Unquenched simulations with $N_f = 2$ light quark flavours

qq+q - Collaboration

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Talk given by
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Lattice 2004
Fermilab

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- GOAL: estimates for GASSER-LEUTWYLER-low energy constants
- last year showed results for $L^3 \times T = 16^3 \times 16$, three simulation points

  qq+q Coll., Eur. Phys. J. **C 31** (2003) 227, and Tsukuba 2003
- redone the simulations at $L^3 \times T = 16^3 \times 32$, four simulation points
  - ∗ using valence quark (partially quenched) down to $m_{\text{val}} \simeq \frac{1}{2} m_{\text{sea}}$
  - ∗ advantage of used ratios becomes visible
  - ∗ NNLO vs. $\mathcal{O}(a)$

Simulation Parameters

- $L^3 \times T = 16^3 \times 32$, $\beta = 5.1$ (hep-lat 0403014, to appear in Eur. Phys. J. C)
- 4 simulation points: $\frac{1}{4} m_{\text{strange}} \leq m_{\text{sea}} \leq \frac{2}{3} m_{\text{strange}}$ ($\kappa_{\text{sea}} = 0.1760, 0.1765, 0.1768, 0.1770$)
- ≈ 1000 independent configurations after thermalization at each κ_{sea}
- using Two-Step Multi-Boson (TSMB) algorithm
- cost of the algorithm: $C_{\tau_{\text{int}}} \simeq F\Omega(am_q)^{-2}$, $F_{\text{plaquette}} \simeq 7 \cdot 10^6$, $Fm_\pi \simeq 10^6$, $F_{f_\pi} < 4 \cdot 10^5$
- large volume ($L \simeq 3$fm), but coarse lattice ($a \simeq 0.195(4)$fm)

κ_{sea}	0.1760	0.1765	0.1768	0.1770
r_0/a	2.229(63)	2.212(44)	2.621(46)	2.528(51)
am_π	0.6542(10)	0.5793(17)	0.3919(46)	0.3657(24)
$M_r = (r_0 m_\pi)^2$	2.13(12)	1.642(72)	1.055(36)	0.855(34)
$Z_q a m_q$	0.07092(27)	0.05571(30)	0.02566(27)	0.02208(21)
$\sigma_i = m_{qi}/m_{q0}$	1.0	0.7856(56)	0.3618(44)	0.3113(31)
$Z_A^{-1} a f_\pi$	0.2819(15)	0.2590(14)	0.2008(17)	0.1936(16)

Partially Quenched Chiral Perturbation Theory

[Sharpe,Shoresh]

- including chiral symmetry breaking due to Wilson-term into analysis: $\boldsymbol{\rho}$
- Lagrangean in terms of

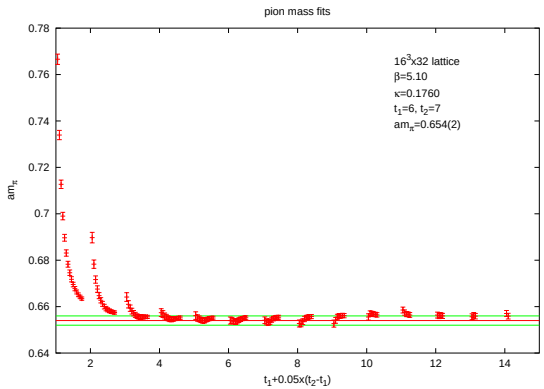
$$\Sigma = \exp\left[\frac{2i\Pi}{f}\right], \quad \chi = \frac{2B_0}{f_0^2}\mathrm{diag}(m_q), \quad \rho = \frac{2W_0 a c_{\mathrm{SW}}}{f_0^2}$$

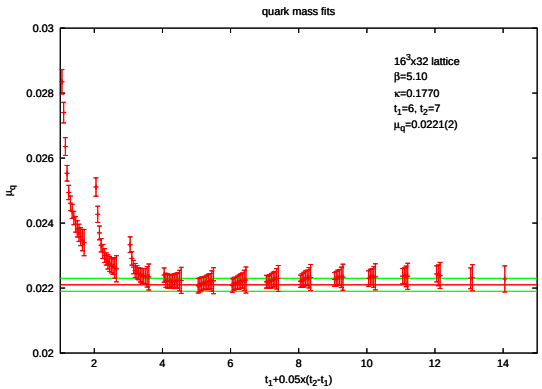
$$\mathcal{L} \quad = \quad \frac{f^2}{4}\mathrm{tr}\Big[\partial\Sigma\partial\Sigma^\dagger\Big] - \frac{f^2}{4}\mathrm{tr}\Big[(\chi+\rho)\Sigma^\dagger + \Sigma(\chi+\rho)^\dagger\Big] \; + \; \mathcal{L}_{\mathrm{NLO}}(L_i, W_i) \; + \; \ldots$$

