Dynamical simulations with twisted mass fermions including the strange quark

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- twisted-mass Wilson fermions for $N_f = 2$ viable alternative

- "realistic" QCD-simulations should include the strange quark

- no "single twisted fermion"

- different approaches possible with twisted mass
  * use untwisted (standard Wilson) strange-quark
  * use another doublet ($N_f = 2 + 2$) (works only for quenched studies)
  - use mass-splitting a'la Frezzotti-Rossi for 2nd doublet

$$\boldsymbol{N_f \ = \ 2 + 1 + 1}$$

degenerate up, down; non-degenerate strange, charm ("charm as bonus")

Mass-split doublets

fermionic action with twisted mass term and mass-splitting term [Frezzotti, Rossi, 2004]

χ-basis: $S \; = \; \sum_{xy} \bar{\chi}_x \, Q^{\chi}_{x,y} \, \chi_y$

$$Q^{\chi}_{x,y} \;=\; \delta_{x,y}\Big[\mu_\kappa \;+\; i\gamma_5\tau_1 a\mu_\sigma \;+\; \tau_3 a\mu_\delta\Big] \underbrace{-\frac{1}{2}\sum_{\mu=\pm 1}^{4}\delta_{x,y+\hat{\mu}}\gamma_\mu U_{y\mu}}_{\equiv N_{x,y}} \underbrace{-\frac{r}{2}\sum_{\mu=\pm 1}^{4}\delta_{x,y+\hat{\mu}} U_{y\mu}}_{\equiv R_{x,y}}$$

ψ-basis: $\psi_x = \frac{1}{\sqrt{2}}(1+i\gamma_5\tau_1)\chi_x, \qquad \bar{\psi}_x = \bar{\chi}_x \frac{1}{\sqrt{2}}(1+i\gamma_5\tau_1)$

$$Q^{\psi}_{x,y} \;=\; \frac{1}{2}(1-i\gamma_5\tau_1)Q^{\chi}_{x,y}(1-i\gamma_5\tau_1) \;=\; a\mu_\sigma \;+\; \tau_3 a\mu_\delta \;+\; N \;-\; i\gamma_5\tau_1(\mu_\kappa + R)$$

physical basis ψ^{phys}: $\psi^{\text{phys}}_x = \exp\left[\frac{i}{2}\left(\omega - \frac{\pi}{2}\right)\gamma_5\tau_1\right]\psi_x, \qquad \bar{\psi}^{\text{phys}}_x = \bar{\psi}_x \exp\left[\frac{i}{2}\left(\omega - \frac{\pi}{2}\right)\gamma_5\tau_1\right]$

twist angle ω: (tuning to full twist. . .)

$$\text{“}\ \tan\omega = \frac{a\mu_\sigma}{\mu_\kappa - \mu_{\kappa\text{crit}}}\ \text{”}$$

Set-up for dynamical $N_f = 2 + 1 + 1$-simulations

- light doublet: $\mu_\delta = 0$ representing degenerate up- and down-quarks ($N_f = 2$)
  - parameters: $\mu_{\kappa,l} = 1/(2\kappa_l)$, $a\mu_l = a\mu_{\sigma,l}$ more convenient: $\tau_1 \to \tau_3$
  - tune κ_l to $\kappa_{l,\text{crit}}$
- heavy doublet: $\mu_\delta \neq 0$ representing *non*-degenerate strange- and charm-quarks
  - parameters: $\mu_{\kappa,h} = 1/(2\kappa_h)$, $a\mu_\sigma$, $a\mu_\delta$
  - tune κ_h to $\kappa_{h,\text{crit}}$
  - based on (parity) $\times$ ($\mu \to -\mu$)-symmetry: PCAC-defined critical quark mass only influenced by $\mathcal{O}(a)$-effects due to TM-terms [Farchioni et al., 2005; Chiarappa et al., 2006]

$$\Rightarrow \quad \kappa_{l,\text{crit}} \approx \kappa_{h,\text{crit}}$$

- gauge action: gauge coupling $\beta = 6/g^2$ (improved gauge actions tree-level Symanzik, Iwasaki, DBW2 preferable to pure Wilson)
- 5 parameters:

$$\beta, \quad \kappa\,(= \kappa_l = \kappa_h), \quad a\mu_l, \quad a\mu_\sigma, \quad a\mu_\delta$$

ultimate goal: $\kappa = \kappa_{\text{crit}}$ & μ's such that renormalized masses close to physical masses

tuning to κ_{crit}

- in light-sector measure *untwisted PCAC quark mass*

$$am_{\chi l}^{\text{PCAC}} \equiv \frac{\langle \partial_\mu^* A_{l,x\mu}^+ P_{l,y}^- \rangle}{2\langle P_{l,x}^+ P_{l,y}^- \rangle}$$

