Lattice QCD for Hadron Structure and Interactions

Y. Chen, X. Feng, C. Liu, T. Luu, M. Petschlies, A. Rusetsky, F. Steffens, and C. Urbach

Beratungsgespräch in Beijing 2010

Supercomputer in Jülich

- first European Petaflop Computer

[(c) FZ Jülich]

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… where we started in 2012

Lattice QCD

- IsoQCD simulations
- $N_f = 2 + 1 + 1$ dynamical quarks
- $M_\pi \geq 250$ MeV
- lattice spacings $a \geq 0.06$ fm

Finite Volume Formalism

- two-particle, single channel formalism developed
- attractive and repulsive interactions

Hadron Interaction Results

- $\pi\pi$ at maximal isospin and ρ for at most a few pion masses and lattice spacings
- scalar mesons with unphysical approximations
- $\pi\Sigma$ or Kp meson-baryon with no control of systematics
- baryon-baryon scattering with no control of systematics
  (at very unphysical pion mass values)

… where we started in 2012

Parton Distribution Functions

- only Mellin moments $\langle x^n \rangle$ were accessible
- x dependence cannot not be calculated directly
- even moments computed mostly with approximations (quenched, no disconnecteds, …)
- nucleon well covered
- little available for pion / kaon

… where we started in 2012

Supercomputer in Jülich

- Juqueen: 5.9 Pflops

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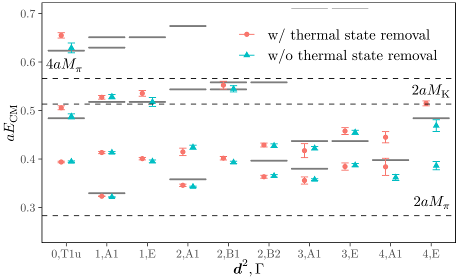
Lüscher Method on One Page

Lattice Energy Levels E



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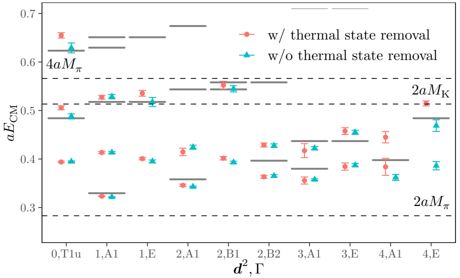

Determinant Equation

$$\det\left[\mathcal{M}^{\Gamma,\mathbf{d}}(E) - \cot(\delta)\right] = 0$$

($\mathcal{M}$ Lüscher function,
δ continuum phase shift)

Lüscher Method on One Page

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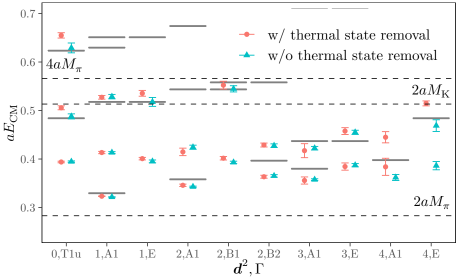

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Continuum Interaction Parameters

obtained via fits to δ at n discrete scattering energies E_i

Lüscher Method: The Simplest Case

- consider only S-wave, no mixing, and assume finite range expansion

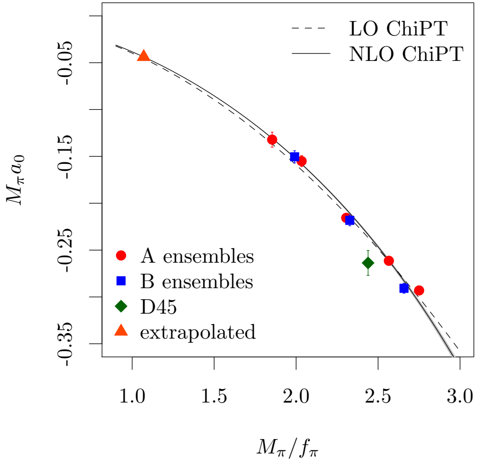
$$\Delta E \;=\; -\frac{2\pi a_0}{\mu L^3}\left(1 + c_1\frac{a_0}{L} + c_2\frac{a_0^2}{L^2} + c_3\frac{a_0^3}{L^3}\ldots\right)$$

- The scattering length a_0 can be determined by inverting this equation!
- c_i known, L the box extent, μ the reduced two particle non-interacting mass
- works excellent e.g. for $\pi\pi$ scattering with $I = 0, 2$

$\pi\pi$-Scattering I

- $\pi\pi$ at $I = 2$ $\Rightarrow$ benchmark system
- weakly repulsive
- parameter free LOChiPT prediction
- three lattice spacings, different volumes
- found only very small deviations from LO chiral perturbation theory

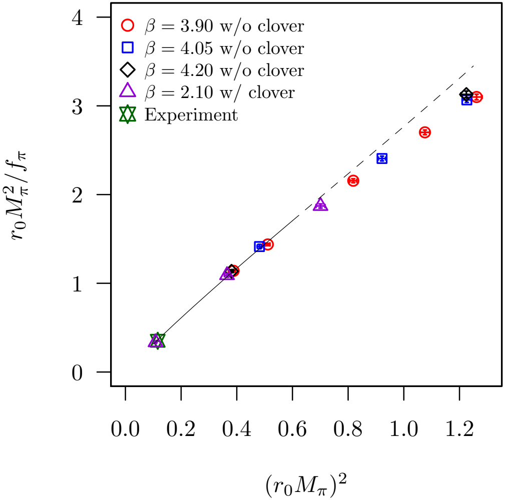
  [ETMC, C. Helmes et al., JHEP 09 (2015) 109]
- similar results for πK and KK scattering



