The limits of the Aoki phase with $N_f = 2$ Wilson fermions at zero and finite temperature

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Lattice QCD simulations via International Research Network

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Overview

- 1. Introduction and motivation
- 2. The Aoki phase at T = 0
 - The proposed phase structure
 - Simulation and observables of interest
 - Numerical results at zero temperature
 - Conclusion: Phase diagram at T = 0
- 3. The finite-temperature case
 - Proposal for T > 0
 - Some preliminary numerical results (2003)
 - More detailed numerical results (2004)
- 4. Conclusion

Results published in :

E.-M. I., W. Kerler, M. Müller-Preussker, A. Sternbeck and H. Stüben, Phys. Rev. D 69 (2004) 074511

and

- A. Sternbeck, E.-M. I., W. Kerler, M. Müller-Preussker and
- H. Stüben, hep-lat/0309059 (Lattice 2003)

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One analytic prediction has been around since long (S. Aoki (1984). Occasionally, observations of unexpected phase transitions are reported :

| | unimproved | clover improved |
|-----------------------|------------------|-----------------|
| | Wilson fermions | Wilson fermions |
| Wilson gauge action | yes [1], yes [3] | yes [2] |
| improved gauge action | | no [2], yes [4] |

- case T = 0
 - 1. $N_f = 2$: F. Farchioni et al., hep-lat/0406039 ; transition at $\beta = 5.2$, at small enough twisted mass $\mu \neq 0$ first order behavior at various κ , a scenario replacing the Aoki phase at higher β .
 - 2. $N_f = 3$: S. Aoki et al. (JLQCD), hep-lat/040916 ; preliminary in S. Aoki et al. (JLQCD), hep-lat/0110088 : unexpected first order bulk transition at $\beta \leq 5.0$, $\kappa \approx 0.135$; does not remain with improved gauge action !
- case $T \neq 0$
 - 3. $N_f = 2$: T. Blum et al., Phys. Rev. D 50, 3377 (1994) : found an unexplained bulk transition
 - 4. $N_f = 2$: A. Ali Khan et al., Phys. Rev. D 63, 034502 (2000) and Phys. Rev. D 64, 074510 (2001) : Aoki phase identified, not unexpected !

Bulk phase transitions render the continuum limit uncertain !

One suspected reason of metastabilities :

unphysical, small eigenvalues of the Wilson-Dirac operator (eventually even stronger in the case of clover-improved Wilson-Dirac operator, if the gauge action does not suppress dislocations) make simulations slow and create metastabilities/hysteresis.

Remedy :

twisted mass lattice QCD formulation, avoids small eigenvalues : Det $[\mathbb{1}(D_W + m_0) + i\mu\gamma_5\tau^3] = \det [(D_W^{\dagger} + m_0)(D_W + m_0) + \mu^2]$ For us :

Exactly this source term, with $h = \mu \rightarrow 0$, is testing the parity-flavor symmetry breaking characterizing the Aoki phase in some part of the β - κ plane.

For all phenomenological purposes :

It seems to be safe to use improved gauge action in conjunction with clover improved Wilson fermions (including non-perturbative tuning of the improvement coefficients) and to take advantage of the "gentleness" of this system even at lattice spacings of $a \simeq 0.1...0.2$ fm.

Why then the interest in Wilson gauge action and (unimproved) Wilson fermions ?

Indeed, new simulations with Wilson gauge action and Wilson fermions, eventually with additional ("twist") terms in the Wilson-Dirac operator (see above).

Reasons for the renewed interest :

- a clean reference case for testing new algorithms;
- theoretical interest: question of localization of the Wilson-Dirac operator, also because this is input to DW fermions and to the overlap Dirac operator;
- interrelation between defects and fermion spectrum;
- analytical predictions exist :
 S. Aoki, Phys. Rev. D 30, 2653 (1984);
- due to the promises of the twisted mass lattice QCD approach; in order to exploit the computational advantages of the twisted mass approach, one should explore the slightly extended parameter space in order to keep away from phase transitions.

For the advantages of the tm lattice QCD approach (e.g. minimized lattice artefacts for twist angle $\omega = \pi/2$) R. Frezzotti, P. A. Grassi, S. Sint and P. Weisz, JHEP 0108 (2001) 058, (hep-lat/0101001)

R. Frezzotti and G. C. Rossi, JHEP 0408 (2004) 007 (hep-lat/0306014)

Our original motivation to study the Aoki phase :

After trying to improve HMC simulations by parallel tempering at β = 5.6 and κ = 0.1550...0.1575 (the range of the T_χL collaboration)
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- also with limited success in the κ -h plane.
- Study of of the autocorrelation matrix (including swaps between neighboring κ or h values) shows: no gain in statistics.
- Swapping is suppressed if HMC is optimized at each parameter set !

Finally, in the production runs of the Aoki phase study, we have used plain HMC !

2 The Aoki phase at T = 0

 $N_f = 2$ dynamical Wilson fermions at T = 0: There is a phase of spontaneously broken parity-flavour-symmetry.



- critical lines of second order phase transition where $m_{\pi^{0\pm}}=0$

• symmetry of the diagram : $m_0 \leftrightarrow -(m_0 + 8)$ $\kappa \leftrightarrow -\kappa$

Regions : A: $\langle \bar{\psi}i\gamma_5\tau^3\psi\rangle = 0$ B: $\langle \bar{\psi}i\gamma_5\tau^3\psi\rangle \neq 0$

Goldstone theorem :

There are two massless states in the broken phase



- Charged pions π^{\pm} are the Goldstone bosons of the broken flavour symmetry, massless for $\kappa_c^{(1)}(\beta) < \kappa < \kappa_c^{(2)}(\beta)$.
- Neutral pion π^0 is massless only at $\kappa_c^{(i)}(\beta)$ (the lower and upper transition lines) due to the 2nd order phase transition.
- $\langle \bar{\psi} i \gamma_5 \tau^3 \psi \rangle \neq 0$ $\langle \bar{\psi} i \gamma_5 \tau^{1,2} \psi \rangle = 0$ in region B

• Aoki phase confirmed at strong coupling:





analytically as well as numerically

extending to $\beta = \infty$?

