Proton electromagnetic form factors and radii from lattice QCD

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[PRD **109**, 094510], [PRL **132**, 211901]
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Outline

Motivation

- Precision matters if lattice QCD is to have an impact on determination of the proton radii
- In lattice QCD as in the context of scattering experiments: electromagnetic radii extracted from the slope of the corresponding form factors at $Q^2 = 0$,

$$\langle r^2 \rangle = -\frac{6}{G(0)} \left. \frac{\partial G(Q^2)}{\partial Q^2} \right|_{Q^2=0} \tag{1}$$

- Full calculation of the proton and neutron form factors separately necessitates explicit treatment of the numerically challenging quark-disconnected contributions
- Neglected in many previous lattice studies, in particular no simultaneous control of all relevant systematics (continuum and infinite-volume extrapolation)
- Accurate determination of proton radii from muonic hydrogen spectroscopy ⇒ other definitions of radii, not previously computed on the lattice, become relevant

Motivation

- Lamb shift
  - LO proton-structure contribution: electric radius
  - NLO: two-photon exchange, dominated by elastic part, depends on third Zemach moment[1],

$$\langle r_E^3 \rangle_{(2)}^p = \frac{24}{\pi} \int_0^\infty \frac{dQ^2}{(Q^2)^{5/2}} \left[(G_E^p(Q^2))^2 - 1 + \frac{1}{3} \langle r_E^2 \rangle^p Q^2 \right] \tag{2}$$

  - Associated radius: Friar radius, $r_F^p = \sqrt[3]{\langle r_E^3 \rangle_{(2)}^p}$
- Hyperfine splitting (HFS)
  - LO proton-structure contribution: Zemach radius[2],

$$r_Z^p = -\frac{2}{\pi} \int_0^\infty \frac{dQ^2}{(Q^2)^{3/2}} \left(\frac{G_E^p(Q^2) G_M^p(Q^2)}{\mu_M^p} - 1 \right) \tag{3}$$

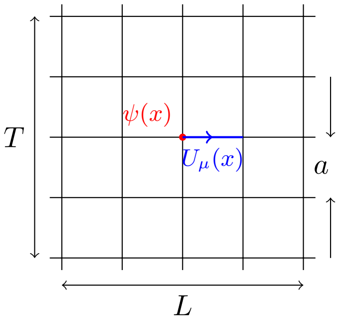
  - First-principles prediction of Zemach radius could be checked by high-precision experiments

[1] Friar 1979 [Ann. Phys. **122**, 151]; [2] Zemach 1956 [Phys. Rev. **104**, 1771].

Outline

QCD on the lattice

- Coupling of QCD is large at large distances / low energies
- Low-energy regime of QCD (typical hadronic scales) is hence inaccessible to perturbative methods
- Powerful tool for the non-perturbative study: lattice QCD
- Replace space-time by a four-dimensional Euclidean lattice
- Gauge-invariant UV-regulator for the quantum field theory due to the momentum cut-off
- Path integral becomes finite-dimensional and can be computed numerically



- Allows a systematic extrapolation to the continuum and infinite-volume limit, $a \to 0$ and $V \to \infty$

Ensembles

Coordinated Lattice Simulations (CLS)[3]

- Non-perturbatively $\mathcal{O}(a)$-improved Wilson fermions
- $N_f = 2 + 1$: 2 degenerate light quarks ($m_u = m_d$), 1 heavier strange quark ($m_s > m_{u,d}$)
- $\mathrm{tr}\, M_q = 2m_l + m_s =$ const.
- Tree-level improved Lüscher-Weisz gauge action
- $\mathcal{O}(a)$-improved conserved vector current

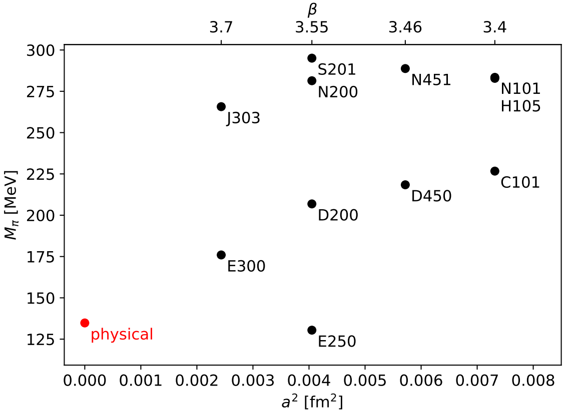
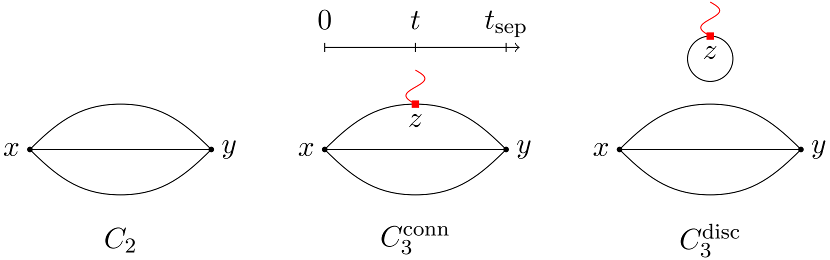


Figure: Overview of the ensembles used in this study

[3] Bruno et al. 2015 [JHEP **2015** (2), 43]; Bruno, Korzec, and Schaefer 2017 [PRD **95**, 074504].