- $\epsilon \sim \frac{p^2}{\Lambda^2} \sim \frac{m_\pi^2}{\Lambda^2}$, $\Lambda \sim 1\mathrm{GeV}$, $\delta \sim \frac{2W_0 a c_{\mathrm{SW}}}{\Lambda^2}$
- $\{\epsilon, \delta\} \ll \{\epsilon^2, \epsilon\delta\} \ll \delta^2$
- all simulations at $\beta = 5.1 \Rightarrow$ only indirect information about lattice artifacts

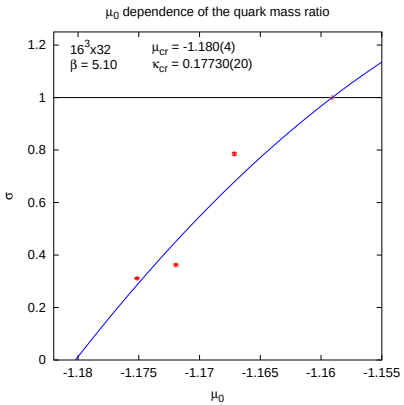
Measurements

- extract pion masses, quark masses, and decay constants



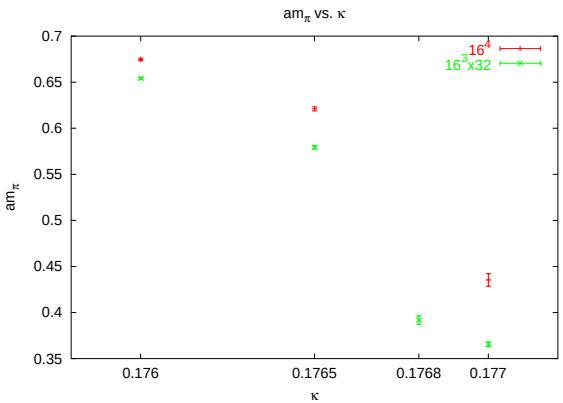


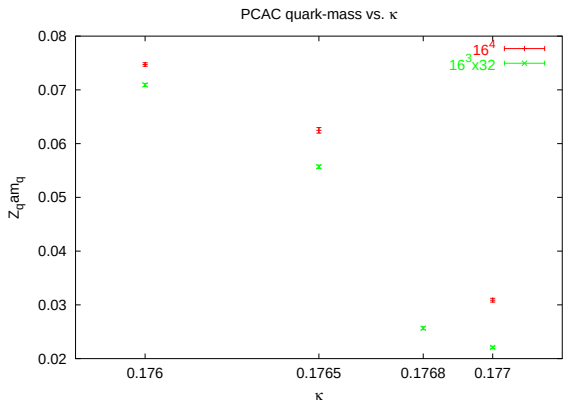
- using PCAC-quark mass ($\chi \propto m_{\text{AWI}\equiv\text{PCAC}}$) is essential
- error estimates by linearization method
- fitting ratios as functions of quark mass ratios $\boldsymbol{\xi} \equiv \frac{\boldsymbol{\chi_V}}{\boldsymbol{\chi_S}}$ ($\Rightarrow \; R(\xi)$)
  - $*$ no renormalization constants
  - $*$ but same "information" about quark mass dependence



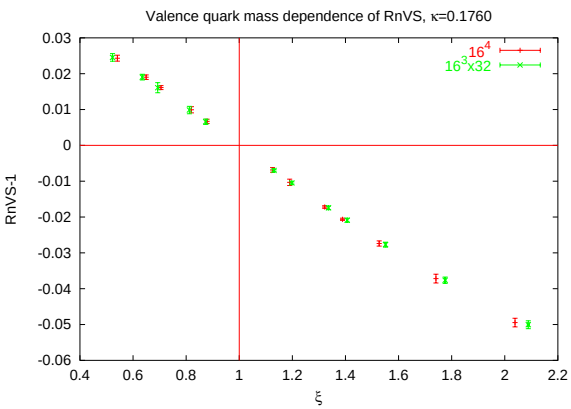
comparison 16^4 vs. $16^3 \times 32$

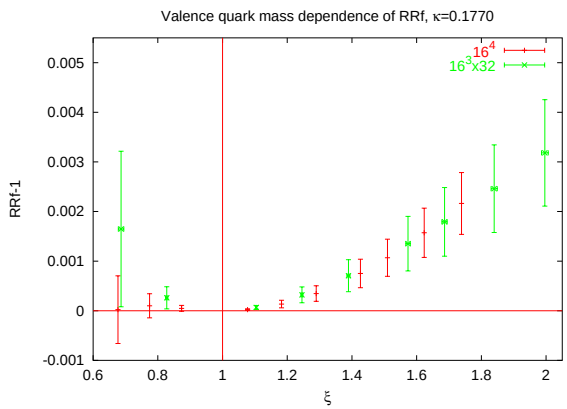
- "raw" data quite different





- but ratios as functions of ratios are stable





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Valence quark mass dependence