- analogously in heavy sector . . . but
- using symmetry of the action:
  - $*$ parity $\times$ $(\mu \to -\mu)$
  - $*$ $\Big(\chi_h \to \exp(i\frac{\pi}{2}\tau_1)\chi_h, \bar\chi_h \to \bar\chi_h \exp(-i\frac{\pi}{2}\tau_1)\Big) \times \Big(\mu_\delta \to -\mu_\delta\Big)$

$$m_{\chi h}^{\text{PCAC}} = m_{\chi l}^{\text{PCAC}} + \mathcal{O}(a)$$

extracting the K's, D's, . . .

- pion-mass and -decay constant like $N_f = 2$
- including the heavy-doublet: Kaon-D-meson sector

$$C_{K^+} = \bar{\chi}_s \Gamma_C \chi_u \qquad C_{D^0} = \bar{\chi}_c \Gamma_C \chi_u$$
$$C_{K^0} = \bar{\chi}_s \Gamma_C \chi_d \qquad C_{D^-} = \bar{\chi}_c \Gamma_C \chi_d$$
$$C = S, P, V, K \qquad \Gamma_C = 1, \gamma_5, \gamma_\mu, \gamma_\mu \gamma_5$$

- expect better signal from scalar correlators

$$\mathcal{V} = (Z_P P_{K^+}, Z_P P_{D^0}, Z_S S_{K^+}, Z_S S_{D^0})^T$$
$$\bar{\mathcal{V}} = (-Z_P P_{K^-}, -Z_P P_{\bar{D}^0}, -Z_S S_{K^-}, -Z_S S_{\bar{D}^0})$$

- correlator-matrix $\mathcal{C} = \langle \mathcal{V} \otimes \bar{\mathcal{V}} \rangle$
- fully renormalised (physical) matrix $\hat{\mathcal{C}}$ from

$$\hat{\mathcal{V}} = \mathcal{M}\mathcal{V} \quad \hat{\bar{\mathcal{V}}} = \bar{\mathcal{V}}\mathcal{M}^{-1}$$

$$\mathcal{M}(\omega_l,\omega_h) \;=\; \begin{pmatrix} \cos\frac{\omega_l}{2}\cos\frac{\omega_h}{2} & -\sin\frac{\omega_l}{2}\sin\frac{\omega_h}{2} & i\sin\frac{\omega_l}{2}\cos\frac{\omega_h}{2} & i\sin\frac{\omega_h}{2}\cos\frac{\omega_l}{2} \\ -\sin\frac{\omega_l}{2}\sin\frac{\omega_h}{2} & \cos\frac{\omega_l}{2}\cos\frac{\omega_h}{2} & i\sin\frac{\omega_h}{2}\cos\frac{\omega_l}{2} & i\sin\frac{\omega_l}{2}\cos\frac{\omega_h}{2} \\ i\sin\frac{\omega_l}{2}\cos\frac{\omega_h}{2} & i\sin\frac{\omega_h}{2}\sin\frac{\omega_l}{2} & \cos\frac{\omega_l}{2}\cos\frac{\omega_h}{2} & -\sin\frac{\omega_h}{2}\sin\frac{\omega_l}{2} \\ i\sin\frac{\omega_h}{2}\cos\frac{\omega_l}{2} & i\sin\frac{\omega_l}{2}\cos\frac{\omega_h}{2} & -\sin\frac{\omega_l}{2}\sin\frac{\omega_h}{2} & \cos\frac{\omega_h}{2}\cos\frac{\omega_l}{2} \end{pmatrix}$$

restore parity- and flavour-symmetry: $\hat{\mathcal{C}} = \mathcal{M}\,\mathcal{C}\,\mathcal{M}^{-1}$ diagonal

