Lattice QCD with $N_f = 2 + 1 + 1$ dynamical quarks: recent results from the ETM collaboration

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Grenoble, June 2014

Quantum Chromodynamics (QCD):

The theory of strong interactions

asymptotic freedom	$\longleftrightarrow$	confinement
small distances		large distances
energies $\gg 1\mathrm{GeV}$		energies $\leq 1\mathrm{GeV}$
coupling $\alpha_s < 1$		coupling $\alpha_s \approx 1$
perturbative treatment possible		non-perturbative treatment needed

- QCD Lagrange density

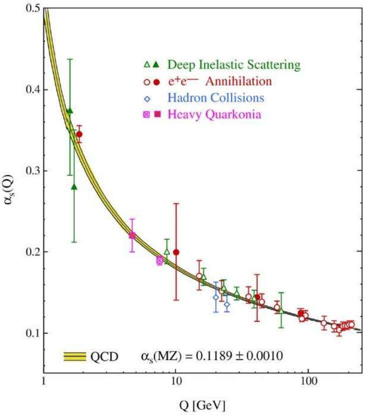
$$\mathcal{L}_{\mathrm{QCD}} = \sum_f \bar\psi_f (i\not{D} - m_f)\psi_f - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}$$

$\bar\psi, \psi$: quarks, $F_{\mu\nu}$: Gluons

- strongly coupled at low energies
  - hadron masses, decay constants
  - SM parameters
  - scattering/resonance properties
  - parton distributions
  - ...

$\Rightarrow$ need a non-perturbative method

QCD running coupling



[Bethke, 2006]

Motivation

fundamental question:

can we compute these quantities from first principles?

Outline

1. Lattice QCD in a nutshell
2. results from the pion sector: quark masses
3. flavour singlets: η and η' mesons
4. two particle systems: example of $\pi\pi$ scattering
5. average quark momentum fraction: pion $\langle x \rangle_\ell$
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Expectation Values in the Path Integral Formulation

- expectation value of operator $\mathcal{O}$

$$\langle\mathcal{O}\rangle = \int \mathcal{D}A\, \mathcal{D}\bar{\psi}\, \mathcal{D}\psi\, \mathcal{O}\, \exp(iS[\bar{\psi},\psi,A])$$

- Ken Wilson noticed: rotate $t \rightarrow i\tau$ to Euclidean space-time

$$\langle\mathcal{O}\rangle = \int \mathcal{D}A\, \mathcal{D}\bar{\psi}\, \mathcal{D}\psi\, \mathcal{O}\, \exp(-S_{\mathrm{E}}[\bar{\psi},\psi,A])$$

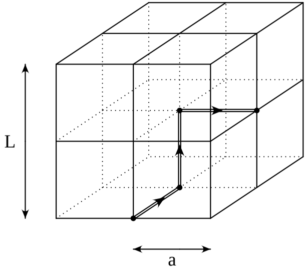
- allows to apply Monte-Carlo methods
  interpreting $\exp(-S_{\mathrm{E}})$ as a probability density

- can still obtain Minkowski space quantities

  [Osterwalder and Schrader (1973,1975)]

$\rightarrow$ source of statistical errors

- lattice regularisation: discretise space-time
  - hyper-cubic $L^3 \times T$-lattice with lattice spacing a
  - $\Rightarrow$ momentum cut-off: $k_{\mathrm{max}} \propto 1/a$
  - derivatives $\Rightarrow$ finite differences
  - integrals $\Rightarrow$ sums
  - gauge potentials A_μ in $G_{\mu\nu} \Rightarrow$ link matrices U_μ ('•⟶•')



- need to remove the cut-off

$\Rightarrow$ continuum limit $a \rightarrow 0$

$\rightarrow$ source of systematic errors

- need to take thermodynamic limit

$\Rightarrow$ study $1/L \rightarrow 0$

Quark Mass Dependence

- lattice calculations still mostly at larger than physical up/down quark masses

- need to extrapolate to physical up/down quark masses

$\Rightarrow$ guidance by chiral perturbation theory (χPT)

