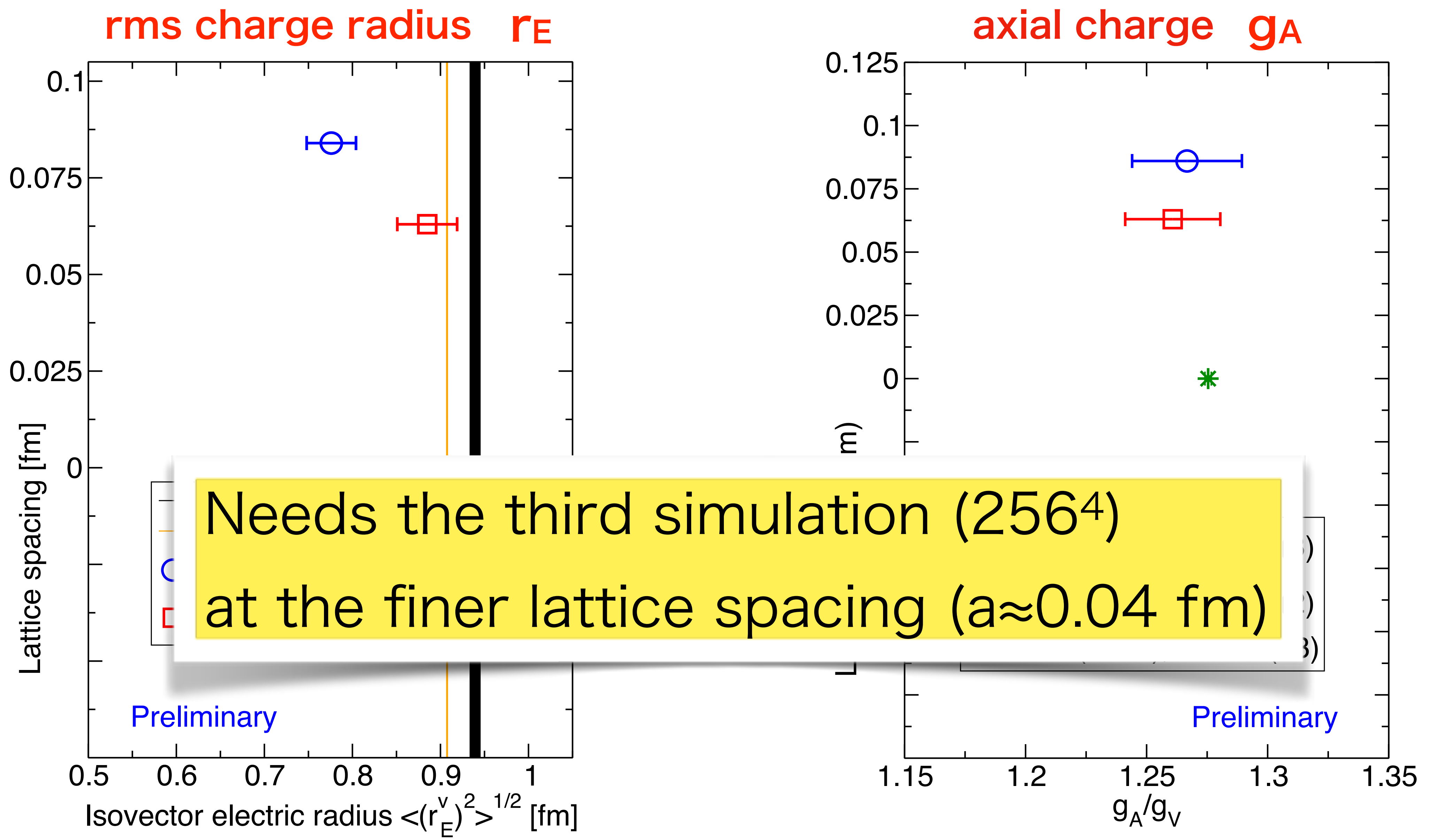
Significantly large(~10%)



Negligibly small (< 1%)

Summary (Cont.)

- **Lattice discretization uncertainties** on r_E and g_A



Significantly large(~10%)

Negligibly small (< 1%)

Back up slides

Why is the spatial size so large?

There are three reasons to pay special attention to our **large spatial volume of (10 fm)^3** at the physical point.

- To avoid relatively large finite size effect on nucleon observables

  ✓ $L - 2R \gg 1/m_\pi$ ($R \sim 0.85$ fm) $\rightarrow L > 3$ fm

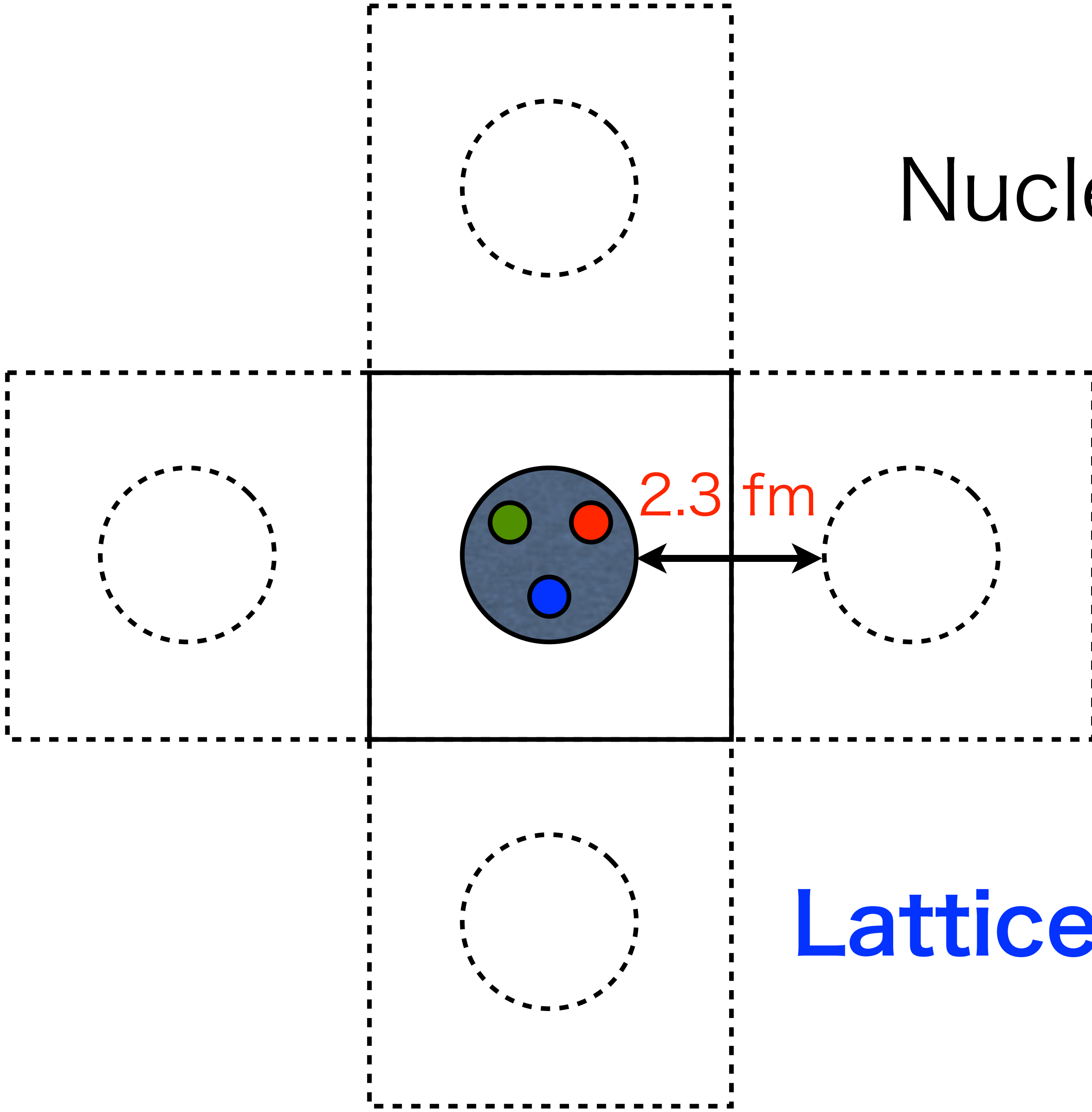
- The spatial charge distribution falls exponentially