Nucleon two- and three-point correlation functions



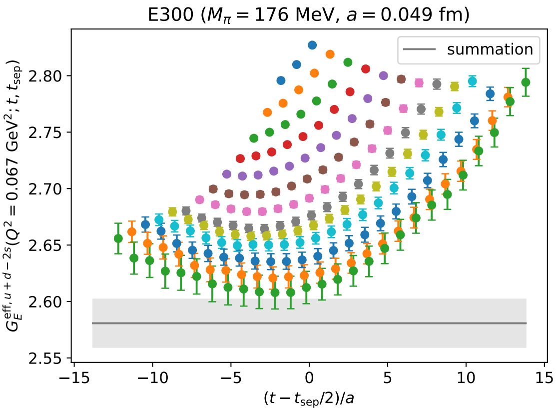
- Measure the two- and three-point correlation functions of the nucleon
- For three-point functions, Wick contractions yield connected and disconnected contribution
- Compute the quark loops via a stochastic estimation using a frequency-splitting technique[4]
- Extract the effective form factors $G_{E,M}^{\text{eff}}$ using the ratio method[5]

[4] Giusti et al. 2019 [EPJC **79**, 586]; Cè et al. 2022 [JHEP **2022** (8), 220]; [5] Korzec et al. 2009 [PoS **066**, 139].

Outline

Excited-state analysis

- Cannot construct exact interpolating operator for the proton (any hadron) on the lattice
- All possible states with the same quantum numbers contribute
- Effect of heavier excited states suppressed exponentially with the distance between operators in Euclidean time
- For baryons, the relative statistical noise grows also exponentially with the source-sink separation $t_{\mathrm{sep}} = y_0 - x_0$



Excited-state analysis: summation method

- Explicit treatment of the excited-state systematics required
- Summation of the effective form factors over the operator insertion time,

$$S_{E,M}(Q^2;t_{\mathrm{sep}}) = \sum_{t=t_{\mathrm{skip}}}^{t_{\mathrm{sep}}-t_{\mathrm{skip}}} G^{\mathrm{eff}}_{E,M}(Q^2;t,t_{\mathrm{sep}}), \quad t_{\mathrm{skip}} = 2a \tag{4}$$

- Parametrically suppresses the effects of excited states ($\propto e^{-\Delta t_{\mathrm{sep}}}$ instead of $\propto e^{-\Delta t}$, $e^{-\Delta(t_{\mathrm{sep}}-t)}$ [Δ: energy gap to lowest-lying excited state]) $\rightarrow$ "summation method"
- For $t_{\mathrm{sep}} \rightarrow \infty$, the slope as a function of t_{sep} is given by the ground-state form factor,

$$S_{E,M}(Q^2;t_{\mathrm{sep}}) \xrightarrow{t_{\mathrm{sep}}\rightarrow\infty} C_{E,M}(Q^2) + \frac{1}{a}(t_{\mathrm{sep}} + a - 2t_{\mathrm{skip}})G_{E,M}(Q^2) \tag{5}$$

Excited-state analysis: window average

- Apply summation method with varying starting values $t_{\mathrm{sep}}^{\mathrm{min}}$ for the linear fit
- Perform a weighted average over $t_{\mathrm{sep}}^{\mathrm{min}}$, where the weights are given by a smooth window function[6],

$$\hat{G} = \frac{\sum_i w_i G_i}{\sum_i w_i}, \qquad w_i = \tanh \frac{t_i - t_w^{\mathrm{low}}}{\Delta t_w} - \tanh \frac{t_i - t_w^{\mathrm{up}}}{\Delta t_w}, \tag{6}$$

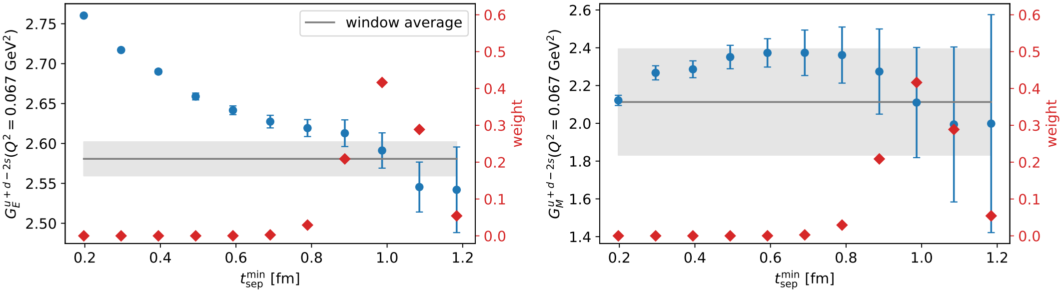
where t_i is the value of $t_{\mathrm{sep}}^{\mathrm{min}}$ in the i-th fit, $t_w^{\mathrm{low}} = 0.9\,\mathrm{fm}$, $t_w^{\mathrm{up}} = 1.1\,\mathrm{fm}$ and $\Delta t_w = 0.08\,\mathrm{fm}$

[6] Djukanovic et al. 2022 [PRD **106**, 074503]; Agadjanov et al. 2023 [PRL **131**, 261902].

Excited-state analysis: window average

- Apply summation method with varying starting values $t_{\mathrm{sep}}^{\mathrm{min}}$ for the linear fit
- Perform a weighted average over $t_{\mathrm{sep}}^{\mathrm{min}}$, where the weights are given by a smooth window function[6]

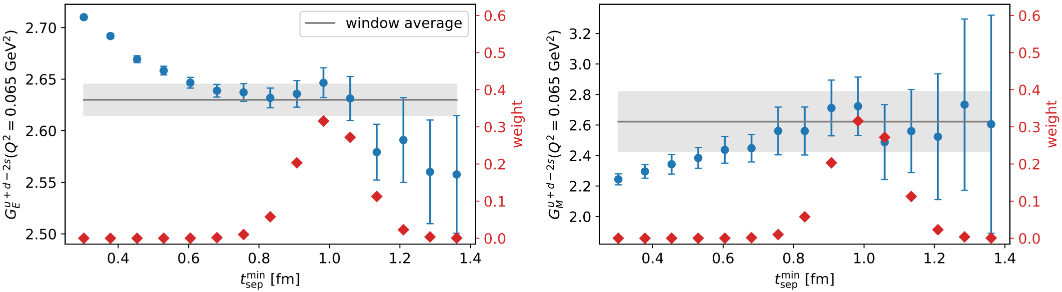
E300 ($M_\pi = 176$ MeV, $a = 0.049$ fm)



[6] Djukanovic et al. 2022 [PRD **106**, 074503]; Agadjanov et al. 2023 [PRL **131**, 261902].