… arriving at the physical point in 2015

- inclusion of clover term in ETMC ensembles
- further reduction in lattice artefacts made physical point possible
- proof of concept in $N_f = 2$ flavour QCD at single lattice spacing value

  [ETMC, Abdel-Rehim et al., Phys.Rev.D 95 (2017) 9, 094515]
- actual goal: $N_f = 2 + 1 + 1$ physical point



$\pi\pi$-Scattering II

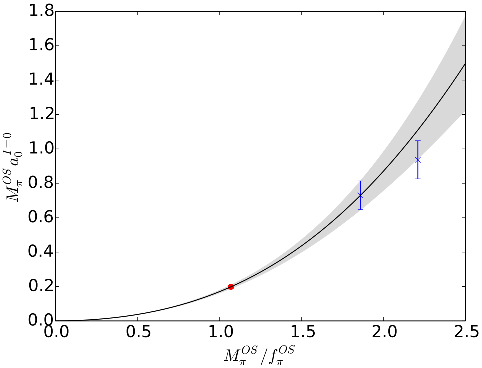
- $I = 0$ two pion scattering
- much more challenging due to fermionic disconnected contributions
- mixed action due to flavour symmetry breaking in Wilson twisted mass

[Liu et al., Phys.Rev.D 96 (2017) 5, 054516]

$$M_\pi a_0^{I=1} \;=\; 0.198(9)(6)$$

- significant systematic effects expected

[Draper, Sharpe, Phys.Rev.D 105 (2022) 3, 034508]

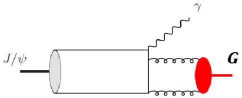


Balls with Glue? Radiative J/ψ Decays

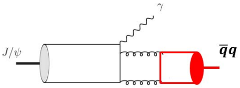
- can one identify one of the ten scalar mesons as predominantly a glueball?
- highly non-trivial question (and maybe not well defined)
- radiative decays of J/ψ might be a good place to look for scalar glueballs
- decay into $\bar{q}q$ naïvly suppressed by α_s^2
- here: exploratory quenched study, two lattice spacings

  [L.Gui, et al. (CLQCD), Phys. Rev. Lett. 110, 021601 (2013)]
- for tensor glueballs see

  [Y.B. Yang et al .(CLQCD), Phys. Rev. Lett. 111, 091601 (2013)]



$O(1)$



$O(\alpha_s^2)$

- **not** based on Lüscher method
- matrix element

$$\propto \langle G | j^\mu | J/\psi \rangle$$

estimated from three-point function

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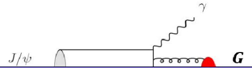

(1)

α_s^2)

d

estimated from three-point function

Main conclusion

$\Gamma(J/\psi \rightarrow \gamma \rightarrow G_{0^+})/\Gamma_{\text{tot}} = 3.8(9) \times 10^{-3}$ from LQCD

consistent with $f_0(1710)$ PDG production rate

BR$(J/\psi \rightarrow \gamma \rightarrow \gamma f_0(1710)) = 1.9 \times 10^{-3}$

and inconsistent with rates of other scalar mesons.

Quenched, so systematics are uncontrolled!

... second funding period 2016

Supercomputer in Jülich

- still Juqueen: 5.9 Pflops

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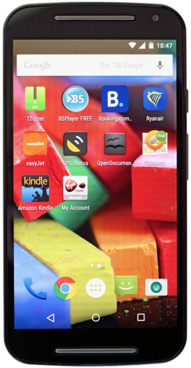

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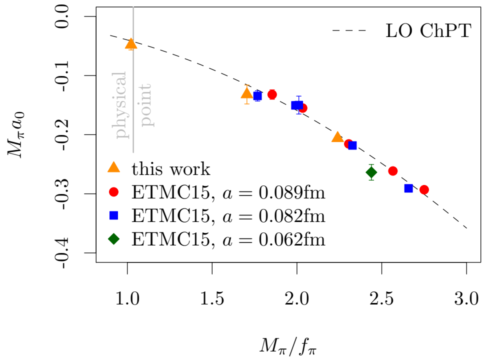
$\pi\pi$-Scattering III

- $N_f = 2$ results for the $I = 2$ scattering length
- confirm the previous extrapolation
- and mass dependence

  [Fischer et al., Eur.Phys.J.C 81 (2021) 5, 436]
- physical point ensemble significantly noisier



A Third Particle Enters the Game

- Three particle decays highly relevant
- Three-pion decays of $K, \eta, \omega, a_1(1260), a_1(1420)$
- Decays of exotica, e.g.: $X(3872) \to \bar{D}^* D \to \bar{D} D\pi$, $Y(4260) \to J/\psi\,\pi\pi$
- Roper resonance $\to \pi N$ and $\pi\pi N$
- Few-body physics: reactions with the light nuclei