  ✓ $L > 2r_{cut} = 6.4\,R$ ($r_{cut} = 3.2\,R$) $\rightarrow L > 6$ fm

- To access the small momentum transfer region

  ✓ $|\mathbf{q}|_{min} = 2\pi / L$, $q_{min} < 2m_\pi$ $\rightarrow L > 4.5$ fm

How Large Spatial Size is Necessary?



Nucleon's size (2R~1.7 fm)

R=RMS radius

Periodic boundary condition

Lattice size (4 fm) > 2R + r_π

Compton wavelength of the pion (r_π~1.4 fm)

How Large Spatial Size is Necessary?

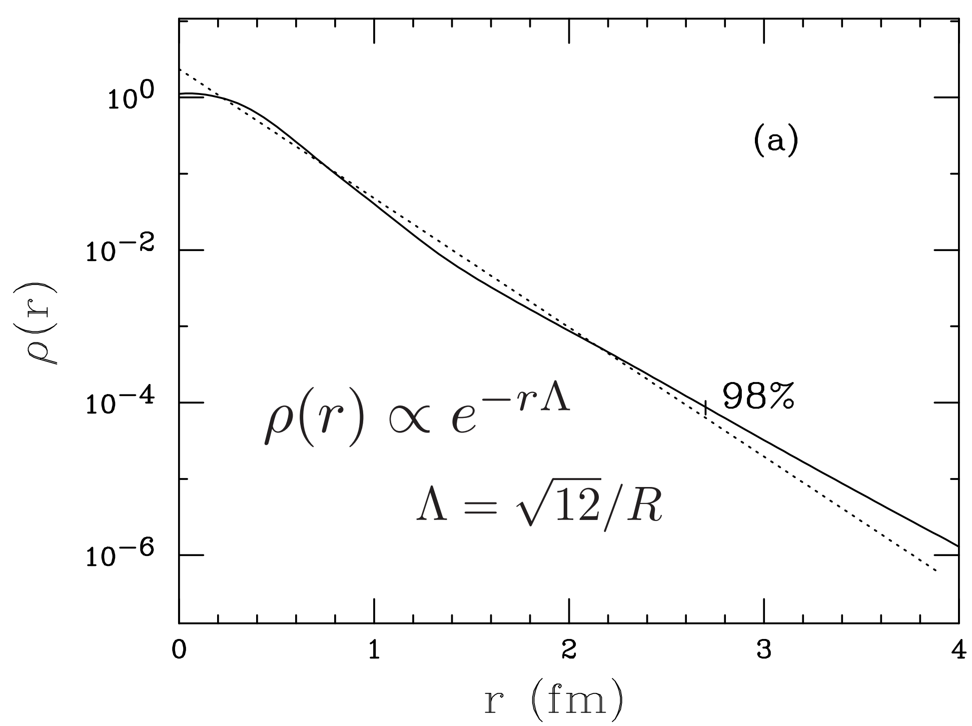
Sick, Atoms 6(2018)2

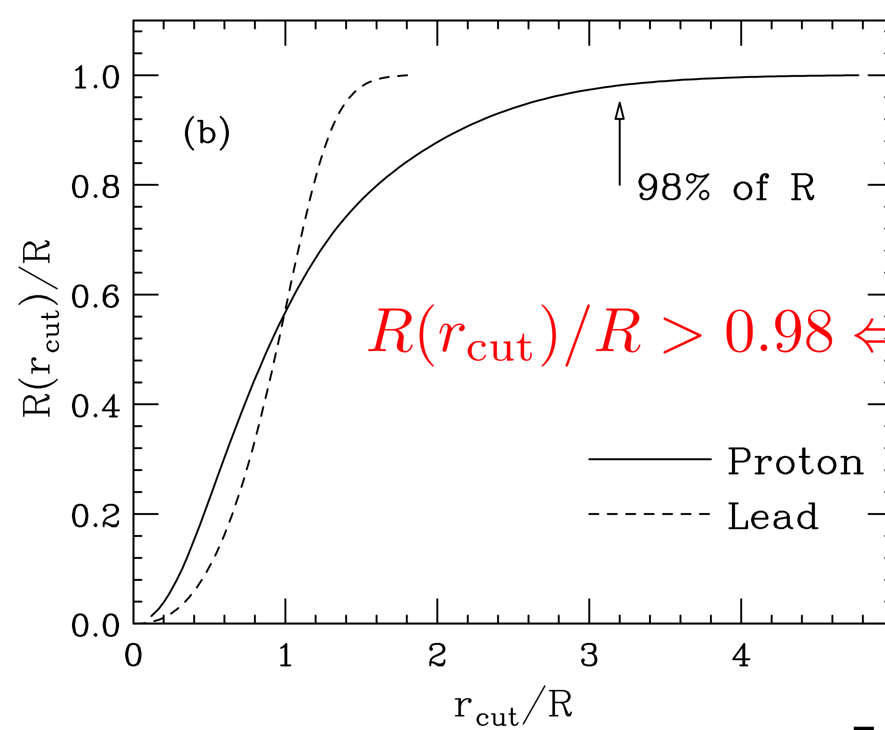
Charge RMS radius

$$R^2 \equiv 4\pi \int_0^\infty \rho(r) r^4 dr$$

exp-form $\rho(r) \propto e^{-r\Lambda}$ ⟷ (3d-FT) **dipole-form** $G_E(q^2) \propto \frac{1}{(q^2+\Lambda^2)^2}$

$$R(r_{\rm cut})/R = \left[\int_0^{r_{\rm cut}} \rho(r) r^4 dr \Big/ \int_0^\infty \rho(r) r^4 dr \right]^{1/2}$$