Excited-state analysis: window average

D450 ($M_\pi = 218$ MeV, $a = 0.076$ fm)



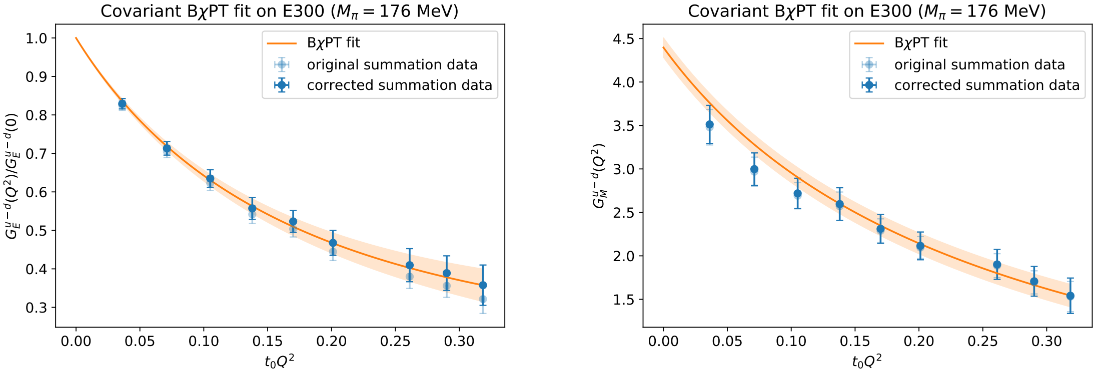
- Reliable detection of the plateau with reduced human bias (same window on all ensembles)
- Conservative error estimate

Direct Baryon χPT fits

- $\langle r^2 \rangle = -\frac{6}{G(0)} \frac{\partial G(Q^2)}{\partial Q^2}\Big|_{Q^2=0}$, $\mu_M = G_M(0) \Rightarrow$ parametrize Q^2-dependence of FFs
- Combine this with the chiral, continuum, and infinite-volume extrapolation
- Use expressions from covariant chiral perturbation theory[7] to perform a simultaneous fit to the pion-mass, Q^2-, lattice-spacing, and finite-volume dependence of the form factors
- Include contributions from the ρ (ω and ϕ) mesons in the isovector (isoscalar) channel
- Reconstruct proton and neutron observables from separate fits to the isovector and isoscalar form factors
- Perform fits with various cuts in M_π and Q^2, as well as with different models for the lattice-spacing and finite-volume dependence, in order to estimate systematic uncertainties
- Large number of degrees of freedom $\Rightarrow$ improved stability against lowering the Q^2-cut

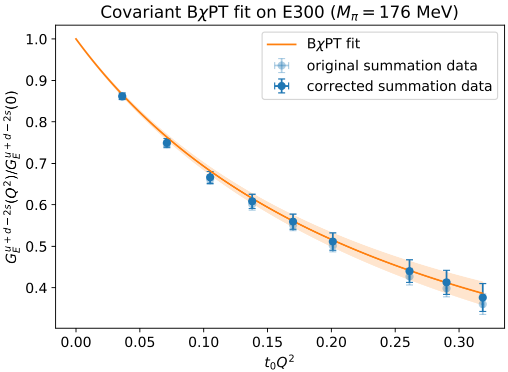
[7] Bauer, Bernauer, and Scherer 2012 [PRC **86**, 065206].

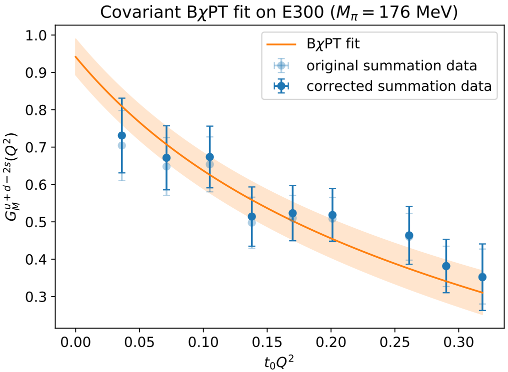
Q^2-dependence of the isovector form factors on E300



- Direct BχPT fit describes data very well
- Reduced error due to the inclusion of several ensembles in one fit

Q^2-dependence of the isoscalar form factors on E300





Zemach and Friar radii from the lattice

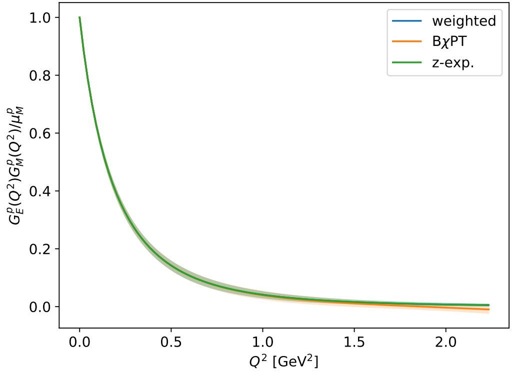
- BχPT including vector mesons only trustworthy for $Q^2 \lesssim 0.6\,\text{GeV}^2$
- Tail of the integrands suppressed: contribution of the form factors above $0.6\,\text{GeV}^2$ to r_Z^p less than $0.9\,\%$, to $\langle r_E^3\rangle_{(2)}^p$ less than $0.3\,\%$
- Extrapolate BχPT fit results using a z-expansion[8] *ansatz*
- Incorporate the large-Q^2 constraints on the form factors[9]
- For integration, smoothly replace BχPT parametrization of the form factors by z-expansion-based extrapolation ($\Delta Q_w^2 = 0.1\,\text{GeV}^2$),