[Weinberg (1979), Gasser and Leutwyler (1984,1985)]

- in particular for (pseudo) Goldstone bosons at LO
  - $M_\pi^2 \;\propto\; m_\ell \quad\leftarrow\quad M_\pi^2$ proxy for m_ℓ
  - others $M^2 \;\equiv\; f(m_\ell, m_s)$

- η' more involved: $M_{\eta'} = const + g(m_\ell, m_s)$

$\rightarrow$ source for systematic errors

- let $O(x,t)$ be an operator with quantum numbers of a given state
- for instance for the pion it is given by

$$O(x,t) = \bar{u} i\gamma_5 d(x,t)\,, \qquad O(t) = \sum_x O(x,t)$$

  projected to zero momentum
- create pion at time 0 and annihilate at t

$$C_\pi(t) = \langle O(0)\, O(t)\rangle \propto \sum_n \langle 0|O(0)|n\rangle\langle n|e^{-Ht}O(0)e^{+Ht}|0\rangle$$

  inserting a complete set of states $|n\rangle$ and using the time evolution operator $\exp -Ht$

- which leads to

$$C_\pi(t) \propto \sum_n |\langle 0|\, O\, |n\rangle|^2\, e^{-(E_n - E_0)t}$$

- and for large times the lowest state dominates

$$\lim_{t\to\infty} C_\pi(t) \propto e^{-(E_1 - E_0)t}$$

- $E_1 - E_0$ corresponds at zero momentum to the mass M_π

- and matrix elements of the pion for $n = 1$

$$\langle 0|\, O\, |\pi\rangle$$

- also define effective masses

$$M = -\frac{d}{dt} \log C_\pi(t)$$

- $2+1+1$ quark flavour ensembles from ETM Collaboration
  $m_u = m_d < m_s < m_c$ Wilson twisted mass fermions
  [ETMC, R. Baron et. al., JHEP 06 111 (2010)]

- collaborative effort with more than 30 scientists all over Europe
- charged pion masses range from $\approx 230\ \mathrm{MeV}$ to $\approx 500\ \mathrm{MeV}$

- $L \geq 3\ \mathrm{fm}$ and $M_\pi \cdot L \geq 3.5$ for most ensembles

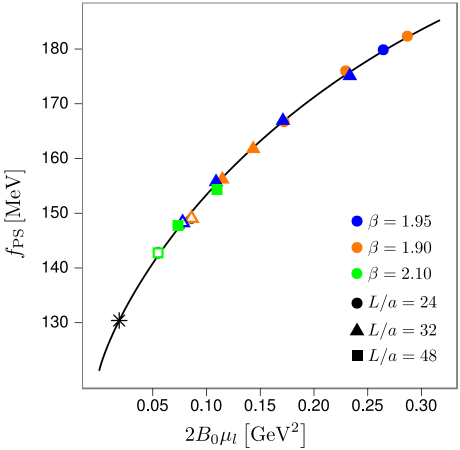
- different volumes to check for finite size effects

- bare m_s and m_c fixed for each lattice spacing

Ensemble-Details

- three lattice spacings (A, B and D ensembles): $a_A = 0.086\ \mathrm{fm}$, $a_B = 0.078\ \mathrm{fm}$ and $a_D = 0.061\ \mathrm{fm}$ $\beta = 1.90, 1.95, 2.10$
- use $r_0 = 0.45(2)\ \mathrm{fm}$ (from f_π) throughout the talk r_0 Sommer scale determined from static $\bar{q}q$ potential

$\Rightarrow$ $r_0 M$ is dimensionless (with M a mass)



[ETMC, R.Baron, C.U., et al., 2010, 2011]

Why Wilson Twisted Mass Fermions?