Lattice Energy Levels E
Finite Volume, discrete, real

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Lattice Energy Levels E
Finite Volume, discrete, real

↓ EFTs

Interaction Properties
Infinite Volume, possibly complex

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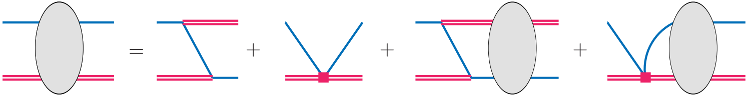
Three equivalent EFTs

- RFT (Relativistic Field Theory)
  [Hansen, Sharpe, 2014]
- NREFT (Non-relativistic EFT)
  [Hammer, Pang, Rusetsky, 2017]
- FVU (Finite Volume Unitarity)
  [Mai, Döring, 2017]

The Quantization Condition in Non-Relativistic EFT



Bethe-Salpeter equation

[Hammer, Pang, Rusetsky, 2017]

$$\mathcal{M}(\mathbf{p},\mathbf{q};E) = Z(\mathbf{p},\mathbf{q};E) + 8\pi\int^{\Lambda}\frac{d^3\mathbf{k}}{(2\pi)^3 2w(\mathbf{k})}\,Z(\mathbf{p},\mathbf{k};E)\tau(\mathbf{k};E)\mathcal{M}(\mathbf{k},\mathbf{q};E)$$

$$Z(\mathbf{p},\mathbf{q};E) = \frac{1}{2w(\mathbf{p}+\mathbf{q})(w(\mathbf{p})+w(\mathbf{q})+w(\mathbf{p}+\mathbf{q})-E)} + \underbrace{\tilde{H}_0}_{\text{data: 3-particle sector}} + \cdots$$

2-body amplitude: $4w(k^*)\tau^{-1}(\mathbf{k};E) = \underbrace{k^*\cot\delta(k^*)}_{\text{data: 2-particle sector}} + \underbrace{\sqrt{\frac{s_2}{4}-m^2}}_{=k^*}$

Finite volume: $\mathbf{p} = \frac{2\pi}{L}\mathbf{n},\ \mathbf{n}\in\mathbb{Z}^3$, poles of the scattering matrix $\Rightarrow$ spectrum

Three Pions at Maximal Isospin

- Three pions in $N_f = 2$ incl. physical point

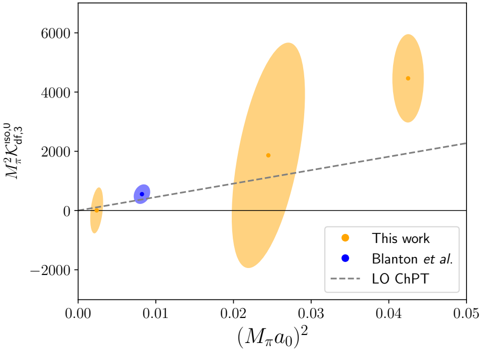
  [Fischer et al., Eur.Phys.J.C 81 (2021) 5, 436]

- analysis using RFT
- det equation

$$\det(F_3^{-1}(E^*, L) + \mathcal{K}_{3,\text{df}}(E^*)) = 0$$

- $\mathcal{K}_{3,\text{df}}$ related to physical scattering amplitude $\mathcal{M}_3$ via integral equations
- isotropic approximation

$$\mathcal{K}_{3,\text{df}} = \mathcal{K}^{\text{iso},0}_{\text{df},3} + \mathcal{K}^{\text{iso},1}_{\text{df},3}\Delta\,, \quad \Delta = \frac{(E^*)^2 - 9M_\pi^2}{9M_\pi^2}\,,$$



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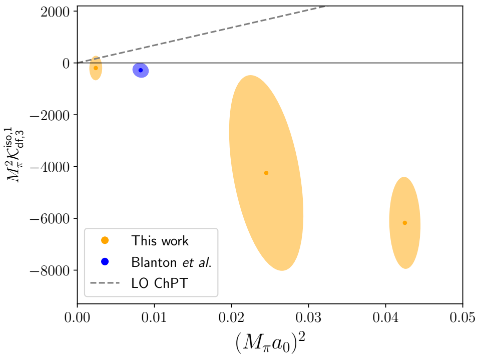
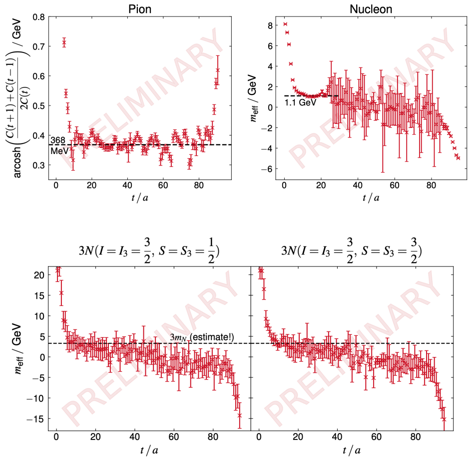


First (and last?) LQCD attempt at the 3-neutron system

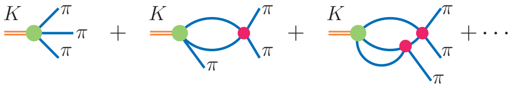
- 3-neutrons: the really hard stuff!
  exponentially error growth
- Developed interpolating operators and contraction codes for p-wave $S = \frac{1}{2}$ and $\frac{3}{2}$ three-neutron system
- Measurements performed on $48^3 \times 96$ Clover lattices with $m_\pi \approx 370$ MeV
- No signal due to noise (not surprising)