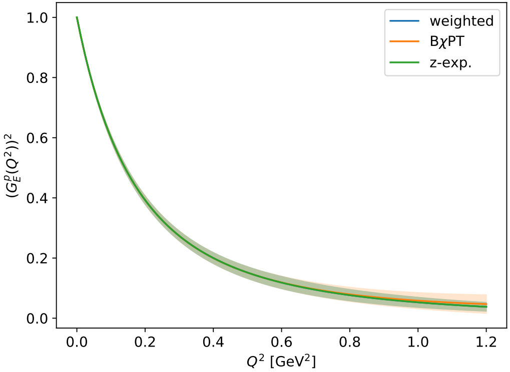
$$F(Q^2) = \frac{1}{2}\left[1 - \tanh\left(\frac{Q^2 - Q_{\text{cut}}^2}{\Delta Q_w^2}\right)\right] F^{\chi}(Q^2) + \frac{1}{2}\left[1 + \tanh\left(\frac{Q^2 - Q_{\text{cut}}^2}{\Delta Q_w^2}\right)\right] F^{z}(Q^2), \tag{7}$$

where $F(Q^2) \equiv G_E(Q^2) G_M(Q^2)/\mu_M$ for r_Z and $F(Q^2) \equiv G_E^2(Q^2)$ for $\langle r_E^3\rangle_{(2)}$, resp.

[8] Hill and Paz 2010 [PRD **82**, 113005]; [9] Lepage and Brodsky 1980 [PRD **22**, 2157]; Lee, Arrington, and Hill 2015 [PRD **92**, 013013].

Integrands for the Zemach radius and third Zemach moment of the proton





- BχPT clearly not reliable for large Q^2
- z-expansion agrees well with BχPT parametrization in region where it is fitted

Outline

Model average

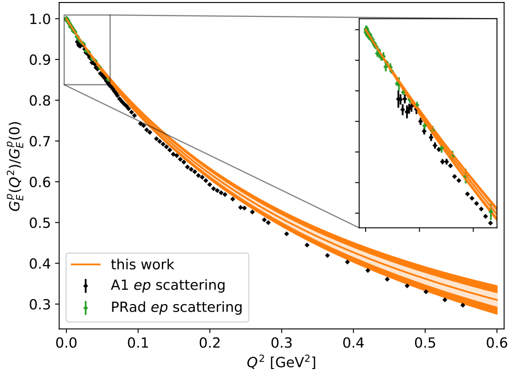
- Perform a weighted average over the results of all fit variations, using weights derived from the Akaike Information Criterion[10],

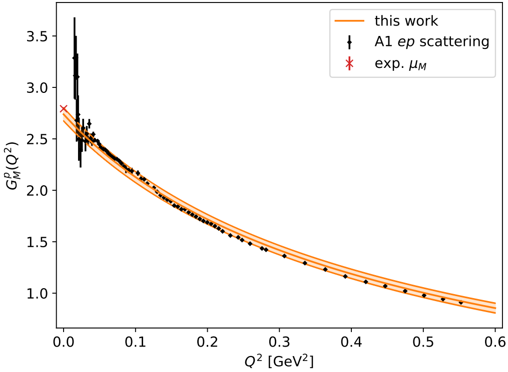
$$w_i = \exp\left(-\frac{1}{2}\mathrm{BAIC}_i\right) \Big/ \sum_j \exp\left(-\frac{1}{2}\mathrm{BAIC}_j\right) , \quad \mathrm{BAIC}_i = \chi^2_{\mathrm{noaug,min},i} + 2n_{f,i} + 2n_{c,i}, \tag{8}$$

  where n_f is the number of fit parameters and n_c the number of cut data points
- Strongly prefers fits with low n_c, *i.e.*, the least stringent cut in Q^2 $\Rightarrow$ apply a flat weight over the different Q^2-cuts to ensure strong influence of our low-momentum data
- Determine the final cumulative distribution function (CDF) from the weighted sum of the bootstrap distributions[11]
- Quote median of this CDF together with the central $68\,\%$ percentiles

[10] Akaike 1974 [IEEE Trans. Autom. Contr. **19**, 716]; Neil and Sitison 2022 [arXiv:2208.14983]; [11] Borsányi et al. 2021 [Nature **593**, 51].

Model-averaged proton form factors at the physical point

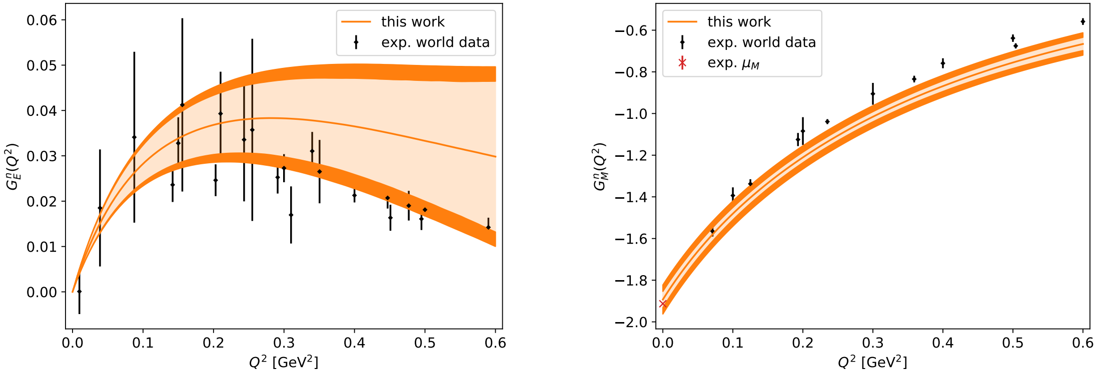




- Slope of the electric form factor closer to that of PRad[12] than to that of A1[13]
- Good agreement with A1 for the magnetic form factor

[12]Xiong et al. 2019 [Nature **575**, 147]; [13]Bernauer et al. 2014 [PRC **90**, 015206].