- added 12 valence quark masses, $0.5 \leq \xi \equiv \frac{\chi_V}{\chi_S} \leq 2.0$
- problems with exceptional configurations at $\xi < 1 \Rightarrow$ restricted fits to $\xi \geq 1$
- performed global (i.e. all sea quark masses together) linear fits
- fitted ratios and double ratios of masses and decay constants

$$Rf_{\mathsf{VV}} \equiv \frac{f_{\mathsf{VV}}}{f_{\mathsf{SS}}} \qquad Rf_{\mathsf{VS}} \equiv \frac{f_{\mathsf{VS}}}{f_{\mathsf{SS}}} \qquad RRf \equiv \frac{f_{\mathsf{VS}}^2}{f_{\mathsf{VV}} f_{\mathsf{SS}}}$$

$$Rn_{\mathsf{VV}} \equiv \frac{m_{\mathsf{VV}}^2}{\xi m_{\mathsf{SS}}{}^2} \qquad Rn_{\mathsf{VS}} \equiv \frac{2m_{\mathsf{VS}}^2}{(\xi+1)m_{\mathsf{SS}}^2} \qquad RRn \equiv \frac{4\xi m_{\mathsf{VS}}^4}{(\xi+1)^2 m_{\mathsf{VV}}^2 m_{\mathsf{SS}}^2}$$

- assume continuum formulas
- include NNLO [Sharpe, Van de Water]

$\Rightarrow$ 11 parameters to fit $\chi_R, \chi_R L_{R5}, \chi_R(2L_{R8} - L_{R5})$ plus 8 NNLO

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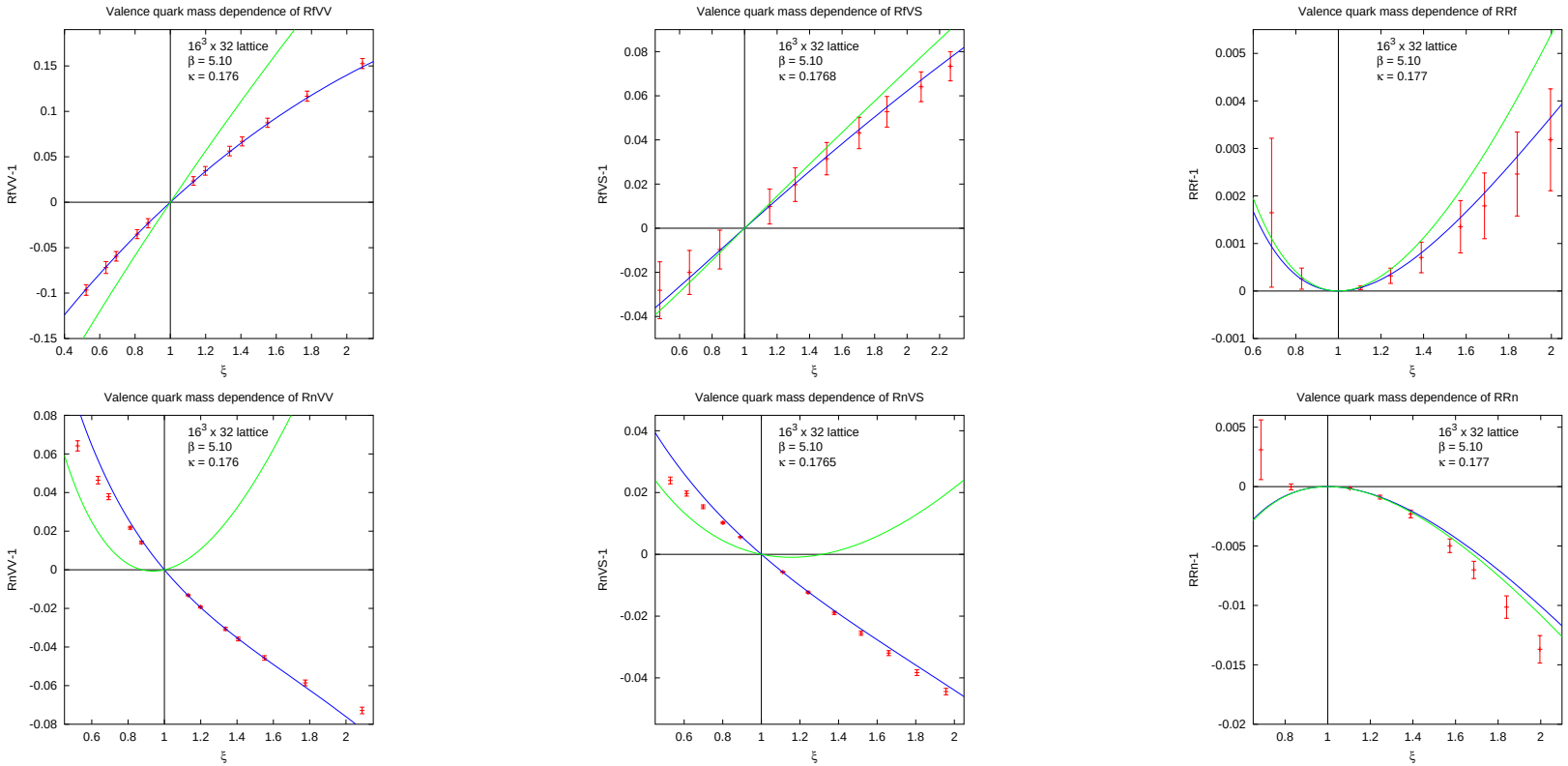
Global Fits