[Wynen, Luu, *et al.*, https://doi.org/10.22323/1.334.0092 (2018)]

The 3-particle analog of the Lellouch-Lüscher formula

- Final-state interactions lead to an irregular L-dependence of the matrix element



[Müller & Rusetsky, 2020]

- The non-relativistic Lagrangian

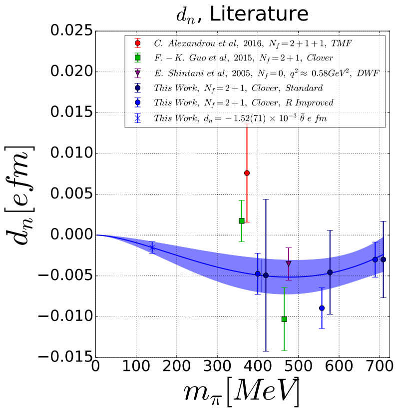
$$\begin{aligned}\mathscr{L} &= \phi^\dagger(i\partial_t - w)(2w)\phi + \frac{C_0}{4}\phi^\dagger\phi^\dagger\phi\phi + \cdots + \frac{D_0}{36}\phi^\dagger\phi^\dagger\phi^\dagger\phi\phi\phi \\ &+ K^\dagger(i\partial_t - w_K)(2w_K)K + g(K^\dagger\phi\phi\phi + \text{h.c.}) + \cdots\end{aligned}$$

- Calculate the decay matrix element in a finite and in the infinite volume, extract g
- Matrix elements are related through

$$|\langle n|H_W|K\rangle_L| = \underbrace{\mathbb{L}_3(L)}_{\text{depends on pion interactions}} |\langle\pi\pi\pi; out|H_W|K\rangle_\infty|$$

Nucleon EDM and the Gradient Flow

- Gradient flow (GF) protects us from systematic errors associated with the lattice spacing
- Used GF + LQCD+θ-term to calculate induced nucleon EDM
- Performed chiral + continuum extrapolations
- Accounted for finite-volume mixing of form factors



times $\bar{\theta}$!

[Dragos, Luu, Shindler, de Vries, Yousif, https://doi.org/10.1103/PhysRevC.103.015202 (2019)]

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  systemati
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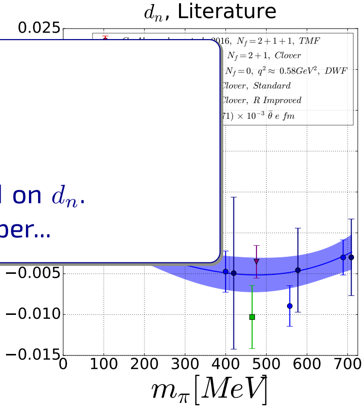
limit on $\bar{\theta}$

$$|\bar{\theta}| < 1.98 \times 10^{-10}$$

using the experimental bound on d_n.
more predictions in the paper...



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... third funding period 2021

Supercomputer in Jülich

- Juwels: 85 Pflops
- including 73 Pflops GPU booster module

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Understanding Systematics of 3pt Quantisation in ϕ^4-Theory

- two scalar fields ϕ_0, ϕ_1

  [Garofalo, Romero-López, Rusetsky, Urbach, 2023]

- include interaction term

$$S_{\text{int}} = +\frac{g}{2}\phi_0\phi_1^3$$

- allows decay $\phi_0 \to 3\phi_1$

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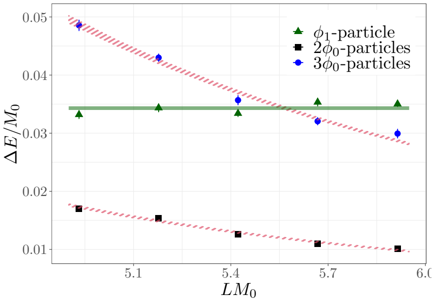

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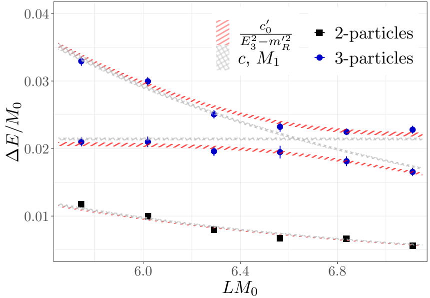
$$S_{\text{int}} = +\frac{g}{2}\phi_0\phi_1^3$$

- allows decay $\phi_0 \to 3\phi_1$
- at $g = 0$ no coupling
- at $g > 0$ avoided level crossing

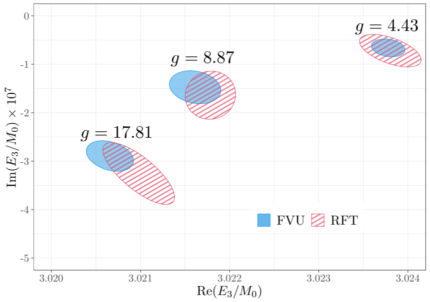


First observation in
a Lattice calculation

Understanding Systematics of 3pt Quantisation in ϕ^4-Theory

- can go further in this model

  [Garofalo, Mai, Romero-López, Rusetsky, Urbach, 2023]
- reconstruct complex mass
- compare FVU and RFT approaches
- we find good agreement!
- but systematics visible