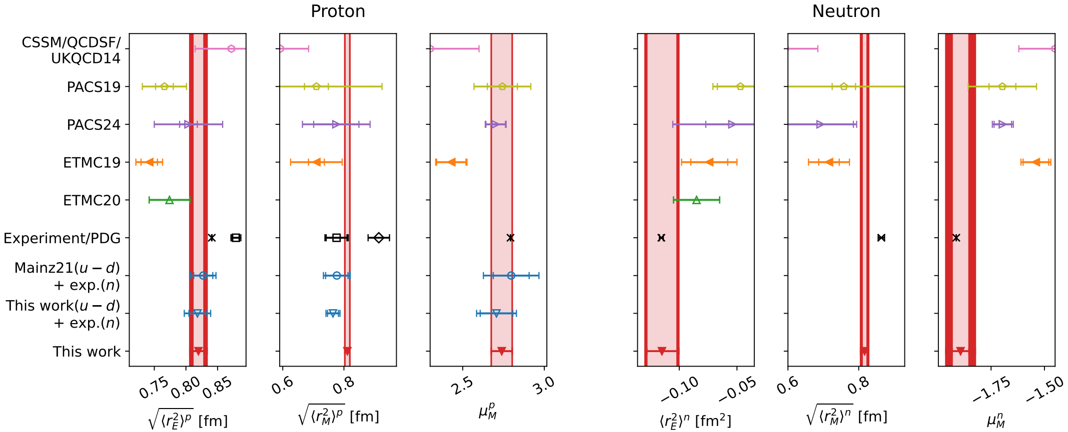
Model-averaged neutron form factors at the physical point



(Mostly) compatible with the collected experimental world data[14] within our errors

[14] Ye et al. 2018 [PLB **777**, 8].

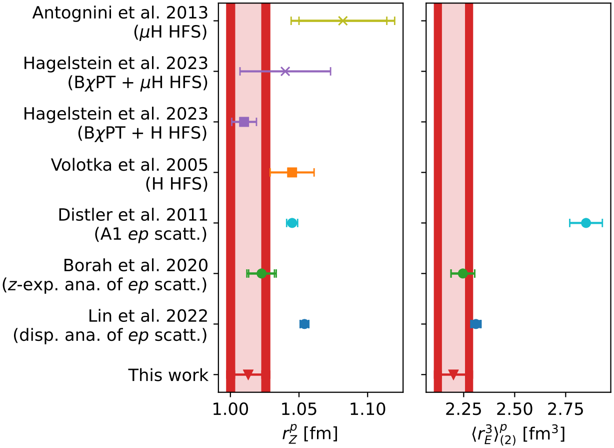
Electromagnetic radii and magnetic moments



Magnetic moments reproduced, low value for $\sqrt{\langle r_E^2\rangle^p}$ clearly favored, $\sqrt{\langle r_M^2\rangle^p}$ agrees with A1

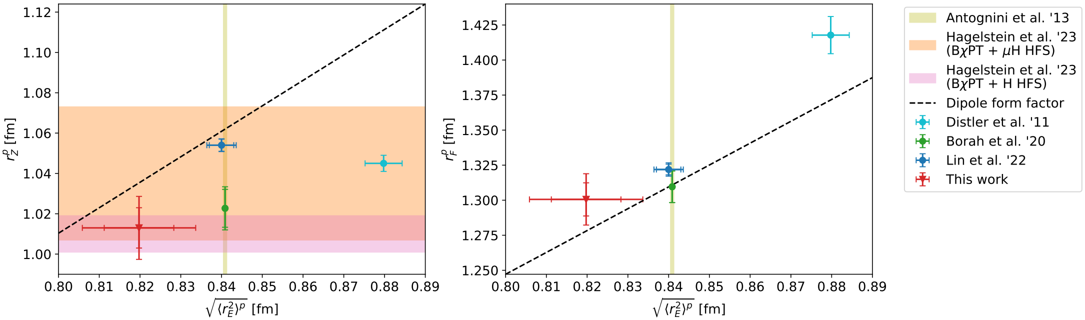
Zemach radii and third Zemach moments

- r_Z^p: low value favored, but agrees within $2\,\sigma$ with most other determinations (except for dispersive analysis)
- $\langle r_E^3 \rangle_{(2)}^p$: low value favored, good agreement with dispersive analysis, clear tension with A1
- Our estimates are $\sim 80\,\%$ and $\sim 95\,\%$, respectively, correlated with electromagnetic radii
- Low results for r_Z^p and $\langle r_E^3 \rangle_{(2)}^p$ expected, no independent puzzle



- Neutron results agree with z-expansion analysis of world en-scattering data, larger error

Correlations between different proton radii



- Large correlation of Zemach and Friar radii with electromagnetic radii also in experiment
- Lattice results seem to confirm trend observed in data-driven evaluations

Outline

Conclusions

- Determination of the electromagnetic form factors of the proton and neutron from lattice QCD including connected and disconnected contributions, as well as a full error budget
- Magnetic moments of the proton and neutron agree well with the experimental values
- Small electric *and* magnetic radii of the proton favored
- Accordingly also small values for Zemach and Friar radii of the proton favored (large correlation with electromagnetic radii)
- Good agreement with dispersive approaches for electric properties of the proton (electric and Friar radii), tension regarding its magnetic properties (magnetic and Zemach radii)
- Competitive errors, in particular for the magnetic radii
- Further investigations required, in particular for the proton's magnetic and Zemach radii