full fit / only NLO contribution

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- NNLO important at two highest m_{sea}

  without NNLO: just small range around $\xi = 1$ possible
- global fit: $\chi^2_{\text{fit}} \simeq 200 (\simeq \text{d.o.f.})$
- $\chi_R = 35.8(3.3)$ (@ reference sea quark mass)

  tree-level estimate: $\frac{(r_0 m_\pi)^2}{(r_0 f_0)^2} \approx 40$
- $\alpha_5 = 2.06(42)$ (@ $4\pi f_0 = \Lambda_\chi$)
- $2\alpha_8 - \alpha_5 = 0.583(45)$ (@ $4\pi f_0 = \Lambda_\chi$)

  previous 16^4: $\chi_R = 33.5(2.4)$, $\alpha_5 = 2.24(20)$, $2\alpha_8 - \alpha_5 = 0.762(49)$

$$\begin{aligned} \alpha_5 &= 128\pi^2 L_{R5} + \log \frac{\chi_R}{16\pi^2} \\ 2\alpha_8 - \alpha_5 &= 128\pi^2 (2L_{R8} - L_{R5}) - \log \frac{\chi_R}{16\pi^2} \end{aligned}$$

Sea quark mass dependence

- first fit sea quark mass dependence alone ($\chi^2_{\text{fit}} = 0.8$):

$$\chi_R = 30.8(9.4),\ \frac{\Lambda_4}{f_0} = 23.3(8.2),\ \frac{\Lambda_3}{f_0} = 7.64(14)$$

- take value $\chi_R = 35.8(3.3)$ from valence quark mass dependence:

$$\frac{\Lambda_4}{f_0} = 21.4(1.5),\ \frac{\Lambda_3}{f_0} = 8.21(27)$$

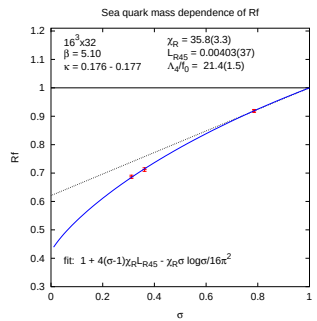
$$\Lambda_4 = 1.99(14)\text{GeV},\ \Lambda_3 = 0.76(3)\text{GeV}$$

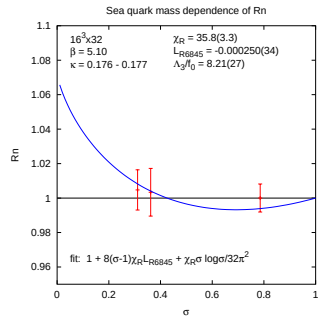
prev. 16^4: $\frac{\Lambda_4}{f_0} = 22.9(1.5),\ \frac{\Lambda_3}{f_0} = 6.51(57)$

CP-PACS, `hep-lat 0404014`: $\Lambda_4 = 2.44(13)\text{GeV}, \Lambda_3 = 0.15(15)\text{GeV}$

- $m_q \to 0$: $Rf_0 = 0.4228(60),\ Rn_0 = 1.0717(69)$

$$Z_A^{-1} f_0 = 121(5)\text{MeV}$$





$$Rn \propto \frac{m_\pi^2}{m_q}$$

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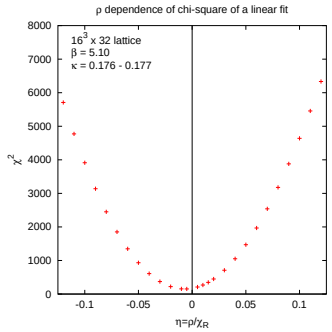
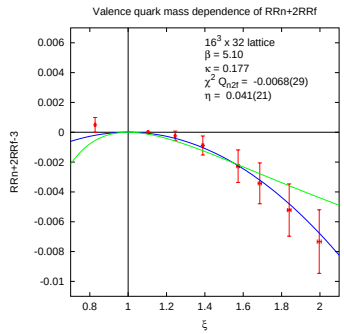
$\mathcal{O}(a)$-contributions