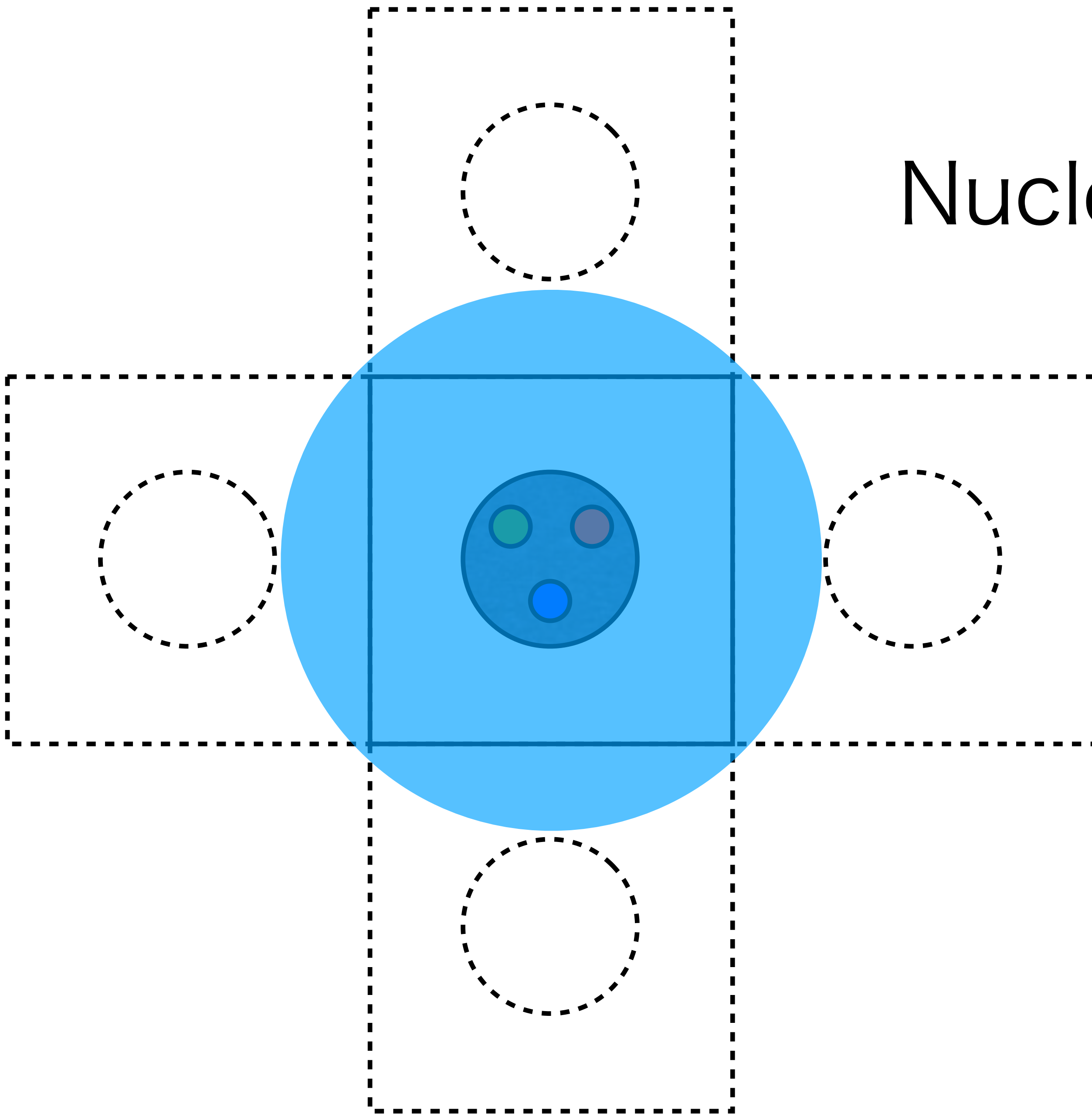




$R(r_{\rm cut})/R > 0.98 \Leftrightarrow r_{\rm cut} > 3.2R$

Integration up to $r_{\rm cut}$=2.7 fm ⇒ Only 98% of charge RMS radius

How Large Spatial Size is Necessary?



Nucleon's size (2R~1.7 fm)