Backup slides

From correlation functions to form factors

- Average over the forward- and backward-propagating nucleon and over x-, y-, and z-polarization for the disconnected part
- Calculate the ratios

$$R_{V_\mu}(\mathbf{q}; t_{\text{sep}}, t) = \frac{C_{3,V_\mu}(\mathbf{q}; t_{\text{sep}}, t)}{C_2(\mathbf{0}; t_{\text{sep}})} \sqrt{\frac{\bar{C}_2(\mathfrak{q}; t_{\text{sep}} - t) C_2(\mathbf{0}; t) C_2(\mathbf{0}; t_{\text{sep}})}{C_2(\mathbf{0}; t_{\text{sep}} - t) \bar{C}_2(\mathfrak{q}; t) \bar{C}_2(\mathfrak{q}; t_{\text{sep}})}}, \tag{9}$$

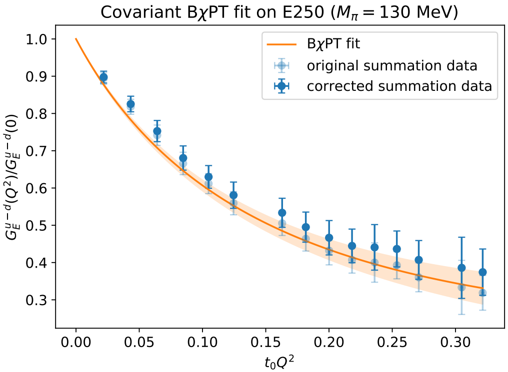
where $t_{\text{sep}} = y_0 - x_0$, $t = z_0 - x_0$, and $\bar{C}_2(\mathfrak{q}; t_{\text{sep}}) = \sum_{\tilde{\mathbf{q}} \in \mathfrak{q}} C_2(\tilde{\mathbf{q}}; t_{\text{sep}}) \Big/ \sum_{\tilde{\mathbf{q}} \in \mathfrak{q}} 1$

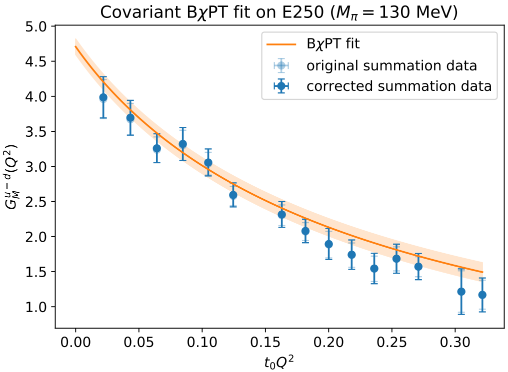
- At zero sink momentum, the effective form factors can be computed from the ratios as

$$G_E^{\text{eff}}(Q^2; t_{\text{sep}}, t) = \sqrt{\frac{2E_{\mathbf{q}}}{m + E_{\mathbf{q}}}} R_{V_0}(\mathbf{q}; t_{\text{sep}}, t), \tag{10}$$

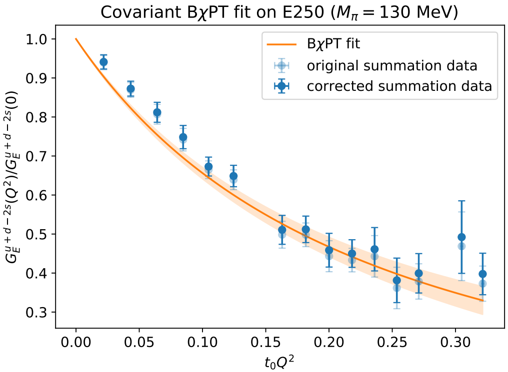
$$G_M^{\text{eff}}(Q^2; t_{\text{sep}}, t) = \sqrt{2E_{\mathbf{q}}(m + E_{\mathbf{q}})} \frac{\sum_{j,k} \epsilon_{ijk} q_k \operatorname{Re} R_{V_j}^{\Gamma_i}(\mathbf{q}; t_{\text{sep}}, t)}{\sum_{j \neq i} q_j^2} \tag{11}$$

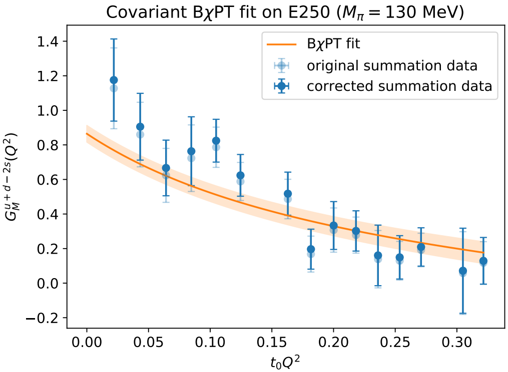
Q^2-dependence of the isovector form factors on E250



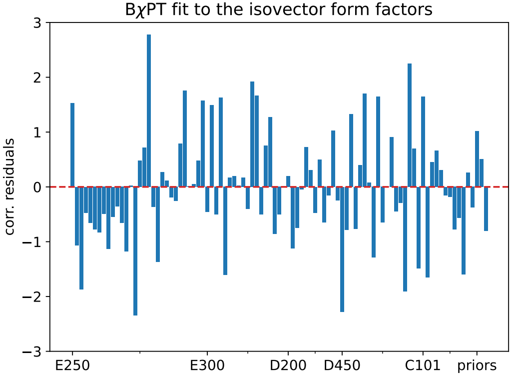


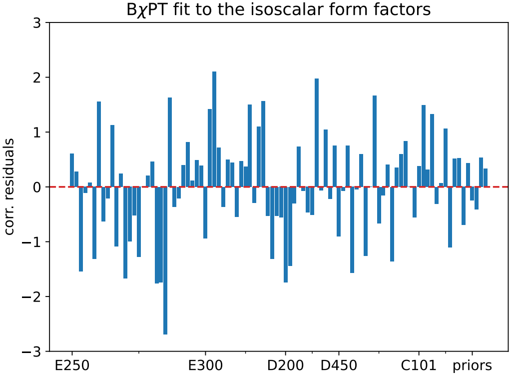
Q^2-dependence of the isoscalar form factors on E250



