Phase Structure of Wilson-Twisted-Mass-Lattice-QCD with three Quark Flavours by Means of Chiral Perturbation Theory

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QCD-Lagrangian

QCD is the gauge theory of strong interaction with colour SU(3) as underlying gauge group.

QCD-Lagrangian

$$\mathcal{L}_{QCD} = \sum_f \bar{q}_f \left(i\gamma^\mu D_\mu - m_f \right) q_f - \frac{1}{4} F_{\mu\nu,a} F_a^{\mu\nu}$$

Covariant derivative and field strength tensor

$$D_\mu = \partial_\mu - ig \sum_{a=1}^{8} \frac{\lambda_a}{2} A_{\mu,a}$$

$$F_{\mu\nu,a} = \partial_\mu A_{\nu,a} - \partial_\nu A_{\mu,a} + g f_{abc} A_{\mu,b} A_{\nu,c}$$

- q_f: quark fields
- D_μ: covariant derivative
- $A_{\mu,a}$: gauge fields
- g: coupling constant
- $F_{\mu\nu,a}$: field strength tensor
- m_f: quark mass

QCD-Lagrangian in the chiral limit

two groups of quark flavours:

$$\begin{pmatrix} m_u = 0.005\,GeV \\ m_d = 0.009\,GeV \\ m_s = 0.175\,GeV \end{pmatrix} \ll 1\,GeV \leq \begin{pmatrix} m_c = (1.15 - 1.35)\,GeV \\ m_b = (4.0 - 4.4)\,GeV \\ m_t = 174\,GeV \end{pmatrix}$$

low energy QCD:

- restriction to light quarks q_u, q_d and q_s
- chiral limit $m_u, m_d, m_s \to 0$
  $\Rightarrow SU(3)_L \times SU(3)_R \times U(1)_V$

QCD-Lagrangian in the chiral limit

$$\mathcal{L}_{QCD} = \sum_{f=u,d,s} \left(\bar{q}_{R,f} i\gamma^\mu D_\mu q_{R,f} + \bar{q}_{L,f} i\gamma^\mu D_\mu q_{L,f} \right) - \frac{1}{4} F_{\mu\nu,a} F_a^{\mu\nu}$$

- non-zero quark masses: $\mathcal{L}_M = -\bar{q}Mq = -\bar{q}_R M q_L - \bar{q}_L M q_R$
  result in an explicit breaking of the chiral symmetries

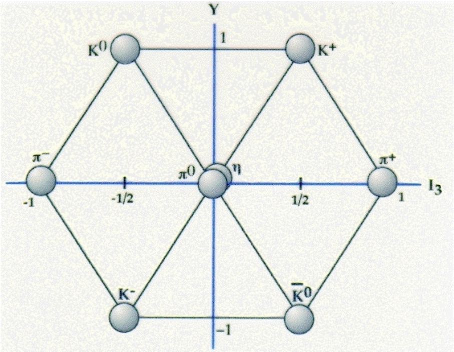
Symmetry breaking in QCD

Spontaneous symmetry breaking in QCD in the chiral limit

ground state of QCD is necessarily invariant under $SU(3)_V \times U(1)_V$

Vafa and Witten (1984)

- $SU(3)_A$ is not a symmetry of the ground state
  $\longrightarrow$ symmetry spontaneously broken
- 8 Goldstone-Bosones have to exist
- explicit breaking of symmetry due to the mass
  $\longrightarrow$ Goldstone-Bosones gain mass
- the pseudo scalar mesons are candidates for these Goldstone-Bosones



Lattice-QCD - Wilson action and Symanzik action

Wilson action

$$S_{Wilson} = a^4 \sum_x \bar{\psi}(x)(D_W + m_0)\psi(x) + \frac{1}{g_0^2} \sum_p Tr[1 - U(p)]$$

$$D_W = \frac{1}{2}\left[\gamma_\mu \left(\nabla_\mu^* + \nabla_\mu\right) - a\nabla_\mu^*\nabla_\mu\right]$$