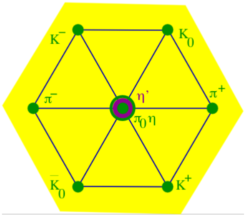
- there is large freedom on how to chose the discretisation!
- advantages of twisted mass at maximal twist
  - improved continuum scaling: $\mathcal{O}(a)$ artifacts absent in physical quantities
  - only modest tuning effort
  - simplified renormalisation patterns
- disadvantages:
  - flavour and parity broken at finite lattice spacing value

  $\Rightarrow$ only M_{π^0} strongly affected
- quite successful in the recent past

[Frezzotti, Rossi, 2003; Jansen, CU, et al., 2004, 2005, ETMC...]

Outline

- nine lightest pseudo-scalar mesons show a peculiar spectrum:
  - 3 very light pions (140 MeV)
  - kaons and the η around 500 MeV
  - η' around 1 GeV



- pions, kaons and eta (pseudo) Goldstone bosons of chiral symmetry

$\Rightarrow$ motivates chiral perturbation theory

- heavy η': this was called the $U(1)$-problem

- solution:

$\Rightarrow$ the large mass of the η' meson is thought to be caused by the QCD vacuum structure and the $U_A(1)$ anomaly

[Weinberg (1975), Belavin et al. (1975), 't Hooft (1976), Witten (1979), Veneziano (1979)]

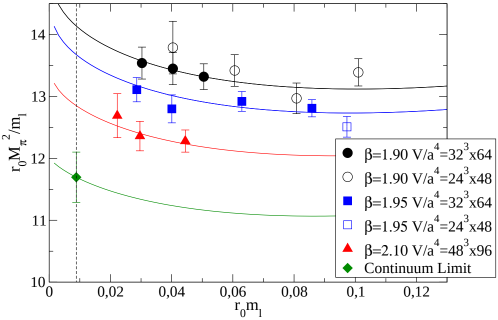
- chiral perturbation theory χPT: low energy effective theory
- describe mass dependence with $n_f = 2$ NLO χPT
  plus leading lattice artifacts

$$\begin{aligned} M_{\mathrm{PS}}^2 &= \chi_\mu \left[1 + \xi \log(\chi_\mu/\Lambda_3^2 + D_m a^2)\right] \quad K_m^2(L) \\ f_{\mathrm{PS}} &= f_0 \quad \left[1 - 2\xi \log(\chi_\mu/\Lambda_4^2) + D_f a^2\right] K_f(L) \end{aligned}$$

with $\chi_\mu = 2\hat{B}_0 Z_\mu \mu_q$ and $\xi = \chi_\mu/(2\pi f_0)^2$

- finite size corrections $K_m(L), K_f(L)$ from continuum χPT
  [Gasser, Leutwyler, 1987, 1988; Colangelo, Dürr, Haefeli, 2005, Colangelo, Wenger, Wu, 2010]
- fit simultaneously to our data at all lattice spacing values
- 15 ensembles $\rightarrow$ 30 data points

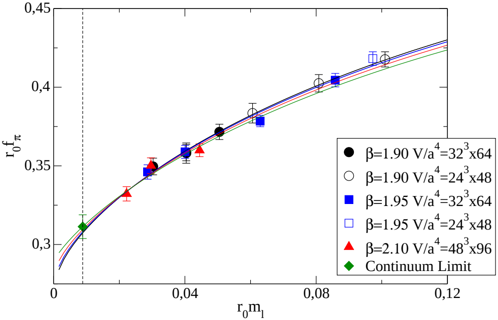
- at first glance completely linear
- in ratio sensitivity to Λ_3 clearly visible
- sizable lattice artifacts
- data finite size corrected



- a constant extrapolation cannot be ruled out

[ETMC, Carrasco, CU, et al., 2014, arXiv:1403.4504]

- clearly finite in the chiral limit
- lattice artifacts less pronounced
- data finite size corrected



- also here a linear extrapolation is not completely excluded

$\Rightarrow$ still sizable systematic errors from chiral extrapolation

[ETMC, Carrasco, CU, et al., 2014, arXiv:1403.4504]

Quark Masses, Decay Constants

- perform NLO χPT fit and polynomial fits with different fit ranges
- set the scale by $f_{\mathrm{PS}} = f_\pi$ where $M_{\mathrm{PS}}/f_{\mathrm{PS}}$ assumes its physical value