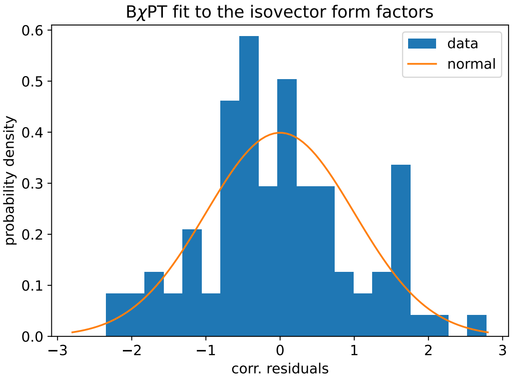


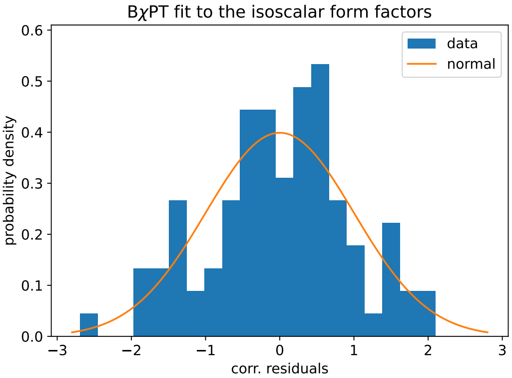
Residuals of the BχPT fits





Histograms


BχPT fit to the isovector form factors
data
normal
probability density
corr. residuals
0.0
0.1
0.2
0.3
0.4
0.5
0.6
−3
−2
−1
0
1
2
3


BχPT fit to the isoscalar form factors
data
normal
probability density
corr. residuals
0.0
0.1
0.2
0.3
0.4
0.5
0.6
−3
−2
−1
0
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2
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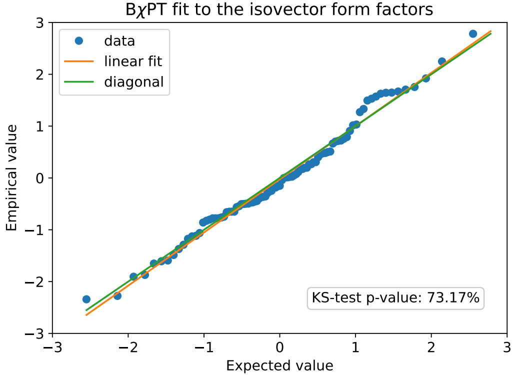
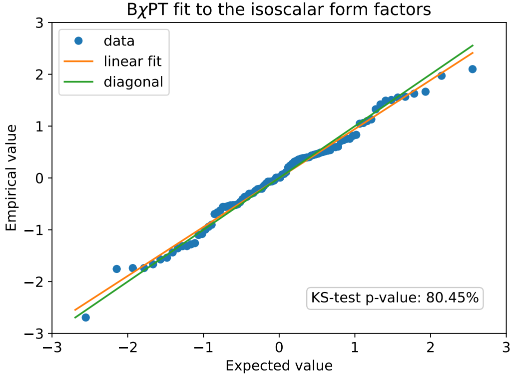
Q-Q plots



BχPT fit to the isovector form factors
data
linear fit
diagonal
KS-test p-value: 73.17%
Empirical value
Expected value



BχPT fit to the isoscalar form factors
data
linear fit
diagonal
KS-test p-value: 80.45%
Empirical value
Expected value

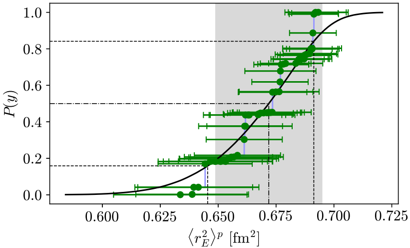
Disambiguating the statistical and systematic uncertainties

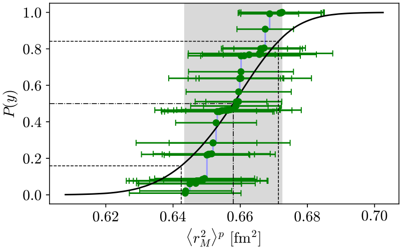
- Scale the statistical variances of the individual fit results by a factor of $\lambda = 2$
- Repeat the model averaging procedure
- Assumptions:
  - Above rescaling only affects the statistical error of the averaged result
  - Statistical and systematic errors add in quadrature
- Contributions of the statistical and systematic errors to the total error,

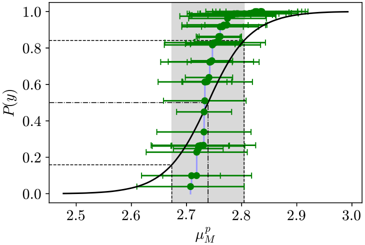
$$\sigma_{\mathrm{stat}}^2 = \frac{\sigma_{\mathrm{scaled}}^2 - \sigma_{\mathrm{orig}}^2}{\lambda - 1}, \qquad \sigma_{\mathrm{syst}}^2 = \frac{\lambda\sigma_{\mathrm{orig}}^2 - \sigma_{\mathrm{scaled}}^2}{\lambda - 1} \tag{12}$$

- Consistency check: results are almost independent of λ (if it is chosen not too small)