- Wilson-Term breaks chiral symmetry explicitly

Symanzik effective action

$$S = S_0 + aS_1 + a^2 S_2 + \cdots . \qquad S_k = \int d^4x \mathcal{L}_k(x)$$

Improved lattice action

$$S_{imp} = S_{Wilson} + a^5 \sum_x c_{SW} \bar{\psi} \sigma_{\mu\nu} \hat{F}_{\mu\nu} \psi$$

Effective lattice action

$$S = S_0 + a c_{SW} \bar{\psi} \sigma_{\mu\nu} F_{\mu\nu} \psi$$

- $\mathcal{O}(a)$ term breaks chiral symmetry as well as the mass term

Twisted Mass QCD

- Twisted Mass in the continuum preserves physics

$$\mathcal{L}_{QCD,m} = \bar{\chi} M \mathrm{e}^{\mathrm{i}\omega\gamma_5\tau^3} \chi = \bar{\chi}(\tilde{m} + \mathrm{i}\gamma_5\mu)\chi = \bar{\psi} M \psi$$

Wilson Twisted Mass

$$S_F^{tw} = a^4 \sum_x \bar{\chi}(x) \left(\frac{1}{2} \left(\gamma_\mu \left(\nabla_\mu^* + \nabla_\mu \right) - ar \nabla_\mu^* \nabla_\mu \right) + m_0 \mathrm{e}^{\mathrm{i}\omega\gamma_5\tau^3} \right) \chi(x)$$

$$S_F^{ph} = a^4 \sum_x \bar{\psi}(x) \left(\frac{1}{2} \left(\gamma_\mu \left(\nabla_\mu^* + \nabla_\mu \right) - ar \nabla_\mu^* \nabla_\mu \mathrm{e}^{-\mathrm{i}\omega\gamma_5\tau^3} \right) + m_0 \right) \psi(x)$$

- Wilson term is not invariant under axial flavour transformations

Advantages of tmQCD

- a twist of $\omega = \frac{\pi}{2}$ results in an automatic $\mathcal{O}(a)$ improvement
- tmQCD avoids quark zero modes of the Wilson-Dirac operator

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Chiral Perturbation Theory

Effective field theory for QCD at low energies

- the effective Lagrangian is expressed in terms of hadronic degrees of freedom
- at low energies these are the members of the pseudoscalar octet (π, K, η)
- they are regarded as the Goldstone bosons of the spontaneous breaking of the chiral $SU(3)_L \times SU(3)_R$ symmetry down to $SU(3)_V$
- the explicit symmetry breaking by the mass term in QCD is related to the masses of light pseudoscalars in the "real" world
- in addition to the mass term, Pauli-Term also breaks chiral symmetry.

Transformation properties of the Goldstone bosons

- $\vec{\Pi}$ Goldstone fields
- symmetry group of the Lagrangian G and of the ground state H:

$$G = \mathrm{SU}(3)_L \times \mathrm{SU}(3)_R = \{(L,R) | L \in \mathrm{SU}(3)_L, R \in \mathrm{SU}(3)_R\}$$
$$H = \{(V,V) | V \in \mathrm{SU}(3)_V\} \cong \mathrm{SU}(3)_V$$

- definition: left coset of H: $gH = \{gh | h \in H\}$
- element $\tilde{g} = (\tilde{L}, \tilde{R}) \in G$
- left coset $\tilde{g}H = (\tilde{L}V, \tilde{R}V)$ is isomorphic to one $\vec{\Pi}$
- $\tilde{g}H$ is uniquely characterized through the SU(3) matrix $U = \tilde{R}\tilde{L}^\dagger$

$$(\tilde{L}V, \tilde{R}V) = (\tilde{L}V, \tilde{R}\tilde{L}^\dagger\tilde{L}V) = (1, \tilde{R}\tilde{L}^\dagger)\underbrace{(\tilde{L}V, \tilde{L}V)}_{\in H} \quad \Rightarrow \quad \tilde{g}H = (1, \underbrace{\tilde{R}\tilde{L}^\dagger}_{=U})H$$

