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Lattice Quantum Chromodynamics with a chirally twisted mass term

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1. Introduction

Quantum Chromodynamics

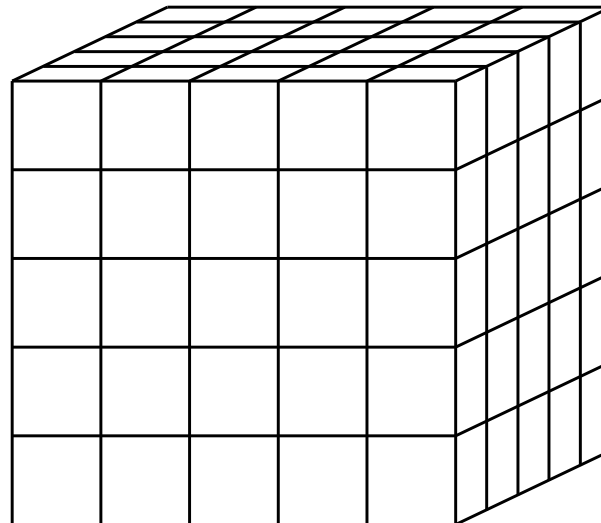
Continuum:

$$\mathcal{L}_{\text{QCD}} = \sum_f \bar{\psi}_f \{ \gamma_\mu (\partial_\mu - i g A_\mu) + m_f \} \psi_f + \frac{1}{4} F_{\mu\nu}^i F_{\mu\nu}^i, \quad f = 1, \dots, N_f \quad \text{flavours}$$

Perturbation theory \sim expansion in g \rightarrow high energy regime

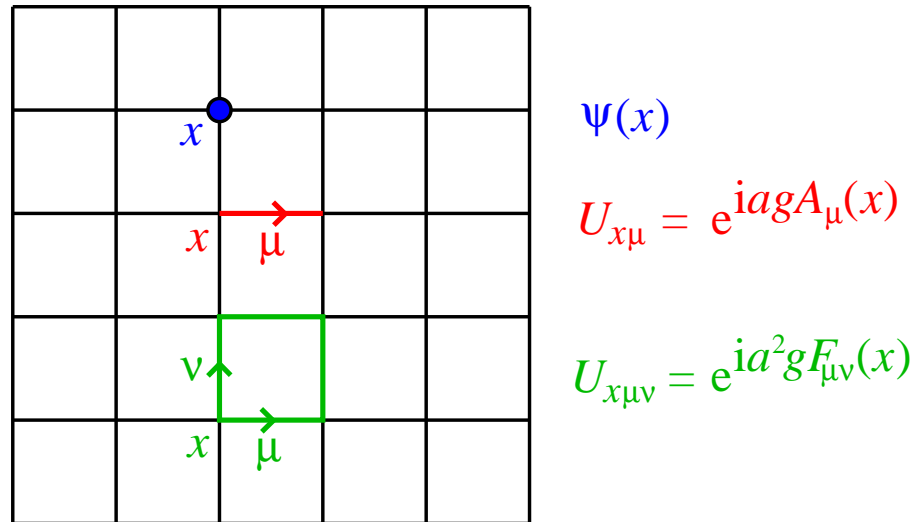
Non-perturbative problems: spectrum, matrix elements, ...

\rightarrow QCD on the lattice



lattice spacing a

Lattice QCD



Wilson action:

$$\begin{aligned}
 \mathcal{L} &= \left(m_0 + \frac{4}{a}\right) \bar{\psi}_x \psi_x - \frac{1}{2a} \sum_{\mu} \left\{ \bar{\psi}_{x+\mu} (1 + \gamma_\mu) U_{x\mu} \psi_x + \bar{\psi}_x (1 - \gamma_\mu) U_{x\mu}^\dagger \psi_{x+\mu} \right\} \\
 &\quad - \frac{2}{a^4 g^2} \sum_{\mu < \nu} \text{Re Tr } U_{x\mu\nu} \\
 &\simeq \bar{\psi} (\gamma_\mu D_\mu + m_q) \psi - \frac{1}{2a} \bar{\psi} D_\mu D_\mu \psi + \frac{1}{4} F_{\mu\nu}^i F_{\mu\nu}^i
 \end{aligned}$$

quark mass $m_0 = m_c + m_q$

Numerical investigations of **Quantum Chromodynamics** on the **lattice** have to fight against problems from

- finite a (lattice spacing) effects,
- finite L (lattice size) effects,
- small **quark masses**

Quark masses: $m_u = 5 \text{ MeV}$, $m_d = 9 \text{ MeV}$, $m_s = 175 \text{ MeV}$

Monte Carlo: slowing down $\propto m_q^p$, $p = 2 - 3$

Extrapolation to small $m_q \rightarrow$ **chiral perturbation theory** (χ PT)

(Weinberg; Gasser, Leutwyler, ...): expansion around chiral limit, $m_q = 0$

Lattice spacing a

$$X(a) = X(\text{continuum}) + c_1 a + c_2 a^2 + \dots$$

Symanzik's improvement program: $c_1 \rightarrow 0, c_2 \rightarrow 0, \dots$

Ansatz:

Twisted mass lattice QCD (Frezzotti, Grassi, Sint, Weisz, Rossi)

$\rightarrow \mathcal{O}(a)$ improvement

ETMC: European Twisted Mass Collaboration

O. Bär, D. Bećirević, B. Blossier, Ph. Boucaud, T. Chiarappa, F. De Soto, P. Dimopoulos, F. Farchioni, R. Frezzotti, V. Giménez, G. Herdoiza, K. Jansen, J.P. Leroy, M.P. Lombardo, V. Lubicz, G. Martinelli, C. McNeile, F. Mescia, C. Michael, I. Montvay, G. Münster, K. Nagai, D. Palao, M. Papinutto, O. Pène, J. Pickavance, J. Rodríguez-Quintero, G.C. Rossi, S. Schäfer, L. Scorzato, A. Shindler, S. Simula, T. Sudmann, C. Tarantino, C. Urbach, A. Vladikas, U. Wenger