R=RMS radius

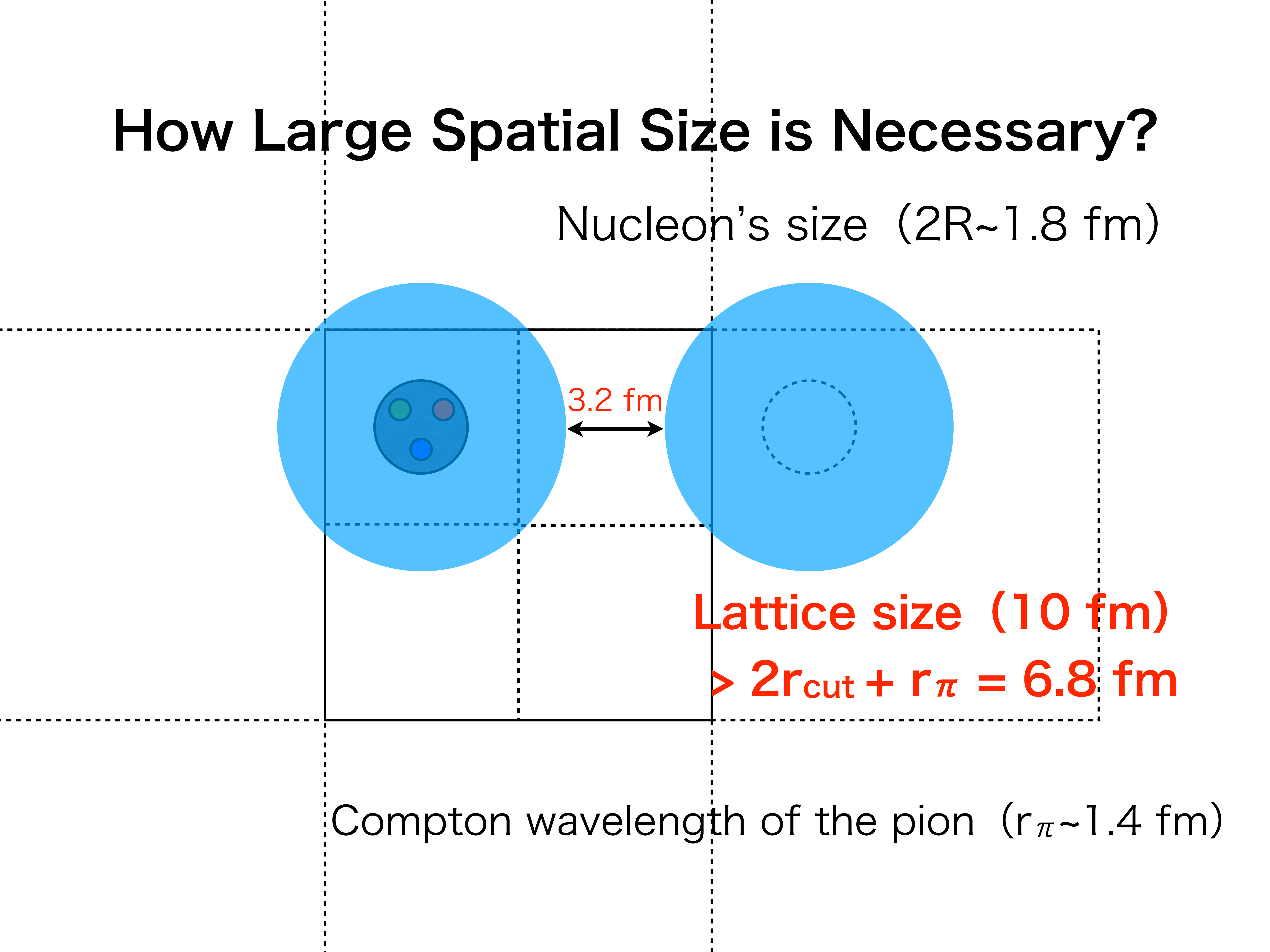
Periodic boundary condition

Lattice size (4 fm)

$< 2r_{cut}$=6.4R=5.4 fm

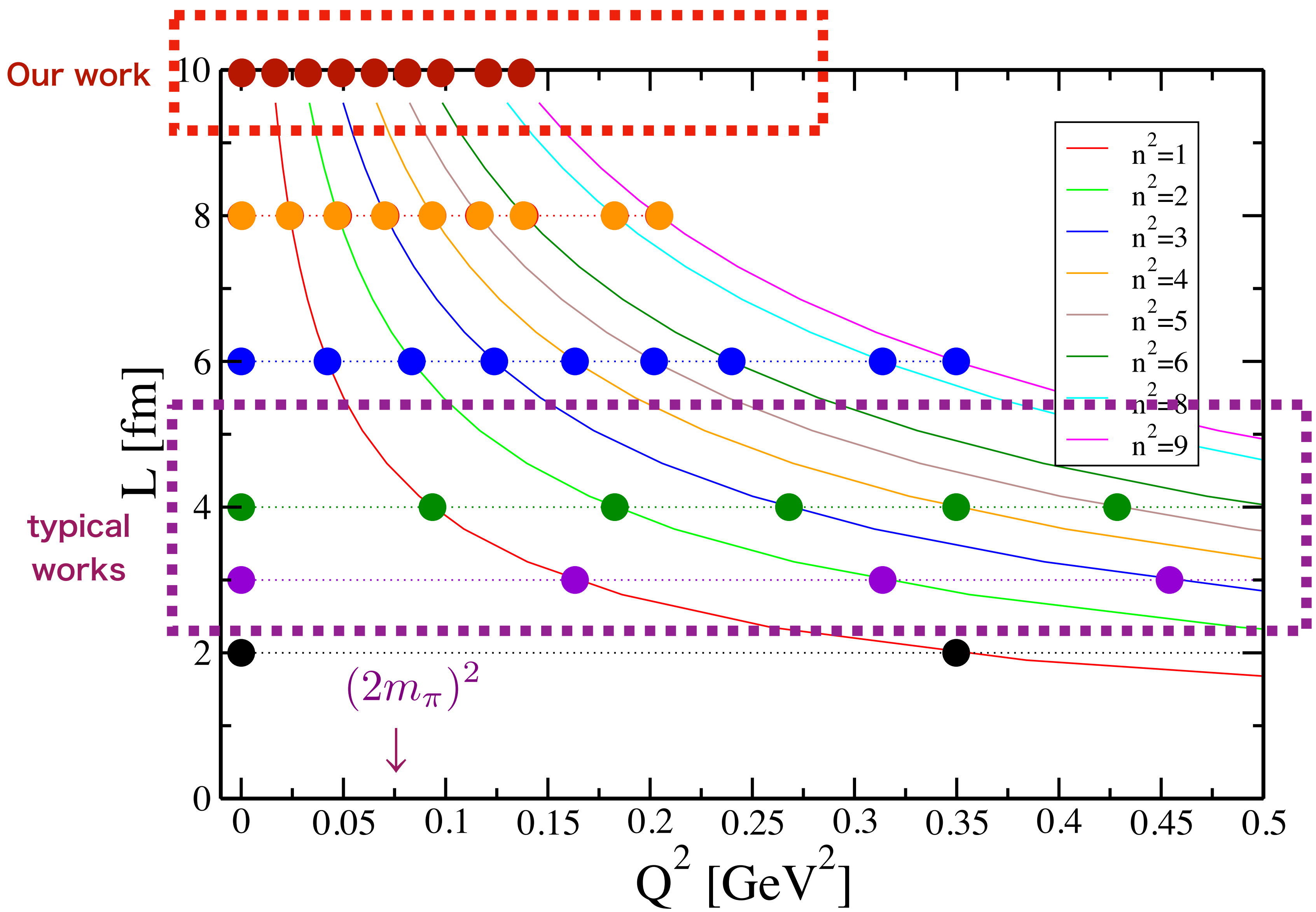
4 fm is not large enough for nucleon physics