CDFs of the electromagnetic radii and magnetic moment of the proton







Final results

Observable	Isovector	Isoscalar	Proton	Neutron
$\langle r_E^2 \rangle$ [fm^2]	$0.785(22)(26)$	$0.554(18)(13)$	$0.672(14)(18)$	$-0.115(13)(7)$
$\langle r_M^2 \rangle$ [fm^2]	$0.663(11)(8)$	$0.657(30)(31)$	$0.658(12)(8)$	$0.667(11)(16)$
μ_M	$4.62(10)(7)$	$2.47(11)(10)$	$2.739(63)(18)$	$-1.893(39)(58)$
r_Z [fm]	–	–	$1.013(10)(12)$	$-0.0411(56)(40)$
$\langle r_E^3 \rangle_{(2)}$ [fm^3]	–	–	$2.200(60)(71)$	$0.0078(20)(12)$

- z-expansion: model-independent description of the Q^2-dependence of the form factors
- Map domain of analyticity of the form factors onto the unit circle,

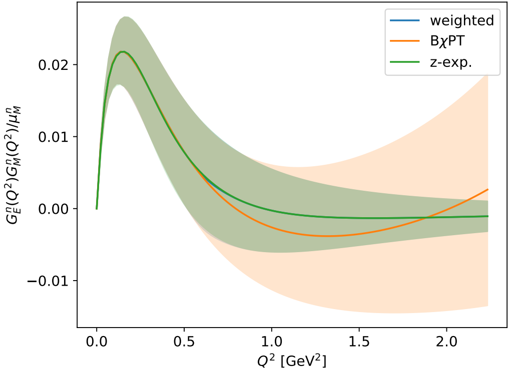
$$z(Q^2) = \frac{\sqrt{\tau_{\text{cut}} + Q^2} - \sqrt{\tau_{\text{cut}} - \tau_0}}{\sqrt{\tau_{\text{cut}} + Q^2} + \sqrt{\tau_{\text{cut}} - \tau_0}}, \tag{13}$$

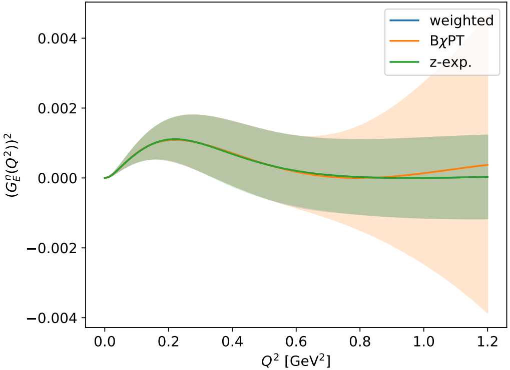
  where $\tau_{\text{cut}} = 4M_{\pi,\text{phys}}^2$, and we employ $\tau_0 = 0$
- Expand the form factors as

$$G_E^{p,n}(Q^2) = \sum_{k=0}^{m} a_k^{p,n} z(Q^2)^k, \quad G_M^{p,n}(Q^2) = \sum_{k=0}^{m} b_k^{p,n} z(Q^2)^k \tag{14}$$

- We fix $G_E^p(0) = a_0^p = 1$ and $G_E^n(0) = a_0^n = 0$, respectively, use $m = 9$, and incorporate the 4 sum rules for each form factor

Integrands for the Zemach radius and third Zemach moment of the neutron

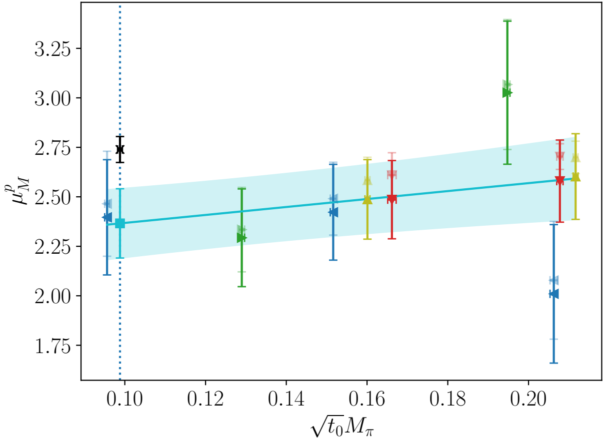




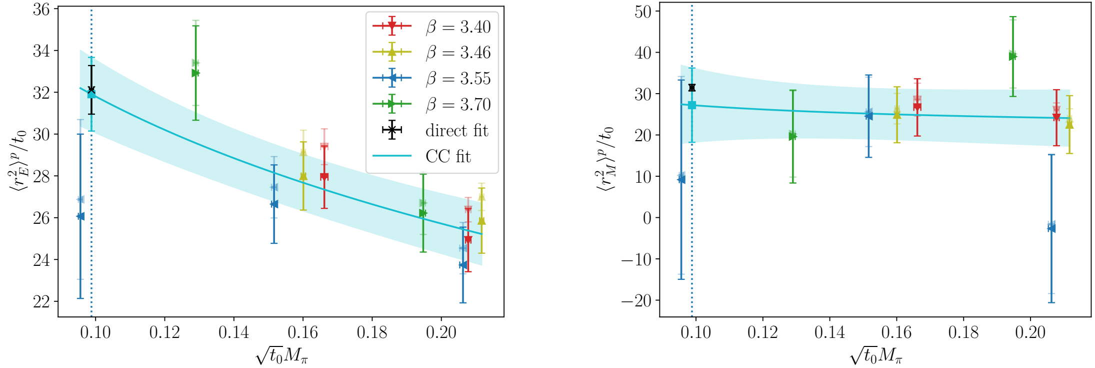
z-expansion agrees also here well with BχPT parametrization in region where it is fitted

Crosscheck of direct fits with z-expansion: proton magnetic moment

- Use $m = 2$ and no sum rules (focus on low-momentum region)
- Magnetic moment significantly smaller than direct fits which are compatible with experiment
- Direct fits use more data in one fit $\Rightarrow$ increased stability against statistical fluctuations



Crosscheck of direct fits with z-expansion: proton electromagnetic radii



Radii in good agreement with direct fits, albeit with significantly larger errors