Berlin, Frascati, Grenoble, Hamburg, Huelva, Liverpool, Milano, München, Münster, Paris XI, Roma III, Roma “La Sapienza”, Roma Tor Vergata, València, Villazzano, Zeuthen, Zürich

2. Chiral symmetry of Quantum Chromodynamics

Continuum:

$$\mathcal{L}_{\text{QCD}} = \sum_f \bar{\psi}_f \{ \gamma_\mu (\partial_\mu - i g A_\mu) + m_f \} \psi_f + \frac{1}{4} F_{\mu\nu}^i F_{\mu\nu}^i, \quad f = 1, \dots, N_f \quad \text{flavours}$$

$$\psi_L \equiv \frac{1}{2} (1 - \gamma_5) \psi, \quad \psi_R \equiv \frac{1}{2} (1 + \gamma_5) \psi$$

$$\rightarrow \mathcal{L}_q = \bar{\psi}_L \gamma_\mu D_\mu \psi_L + \bar{\psi}_R \gamma_\mu D_\mu \psi_R + m_q (\bar{\psi}_L \psi_R + \bar{\psi}_R \psi_L)$$

$$m_q = 0 \quad \rightarrow \quad \text{chiral symmetry} \quad \text{SU}(N_f)_L \otimes \text{SU}(N_f)_R \otimes \text{U}(1)_V \otimes \text{U}(1)_A$$

$$\psi_L \rightarrow L \psi_L, \quad \psi_R \rightarrow R \psi_R \quad \text{with} \quad L \in \text{SU}(N_f)_L, \quad R \in \text{SU}(N_f)_R$$

spontaneously broken to $\text{SU}(N_f)_V$, $(L \equiv R)$

Goldstone bosons = pseudoscalar mesons: pions, Kaons, η

explicitly broken by quark masses $m_q \neq 0$

Goldstone bosons \rightarrow light Pseudo-Goldstone bosons

For $N_f = 2$: Pseudo-Goldstone bosons = pions π_b , $b = 1, 2, 3$

Gell-Mann, Oakes, Renner: $m_\pi^2 = B_0(m_u + m_d)$

3. Twisted mass lattice QCD

Frezzotti, Grassi, Sint, Weisz, Rossi

Consider $N_f = 2$, $m_u = m_d \equiv m_q$

Parameters: quark mass m_q , gauge coupling g

Mass term $\bar{\psi} M(\omega) \psi$ with

$$M(\omega) = m_q e^{i\omega\gamma_5\tau_3} = m + i\mu\gamma_5\tau_3, \quad \text{where } m = m_q \cos(\omega), \mu = m_q \sin(\omega)$$

Continuum: no effect, remove ω by chiral rotation: $\psi = e^{-i\omega\gamma_5\tau_3/2} \psi'$

Lattice: dependence on ω due to explicit breaking of chiral symmetry through Wilson term

Promising approach for reducing lattice effects in numerical simulations

Full $\mathcal{O}(a)$ improvement for $\omega = \frac{\pi}{2}$ (Frezzotti, Rossi)

4. Low-energy effective Lagrangean for pions

Phase structure, chiral perturbation theory

→ Low-energy effective Lagrangean

in terms of $U(x) = \exp\left(\frac{i}{F_0} \pi_b(x) \tau_b\right)$

transforms as $U \rightarrow LUR^{-1}$, $(L, R) \in \text{SU}(N_f)_L \otimes \text{SU}(N_f)_R$

Continuum:

Leading order $\mathcal{L}_2 = \frac{F_0^2}{4} \text{Tr} (\partial_\mu U^\dagger \partial^\mu U) - \frac{F_0^2}{4} \text{Tr} (\chi U^\dagger + U \chi^\dagger)$

$$\chi = 2B_0 M, \quad M = \begin{pmatrix} m_u & 0 \\ 0 & m_d \end{pmatrix}$$

Expansion: $\mathcal{L}_2 = \frac{1}{2} (\partial_\mu \pi_a) (\partial_\mu \pi_a) + \frac{1}{2} B_0 (m_u + m_d) \pi_a \pi_a + \dots$

with pion masses $m_\pi^2 = B_0 (m_u + m_d)$ $(F_0^2 B_0 = -\langle \bar{u}u \rangle)$

Higher orders: terms with more fields and/or derivatives

Next-to-leading order (NLO)

$$\begin{aligned}\mathcal{L}_4 = & \frac{F_0^2}{4} \text{Tr} (\partial_\mu U \partial_\mu U^\dagger) - \frac{F_0^2}{4} \text{Tr} (\chi U^\dagger + U \chi^\dagger) \\ & - L_1 [\text{Tr} (\partial_\mu U \partial_\mu U^\dagger)]^2 - L_2 \text{Tr} (\partial_\mu U \partial_\nu U^\dagger) \text{Tr} (\partial_\mu U \partial_\nu U^\dagger) \\ & - L_3 \text{Tr} \left([\partial_\mu U \partial_\mu U^\dagger]^2 \right) + L_4 \text{Tr} (\partial_\mu U \partial_\mu U^\dagger) \text{Tr} (\chi U^\dagger + U \chi^\dagger) \\ & + L_5 \text{Tr} (\partial_\mu U \partial_\mu U^\dagger [\chi U^\dagger + U \chi^\dagger]) - L_6 [\text{Tr} (\chi U^\dagger + U \chi^\dagger)]^2 \\ & - L_7 [\text{Tr} (\chi U^\dagger - U \chi^\dagger)]^2 - L_8 \text{Tr} (\chi U^\dagger \chi U^\dagger + U \chi^\dagger U \chi^\dagger)\end{aligned}$$