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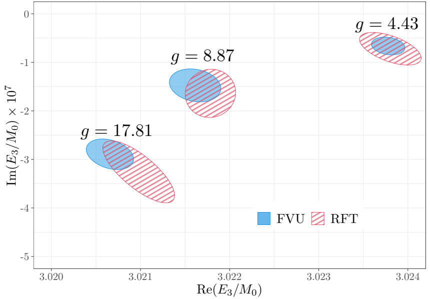


Equivalence of FVU and RFT shown in practice in controlled model

J/ψ decays in $N_f = 2$ Flavour Lattice QCD

$J/\psi \to \eta_2$ decay

- similar methodology as the quenched radiative J/ψ decay study
- result

$$\Gamma(J/\psi \to \gamma\eta_2) = 0.385(45)\ \text{keV}$$

[X. Jiang et al., Phys. Rev. Lett. 130, 061901 (2023)]

- assume $U_A(1)$ anomaly and particular value of the mixing angle θ: predictions for η/η' consistent with PDG
- see also other η_2 CRC110 study

[Dimopoulos et al., Phys.Rev.D 99 (2019) 3, 034511]

$J/\psi \to 3\gamma$ decay

- rare decay as precision QCD test
- calculation involves Euclidean 4-point function
- only decay width calculated

$$\Gamma \approx 1.5(3)\ \text{eV}$$

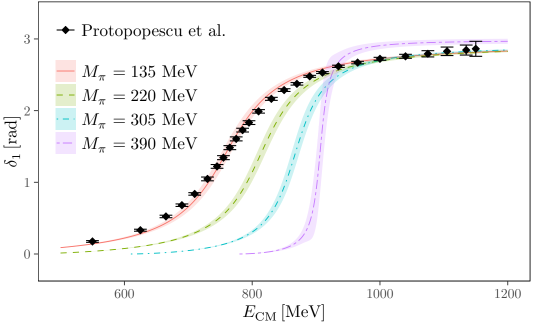
[Meng et al., Phys.Rev.D 102 (2020) 5, 054506]

- agreement with experiment within errors
- Lattice Dalitz plot can be directly compared

ρ -Meson to the Limits

- ρ -resonance a poster Breit-Wigner resonance
- best studied resonance from Lattice QCD
- first continuum extrapolated analysis performed in CRC110

  [Werner et al., Phys.Lett.B 819 (2021) 136449]
- chiral extrapolation based on VMEFT
- still: large systematic effects expected

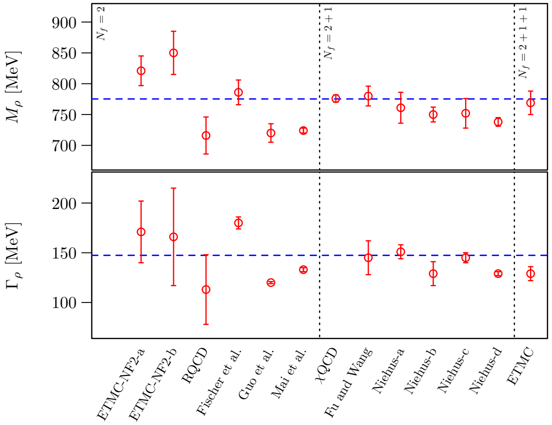


ρ -Meson Summary

- comprehensive comparison in CRC110 review paper

  [Mai, Meißner, Urbach, Phys. Rept. 1001 (2023) 1-66]

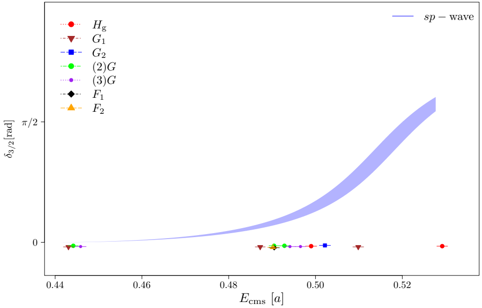
- uncertainties shrink over time
- but there are still discrepancies
- calculation at physical pion mass with several lattice spacings needed!



Elastic πN-scattering and the Δ Resonance

- Δ: lowest lying baryon resonance
- determination at physical pion mass
- single lattice spacing / volume
- includes S- and P-wave mixing
- example P-wave phase shift
- they obtain

$$M_\pi a_0^{3/2} = 0.13(4)$$
$$M_R = 1269(45)\text{MeV}$$
$$\Gamma_R = 144(181)\text{MeV}$$



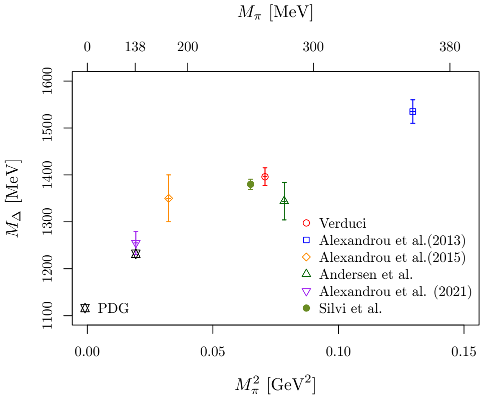
[Alexandrou et al., Phys.Rev.D 109 (2024) 3, 3]