Transformation behavior of U

$$g\tilde{g}H = (L, R\tilde{R}\tilde{L}^\dagger)H = (1, R\tilde{R}\tilde{L}^\dagger L^\dagger)(L,L)H = (1, R(\tilde{R}\tilde{L}^\dagger)L^\dagger)H$$

$$U' \mapsto RUL^\dagger$$

Exponential parameterization of U

Matrix U

$$U(x) = exp\left(i\frac{\phi(x)}{F_0}\right)$$

$$\phi(x) = \sum_{a=1}^{8} \lambda_a \phi_a \equiv \begin{pmatrix} \pi^0 + \frac{1}{\sqrt{3}}\eta & \sqrt{2}\pi^+ & \sqrt{2}K^+ \\ \sqrt{2}\pi^- & -\pi^0 + \frac{1}{\sqrt{3}}\eta & \sqrt{2}K^0 \\ \sqrt{2}K^- & \sqrt{2}\bar{K}^0 & -\frac{2}{\sqrt{3}}\eta \end{pmatrix}$$

The result for $N_f = 2$ reads:

$$\phi(x) = \sum_{i=}^{3} \tau_i \phi_i \equiv \begin{pmatrix} \pi^0 & \sqrt{2}\pi^+ \\ \sqrt{2}\pi^- & -\pi^0 \end{pmatrix}$$

- transformation behavior of the ground state $U_0 = 1$:

$$VU_0V^\dagger = VV^\dagger = 1 = U_0$$

$$AU_0A = AA \neq U_0$$

Weinberg's Power Counting Scheme

Steven Weinberg:
Phenomenological Lagrangians (1979)

"...if one writes down the most general possible Lagrangian, including all terms consistent with assumed symmetry principles, and then calculates matrix elements [...], the result will simply be the most general possible S-matrix consistent with analyticity, perturbative unitarity, cluster decomposition and the assumed symmetry principles."

$\longrightarrow$ dynamics of the Goldstone bosons is organized as a string of terms:

$$\mathcal{L} = \mathcal{L}_2 + \mathcal{L}_4 + \mathcal{L}_6 + \cdots$$

expanding parameters are:

- quark mass m_0
- lattice parameter a
- momenta p^2

$$\text{LO:} \quad \mathcal{L}_2 \sim \mathcal{O}(p^2, m, a)$$

$$\text{NLO:} \quad \mathcal{L}_4 \sim \mathcal{O}(p^4, m^2, a^2, am, p^2 m)$$

Construction of the chiral Lagrangian

invariant terms of invariant objects (building blocks: A, B, C,...) are of the form:

$$\text{LO:} \quad \mathrm{Tr}(AB^\dagger) \qquad \text{NLO:} \quad \mathrm{Tr}(AB^\dagger CD^\dagger), \quad Tr(AB^\dagger)Tr(CD^\dagger), \quad \ldots$$

building blocks:

- matrix U and $\partial_\mu U$ are invariant objects:

$$U \mapsto RUL^\dagger$$
$$\partial_\mu U \mapsto R\partial_\mu UL^\dagger$$

- not invariant objects, using spurion analysis:

$$\text{mass:} \quad \chi \mapsto R\chi L^\dagger$$
$$\text{discretization errors:} \quad ac_{SW} \sim A \mapsto RAL^\dagger$$

Possible non-zero or non-constant terms up to $\mathcal{O}(p^2)$

$$\mathrm{Tr}[\partial_\mu U(\partial^\mu U)^\dagger], \quad \mathrm{Tr}(\chi U^\dagger), \quad \mathrm{Tr}(U\chi^\dagger), \quad \mathrm{Tr}(AU^\dagger), \quad \mathrm{Tr}(UA^\dagger)$$

LO chiral Lagrangian and Twisted-Mass

with

$$\chi = 2B_0 M, \qquad M = \mathrm{diag}(m_u, m_d, m_s), \qquad A = \rho = 2W_0 a\mathbf{1}$$

LO chiral Lagrangian for WχPT

$$\mathcal{L}_2 = \frac{F_0^2}{4}\left\langle \partial_\mu U \partial^\mu U^\dagger \right\rangle - \frac{F_0^2}{4}\left\langle \chi U^\dagger + U\chi^\dagger \right\rangle - \frac{F_0^2}{4}\left\langle \rho U^\dagger + U\rho^\dagger \right\rangle .$$

next-to-leading order (NLO):