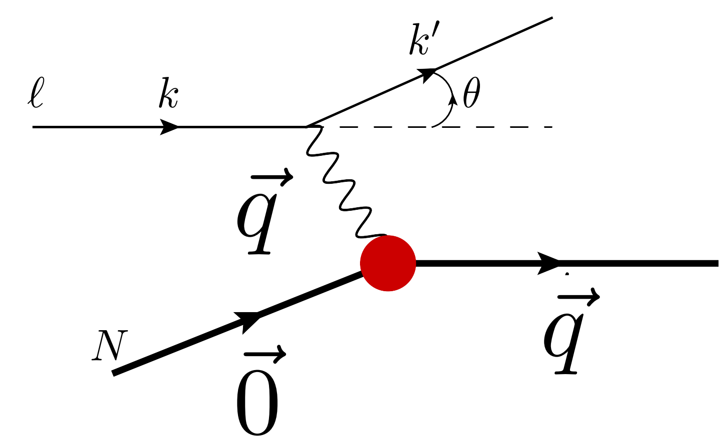
How Large Spatial Size is Necessary?



How Large Spatial Size is Necessary?

Discrete momenta on the lattice are related to the size of the spatial extent L





$$Q^2 = -q^2 = 2M_N(E(\vec{q}) - M_N)$$

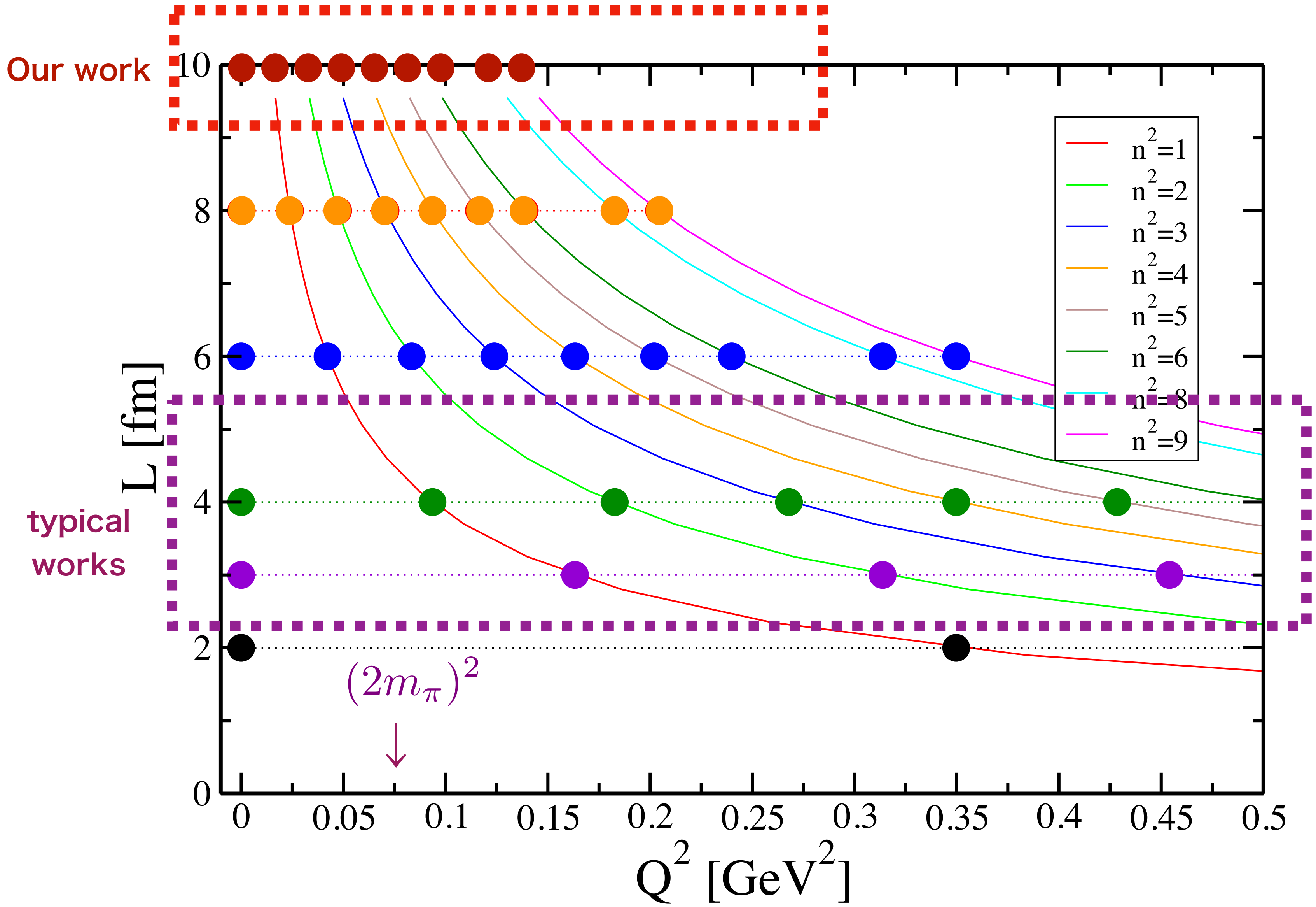
$$E(\vec{q}) = \sqrt{M_N^2 + \vec{q}^2}$$

$$\vec{q}^2 = \left(\frac{2\pi}{L}\right)^2 \vec{n}^2$$

✓can access the **small** momentum transfer **up to 114 MeV < 2m$_\pi$**

How Large Spatial Size is Necessary?

Discrete momenta on the lattice are related to the size of the spatial extent L



$$\langle r_E^2 \rangle = -\frac{6}{G_E(0)} \frac{dG_E(q^2)}{dq^2}\bigg|_{q^2=0}$$