- so far used continuum formulas
- $\eta_S \equiv \frac{\rho_S}{\chi_S}, \quad \rho \equiv \frac{2W_0 a c_{\mathrm{SW}}}{f_0^2}$
- from 16^4: $0.02 \leq \eta_S \leq 0.07$
- χ^2 of global fits with η (plus add. LEC)
  $\rightarrow$best fit: $\frac{\rho}{\chi_R} \simeq -0.01$ ($|\rho| \simeq 0.5$MeV)



- $RRn + 2\,RRf - 3 = \begin{cases} \text{NNLO} \\ \mathcal{O}(a) \end{cases}$

  at our smallest quark mass: $\chi^2_{\text{fit, NNLO}} = 1.3$, $\chi^2_{\text{fit, }\mathcal{O}(a)} = 7.2$
- $\mathcal{O}(a^2)$ for m^2_{XX} known [Bär et al., Aoki], but in ratios just redef. of $\mathcal{O}(a)$, decay const. similar???



in our fits:

$\Rightarrow$ $\mathcal{O}(a)$ not important, but NNLO is!

(but including simulations at various β could change this...

on the other hand: did not see large scaling effects $\beta = 4.68 \rightarrow 5.10$, cf. qq+q, Tsukuba 2003)

Conclusions

- previous results on 16^4 confirmed
- improved sea quark analysis by including one more simulation point
- use of m_{PCAC} is essential
- "Ratios of ratios" are stable
- combined fitting procedure works
  - ∗ take $\chi_R, \ldots$ from (global) valence quark mass dependence
  - ∗ use it for sea quark mass dependence $\longrightarrow$ Λ_3, Λ_4
  - ∗ but maybe reached limit of PQχPT (exceptional configurations) $\Rightarrow$ simulation at lighter sea quark mass is necessary
- lattice artefacts are negligible compared to NNLO at least at fixed β
-

$$\alpha_5 \;=\; 2.06(42) \qquad (2\alpha_8 - \alpha_5) \;=\; 0.583(45) \quad (@4\pi f_0 = \Lambda_\chi)$$

$$\Lambda_3 \;=\; 0.76(3)\text{GeV} \qquad \Lambda_4 \;=\; 1.99(14)\text{GeV}$$

Outlook

- starting to use twisted-mass fermions for light quarks
  $\longrightarrow$ talks by FARCHIONI & URBACH this conference (also cf. DESY 04-098)
  - provide a lower bound to the eigenvalue-spectrum
  - automatic $\mathcal{O}(a)$-improvement
- PQχPT with twisted mass term: MÜNSTER, SCHMIDT, ES (hep-lat 0402003), also talk by MÜNSTER this conference
  - e.g.:

$$
\begin{aligned}
Rf_{\mathrm{VV}} \quad = \quad & 1 + 4L_{S5}\chi_S(\xi - 1) + 4W_{S5}\chi_S\eta(\cos\omega_V - \cos\omega_S) + \frac{\chi_S}{32\pi^2}\Big\{2\Big[1 + \eta\cos\omega_S\Big]\log[1 + \eta\cos\omega_S] \\
& -\Big[1 + \xi + \eta(\cos\omega_S + \cos\omega_V)\Big]\log\left[\frac{1 + \xi + \eta(\cos\omega_S + \cos\omega_V)}{2}\right]\Big\} + \mathcal{O}(\eta^2)
\end{aligned}
$$