Gasser-Leutwyler coefficients L_i

\mathcal{L} non-renormalizable, Weinberg power counting scheme

Lattice:

Symanzik's effective action: $\mathcal{L}_{\text{LQCD}} = \mathcal{L}_{\text{QCD}} + a \mathcal{L}_1 + \dots$ in the continuum

→ effective chiral Lagrangean \mathcal{L} including lattice artifacts

~ terms in \mathcal{L} proportional to powers of a

$$\mathcal{L}_2 = \frac{F_0^2}{4} \text{Tr} (\partial_\mu U^\dagger \partial^\mu U) - \frac{F_0^2}{4} \text{Tr} (\chi U^\dagger + U \chi^\dagger) - \frac{F_0^2}{4} \text{Tr} (\rho U^\dagger + U \rho^\dagger)$$

where

$$\chi = 2B_0 m'_q, \quad \rho = 2W_0 a$$

Expansion:
$$\mathcal{L}_2 = \frac{1}{2} (\partial_\mu \pi_a) (\partial_\mu \pi_a) + \frac{1}{2} m_\pi^2 \pi_a \pi_a + \dots$$

with pion masses
$$m_\pi^2 = 2B_0 m'_q + 2W_0 a = 2B_0 m_q$$

Calculate m_π^2 , F_π , etc. in powers of $m_q \sim \chi$ (modified by logarithms)

and $a \sim \rho$

Next-to-leading order: Rupak, Shoresh $\mathcal{O}(a)$; Bär, Rupak, Shoresh $\mathcal{O}(a^2)$

Monte Carlo → Gasser-Leutwyler coefficients of χ PT

twisted mass lattice QCD:

Twisting of the mass term

$$\chi \rightarrow \chi(\omega) = 2B_0 m'_q e^{-i\omega\tau_3}$$

Leading order

$$\mathcal{L}_2 = \frac{F_0^2}{4} \text{Tr} (\partial_\mu U^\dagger \partial^\mu U) - \frac{F_0^2}{4} \text{Tr} ((\chi(\omega) + \rho) U^\dagger + U(\chi(\omega) + \rho)^\dagger)$$

Next-to-leading order (NLO) to $\mathcal{O}(a^2)$

$$\begin{aligned}
\mathcal{L}_4 = & \frac{F_0^2}{4} \text{Tr} (\partial_\mu U \partial_\mu U^\dagger) - \frac{F_0^2}{4} \text{Tr} (\chi U^\dagger + U \chi^\dagger) - \frac{F_0^2}{4} \text{Tr} (\rho U^\dagger + U \rho^\dagger) \\
& - L_1 [\text{Tr} (\partial_\mu U \partial_\mu U^\dagger)]^2 - L_2 \text{Tr} (\partial_\mu U \partial_\nu U^\dagger) \text{Tr} (\partial_\mu U \partial_\nu U^\dagger) \\
& - L_3 \text{Tr} \left([\partial_\mu U \partial_\mu U^\dagger]^2 \right) \\
& + L_4 \text{Tr} (\partial_\mu U \partial_\mu U^\dagger) \text{Tr} (\chi U^\dagger + U \chi^\dagger) \\
& + W_4 \text{Tr} (\partial_\mu U \partial_\mu U^\dagger) \text{Tr} (\rho U^\dagger + U \rho^\dagger) \\
& + L_5 \text{Tr} (\partial_\mu U \partial_\mu U^\dagger [\chi U^\dagger + U \chi^\dagger]) + W_5 \text{Tr} (\partial_\mu U \partial_\mu U^\dagger [\rho U^\dagger + U \rho^\dagger]) \\
& - L_6 [\text{Tr} (\chi U^\dagger + U \chi^\dagger)]^2 \\
& - W_6 \text{Tr} (\chi U^\dagger + U \chi^\dagger) \text{Tr} (\rho U^\dagger + U \rho^\dagger) - W_6' [\text{Tr} (\rho U^\dagger + U \rho^\dagger)]^2 \\
& - L_7 [\text{Tr} (\chi U^\dagger - U \chi^\dagger)]^2 \\
& - W_7 \text{Tr} (\chi U^\dagger - U \chi^\dagger) \text{Tr} (\rho U^\dagger - U \rho^\dagger) - W_7' [\text{Tr} (\rho U^\dagger - U \rho^\dagger)]^2 \\
& - L_8 \text{Tr} (\chi U^\dagger \chi U^\dagger + U \chi^\dagger U \chi^\dagger) \\
& - W_8 \text{Tr} (\chi U^\dagger \rho U^\dagger + U \rho^\dagger U \chi^\dagger) - W_8' \text{Tr} (\rho U^\dagger \rho U^\dagger + U \rho^\dagger U \rho^\dagger)
\end{aligned}$$

Vacuum \sim minimum of \mathcal{L}

at **non-vanishing pion field** (explicit flavour and parity breaking)

Pion mass **splitting** at $\mathcal{O}(a^2)$

Expansion around vacuum

\rightarrow chiral perturbation theory for twisted mass lattice **QCD**

(Münster, Schmidt, Scholz, Hofmann, Sudmann,
Scorzato, Sharpe, Wu, Aoki, Bär ...)