- up to $\mathcal{O}(p^4)$
- 16 additional terms with 16 Low-Energy-Constants L_i, W_i, W_i'

---

with a twist of the mass Term ($m_u = m_d = m_q \neq m_s$):

$$\mathrm{N}_f = 2: \quad \chi \mapsto \chi(\omega) = 2B_0 m_q \mathrm{e}^{-\mathrm{i}\omega\tau_3} = \tilde{\chi}\mathbf{1} + \mathrm{i}\chi_3' \tau_3$$

$$\mathrm{N}_f = 3: \quad \chi \mapsto \chi(\omega) = \chi e^{-\mathrm{i}\omega\lambda_3} = 2B_0(\mathrm{diag}(\tilde{m}, \tilde{m}, m_s) - \mathrm{i}\mu\lambda_3)$$

Potential in NLO

$$
\begin{aligned}
V(U) = &-\frac{F_0^2}{4}\left\langle \chi U^\dagger + U\chi^\dagger \right\rangle - \frac{F_0^2}{4}\left\langle \rho U^\dagger + U\rho^\dagger \right\rangle \\
&- L_6 \left\langle \chi U^\dagger + U\chi^\dagger \right\rangle^2 - W_6 \left\langle \chi U^\dagger + U\chi^\dagger \right\rangle \left\langle \rho^\dagger U + U^\dagger \rho \right\rangle \\
&- W_6' \left\langle \rho^\dagger U + U^\dagger \rho \right\rangle^2 - L_7 \left\langle \chi U^\dagger - U\chi^\dagger \right\rangle^2 \\
&- W_7 \left\langle \chi U^\dagger - U\chi^\dagger \right\rangle \left\langle \rho^\dagger U - U^\dagger \rho \right\rangle - W_7' \left\langle \rho^\dagger U - U^\dagger \rho \right\rangle^2 \\
&- L_8 \left\langle \chi^\dagger U \chi^\dagger U + U^\dagger \chi U^\dagger \chi \right\rangle - W_8 \left\langle \rho^\dagger U \chi^\dagger U + U^\dagger \rho U^\dagger \chi \right\rangle \\
&- W_8' \left\langle \rho^\dagger U \rho^\dagger U + U^\dagger \rho U^\dagger \rho \right\rangle
\end{aligned}
$$

$$
L_i \sim \mathcal{O}(m^2), \qquad W_i \sim \mathcal{O}(am), \qquad W_i' \sim \mathcal{O}(a^2)
$$

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Potential of two flavour χPT

direction of the vacuum: τ_3

$$\Rightarrow U = e^{i\omega_3\tau_3} = \begin{pmatrix} \cos\omega_3 - i\sin\omega_3 & 0 \\ 0 & \cos\omega_3 + i\sin\omega_3 . \end{pmatrix}$$

choose parameterization:

$$U = u_0 \mathbf{1} + i u_3 \tau_3 \quad \Rightarrow \quad \boxed{u_0 = \cos\omega_3, \quad u_3 = \sin\omega_3}$$

Potential in NLO

$$V(u_0, u_3) = -c_1 u_0 + c_2 u_0^2 + c_3 u_3 + c_4 u_3^2 + c_5 u_0 u_3 + L_{const}.$$

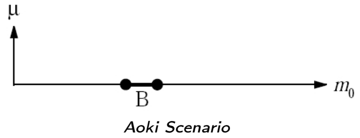
$$c_1 = 2F_0^2(B_0 m_{q0} + W_0 a) = 2F_0^2 B_0 m_0' \propto \tilde{m}', \qquad c_3 = 2F_0^2 B_0 \mu \propto \mu$$

- restrict discussion to $V(u_0, u_3) = -c_1 u_0 + c_2 u_0^2 + c_3 u_3$
- c_1 is proportional to the shifted u- and d-quark mass $\tilde{m}'$
- c_3 is proportional to the twisted mass μ
- sign of c_2 is not known - two possible scenarios