  - important to measure ω

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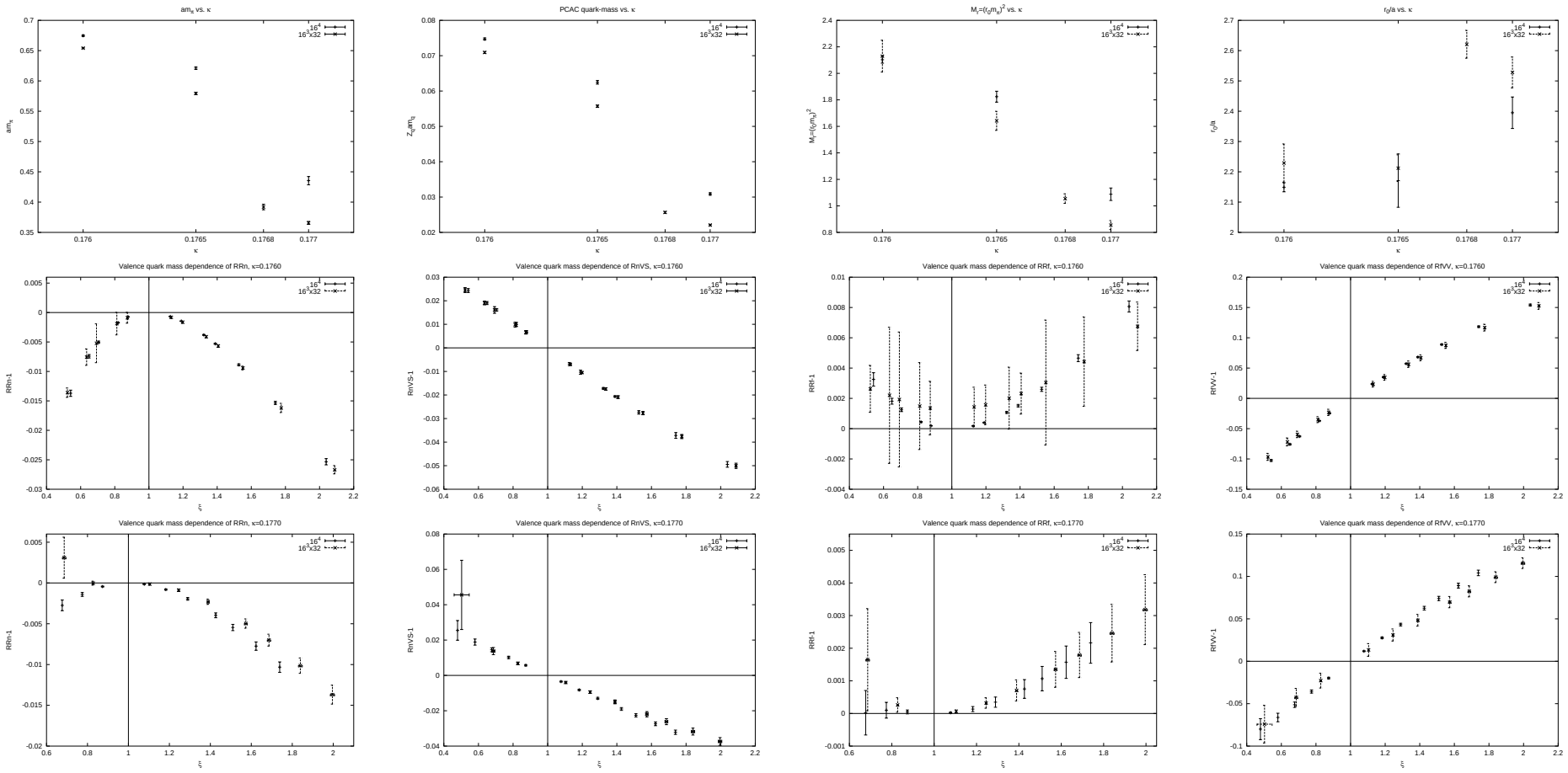
computations were done at:

- APEmille @ NIC/DESY Zeuthen
- Cray T3E @ NIC Jülich
- PC clusters @ DESY Hamburg
- PC clusters @ University of Münster
- Sun Fire SMP-Cluster @ Rechenzentrum RWTH Aachen

APPENDIX

the following transparencies are just for special questions

more comparison 16^4 vs. $16^3 \times 32$...



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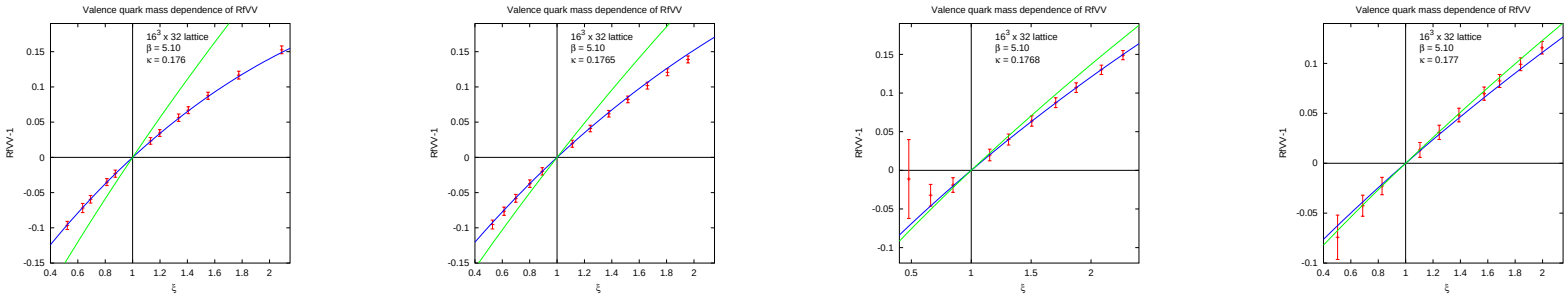
$$Rf_{VV} \equiv \frac{f_{VV}}{f_{SS}}$$