$\Rightarrow$ extract the bare light quark mass μ_ℓ

- compute renormalisation constant using RI-MOM scheme
- in the $\overline{\mathrm{MS}}$ scheme at 2 GeV

$$m_\ell = \frac{1}{Z_P}\mu_\ell = 3.70(17)\ \mathrm{MeV}$$

- errors include systematic effects from fit form, finite size, continuum extrapolation
- similarly for m_s, m_c and quark mass ratios
  for details see arXiv:1403.4504

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- the $U(1)$ axial current is anomalous at quantum level

  [Adler (1969), Jackiw and Bell (1969)]

$$\partial^\mu A^{0q}_\mu = \partial^\mu(\bar{q}\gamma_\mu\gamma_5 q) = 2m_q(\bar{q}i\gamma_5 q) + \frac{\alpha_s}{4\pi}F\tilde{F}$$

  and not spontaneously broken

- anomaly vanishes to all orders in perturbation theory at zero momentum

$\Rightarrow$ need additional mechanism

- instantons with non-trivial topology allow to explain η' mass

  [Belavin et al. (1975), 't Hooft (1976)]

$\Rightarrow$ suggests consistency of QCD with nature

- for exact SU(3) flavour symmetry ($m_u = m_d = m_s$) define (considering only $\bar{q}q$ states ...)

- the flavour octet state η_8

$$\eta_8 \quad \equiv \quad \frac{1}{\sqrt{6}}(\bar{u}i\gamma_5 u + \bar{d}i\gamma_5 d - 2\bar{s}i\gamma_5 s)$$

$\Rightarrow$ a (pseudo) Goldstone boson

- the flavour singlet state η_0

$$\eta_0 \quad \equiv \quad \frac{1}{\sqrt{3}}(\bar{u}i\gamma_5 u + \bar{d}i\gamma_5 d + \bar{s}i\gamma_5 s)$$

$\Rightarrow$ related to $U(1)_A$ anomaly

- SU(3) flavour symmetry broken by larger m_s: $m_s \gg m_u = m_d = m_\ell$

$\Rightarrow$ physical states will be a mixture, e.g.

$$\begin{pmatrix} |\eta\rangle \\ |\eta'\rangle \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix} \cdot \begin{pmatrix} |\eta_\ell\rangle \\ |\eta_s\rangle \end{pmatrix}$$

in the quark flavour basis

$$\eta_\ell \equiv \frac{1}{\sqrt{2}}(\bar{u} i\gamma_5 u + \bar{d} i\gamma_5 d)\,, \qquad \eta_s = \bar{s} i\gamma_5 s$$

- in nature $m_u \neq m_d$ $\quad\Rightarrow\quad$ also π_0 mixes
- how did nature arrange the mixing pattern?
- can one determine the mixing angle(s)?

- mixing can hardly be defined via Fock states

$\Rightarrow$ use matrix elements instead

$$\begin{pmatrix} \mathbf{P}^\ell_\eta & \mathbf{P}^s_\eta \\ \mathbf{P}^\ell_{\eta'} & \mathbf{P}^s_{\eta'} \end{pmatrix} = \begin{pmatrix} c_\ell \cos\phi & -c_s \sin\phi \\ c_\ell \sin\phi & c_s \cos\phi \end{pmatrix}$$

defined via pseudo-scalar matrix elements

$$\mathbf{P}^q_P = \langle 0|\bar{q} i\gamma_5 q|P\rangle\,, \qquad P = \eta, \eta'\,, \qquad q = \ell, s$$

- note: usually defined via decay constants obtained from

$$\langle 0|A^q_\mu|P(p)\rangle = i f^q_P p_\mu$$

with

$$A^\ell_\mu = \frac{1}{\sqrt{2}}(\bar{u}\gamma_\mu\gamma_5 u + \bar{d}\gamma_\mu\gamma_5 d)\,, \qquad A^s_\mu = \bar{s}\gamma_\mu\gamma_5 s$$