Aoki scenario, $c_2 < 0$

A. Twisted mass $\mu = 0$

- $V(u_0) = -c_1 u_0 + c_2 u_0^2$
- minimum at $\epsilon = \frac{c_1}{2|c_2|}$



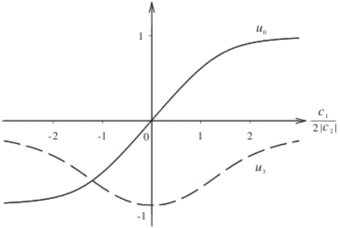
1. $|\epsilon| > 1$

- minimum at:
  $\tilde{m}' > 0: \quad u_0 = 1, \quad U = \mathbf{1}$
  $\tilde{m}' < 0: \quad u_0 = -1, \; U = -\mathbf{1}$
- symmetry of the ground state: $SU(2)_V$
- Pion masses:
  $m_\pi^2 = \frac{1}{F_0^2}(|c_1| - 2c_2)$

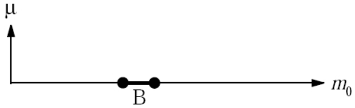
2. $|\epsilon| < 1$

- minimum at: $u_0 = \epsilon$ and $u_3 = \sqrt{1-\epsilon^2}$
- symmetry spontaneously broken to U(1) $\rightarrow$ Aoki phase
- non-vanishing u_3 corresponds to $\langle \bar{\chi}\gamma_5\tau_3\chi \rangle \neq 0$
- π_1, π_2 massless,
  $m_{\pi_3}^2 = \frac{2c_2}{F_0^2}(1-\epsilon^2)$

Aoki scenario, $c_2 < 0$



Aoki Scenario



Aoki Scenario

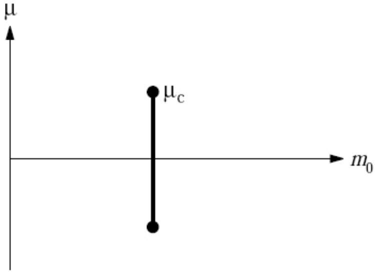
B. Twisted mass $\mu \neq 0$, positive

- $V(u_0, u_3) = -c_1 u_0 + c_2 u_0^2 + c_3 u_3$
- shift of the minimum in τ_3 direction
- SU(2) symmetry explicitly broken
- all pions are massive
- u_0 changes continuously
- u_3 jumps crossing the Aoki phase
- for $\mu \neq 0$ no phase transition

Normal scenario, $c_2 > 0$

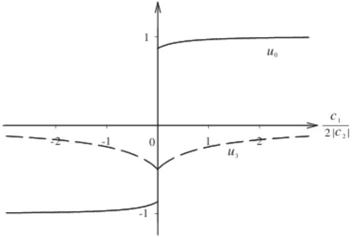
A. Twisted mass $\mu = 0$

- $V(u_0) = -c_1 u_0 + c_2 u_0^2$
- minimum at: $u_0 = 1$ for $\tilde{m}' > 0$
  $u_0 = -1$ for $\tilde{m}' < 0$
- $\tilde{m}' = 0 \to u_0$ jumps from +1 to -1
- SU(2), pion masses are non-zero



B. Twisted mass $\mu \neq 0$

- $V(u_0, u_3) = -c_1 u_0 + c_2 u_0^2 + u_3 c_3$
- minimum at: $|u_0| < 1$ and $u_3 \neq 0$
- SU(2) symmetry explicitly broken
- for $\tilde{m}' = 0$ and $\mu_c < \frac{|c_2|}{F_0^2 B_0} \sim a^2$ jumps u_0
- all pions are massive



normal scenario

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Ground state for $N_f = 3$

minimum may have components in λ_3 and λ_8 direction:

ground state for $N_f = 3$

$$U = \mathrm{e}^{\mathrm{i}(\phi_3\lambda_3 + \phi_8\lambda_8)}$$

$$= \begin{pmatrix} \cos(\phi_3 - \phi_8) - \mathrm{i}\sin(\phi_3 - \phi_8) & 0 & 0 \\ 0 & \cos(\phi_3 + \phi_8) + \mathrm{i}\sin(\phi_3 + \phi_8) & 0 \\ 0 & 0 & \cos(2\phi_8) - \mathrm{i}\sin(2\phi_8) \end{pmatrix}$$

$$\Rightarrow \quad \boxed{U = u_0 \mathbf{1} + \mathrm{i}(u_3\lambda_3 + u_8\lambda_8)}$$