$$\Rightarrow \quad \omega_h$$

extract masses from $\hat{\mathcal{C}}$

Mass-splitting in K-D-sector

using combined *parity-isospin* symmetry of the heavy-light action

$$Q_l^{\psi} = a\mu_l + N - i\gamma_5\tau_3(\mu_{\kappa l} + R) \qquad Q_h^{\psi} = a\mu_\sigma + \tau_3 a\mu_\delta + N - i\gamma_5\tau_1(\mu_{\kappa h} + R)$$

light :	heavy :
Parity $\otimes\ \tau_1$	Parity $\otimes\ \tau_3$
$u(x) \longrightarrow \gamma_0 d(Px)$	$c \longrightarrow \gamma_0 c(Px)$
$d(x) \longrightarrow \gamma_0 u(Px)$	$s \longrightarrow -\gamma_0 s(Px)$

no mass splittings in Kaon- or D-meson-doublets

recent (quenched) study by Abdel-Rehim, Lewis et al.:
same isospin-direction in both doublets leads to observed splitting

Polynomial Hybrid Monte Carlo (PHMC)-algorithm

- HMC with mass preconditioning efficient algorithm for unsplit-TM. . .
- . . . but unfortunately not applicable to $\mu_\delta \neq 0$-case.
  $\det(Q)$ cannot be written as single flavor $\det(Q'^2)$
- use polynomial approximation $P_1(Q^2) \simeq (Q^2)^{-\frac{1}{2}}$ of order n_1 [Frezzotti, Jansen, 1997-99]
- combine with stochastic correction step (noisy correction) [Montvay, EES, 2005]

$$P_1(x)P_2(x) \simeq x^{-\frac{1}{2}}, \quad n_2 > n_1$$

(further correction steps and/or "polynomial mass preconditioning" may be useful at smaller masses. . .)

- adjusting step-size(s) in HMC-step plus polynomial orders n_1, n_2 allows for good tuning properties
- improvement: mixed (P)HMC: heavy doublet–PHMC, light doublet–HMC
  [Chiarappa et al., 2005]
- other possible algorithms for heavy doublet
  - ∗ Rational-HMC (did not try yet for TM)
  - ∗ Two-Step Multi-Boson or Multi-Step Multi-Boson (less efficient than PHMC)
    [Montvay, 1995; Montvay, EES, 2005]
  - ∗ in principle every algorithm capable of odd N_f . . .

Dynamical Simulations

CHIARAPPA,. . . , EES, . . . , URBACH, hep-lat/0606011

- tree-level Symanzik gauge action, two lattice spacings (fixed physical volume: $aL \simeq 2.4$fm)

  * $a \simeq 0.20$fm ($\beta = 3.25$, $L^3 \times T = 12^3 \times 24$)
    $a\mu_l = 0.01$, $a\mu_\sigma = 0.315$, $a\mu_\delta = 0.285$, $\kappa \in [0.1740, 0.1755]$ (7 values, 10 runs)

  * $a \simeq 0.15$fm ($\beta = 3.35$, $L^3 \times T = 16^3 \times 32$)
    $a\mu_l = 0.0075$, $a\mu_\sigma = 0.2363$, $a\mu_\delta = 0.2138$, $\kappa \in [0.1690, 0.1710]$ (9 values)

- varied $\kappa (= \kappa_l = \kappa_h)$ to find κ_{crit}, explore phase-structure

- lattice-spacing, light-doublet similar to previous studies (DBW2 and pure Wilson gauge action)