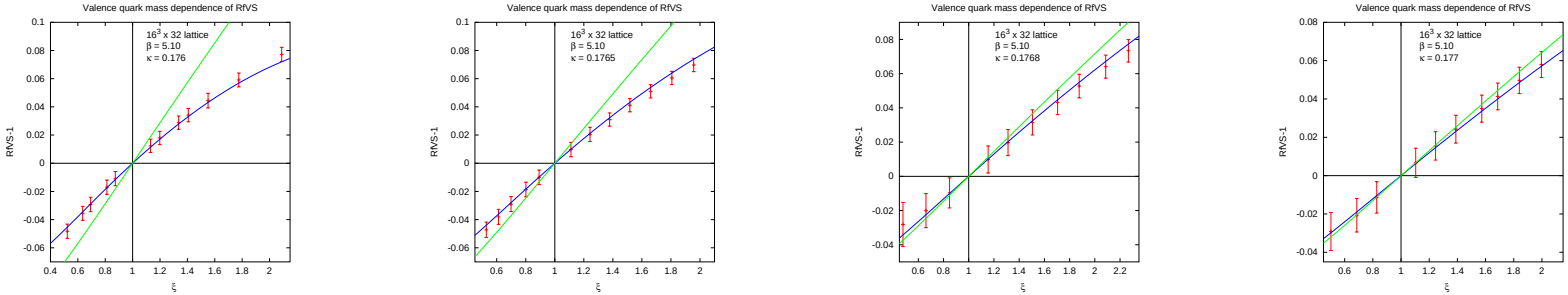
$$= 1 + 4(\xi - 1)\chi_S L_{S5} - \frac{N_s \chi_S}{64\pi^2}(1+\xi)\log\frac{1+\xi}{2} + D_{fVV}\chi_S^2(\xi-1) + Q_{fVV}\chi_S^2(\xi-1)^2 + \mathcal{O}(\chi_S^2 \log\xi, \chi_S^3)$$



full fit / only NLO contribution

$$Rf_{VS} \equiv \frac{f_{VS}}{f_{SS}}$$

$$= 1 + 2(\xi - 1)\chi_S L_{S5} + \frac{\chi_S}{64 N_s \pi^2}(\xi - 1 - \log\xi) - \frac{N_s \chi_S}{128\pi^2}(1+\xi)\log\frac{1+\xi}{2} + \frac{1}{2}D_{fVV}\chi_S^2(\xi-1) + Q_{fVS}\chi_S^2(\xi-1)^2$$
$$+\mathcal{O}(\chi_S^2 \log\xi, \chi_S^3)$$



full fit / only NLO contribution

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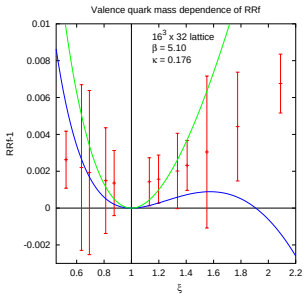
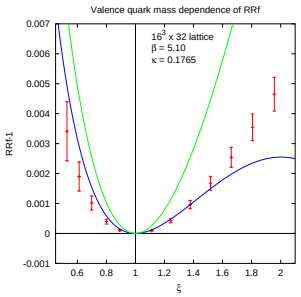
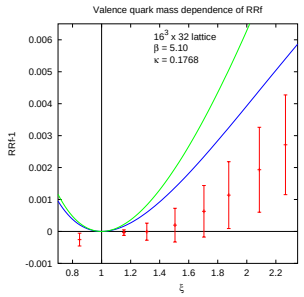
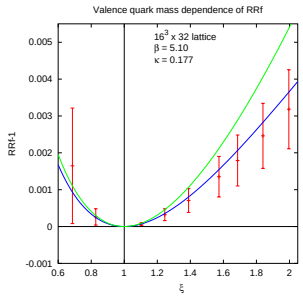
$$RRf \equiv \frac{f_{VS}^2}{f_{SS} f_{VV}}$$
$$= 1 + \frac{\chi_S}{32 N_s \pi^2}(\xi - 1 - \log\xi) + Q_{fd}\chi_S^2(\xi - 1)^2 + \mathcal{O}(\chi_S^2 \log\xi, \chi_S^3)$$