- potential too complicated $\rightarrow$ choose a different parameterization

New Parameterization

$$U = \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix} = \begin{pmatrix} a_1 + \mathrm{i}a_2 & 0 & 0 \\ 0 & b_1 + \mathrm{i}b_2 & 0 \\ 0 & 0 & c_1 + \mathrm{i}c_2 \end{pmatrix}$$

Potential in terms of the parameters *a*, *b*, *c*

- $a_2 = u\sqrt{1-a_1^2}, \qquad b_2 = v\sqrt{1-b_1^2}, \qquad c_2 = w\sqrt{1-c_1^2}$
  $c_1 = -a_2 b_2 + a_1 b_1$
- ambiguity of the signs: $|u| = |v| = |w| = 1$

$$\boxed{V(a_1,a_2,b_1,b_2,c_1,c_2) = V(a_1,b_1,u,v,w)}$$

Full potential in NLO

$$\begin{aligned}
V(a,b,c) = {} & A(\tilde{m}')(a_1+b_1) + A_c(m_s')c_1 + B(\tilde{m}',\mu)(a_1^2+b_1^2) + B_c(m_s')c_1^2 \\
& + C(\tilde{m}',\mu)a_1 b_1 + C_c(\tilde{m}',m_s')(a_1+b_1)c_1 + D(\mu)(a_2-b_2) \\
& + E(\tilde{m}',\mu)a_1 a_2 + F(\tilde{m}',\mu)a_2 b_1 + F_c(m_s',\mu)c_1(a_2-b_2) \\
& + G(\tilde{m}',\mu)a_1 b_2 + G_c(m_s',\mu)c_2(a_1-b_1) + H(\tilde{m}',\mu)b_1 b_2 \\
& + J(\tilde{m}',\mu)a_2 b_2 + J_c(\tilde{m}',m_s')c_2(a_2+b_2) + Const.
\end{aligned}$$

Approximation of $V(a,b,c)$

- $V(a,b,c)$ depends on 3 known and 6 unknown LECs
- approximation for small masses cancels 6 terms
- shift of the masses by $\rho_0 \sim a$

$$\chi_0' = \chi_0 + \rho_0 = 2B_0 \tilde{m}'$$
$$\chi_s' = \chi_s + \rho_0 = 2B_0 m_s'$$

- standardization with $F_0^2 B_0$

Potential for small masses

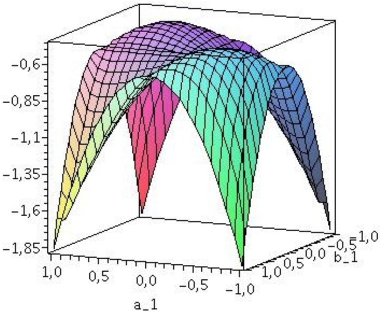
$$V(a,b,c) = -\tilde{m}'(a_1 + b_1) - m_s' c_1 + \mu(a_2 - b_2) - K_0(a_1^2 + b_1^2) - K_0 c_1^2 - 2K_1 a_1 b_1 - 2K_1(a_1 + b_1)c_1 + 2K_2 a_2 b_2 + 2K_2 c_2(a_2 + b_2)$$

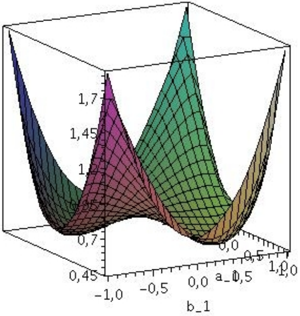
$$K_0 \sim 2K_1 \sim 2K_2 = 4X_{LW} \frac{\rho_0^2}{F_0^2 B_0} \sim a^2$$

Restriction to the predominant constant K_0

potential for $K_1 = K_2 = 0$

$$V(a_1,b_1,u,v) = -\tilde{m}'(a_1+b_1) - m_s'(-uv\sqrt{1-a_1^2}\sqrt{1-b_1^2} + a_1 b_1) + \mu(u\sqrt{1-a^2} - v\sqrt{1-b_1^2}) - K_0(a_1^2+b_1^2) - K_0(-uv\sqrt{1-a_1^2}\sqrt{1-b_1^2} + a_1 b_1)^2$$

