The finite-T phase structure of lattice QCD with twisted-mass Wilson fermions

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EMMI Workshop, St. Goar, August 31 – September 3, 2009

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Reference:

- E.-M. I., K. Jansen, M.-P. Lombardo, M. Müller-Preussker,
- M. Petschlies, O. Philipsen, L. Zeidlewicz, arXiv:0905.3112.

1. Motivation

Why Wilson fermions ?

- advantages/disadvantages
 - + locality satisfied
 - + almost competing algorithms developed
 - chiral symmetry explicitely broken, subtle chiral behavior
 - complicated phase structure, both at $T=\mathbf{0}$ and finite T
 - continuum limit slow
 - + the latter can be cured by improvement

Phases of Wilson fermions: early lattice results



For $N_f = 2$ Wilson fermions apparently compatible with O(4) scaling (cf. F. Karsch's talk).

Main arguments for the twisted-mass approach

- Prevents the occurrence of small eigenvalues of the Dirac operator by lifting eigenvalues, also zero modes. (Gattringer, Solbrig 2005).
- This should allow to work at smaller quark masses.
- With the hopping parameter κ tuned to its critical value κ_c(β) ("maximal twist"), the twisted-mass term behaves as a conventional quark mass.
- In this case automatic O(a) improvement is guaranteed (See Farchioni et al. '05, Urbach '07).

Goal of the tmfT collaboration: Extensive study of the phase diagram of tmQCD in the (κ,β,μ_0) -space at non-zero temperature – a prerequisite for QCD finite-T simulations at maximal twist. **Price to pay:** A 3-dimensional phase diagram with a complicated structure due to $O(a^2)$ parity/flavor violating effects.

2. Set-up

The gauge action :

$$S_G = \beta \sum_x \left[c_0 \sum_{\mu < \nu} \left(1 - \frac{1}{3} \operatorname{Re} \operatorname{Tr} U_{x\mu\nu}^{1 \times 1} \right) + c_1 \sum_{\mu \neq \nu} \left(1 - \frac{1}{3} \operatorname{Re} \operatorname{Tr} U_{x\mu\nu}^{1 \times 2} \right) \right]$$

tree-level Symanzik action with (inverse) gauge coupling $\beta = 6/g_0^2$, $c_1 = -1/12$ and $c_0 = 1-8$ c_1

The fermion action :

$$S_F = a^4 \sum_x \left\{ \overline{\psi}(x) \left[\left(D[U] + m_0 \right) \mathbb{I}_{2 \times 2} + i \ \mu \ \tau_3 \ \gamma_5 \right] \ \psi(x) \right\}$$

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

Wilson-Dirac fermion action with twisted-mass term for $N_f = 2$ light flavors (in the physical basis $\Psi = (u, d)$)

[Frezzotti, Grassi, Sint, Weisz 2001; Frezzotti, Rossi 2004]

• Hopping parameter κ and twisted mass μ_0 combine into a bare quark mass:

$$m_q = \sqrt{\frac{1}{4} \left(\frac{1}{\kappa} - \frac{1}{\kappa_c}\right)^2 + \mu_0^2} \tag{1}$$

- For maximal twist, i.e. κ = κ_c(β) (obtained at T = 0), automatic O(a) improvement is expected.
 (See Farchioni et al. '05, Urbach '07)
- HMC simulations were performed in a wide range $\beta = 1.80, \ldots, 3.90$ on various spatial lattice sizes $N_s = 16$ (24, 32) and $N_t = 8$.
- For $\mu_0 = 0$ and $N_t = 8$ the phase diagram clearly divides into three regions:

– the Aoki-Phase [Aoki '84] for strong coupling, i.e. at small β ,

– a bulk transition region at intermediate β ,

- and the thermal transition and scaling region at larger β .
- This phase structure is embedded in full (β, κ, μ_0) -space.

• As we will see, in the scaling region, according to eq. (1), the thermal transition forms a conical surface, eventually a closed ellipse in the (κ, μ_0) -plane at each β .

3. Anticipating the phase structure

Twisted mass - an irrelevant rotation in continuum, not so on the lattice !