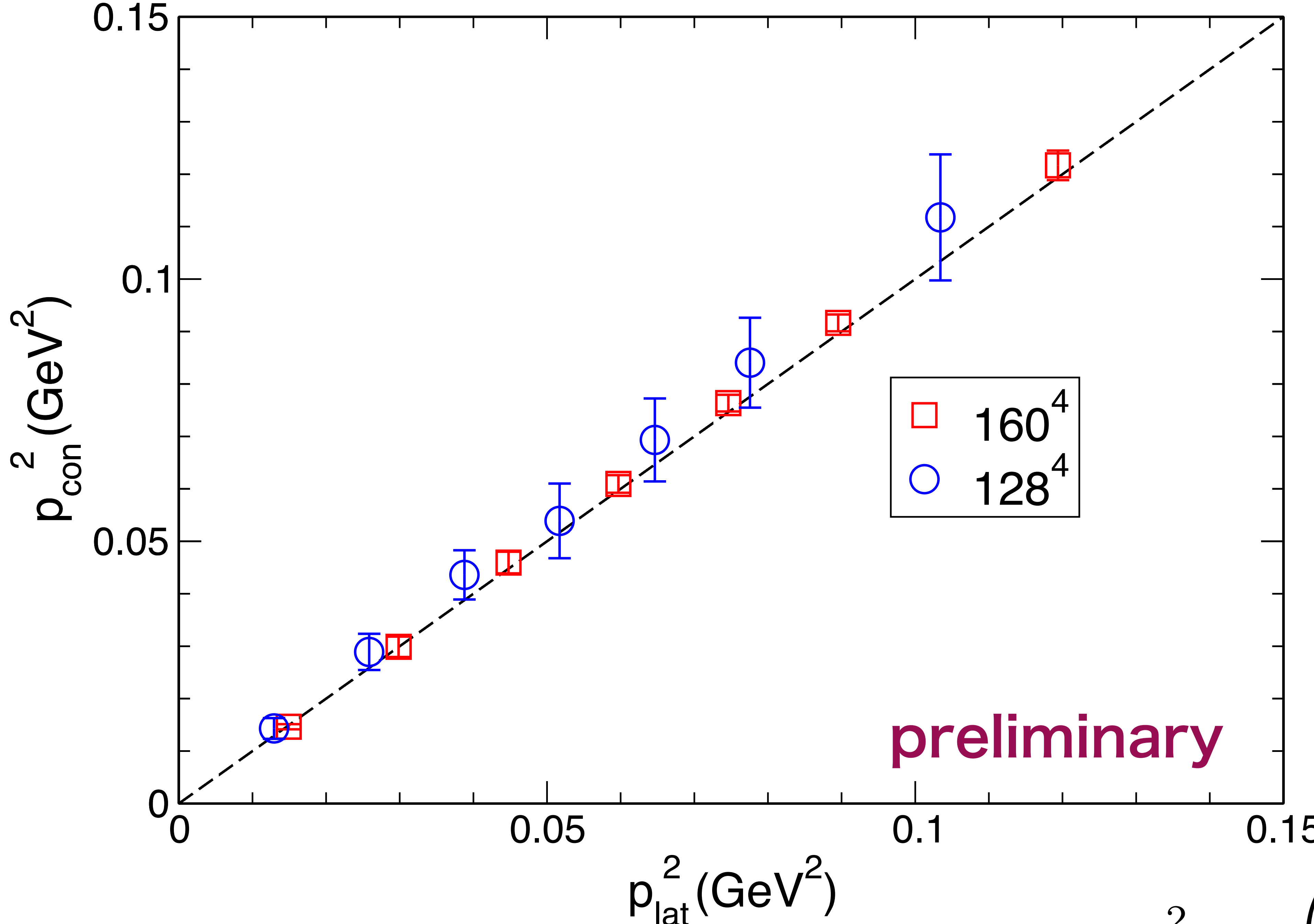
Root-Mean-Square radius

$$R = \sqrt{\langle r_E^2 \rangle} = r_E$$

✓can access the **small** momentum transfer **up to 114 MeV < 2m$_\pi$**

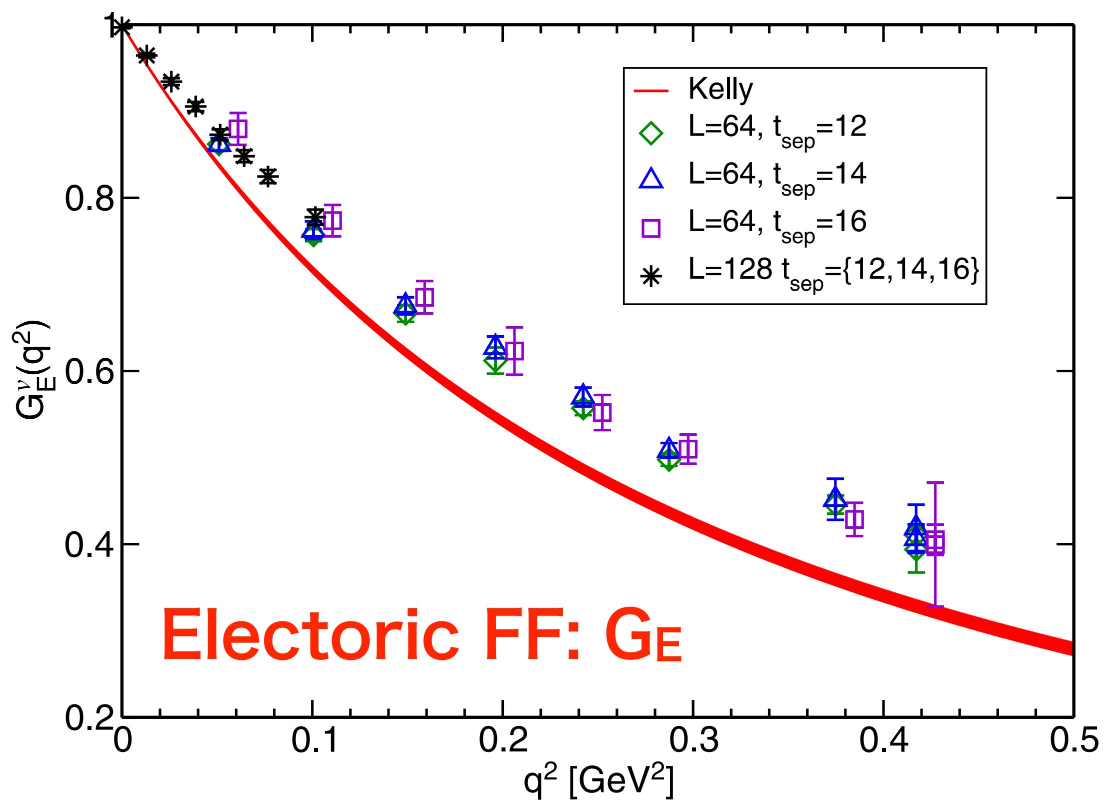