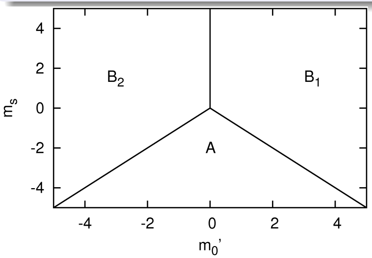




1.a: Potential with $K_0 > 0$, $\mu = 0$

B_1: $U = \mathrm{diag}(1,\ 1,\ 1)$

B_2: $U = \mathrm{diag}(-1,\ -1,\ 1)$



A: $U = \mathrm{diag}(-1,\ 1,\ -1)$ and $U = \mathrm{diag}(1,\ -1,\ -1)$

- border to B: $|\tilde{m}'| = |m_s'|$
- no jump in A for $\tilde{m}' = 0$

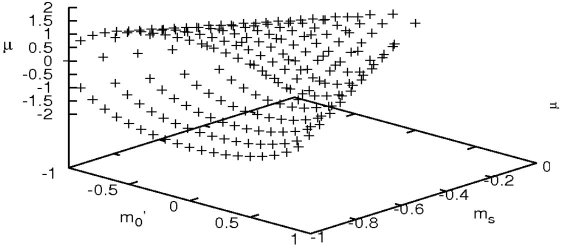
1.b: Potential with $K_0 > 0$, $\mu \neq 0$

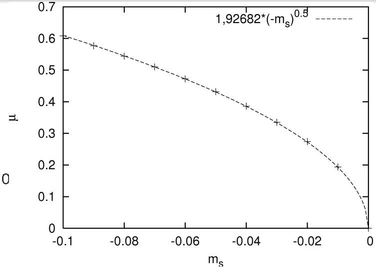
behavior for $\mu \neq 0$

- $\mu \neq 0$ shifts minimum away from $|a| = |b| = |c| = 1$
- jump of the minimum from B_1 to B_2 for $\tilde{m}' = 0$ vanishes for

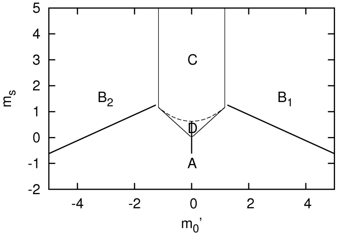
$$|\mu_c| = 2K_0$$

- variation of μ leads to a jump from A to B





2.a: Potential with $K_0 < 0$, $\mu = 0$

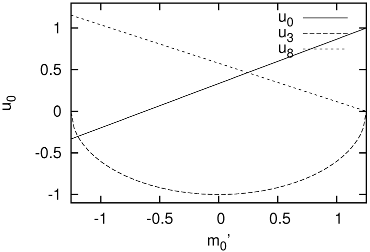


A, B_1 and B_2

- B_1: $U = \mathrm{diag}(1,\,1,\,1)$
  B_2: $U = \mathrm{diag}(-1,\,-1,\,1)$
- A: one minimum at $a_1 = b_1$ $(u = v)$ jump for $m_s' > K_0$
- border A to B_1 and B_2: $m_s' = \pm\frac{1}{2}\tilde{m}' - 3K_0$

C and D

- C: one minimum at $a_1 = b_1$ $(u = -v)$
- D: two minima $|a_1| \neq |b_1|$
- border C and D to B: $m_s' = |\tilde{m}'|$
- jump of the minimum at $\tilde{m}' = 0$ for $m_s' < |K_0|$



behavior of u_i in sector C

2.b: Potential with $K_0 < 0$, $\mu \neq 0$

behavior for $\mu \neq 0$

- $\mu \neq 0$ shifts minimum away from $|a| = |b|$ (sectors A,B,C)
- jump of the minimum at $\mu = 0$ (sectors A,C,D)
- jump of the minimum at $\mu \neq 0$ (sectors A,D)
- jump for $\tilde{m}' = 0$ by $m'_s < 0$ and $\mu \neq 0$ (sector A)