Elastic πN-scattering and the Δ Resonance

- lattice overview for Δ

  [Mai, Meißner, Urbach, Phys, Rept, 1001 (2023) 1-66]

- resonance mass in reasonable agreement with experiment
- width (or coupling) more problematic
- scattering lengths still await precise determinations
- note: Alexandrou 2021 and 2024 are different analysis stages on the same data



[Mai, Meißner, Urbach, Phys. Rept. 1001 (2023) 1-66;]

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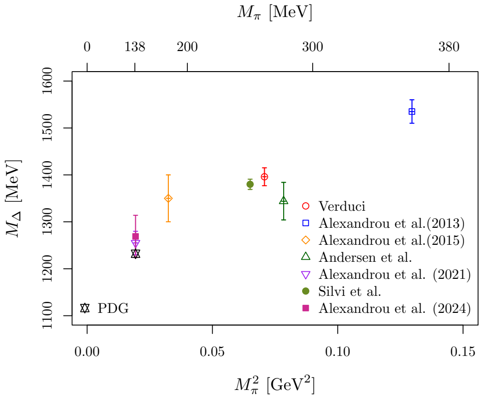

[Mai, Meißner, Urbach, Phys. Rept. 1001 (2023) 1-66; plus update]

$\eta_c \to 2\gamma$ decays

- important in quarkonium physics
- challenging to measure experimentally
- first principle, fully controlled theoretical estimate missing
- new $N_f = 2$ calculation

  [Meng et al., Sci.Bull. 68 (2023) 1880-1885]
- three lattice spacings
- based on a novel method with vastly reduced finite volume effects

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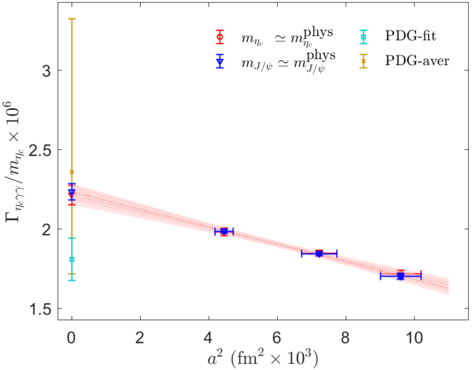

$\eta_c \to 2\gamma$ decays

- important in quarkonium physics
- challenging to measure experimentally
- first principle, fully controlled theoretical estimate missing
- new $N_f = 2$ calculation

  [Meng et al., Sci.Bull. 68 (2023) 1880-1885]
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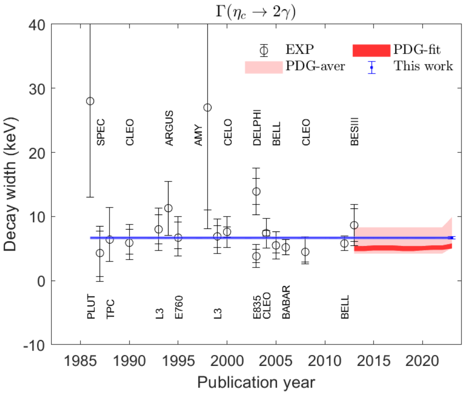
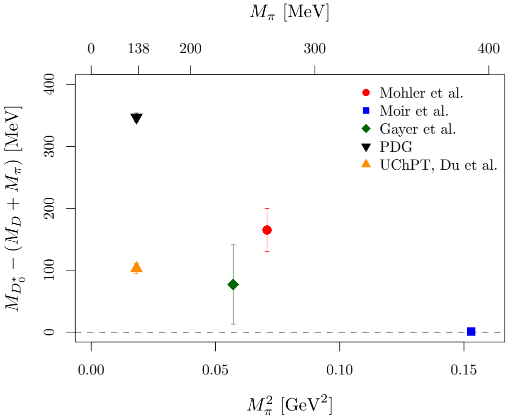


$D\pi$-scattering and the $D_0^*(2300)$

- open charm, $J^P = 0^+$ and $I = 1/2$, decay to $D\pi$
- slightly above $D\pi$ threshold
- expect two pole structure

[Du et al., PRD 98 (9) (2018), 094018]



[Mai, Meißner, Urbach, Phys. Rept. 1001 (2023) 1-66;]

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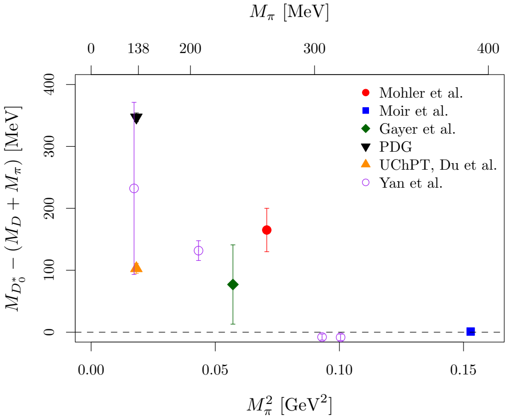
  [Du et al., PRD 98 (9) (2018), 094018]
- new Lattice results by H. Yan (CLQCD)

  [Yan et al, arXiv:2405.13479]
- virtual state below $M_\pi \approx 300$ MeV
- inconclusive at M_π^{phys}!
- requires a coupled channel analysis!