An effective potential study for $T \neq 0$ [Creutz '07]

basic order parameter fields : $\sigma = \overline{\psi}\psi$ $\vec{\pi} = i\overline{\psi}\gamma_5\vec{\tau}\psi$

effective potential including lattice artifacts :

$$V(\vec{\pi},\sigma) = \lambda \left(\sigma^2 + \vec{\pi}^2 - v^2\right)^2 + c_1 \left(\frac{1}{\kappa} - \frac{1}{\kappa_c(\beta)}\right)\sigma + c_2\sigma^2 - \mu\pi_3$$

- λ : O(4) symmetric linear σ model
- c_1 : mass term (changing sign at $\kappa_c(\beta)$)
- c₂: chiral symmetry breaking lattice artifact (changing sign at some β)
- μ : the twisted-mass term

T = 0: Phase diagram for twisted-mass Wilson fermions.



A. Shindler, Phys. Rept. 461 (2008) 37

 $T \neq 0$



Standard view of the phase diagram for non-twisted Wilson fermions in the β - κ plane (cf. CP-PACS).



Schematic phase diagram for twisted-mass QCD in the β - κ - μ_0 space, basically as proposed by Creutz [Creutz '07].

Chiral effective action proposes a unified view of the phase diagram embedded in the β - κ - μ diagram. (Sharpe, Singleton, Creutz)

viewed in the κ - μ plane, going from low β to higher β [Creutz '07]



at low β : discontinuity in μ

at intermediate β : discontinuity in κ



deconfinement inside a disk around $\kappa_c(\beta)$ in the scaling region of β



Contour plots of $m_{\pi^{\pm}}^2$ in the twisted-mass plane (from NLO Lattice χPT) are locating the Aoki phase (left) and the first order bulk transition scenario (right).

4. Aoki phase

An example of an "unphysical phase pocket":

• An external "magnetic field" $h = 2 \kappa \mu_0 \Rightarrow$ induces spontaneous breaking of combined flavor-parity symmetry [Aoki 1984,1987] in some κ interval \Rightarrow order parameter $\lim_{\mu_0 \to 0} \lim_{V \to \infty} \langle \overline{\psi} i \gamma_5 \tau_3 \psi \rangle \neq 0$. (jumps

across $\mu_0 = 0$)

- No phase transition at $\mu_0 \neq 0$ (cf. Ising model at $H \neq 0$)
- Extrapolation to $\mu_0 = 0$ can be studied by Fisher plots. Based on an equation of state

$$h = A_0 \sigma^3 + A_1 (\kappa - \kappa_{c, \text{low}}) \sigma$$
⁽²⁾

with $\sigma = \langle \overline{\psi} i \gamma_5 \tau_3 \psi \rangle$, the would-be order parameter σ^2 is plotted vs. h/σ (requesting a positive intercept).

Evidence for the Aoki phase



 $\beta = 1.8$

 $\beta = 3.0$

 \implies Cusp of the Aoki phase extends at least to $(\beta, \kappa) = (3.0, 0.2035)$.

No evidence for the Aoki phase beyond $\beta = 3.4$



 \Rightarrow No signatures for Aoki phase exist any more for $\beta \geq 3.4$.

5. First order bulk transition

The Sharpe-Singleton scenario [Sharpe-Singleton, '98]

- At intermediate β metastabilities occur signalling a possible 1-st order transition. Represents a remnant of the bulk transition occurring at T = 0 [Münster '04].
- Visible in several observables at $\kappa_c(\beta; T = 0)$ and not too large μ_0 . Data obtained for $\mu_0 \simeq 0.007$, $\beta = 3.40, 3.45$.



Polyakov loop





Other observables go discontinuous



plaquette

Aoki order parameter



6. Thermal transition

- Observables: average plaquette, real part of the Polyakov loop (PL), the pion norm as well as their respective susceptibilities and integrated autocorrelation times.
- Our κ -scans at $\beta \in \{3.4, \ldots, 3.9\}$ and at fixed μ_0 reached statistics of $\mathcal{O}(10^4)$ HMC trajectories per point in the phase diagram.

Consider a κ -scan concentrating on κ above $\kappa_c(\beta)$ (the vertical lines mark $\kappa_c(\beta)$) :

Polyakov Loop :

with $\mu_0 = 0.0068$ for $\beta = 3.4, 3.45, 3.65$; with $\mu_0 = 0.005$ for $\beta = 3.75$. Polyakov Loop susceptibility :

with the same μ_0 values



 \implies At $\kappa > \kappa_c$ the cone is separated from the doubler range.

Next zooming into the cone around $\kappa_c(\beta)$:

(the vertical lines mark $\kappa_c(\beta)$)



The narrow cone itself (around $\kappa_c(\beta)$) can be resolved with large-statistics runs only.