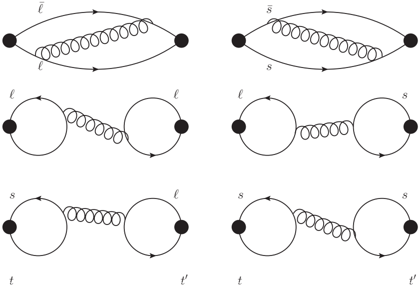
- need to estimate correlator matrix

$$\mathcal{C} = \begin{pmatrix} \eta_{\ell\ell} & \eta_{\ell s} \\ \eta_{s\ell} & \eta_{ss} \end{pmatrix}$$

- η_{XY} correlator of appropriate operators, e.g.

$$\eta_{ss}(t) \quad \equiv \quad \langle \bar{s} i\gamma_5 s(t)\, \bar{s} i\gamma_5 s(0)\rangle$$

- connected and disconnected contributions



- diagonalise matrix $\Rightarrow$ masses M_P and matrix elements $\mathbf{P}_P^q$

- $P = \eta$: lowest state, $P = \eta'$: second state, $P = \eta_c$ ...

- η' mainly the flavour singlet
- disconnected contributions significant

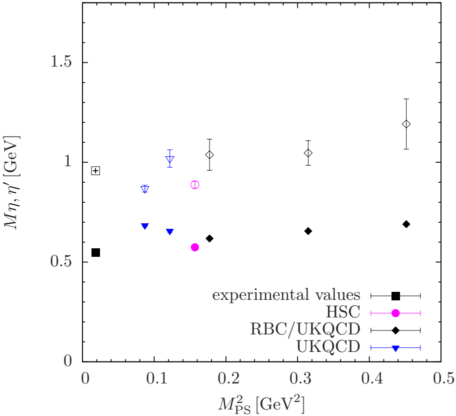
$\Rightarrow$ very noisy

$\Rightarrow$ hard problem

- only little data available
- chiral extrapolation difficult

$\Rightarrow$ no clear picture

- need for improvement



filled symbols: η open: η'

[HSC, J. J. Dudek et al., Phys. Rev. D83 (2011)]
[RBC/UKQCD, N. Christ et al., Phys. Rev. Lett. 105 (2010)]
[UKQCD, E. B. Gregory et al., Phys.Rev. D86 (2012)]

C. Michael, K. Ottnad, C.U., Phys.Rev.Lett. 111 (2013) 18, 181602, SFB/TR 16

η, η' after careful excited state subtraction

[Neff et al. (2001), K.Jansen, C.Michael, C.U. (2008)]

η:

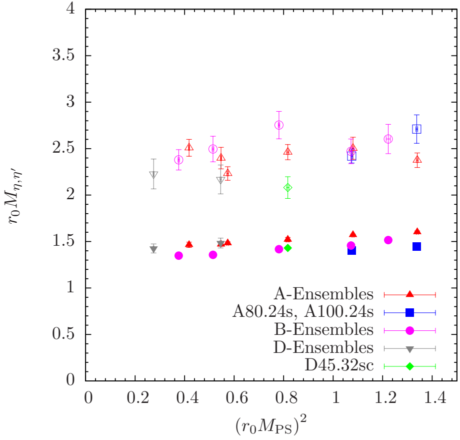
- high statistical precision

$\Rightarrow$ strange quark mass or lattice spacing dependence visible

η':

- reasonable precision

$\Rightarrow$ within errors no strange quark or lattice spacing dependence visible



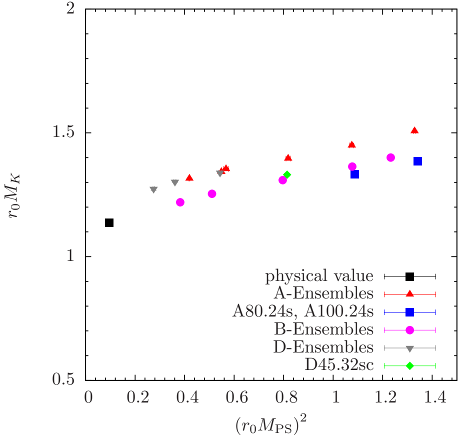
- m_s not perfectly tuned to its physical value
- two re-tuned ensembles for a_A