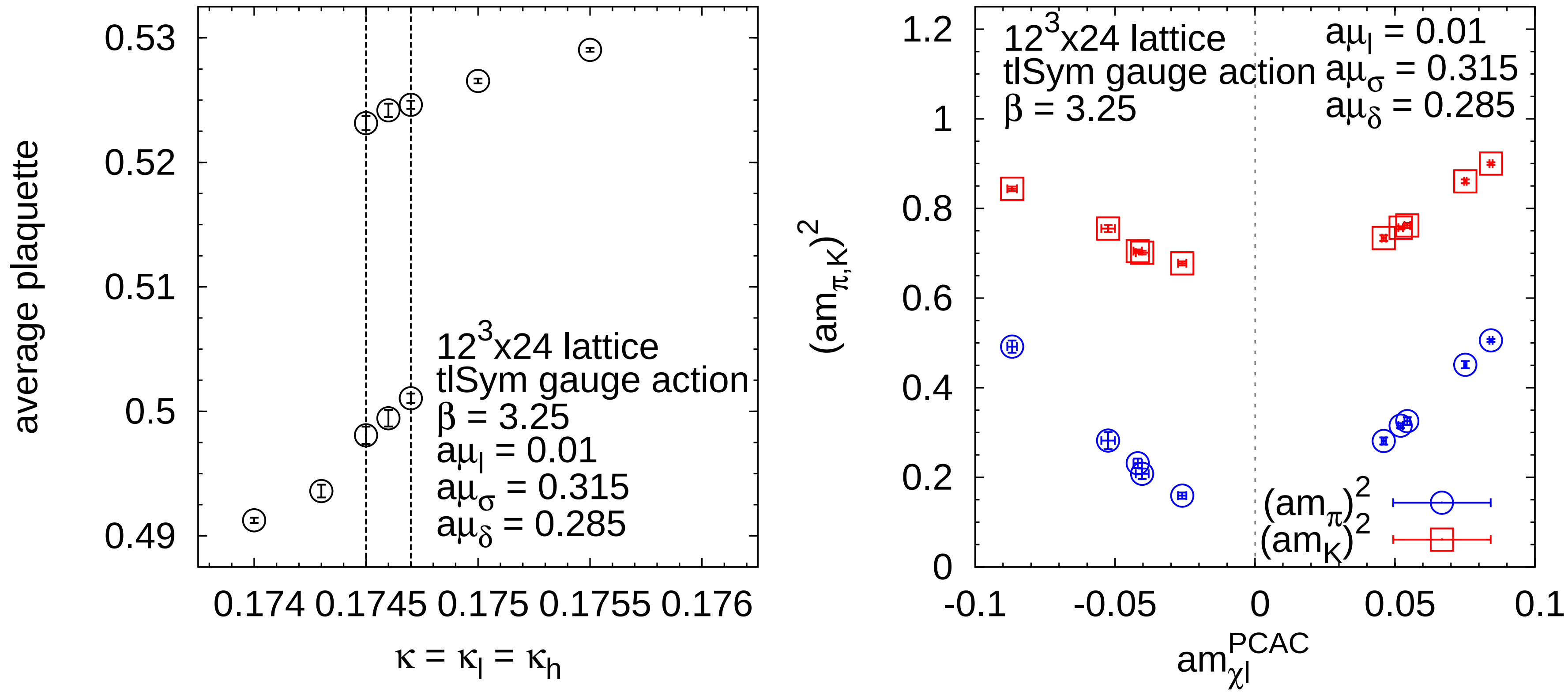
- performed at (ZAM Jülich) (IBM-p690) at (NIC Jülich) and PC-Cluster at (Hamburg)