5. Phase structure

„The first thing to do is to look for phase transitions“ (G. Parisi, 1988)

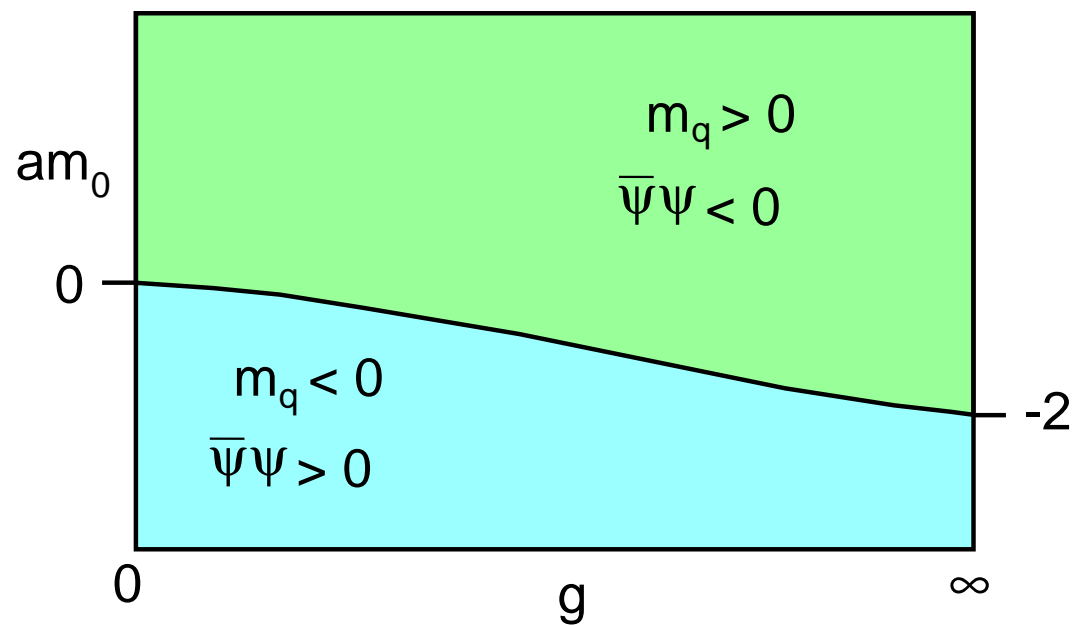
old folklore, see textbooks

$$m_0 = m_c + m_q$$

$$g \rightarrow 0: \quad \text{continuum limit} \sim \text{free quarks} \quad \longleftrightarrow \quad m_c = 0$$

$$\text{perturbation theory for quark self-energy:} \quad m_c = -\frac{1}{a} (0.4340 g^2 + \dots)$$

$$g \rightarrow \infty: \quad m_c = -\frac{1}{a} \cdot 2 \quad \longleftrightarrow \quad m_\pi = 0$$



physical region: $m_q \geq 0, \quad \bar{\psi}\psi \neq 0,$

at m_c : $m_\pi = 0,$ spontaneously broken chiral symmetry

Analogy:

Ising model

QCD

magnetic field h

quark mass m_q

magnetization M

$\bar{\psi}\psi$

This picture is **wrong**.

More careful look (Aoki 1984, ...)

Discuss symmetry breaking.

For $N_f = 2$: $SU(2)_L \otimes SU(2)_R \sim SO(4)$, $SU(2)_V \sim SO(3)$

Z_2 (Ising) \longrightarrow $SO(4)$ (Heisenberg model)

No Goldstone bosons at $m_q = 0$?

Visualize the potential.

SO(4) description: $U = u_0 + iu_a\tau_a$, $|u|^2 = 1$, $2\chi + 2\rho \equiv h_0 + ih_3\tau_3$

$\text{Tr}(U(\chi^\dagger + \rho^\dagger)) = u \cdot h \iff$ magnetic field in O(4) Heisenberg model

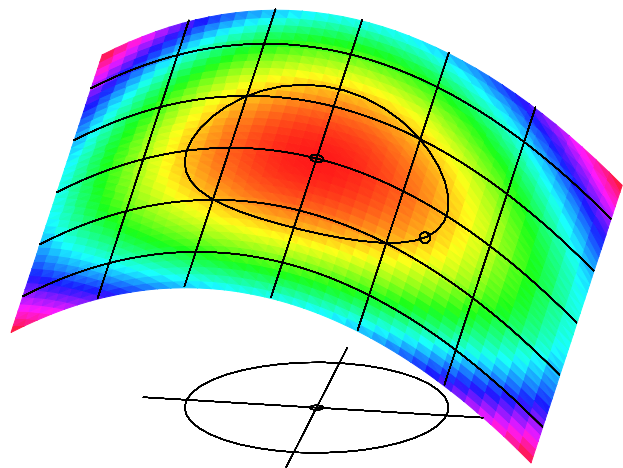
Potential in next-to-leading order:

$$V = -c_1 u_0 + c_2 u_0^2 + c_3 u_3 + c_4 u_3^2 + c_5 u_0 u_3$$

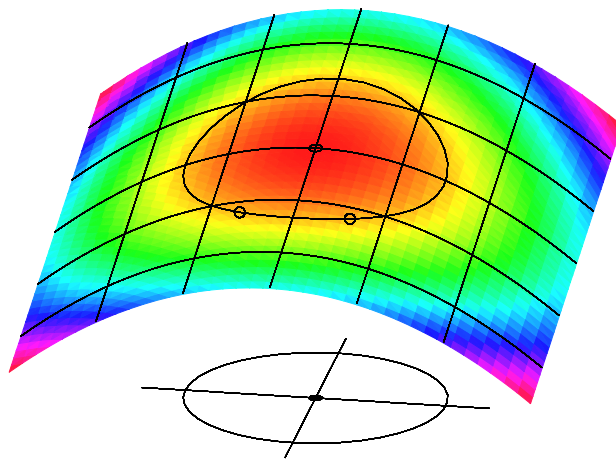
$$c_1 \sim m_q, \quad c_2 = \mathcal{O}(a^2) \quad \text{for small } m_q, \quad c_3 \sim \mu$$

Scenarios at $\mu > 0$:

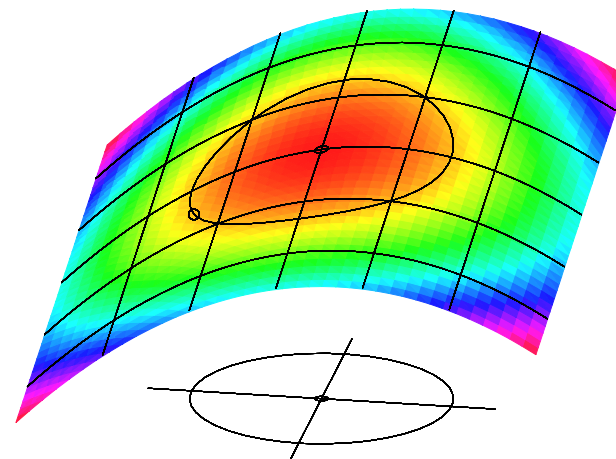
$c_2 < 0$



$$m_q > 0$$



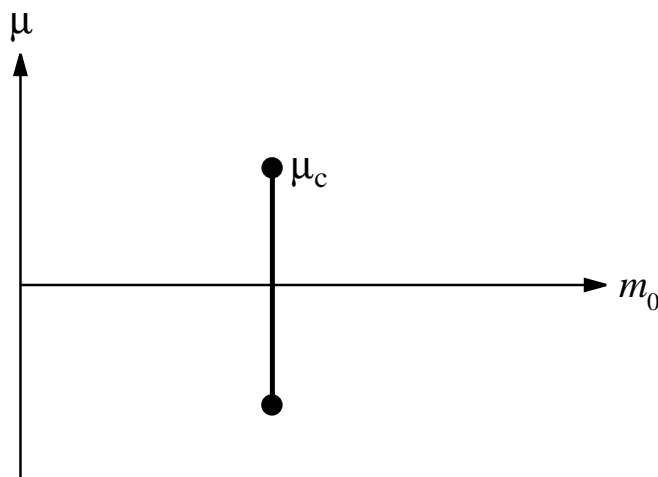
$$m_q = 0$$



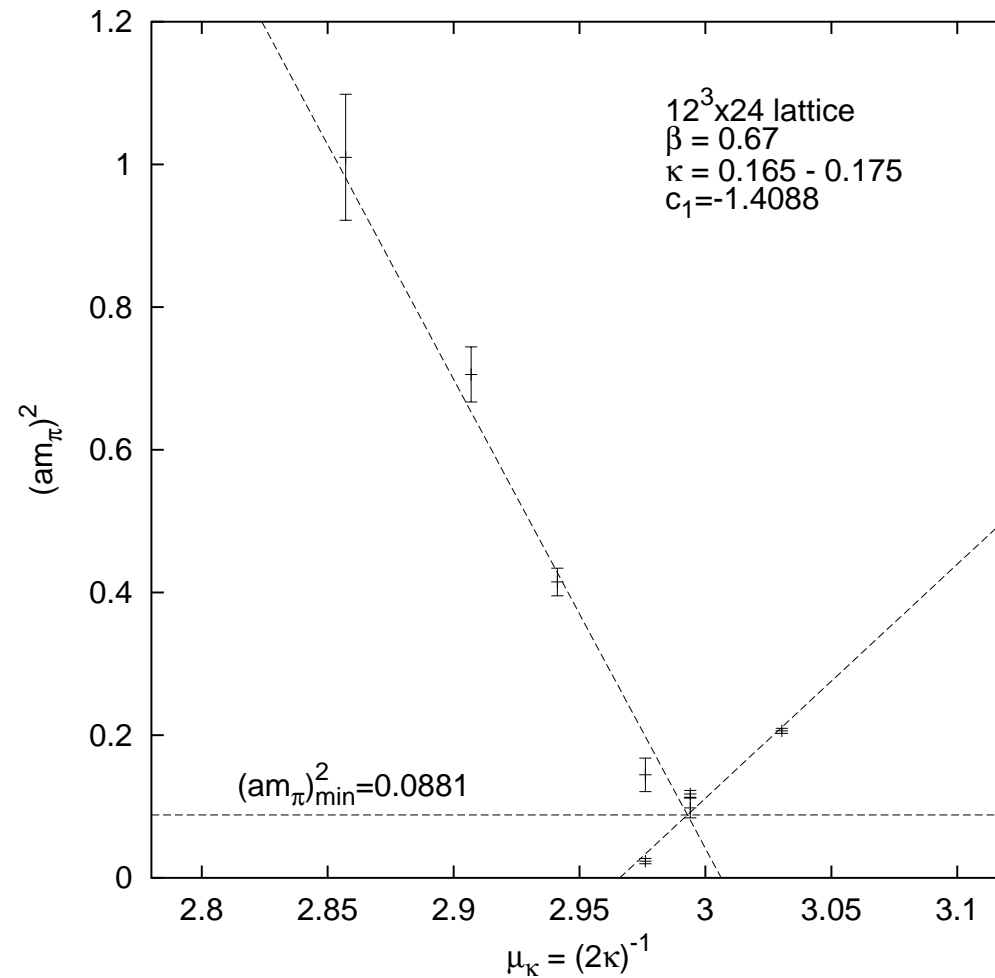
$$m_q < 0$$

1st order phase transition, 2nd order end point $\mu_c \sim a^2$

normal scenario:



minimal $m_\pi^2 \sim a^2$

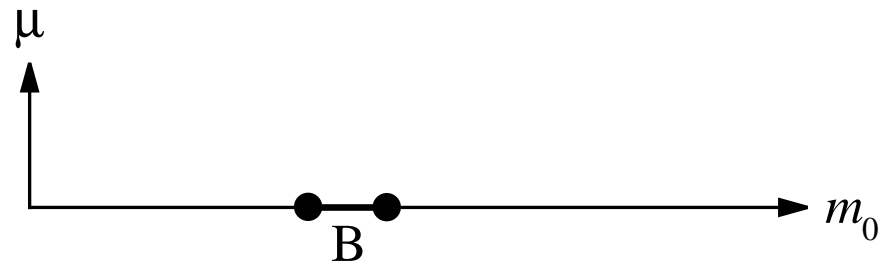


from F. Farchioni et al., Eur. Phys. J. C42 (2005) 73-87
(DBW2 action)