$\Rightarrow$ can estimate m_s dependence

- estimate

$$D_\eta \equiv \frac{d(aM_\eta)^2}{d(aM_\mathrm{K})^2} = 1.47(11)$$

- now assume: D_η independent of a, m_ℓ, m_s, m_c



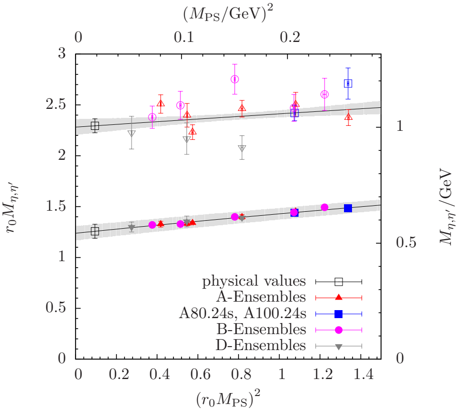
- now correct all $(r_0 M_\eta)^2$ using D_η

$\Rightarrow$ $(r_0 \bar{M}_\eta)^2 \propto const + (r_0 M_{\mathrm{PS}})^2$

- all a-values fall on the same curve!
- extrapolate $(r_0 \bar{M}_\eta)^2$ linearly in $(r_0 M_{\mathrm{PS}})^2$ to $M_{\mathrm{PS}} = M_\pi$
- result

$$M_\eta = 552(10)_{\mathrm{stat}}\ \mathrm{MeV}$$

- similarly with $(\bar{M}_\eta / \bar{M}_{\mathrm{K}})^2$ or GMO relation

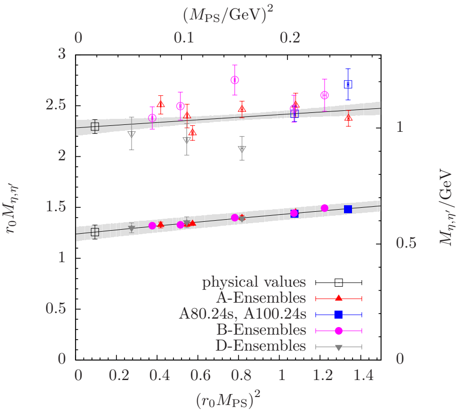


- no clear dependence on
  - lattice spacing
  - strange quark mass
- errors still significant
- include all data in extrapolation
- $(r_0 M_{\eta'})^2 \propto const + (r_0 M_{\mathrm{PS}})^2$

$\Rightarrow$ result

$$M_{\eta'} \;=\; 1005(54)_{\mathrm{stat}}\ \mathrm{MeV}$$

- fitting *A*, *B* and *D* separately gives compatible results

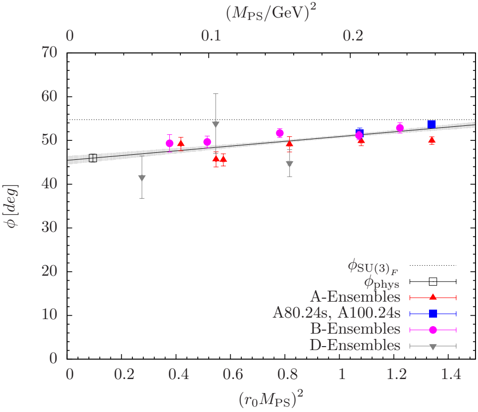


Mixing Angle ϕ

- extrapolate ϕ linearly in $(r_0 M_{\mathrm{PS}})^2$

$\Rightarrow$ $\phi = 46(1)_{\mathrm{stat}}(3)_{\mathrm{sys}}\,^\circ$

- systematic error from fitting different lattice spacings separately
- with $m_\ell = m_s$ we reproduce the SU(3) symmetric value 54.7°



- interpretation: η' meson mainly the flavour singlet state

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Two Particle Scattering

- most of the hadrons are resonances

$\Rightarrow$ a determination of resonance and scattering properties from first principles highly valuable