0.164 0.1648 0.1656 0.1664 0.1627 0.1633 0.1639 0.1645

Fit the peaks $\beta = 3.75$, $\mu_0 = 0.005$ ($\kappa_c(3.75) = 0.166$, $m_\pi \simeq 400$ MeV, $r_0T \simeq 0.5$):





Polyakov Loop susceptibility

Pion norm

- ⇒ Polyakov Loop susceptibility and Pion norm separate the entrance from the exit transition
- \implies The lower transition is slightly below $\kappa_c(3.75)$.
- \implies The chiral and deconfinement signals are seen at the same κ .

Extension of the thermal cone ?

Polyakov Loop expectation values versus κ for $\beta = 3.75$ at various μ_0 :

0.013 0.011 $\mu_0 = 0.005$ LO formula 0.012 NLO formula? 0.01 $\gamma(\text{Re}(L))$ 0.011 0.009 0.01 0.009 Re(<L>) 0.008 04 0.008 0.007 0.007 0.006 0.006 0.005 0.005 0.004 0.003 0.004 0.165 0.166 0.167 0.168 0.165 0.1655 0.166 0.1665 0.167 0.1675 0.168 к к

Expected extension of the ellipse

in the $\kappa - \mu_0$ plane at $\beta = 3.75$:

 \implies No transition seen beyond $\mu_0 = 0.025$ for $\beta = 3.75$.

Adapting the lower and upper (entrance and exit) crossovers to chiral perturbation theory.

Higher order correction are important !

A closer fit of the cone shape:

- Strength and nature of the transition/crossover are subject to discretisation effects, i.e. depend on the twist angle ω . This leads to a distortion of the ellipse and conical shape.
- For sufficiently light quarks, lattice chiral perturbation theory can be applied. The NLO expression for the pion mass allows to estimate the parameters of the ellipse [Sharpe '04]:

$$m_{\pi^{\pm}}^{2} = M' + \frac{16}{f^{2}} \left((2L_{68} - L_{45})(M')^{2} + M'\hat{a}\cos(\omega)(2W - \tilde{W}) + 2\hat{a}^{2}\cos^{2}(\omega)W' \right) + \frac{(M')^{2}}{2\Lambda_{\chi}^{2}} \ln\left(\frac{M'}{\Lambda_{R}}\right).$$

Quark masses are renormalised, $\mu = Z_{\mu}\mu_{0}$, $m = Z_{m}(m_{0} - m_{c})$; $M' = \sqrt{\hat{\mu}^{2} + (\hat{m}')^{2}}$, $\hat{a} = 2W_{0}a$, $\hat{\mu} = 2B_{0}Z_{\mu}\mu_{0}$, $\hat{m}' = 2B_{0}Z_{m}(m_{0} - m_{c})$. The constants *B*'s, *W*'s, *L*'s can in principle be obtained from fits to lattice results at T = 0.

7. Feasibility of a β -scan at maximal twist

Again with $N_t=8$, however with large pion mass, $m_\pi\simeq 1~{
m GeV}$

Consider a β -scan at large π -mass (huge $\mu_0 = 0.040$) with $\kappa \simeq \kappa_c(\beta)$, i.e. at maximal twist :



 \implies Critical point at $\beta_t \simeq 3.88$ (corresponding to $T_c r_0 \simeq 0.66$) where it should be for this m_{π} .

8. Check of O(a) improvement

- In the quenched case with Wilson plaquette action the mesonic pseudoscalar screening mass m_{PS} is determined versus $(a/r_0)^2$ for various lattice sizes $N_s = 24, \ldots, 32$ and $N_t = 6, \ldots, 16$ at fixed $T/T_c = 0.655(5)$ and $m_{PS}/m_V \simeq 0.75$.
- The expected linear behavior in $(a/r_0)^2$ is observed.



9. Conclusions

Summary of scanning the phase structure



Left: All transition points within $\mu_0 \leq 0.007$. Right: The region $\beta \geq 3.75$.

Results and Perspective

- The complicated global (three-dimensional) phase structure of Wilson twisted mass QCD with $N_f = 2$ and improved gauge action has been resolved.
- The conical shape of the thermal transition surface has been confirmed in the scaling region.
- To find the critical or crossover behavior requires very large statistics. A first test to see the crossover for $N_t = 8$ and, correspondingly, at large pion mass was successful.
- O(a) improvement works, as has been demonstrated for the quenched approximation.
- Next we shall run at maximal twist at $N_t = 10$ and 12, where we expect to see the transition down to $m_{\pi} = O(300)$ MeV.