Scenarios at $\mu > 0$:

$$c_2 > 0$$

Aoki scenario:

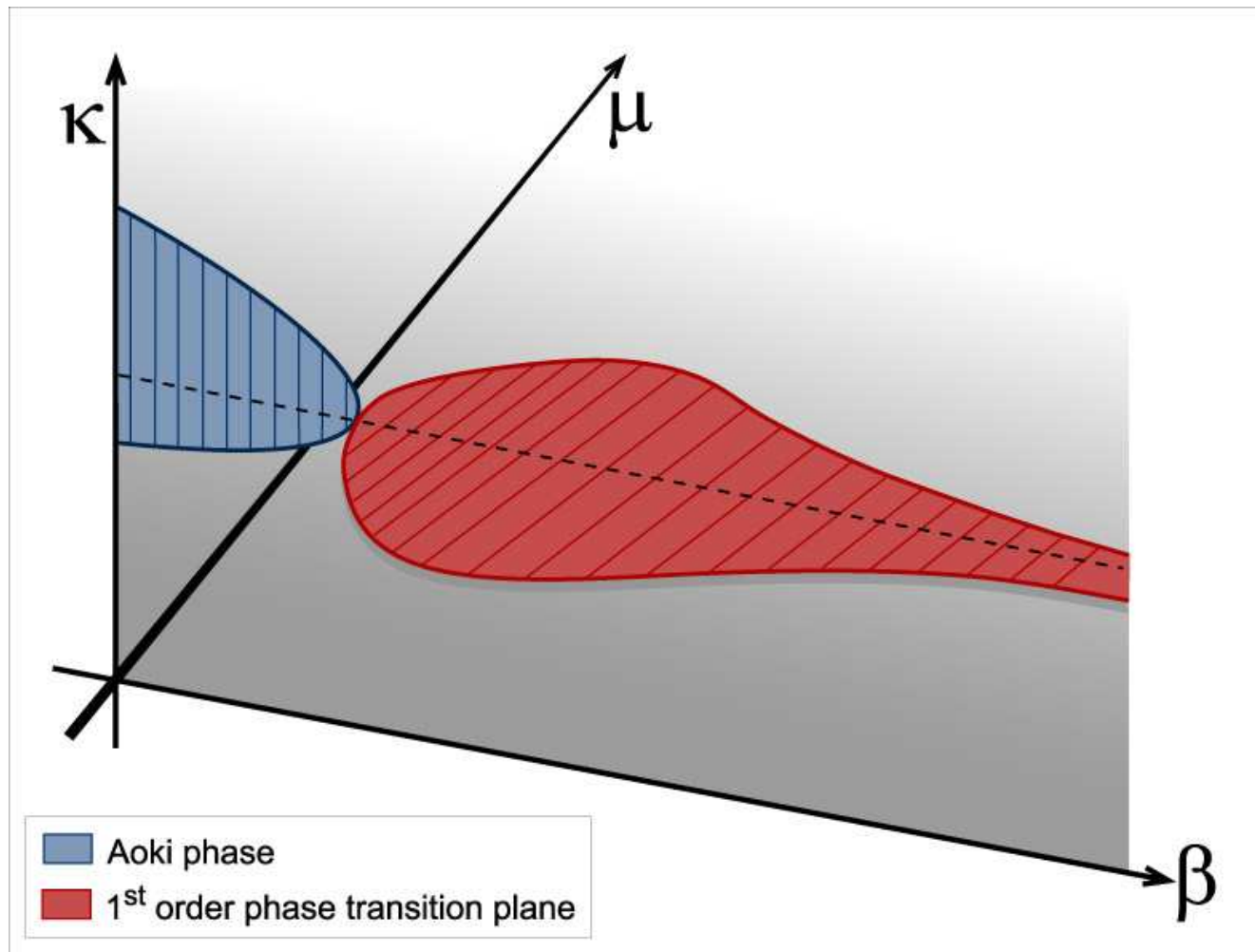


The crucial parameter c_2 depends on g^2 , action

Monte Carlo calculations

Müller-Preußker et al.: large $g^2 \leftrightarrow$ Aoki scenario

QCDTM (Montvay, Farchioni, Jansen et al.): small $g^2 \leftrightarrow$ normal scenario



6. Chiral perturbation theory for twisted mass lattice QCD

Twisting of the mass term

$$\chi \rightarrow \chi(\omega) = 2B_0 m_q e^{-i\omega\tau_3}$$

shifted to the lattice term by chiral rotation

$$\rho \rightarrow \rho(\omega) = e^{i\omega\tau_3} \rho = e^{i\omega\tau_3} 2W_0 a$$

Vacuum \sim minimum of \mathcal{L}

at **non-vanishing pion field**

$$\tilde{\pi}_3 = F_0 \frac{W_0 a}{B_0 m_q} \sin \omega \left[1 - \frac{8\chi_0}{F_0^2} (4L_6 + 2L_8 - 2W_6 - W_8) \right] + \mathcal{O}(a^2)$$