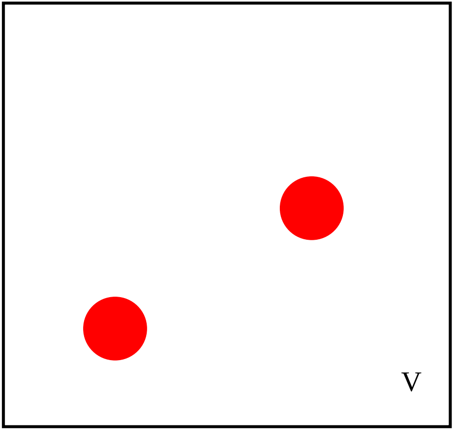
- unfortunately: direct determinations in Euclidean time very difficult

- nuclei bound states of multi nucleon systems

$\Rightarrow$ need to go beyond single hadron masses and matrix elements

$\Leftarrow$ how to treat such systems with Lattice QCD?

... make use of finite size effects!



- for $V \to \infty$:

$\Rightarrow$ interaction probability very low

$\Rightarrow$ $E_{2p}(p = 0) = 2M_{1p}$

- for finite V:

$\Rightarrow$ interaction probability rises

$\Rightarrow$ $E_{2p}(p = 0)$ receives corrections $\propto 1/V$

- Lüscher: correction in $1/V$ related to scattering properties!

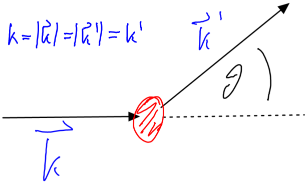
[Lüscher, 1986]

Special Case: Elastic $\pi\pi$ Scattering for $I = 2$

- scattering of two pions below inelastic threshold with isospin $I = 2$
- well described by finite range potential $V(r) = 0 \quad \forall \quad r > R$
- scattering amplitude in the partial wave expansion

$$f_k(\theta) = -\frac{8\pi}{M}\sum_{\ell=0}^{\infty}(2\ell+1)\, f_\ell(k)\, P_\ell(\cos\theta)$$

$k = |\vec{k}| = |\vec{k}'| = k'$



with partial wave amplitude and phase shift δ_ℓ

$$f_\ell(k) = \frac{1}{k\cot\delta_\ell(k) - ik}$$

Special Case: Elastic $\pi\pi$ Scattering for $I = 2$

- at small momenta $k \to 0$ use effective range expansion

$$k^{2\ell+1} \cot \delta_\ell = \frac{1}{a_\ell} - \frac{r_\ell k^2}{2} + \ldots$$

scattering length a_ℓ and effective range r_ℓ

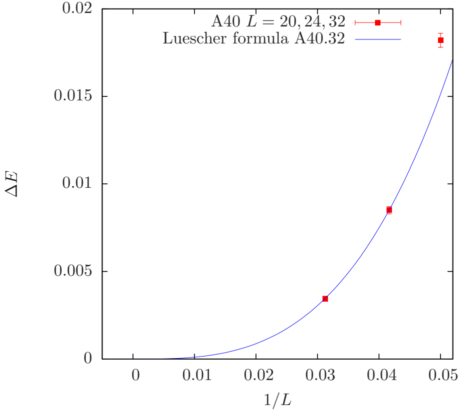
$\Rightarrow$ only S-waves ($\ell = 0$) contribute

- Lüscher:

$$E_{2p}(L) - 2M_{1p} = -\frac{4\pi a_0}{ML^3} \left\{ 1 + \mathcal{O}\left(\frac{1}{L}\right) + \ldots \right\}$$

- translates directly to Quantum Field-theory for $\pi\pi$ systems with $I = 0, 2$ and πN with $I = 1/2, 3/2$

- three volumes $L = 20, 24, 32$
- otherwise fixed parameters
- use the result at $L = 32$ and Lüscher formula to predict $\Delta E(1/L)$
- good agreement to measured data!