ZAM Jülich

NIC Jülich

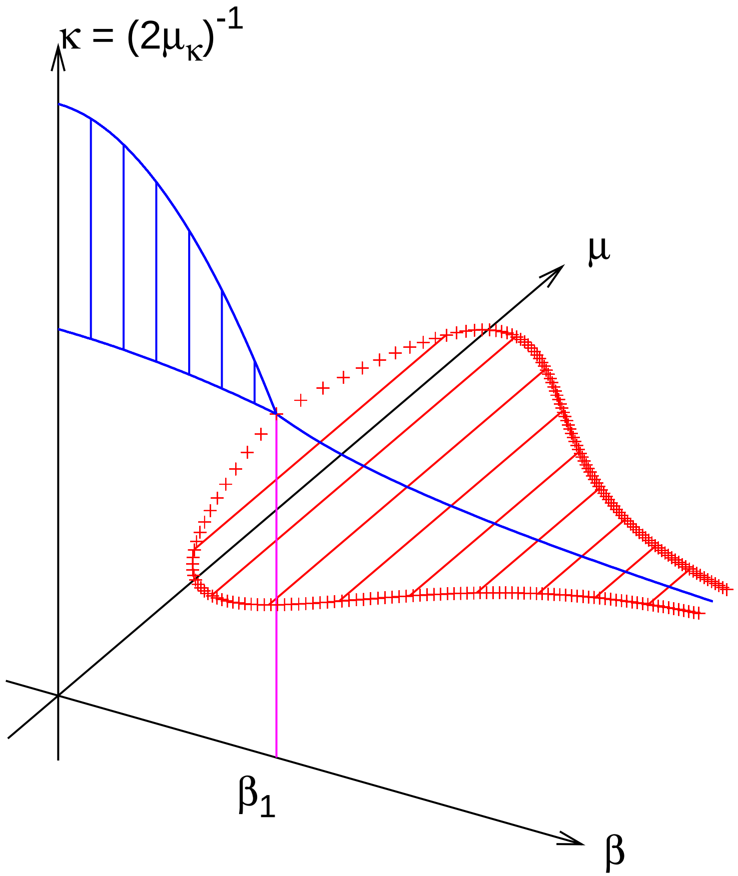
Hamburg

$a \approx \mathbf{0.20}$fm, $\mathbf{12^3 \times 24}$

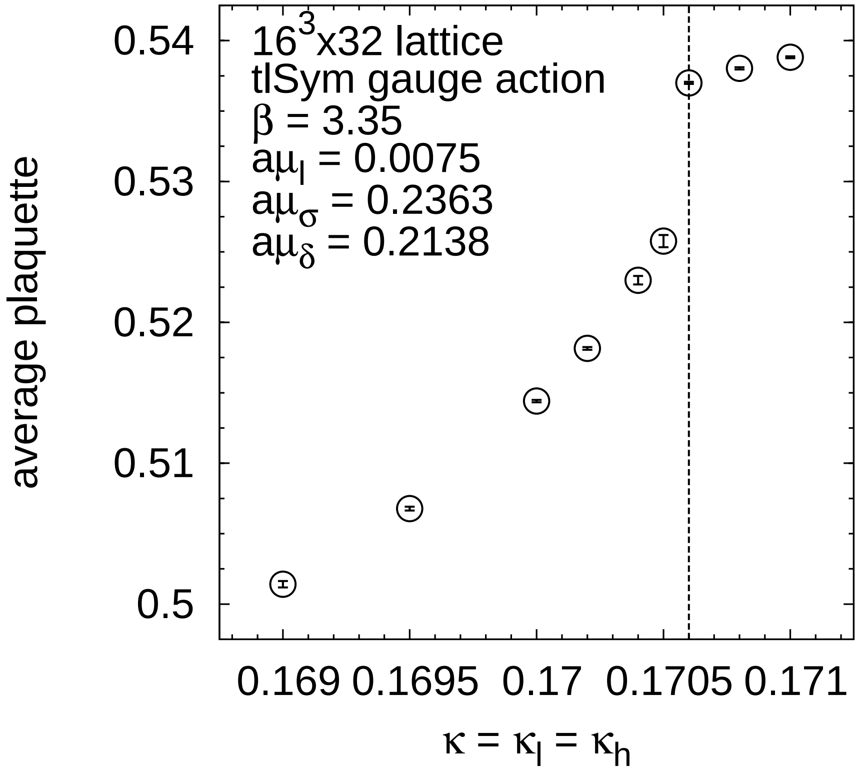


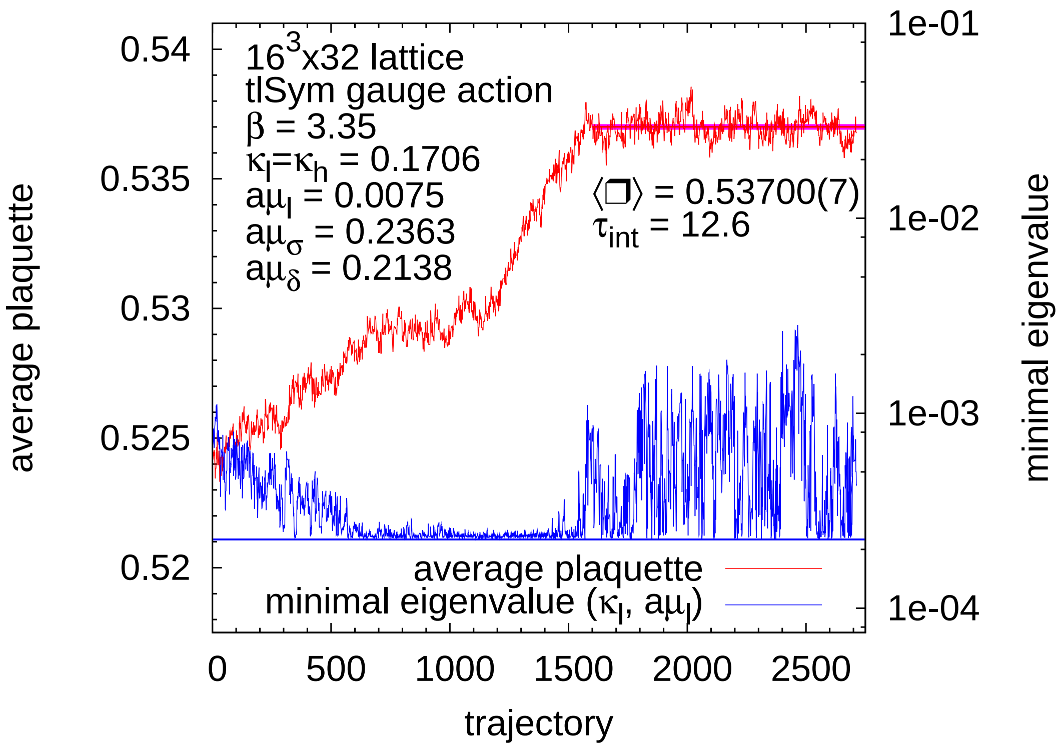
- strong metastability
- minimal pion mass ≈ 670MeV
- minimal $m_K \simeq 920$MeV

. . . just a reminder



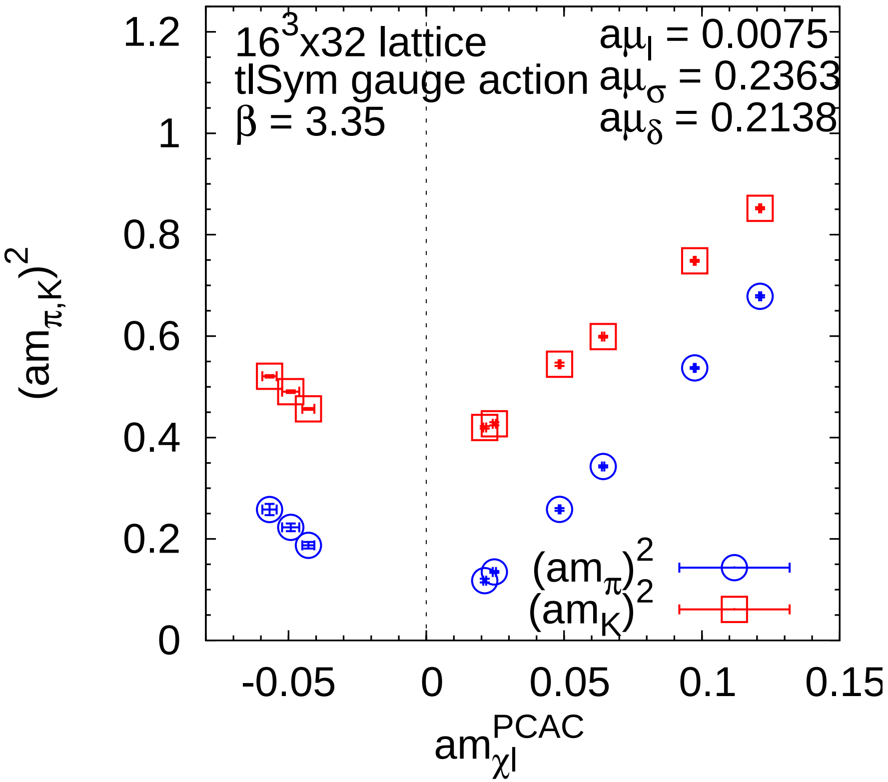
$a \approx 0.15$fm, $16^3 \times 32$





- sharp rise in $\langle\Box\rangle$
  - ? weaker *first order phase transition*
    or
  - ? *cross-over*
  - $\ast$ not distinguishable in finite volume

- not an algorithmic imperfection
  - $\ast$ transition low $\longrightarrow$ high plaquette phase
  - $\ast$ "crossing near origin"
  - $\ast$ lowest EV fluctuating in high plaquette phase