[Mai, Meißner, Urbach, Phys. Rept. 1001 (2023) 1-66; plus update]

The elusive $Z_c(3900)$ (maybe now called $T_{cc1}(3900)$??)

- closed charm, $I^G = 1^+$, $J^{PC} = 1^{+-}$
- rather narrow $\Gamma \approx 30$ MeV
- decay channels
  $J/\psi\pi, \eta_c\pi\pi, D\bar{D}^*, DD^*$
- CLQCD work on $Z_c(3900)$

  [Chen et al., Chin.Phys.C 43 (2019) 10, 103103, Chen et al., Phys.Rev.D 89 (2014) 9, 094506, Liu, Liu, Zhang, Phys.Rev.D 101 (2020) 5, 054502]
- LQCD conclusion so far:
  no evidence for the Z_c was found
- only HAL QCD finds a state at threshold

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We have to control systematics!

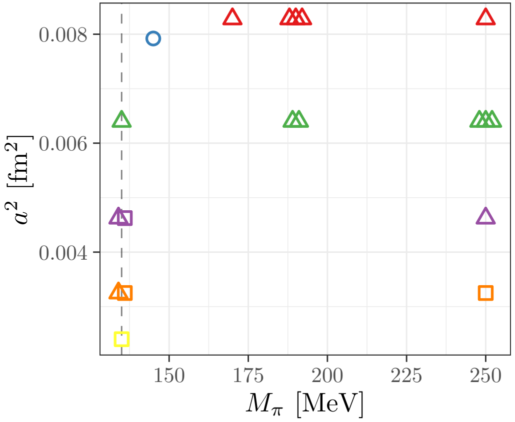
Need to:

- investigate pion mass dependence
- study lattice spacing dependence
- perform a full coupled channel investigation

Physical Point Ensembles at 4 Lattice Spacing Values

- ensemble generation requires significant effort
- major code development and optimisation

  [ETMC, Kostrzewa et al, PoS LATTICE2022 (2023) 340, ...]
- significant investment within CRC110
- many physics results produced and in the pipeline!
- highly competitive set of Lattice QCD ensembles



[B. Kostrzewa]

Physical Point Ensembles at 4 Lattice Spacing Values

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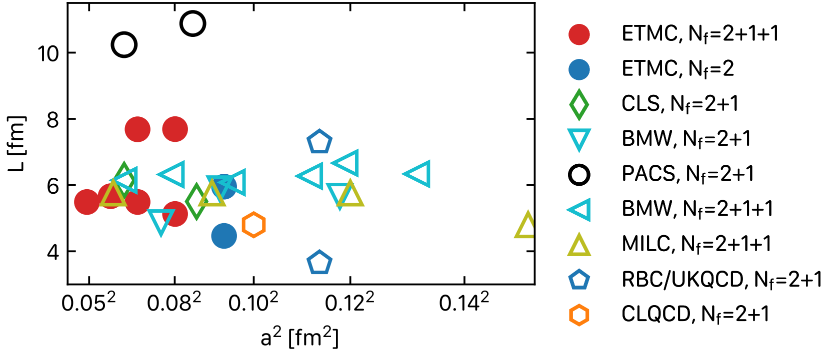
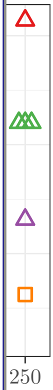
Ensemble Landscape



[G. Koutsou]



Parton Distribution Functions from Lattice QCD

Two approaches available:

Mellin moments of PDFs

- compute moments $\langle x^n \rangle$

  [Martinelli, Sachrajda, Phys.Lett.B 196, (1987)]

$$\langle x^n \rangle = \int_0^1 x^n f(x) \mathrm{d}x$$

- based on local operator matrix elements
- limited to lowest few moments
- full reconstruction of PDF difficult

Quasi/Pseudo PDFs

- compute pseudo/quasi/... PDFs directly

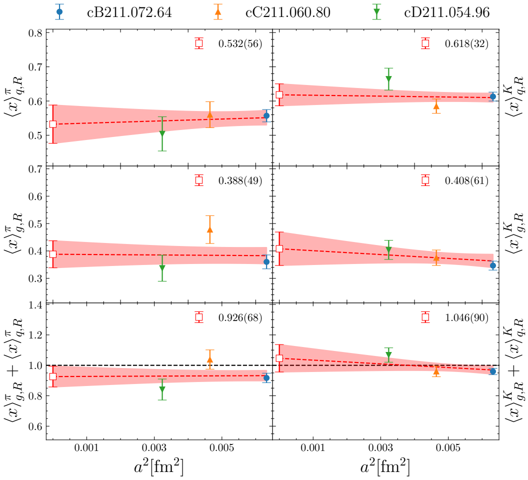
  [Ji, Phys. Rev. Lett. 110, 262002 (2013), ...]