Expansion around vacuum \rightarrow chiral perturbation theory

powers of $m_q \sim \chi$ (modified by logarithms) and

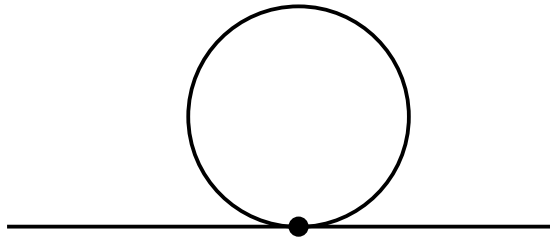
powers of a/m_q , to $\mathcal{O}(a^2)$

6.1 Pion mass

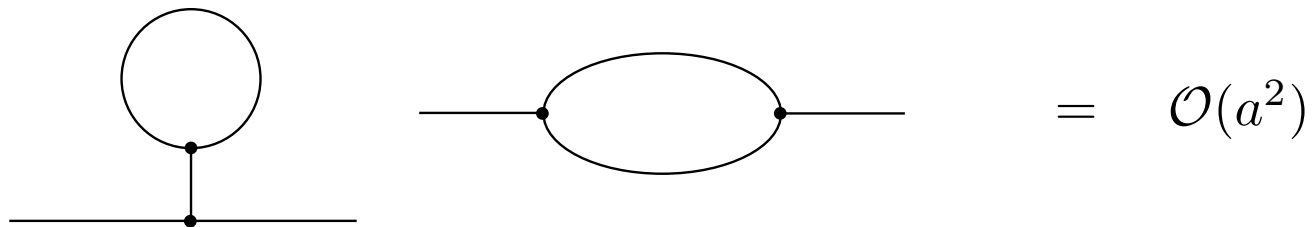
Expansion of \mathcal{L} in pion fields

$$\mathcal{L} = K \frac{1}{2} \{ (\partial_\mu \pi_a) (\partial_\mu \pi_a) + m_\pi^2(\text{tree}) \pi_a \pi_a \} + \dots$$

Loop contributions to the pion propagator from the LO vertices



New vertices from shifted vacuum yield



Result:

$$\begin{aligned} m_\pi^2 &= \chi_0 + \rho_0 + 8 \frac{\chi_0^2}{F_0^2} (4L_6^r + 2L_8^r - 2L_4^r - L_5^r) \\ &\quad + 8 \frac{\chi_0 \rho_0}{F_0^2} (4W_6^r + 2W_8^r - 2W_4^r - W_5^r - 2L_4^r - L_5^r) \\ &\quad + \frac{(\chi_0 + \rho_0)^2}{32\pi^2 F_0^2} \ln \left(\frac{\chi_0 + \rho_0}{\Lambda^2} \right) + \mathcal{O}(a^2) \end{aligned}$$

where

$$\chi_0 = 2B_0 m_q, \quad \rho_0 = 2W_0 a \cos \omega$$

L_k^r, W_k^r : renormalized chiral parameters, Λ = renormalization scale

Dependence on ω : factor $\cos \omega$ (only at $\mathcal{O}(a)$)

Maximal twist, $\omega = \pi/2$ \rightarrow vanishing lattice artifacts, cp. Frezzotti, Rossi

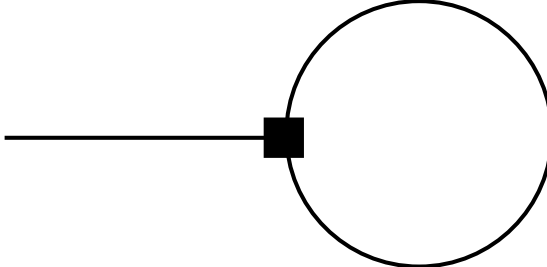
6.2 Pion decay constant

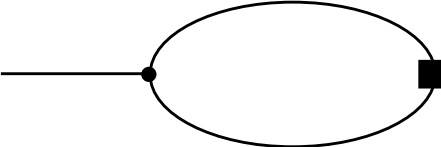
F_π given by $\langle 0 | J_A^{\mu,a} | \pi_b(p) \rangle = iF_\pi p^\mu \delta_{ab}$

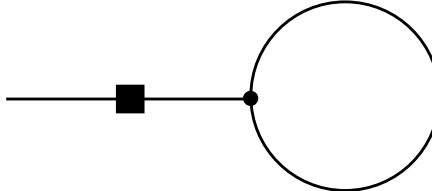
Axial current $J_A^{\mu,a}$: Noether procedure \rightarrow expression in powers of pion fields

Contributions:

tree level: 

loop correction: 

loop corrections at $\mathcal{O}(a^2)$: 



Wave function renormalization:



Result:

$$F_\pi = F_0 \left(1 + \frac{4}{F_0^2} [\chi_0 (2L_4^r + L_5^r) + \rho_0 (2W_4^r + W_5^r)] - \frac{1}{16\pi^2 F_0^2} \left[(\chi_0 + \rho_0) \ln \frac{\chi_0 + \rho_0}{\Lambda^2} \right] \right) + \mathcal{O}(a^2)$$

$$\chi_0 = 2B_0 m_q, \quad \rho_0 = 2W_0 a \cos \omega$$

6.3 Nondegenerate quark masses

G.M., T. Sudmann, JHEP 08 (2006) 085. hep-lat/0603019

a) $N_f = 2, \quad m_u \neq m_d$

Mass term $M = (m_d + m_u)\mathbf{1} + (m_d - m_u)\tau_1$

$$M(\omega) = e^{i\omega\gamma_5\tau_3/2} M e^{i\omega\gamma_5\tau_3/2}$$

b) $N_f = 3, \quad m_u = m_d \neq m_s$

$m_\pi^2, m_K^2, m_\eta^2, F_\pi, F_K, F_\eta$ in chiral perturbation theory

7. Monte Carlo calculations

European Twisted Mass Collaboration

Quenched and unquenched calculations

Phase structure, spectrum, scaling, fits to chiral perturbation theory

Algorithms

improved HMC (Urbach, Jansen, Shindler, Wenger)

PHMC with stochastic correction (Montvay, Scholz)

twisted mass removes small eigenvalues from the fermion matrix

algorithmically favourable: safer and faster

Simulations with $N_f = 2$

improved gauge actions

$(1 - 8b_1)$ (plaquette) + b_1 (double plaquette)