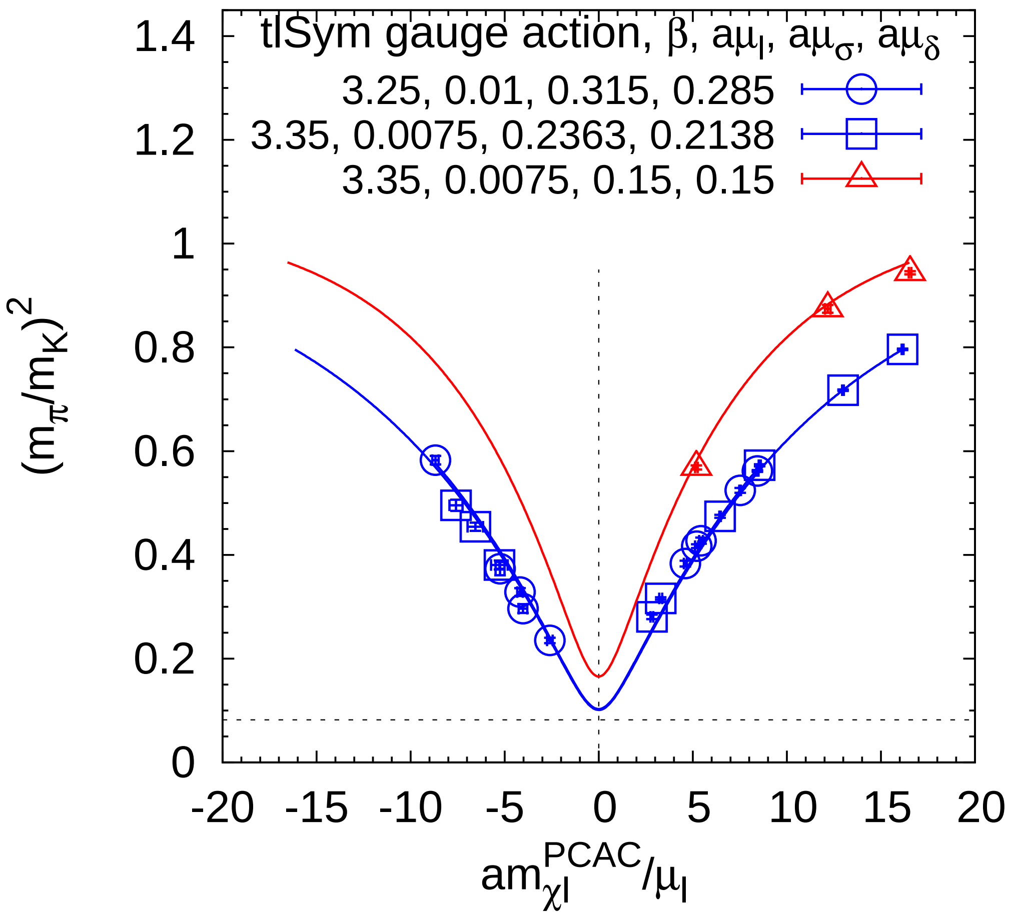


- minimal pion mass $\approx 450\text{MeV}$
- keep in mind: varying κ at fixed μ_l

$\Rightarrow$ $m_\pi > 0$

- minimal $m_K \simeq 850\text{MeV}$
- tuning m_K possible by changing μ_σ, μ_δ

. . . using χPT



$$\frac{m_\pi^2}{m_K^2} = \frac{2m_{ud}}{m_{ud}+m_s}$$

$$m_{ud} = \sqrt{(Z_A m_{\chi l}^{\mathrm{PCAC}})^2 + \mu_l^2}$$

$$m_s = \sqrt{(Z_A m_{\chi h}^{\mathrm{PCAC}})^2 + \mu_\sigma^2} - \frac{Z_P}{Z_S}\mu_\delta$$

fitted $Z_P/Z_S \simeq 0.45$

take Z_A as input

$m_{\chi l}^{\mathrm{PCAC}} \approx m_{\chi l}^{\mathrm{PCAC}}$

minimum close to physical value

Summary

- $N_f = 2 + 1 + 1$-mechanism understood
- dynamical simulations with PHMC-algorithm
- stronger phase-structure compared $N_f = 2$
- minimal pion mass 450MeV
- going to $a \simeq 0.10$fm on $24^3 \times 48$ should allow for pion masses around 300MeV