$\Rightarrow$ this picture suggests higher order corrections in $1/L$ are small

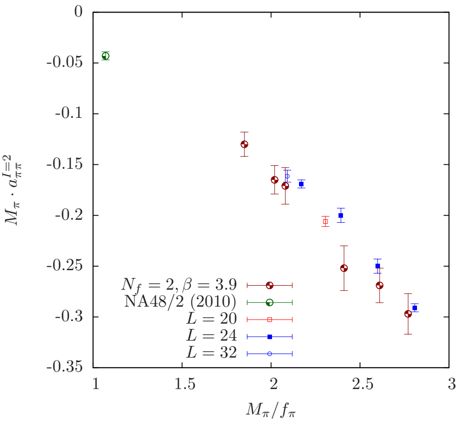
[C. Helmes, C. Jost, B. Knippschild, C.U., M. Werner, SFB/TR 110]

- first $N_f = 2 + 1 + 1$ results (preliminary)

  [see also: Bean et al. NPLQCD, Dudek et al. HSC, ...]

- only one value of the lattice spacing $a = 0.09\ \mathrm{fm}$
- only 100 configurations per ensemble
- agreement with $N_f = 2$ results
- significantly improved statistical precision

$\Rightarrow$ next steps: $\pi\pi$ for $I = 1$, πK and πN



[$N_f = 2$: Xu, Jansen, Renner, Phys.Lett. B684 (2010)]

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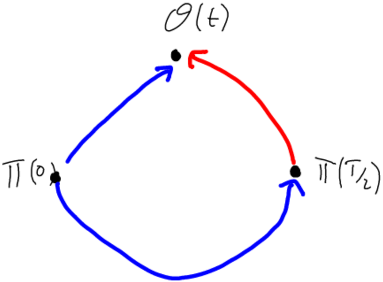
Parton Distribution Functions

- (generalised) parton distribution functions
- important in DIS

$\Rightarrow$ not directly accessible on the lattice

- can compute matrix elements of local operators
- which are related to moments of parton distribution functions
- requires the computation of so-called three point functions of appropriate local operators
- note: there are new ideas on how to compute GPDs directly

- momentum fraction of a (valence) quark in the pion
- matrix element of non-singlet, twist-2 operator
- related to first x-moment of leading twist vector GPD H^{π}

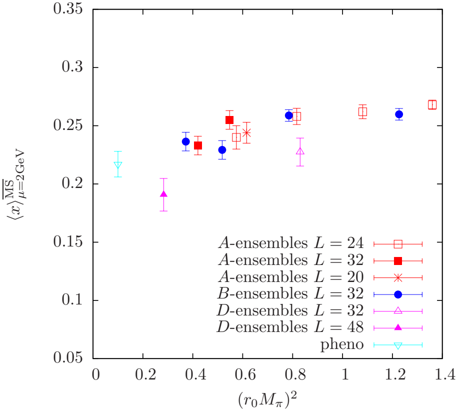


- computed using sequential quark propagators
- and stochastic estimators
- disconnected contributions currently omitted

- renormalised in $\overline{\text{MS}}$ at 2 GeV

  [M. Constantinou, private communication]

- no big finite size effects visible in contrast to old quenched results
- phenomenological status unclear
- curvature at small quark masses needs confirmation
- data preliminary



- phenomenological value from Wijesooriya, Reimer, and Holt, (2005)
- higher moments in progress

Summary

- Lattice QCD with $N_f = 2 + 1 + 1$ dynamical quark flavours
- three lattice spacings and various bare quark mass values
- SM parameters like quark masses determined with precision
- investigation of η and η' for the first time controlling all sources of systematics, where possible
- first results for $\pi\pi$ scattering with $N_f = 2 + 1 + 1$ quarks very encouraging
- $\langle x \rangle_\ell$ of the pion
- ETMC has many more results...

Outlook

- simulation at the physical point ($N_f = 2$, preliminary)
- will significantly reduce systematic uncertainties
- ongoing effort
- will be
  - basis for many physical results
  - allow crosscheck of chiral extrapolations and validity of χPT
  - basis for finite T simulations