Dispersion relation

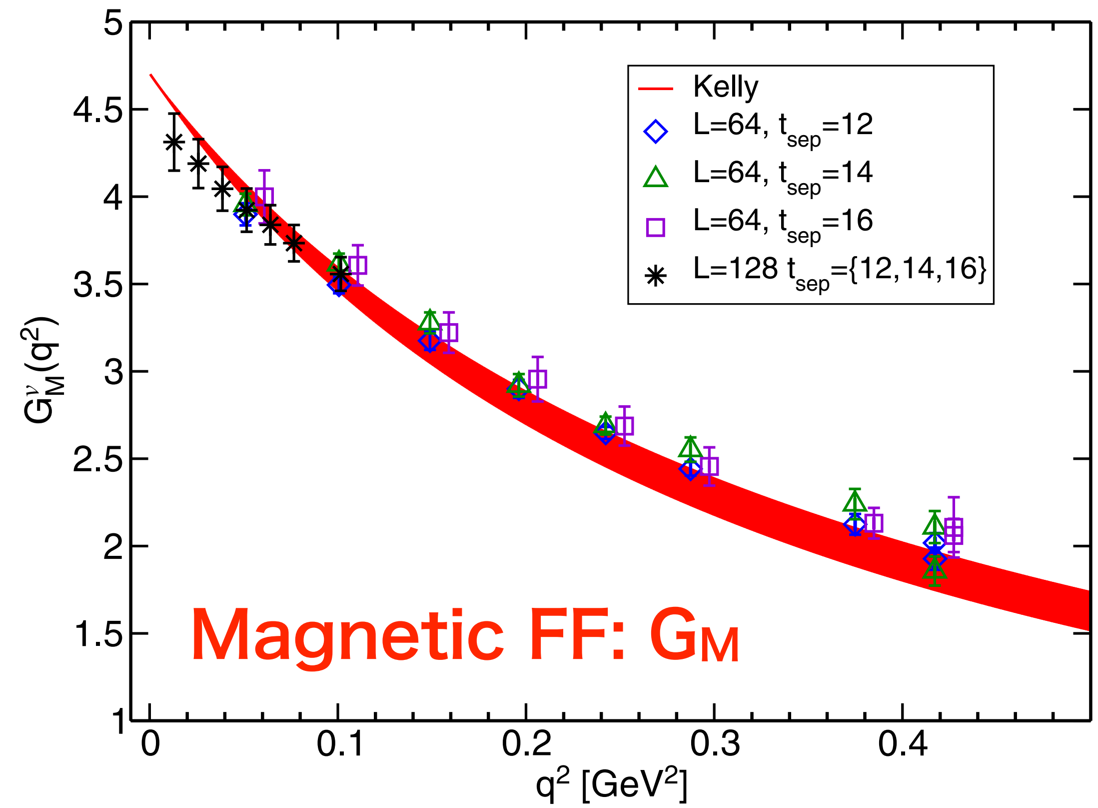
$$p^2_{\mathrm{con}} = E_N^2 - M_N^2$$



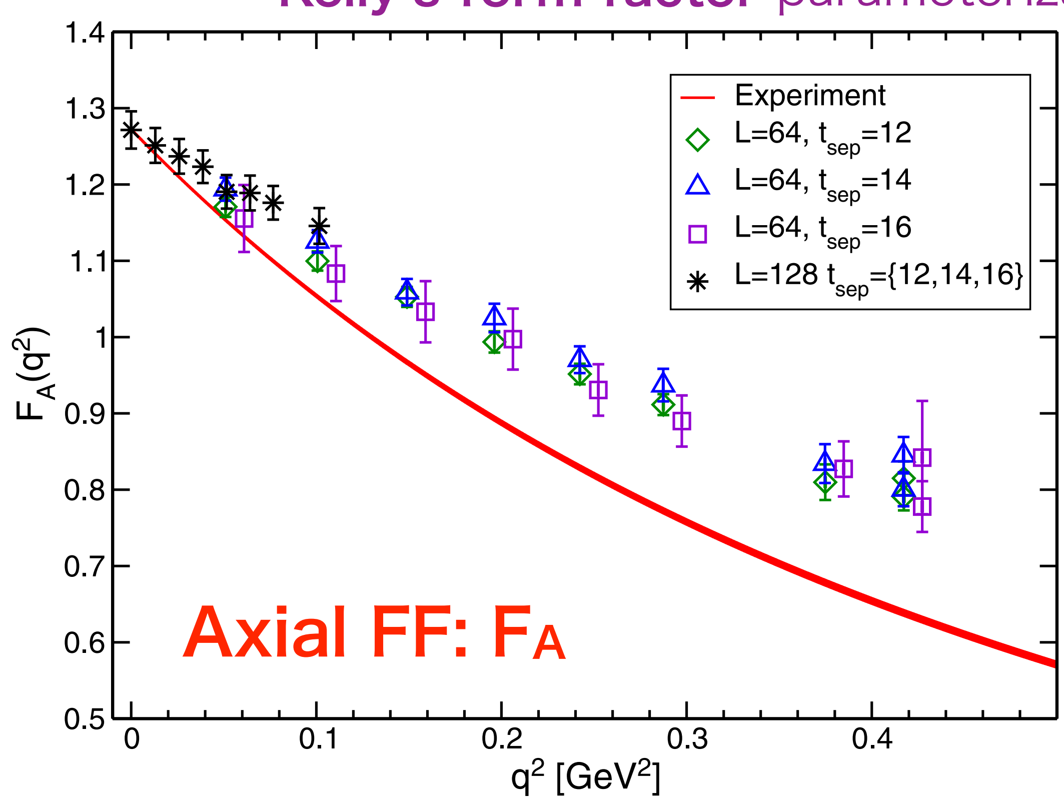
$$p^2_{\mathrm{lat}} = \left(\frac{2\pi}{L}\right)^2 \times n$$