DBW2: $b_1 = -1.4088$

tlSym = tree level Symanzik improved: $b_1 = -\frac{1}{12}$

decrease minimal pion mass $\leftrightarrow \mu_c$

DBW2 action

F. Farchioni et al., Eur. Phys. J. C 47 (2006) 453, hep-lat/0512017

$12^3 \cdot 24$, $a \approx 0.19$ fm, $16^3 \cdot 32$, $a \approx 0.12$ fm,

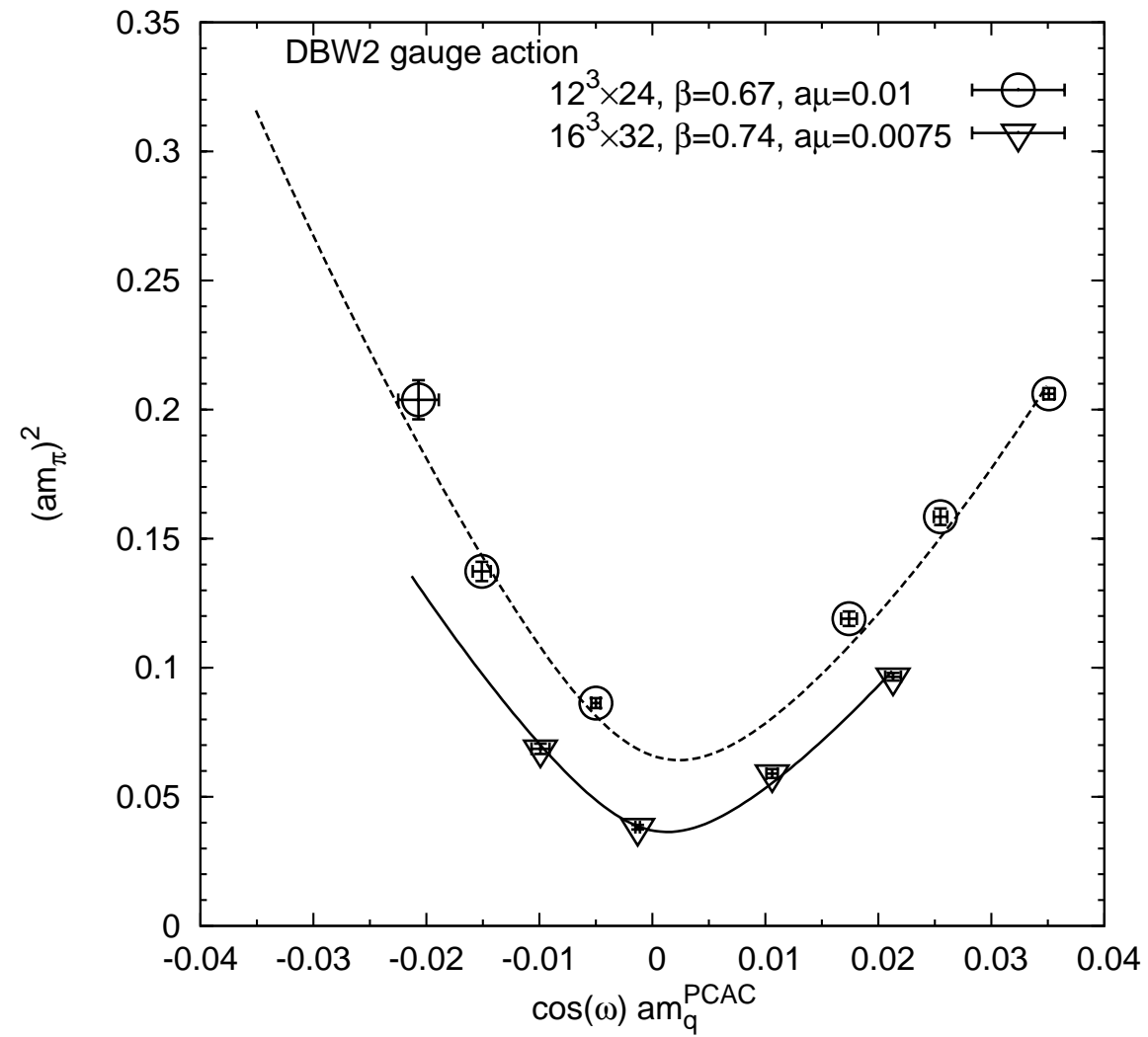
$\mu \approx 11$ MeV

minimal $m_\pi = 320$ MeV

determine m_c : $m_{\text{PCAC}} = 0$

observables: m_π , F_π , G_π , m_{PCAC} , pion mass splitting, ...

Fits to chiral perturbation theory, e.g.:



Estimates of low-energy constants:

$$70 \text{ MeV} \leq F_0 \leq 85 \text{ MeV}$$

$$2.9 \text{ GeV} \leq B \leq 3.5 \text{ GeV}$$

$$4.0 \leq \Lambda_3/F_0 \leq 8.0$$

$$16.0 \leq \Lambda_4/F_0 \leq 19.0$$

phenomenological values (S. Dürr):

$$F_0 \approx 86 \text{ MeV}$$

$$2.3 \leq \Lambda_3/F_0 \leq 23.3$$

$$9.3 \leq \Lambda_4/F_0 \leq 22.1$$

$$\Lambda_3 = 4\pi F_0 \exp(128\pi^2(2L_4 + L_5 - 4L_6 - 2L_8))$$

$$\Lambda_4 = 4\pi F_0 \exp(32\pi^2(2L_4 + L_5))$$

Projects

$N_f = 2$, tlSym gauge action

$24^3 \cdot 48$, $32^3 \cdot 64$

m_π down to 280 MeV

$N_f = 2 + 1 + 1$