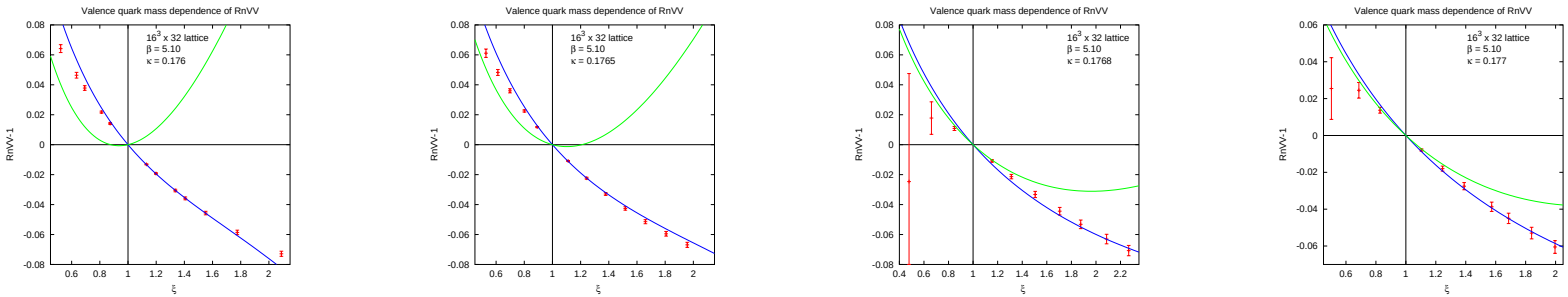




full fit / only NLO contribution

$$Rn_{VV} = \frac{m_{VV}^2}{\xi m_{SS}^2}$$

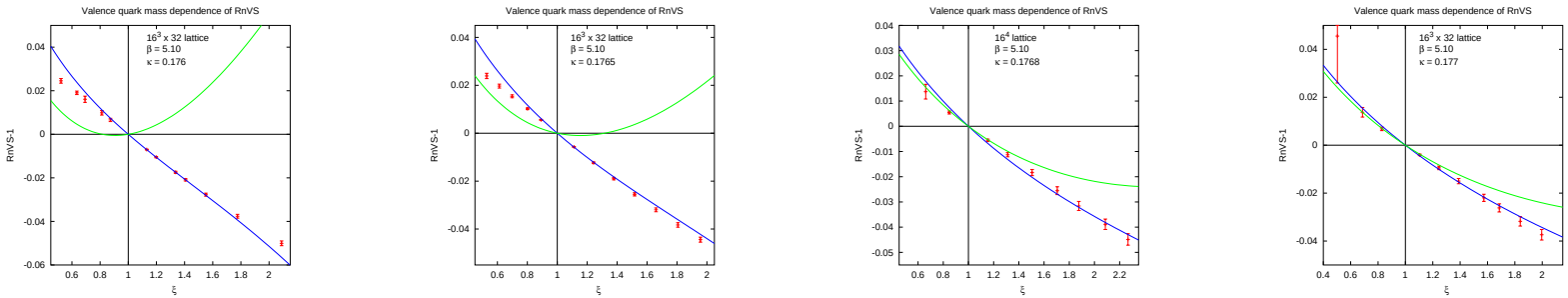
$$= 1 + 8(\xi - 1)\chi_S(2L_{S8} - L_{S5}) + \frac{\chi_S}{16 N_s \pi^2}[\xi - 1 + (2\xi - 1)\log\xi] + D_{nVV}\chi_S^2(\xi - 1) + Q_{nVV}\chi_S^2(\xi - 1)^2 + \mathcal{O}(\chi_S^2 \log\xi, \chi_S^3)$$



full fit / only NLO contribution

$$Rn_{VS} \equiv \frac{2m_{VS}^2}{(\xi+1)m_{SS}^2}$$

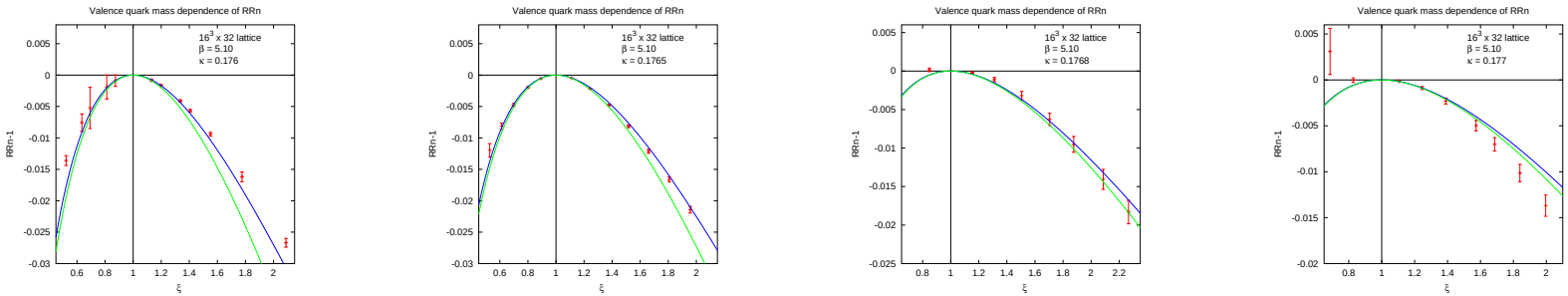
$$1 + 4(\xi-1)\chi_S(2L_{S8} - L_{S5}) + \frac{\chi_S}{16N_s\pi^2}\xi\log\xi + \frac{1}{2}D_{nVV}\chi_S^2(\xi-1) + Q_{nVS}\chi_S^2(\xi-1)^2 + \mathcal{O}(\chi_S^2\log\xi, \chi_S^3)$$



full fit / only NLO contribution

$$RRn \equiv \frac{4\xi m_{VS}^4}{(\xi+1)^2 m_{VV}^2 m_{SS}^2}$$

$$1 - \frac{\chi_S}{16 N_s \pi^2}(\xi - 1 - \log\xi) + Q_{nd}\chi_S^2(\xi-1)^2 + \mathcal{O}(\chi_S^2 \log\xi, \chi_S^3)$$



full fit / only NLO contribution

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