128^4 vs 64^4





Kelly's form factor parameterization, PRC70 (04) 068202

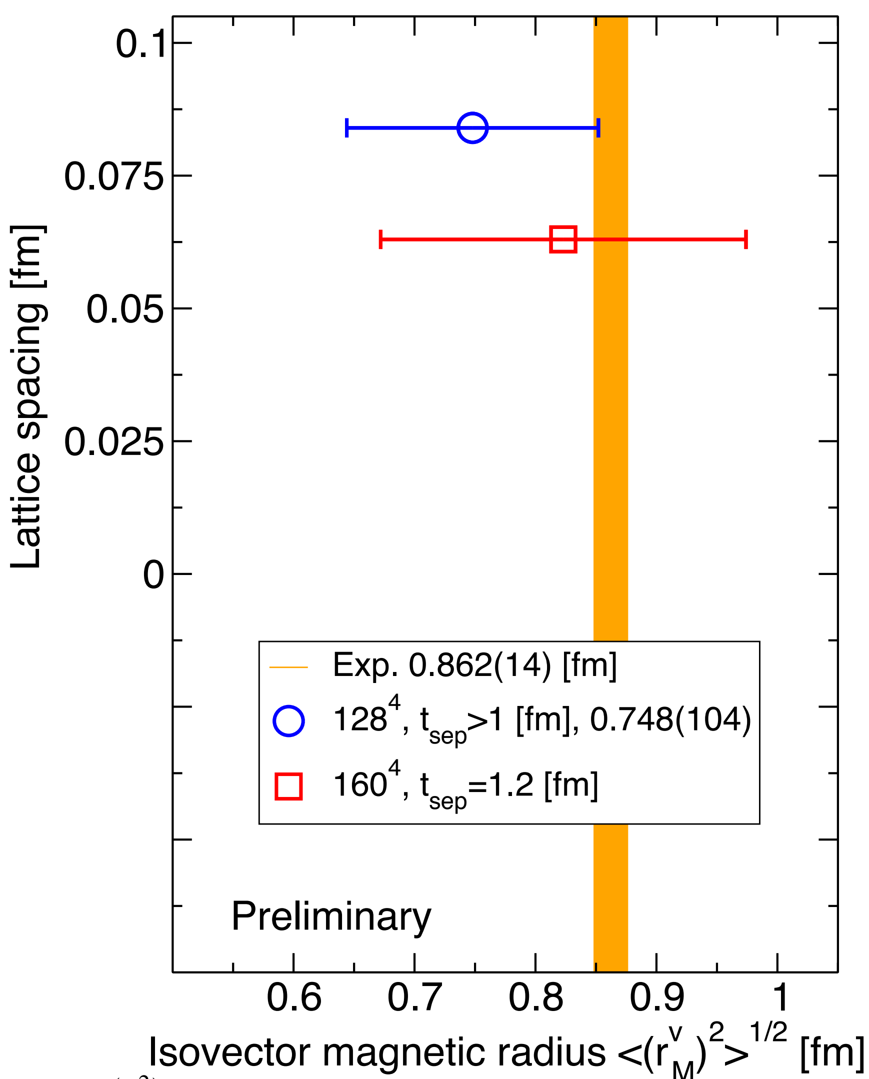


dipole form with r_A=0.67(1) fm

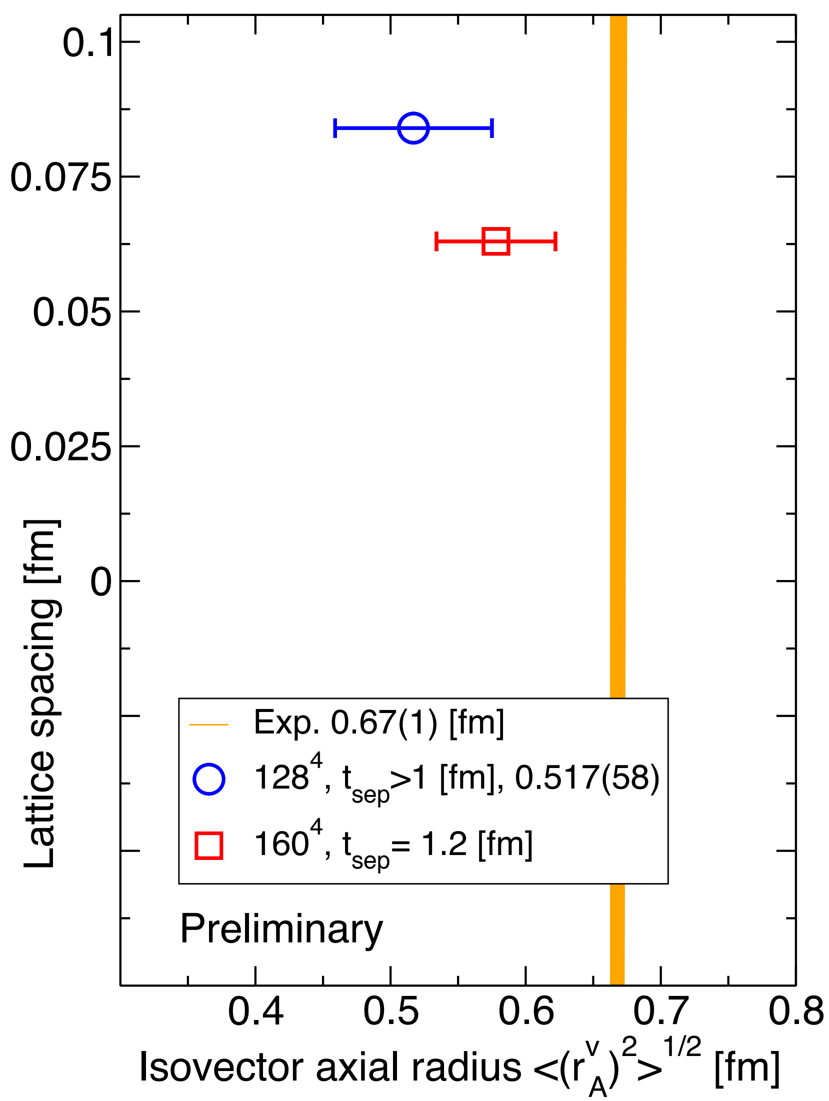
Other rms radii

- **Lattice discretization uncertainties** on r_M and r_A

rms magnetic radius r_M



rms axial radius r_A



$$\langle (r_M^v)^2\rangle \equiv -6\frac{1}{G_M^v(q^2)}\frac{dG_M^v(q^2)}{dq^2}\Big|_{q^2=0} = \frac{\mu_p}{\mu_v}\langle (r_M^p)^2\rangle - \frac{\mu_n}{\mu_v}\langle (r_M^n)^2\rangle,$$

Statistically insignificant

$$\langle r_A^2\rangle = -\frac{6}{F_A(0)}\frac{dF_A}{dq^2}\Big|_{q^2=0}$$

All-mode average

- Compute the combination of correlator with high-precision $O^{(org)}$ and low-precision $O^{(approx)}$

$$O^{(\mathrm{ama})} = \frac{1}{N_{\mathrm{org}}} \sum_{f \in G}^{N_{\mathrm{org}}} \left(O^{(\mathrm{org})f} - O^{(\mathrm{approx})f} \right) + \frac{1}{N_G} \sum_{g \in G}^{N_G} O^{(\mathrm{approx})g}$$

128^4 lattice

t_{sep}/a	N_{org}	N_G	# meas
10	1	128	2, 560
12	1	256	5, 120
14	2	320	6, 400
16	4	512	10, 218