- access to full x-dependence
- intricate renormalisation procedure
- need to match quasi to physical PDFs
- make sure LaMET converges

Pion and Kaon Momentum Decomposition

- ETMC $N_f = 2+1+1$ calculation of $\langle x \rangle$

  [ETMC, Alexandrou et al., arXiv:2405.08529 and Phys.Rev.Lett. 127 (2021) 25, 252001]
- three lattice spacings
- physical pion mass values
- non-perturbative renormalisation
- mixing perturbative
- sum-rule fulfilled within errors for pion/kaon
- marginal difference between pion and kaon



Transverse Momentum Dependent PDFs

- go beyond 1d picture of partons
- relevant in semi-inclusive DIS
- 3d picture via transverse momentum $\vec{k}_T$ (or transverse separation $\vec{b}$)

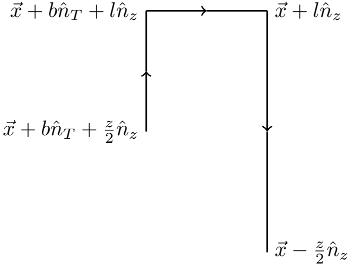
$$f^{\text{TMD}}(x, b, \mu, \zeta)$$

- additional scale ζ to regulate soft radiation
- lattice calculation via quasi PDF $\tilde{f}$

- $\tilde{f}$ related (Fourier Trafo) to purely spatial correlator

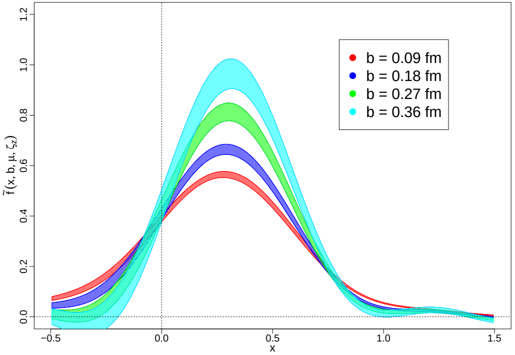
$$\lim_{l\to\infty} \langle H(P_z)|\mathcal{O}(b, l, z)|H(P_z)\rangle$$

- with staple shaped operator $\mathcal{O}$



Transverse Momentum Dependent PDFs

- Soft function, Collins-Soper kernel, perturbative matching all available
  [ETMC, Alexandrou et al., Phys.Rev.D 108 (2023) 11;
  114503, Li et al., Phys.Rev.Lett. 128 (2022) 6, 062002]
- exploratory investigation
- $24^3 \times 48$ lattice at 350 MeV
- $P_z = 1.7$ GeV
- more on GPDs and twist-3
  [Bhattacharya et al.: PRD109 (2024) 3, 034508; PRD106 (2022) 11,114512;
  PRD104 (2021) 11, 114510; PRD108 (2023) 5, 054501]



Hadronic Parity Violation: The $\Delta I = 1$ Coupling h_π

- h_π defined via effective Lagrangian

$$h_\pi \; = \; -\frac{i}{2m_N} \lim_{p_\pi\to 0} \langle n\pi^+ | \mathcal{L}_{\mathrm{PV}} | p\rangle$$

- involves 4-quark operator matrix elements
- one exploratory lattice calculation

[Wasem, Phys.Rev C85, (2012)]

- proposed (again) in the CRC:
use P even matrix elements and PCAC

$$\lim_{p_\pi\to 0} \langle n\pi^+ | \mathcal{L}_{\mathrm{PV}} | p\rangle \; \approx \; -\frac{\sqrt{2}i}{F_\pi} \langle p | \mathcal{L}_{\mathrm{PC}} | p\rangle$$

[Feng, Guo, Seng, Phys.Rev.Lett. 120 (2018)]

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[Feng, Guo, Seng, Phys.Rev.Lett. 120 (2018)]

pros

- matrix elements of stable states
- technically less involved
- less noise

cons

- mixing with lower dimensional operators in twisted mass
- strictly valid only in the chiral limit

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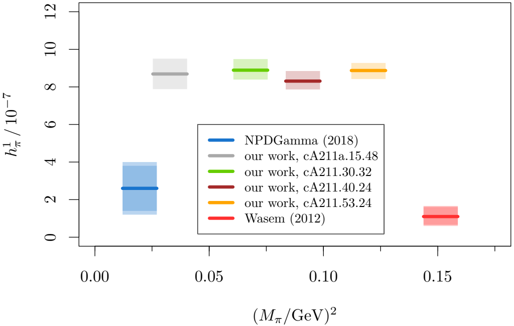

- exploratory investigation

[Petschlies et al., Eur.Phys.J.A 60 (2024) 1]

- renormalisation still missing
- flat pion mass dependence

... final Meeting June 2024

Supercomputer in Jülich

- fall 2024
- Jupiter: ~ 1 Exaflops
- so far only Jedi development partition

[(c) FZ Jülich]

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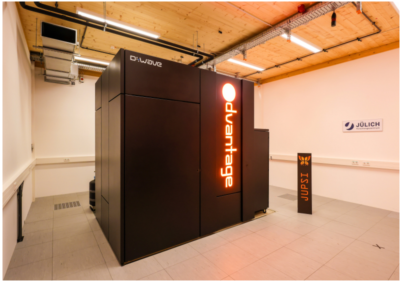
.. and a new era has begun

- quantum annealer
- first calculations as part of CRC110

[e.g. Kim, Luu, Unger, https://doi.org/10.1103/PhysRevD.108.074501 (2023)]



[(c) FZ Jülich]