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 $\beta = 0$

- Numerical simulations $\beta \neq 0$
 - on a (finite) lattice : $\langle \bar{\psi} i \gamma_5 \tau^3 \psi \rangle \equiv 0$

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Another point of view (Bitar et al.)

- Numerical results for $N_f = 2$ Wilson fermions (Bitar 1997/98) on $4^4 - 10^4$ lattices
 - a signal at $\beta = 3.0 4.0$
 - BUT not at $\beta = 5.0 8.0$
 - \Rightarrow We study the leftover interval $\beta = 4.0 5.0$.
- A different interpretation of the condensate $\langle \bar{\psi}i\gamma_5\tau^3\psi\rangle \neq 0$

Signal of chiral symmetry breaking on the lattice

(Bitar *et al.* 1997/98)

No Aoki phase for $\beta \geq 5.0$

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Vafa and Witten : parity and flavor cannot be broken in massless continuum QCD !

A non-vanishing order parameter in the massless continuum theory $\lim_{h\to 0^+} \langle \bar{\psi} i \gamma_5 \tau^3 \psi \rangle = 2\pi \rho(0)$ would signal nothing but chiral symmetry breaking.

No Aoki phase for $\beta \geq 5.0$

Reconciliation (Sharpe, Singleton (1998))

An analytical framework for discussing this scenario at $a \neq 0$ and $m \neq 0$ provided by chiral perturbation theory, with an effective action

$$\mathcal{L}_{\chi} = \frac{f_{\pi}^2}{4} \operatorname{Tr} \left(\partial_{\mu} \Sigma^{\dagger} \partial_{\mu} \Sigma \right) + \mathcal{V}_{\chi}$$

with
$$V_{\chi} = -\frac{c_1}{4} \operatorname{Tr} \left(\Sigma + \Sigma^{\dagger} \right) + \frac{c_2}{16} \left[\operatorname{Tr} \left(\Sigma + \Sigma^{\dagger} \right) \right]^2$$

coefficients are functions of m and a (and the scale $\Lambda = \Lambda_{QCD}$)

$$c_1 \sim m\Lambda^3 + a\Lambda^5$$
 and $c_2 \sim m^2\Lambda^2 + ma\Lambda^4 + a^2\Lambda^6$

 \Rightarrow Main cases : $c_2 > 0$ or $c_2 < 0$

Two possible phases for $c_2 > 0$ (left scenario) : With $\epsilon = \frac{c_1}{2c_2}$ changing, $|\epsilon| \le 1$: then $m_{\pm}^2 = 0$ and $\frac{m_0^2 f_{\pi}^2}{2c_2} = 1 - \epsilon^2$ phase B realized $|\epsilon| \ge 1$: then $\frac{m_{\pm 0}^2 f_{\pi}^2}{2c_2} = |\epsilon| - 1$ phase A realized, enclosing B



No flavor symmetry breaking for $c_2 < 0$ (right) : \Rightarrow three degenerate pions with $\frac{m_{\pm 0}^2 f_{\pi}^2}{2c_2} = 1 + |\epsilon|$ Instead : with driving term $h \neq 0$ (or twisted mass μ) \mathcal{V}_{χ} becomes :

(see Sharpe and Wu, Münster (2004))

$$\begin{split} \mathcal{V}_{\chi} &= -\frac{c_1}{4} \operatorname{Tr} \left(\Sigma + \Sigma^{\dagger} \right) + \frac{c_2}{16} \Big[\operatorname{Tr} \left(\Sigma + \Sigma^{\dagger} \right) \Big]^2 + \frac{c_3}{4} \operatorname{Tr} \left(i (\Sigma - \Sigma^{\dagger}) \tau^3 \right) \\ \text{with } c_3 \sim \mu = h \end{split}$$

- for $c_2 > 0 \Rightarrow 1^{st}$ -order transition line in κ (disc. in $\mu = \pm 0$)
- for $c_2 < 0 \Rightarrow 1^{st}$ -order transition line in μ (disc. in κ , i.e. m_0)



Conclusion :

- Aoki's proposal is realized at $a \neq 0$ if $c_2 > 0$ (at low β).
- A new first order phase transition at a ≠ 0 for c₂ < 0 (found by Farchioni et al. at higher β)
- Will we find the point with $c_2 = 0$? Do we need to go to bigger lattice volume in order to decide this ?
- Bitar's interpretation becomes valid in the continuum limit.

Hybrid MC-simulations for full QCD

stand. Wilson action
$$S[U] = S_G[U] + \log \operatorname{Det} M(U,h) \text{ with } N_f = 2$$

$$S_G = \beta \sum_P \left(1 - \frac{1}{3} \operatorname{Re} \operatorname{tr} \Box_P\right) \quad M = \mathbb{1}(1 - \kappa D) + hi\gamma_5 \tau^3$$

$$\beta = \frac{6}{g^2} \text{ and } \kappa = \frac{1}{2m_0 + 8}$$
order parameter at $h \neq 0$

$$\langle \overline{\psi} i \gamma_5 \tau^3 \psi \rangle_h \simeq \frac{-1}{12V} \langle \operatorname{Tr} \left[i \gamma_5 \tau^3 M^{-1}(U,h)\right] \rangle_U$$
Lattice sizes $4^4 - 12^4$

$$\beta = 4.0 - 5.0$$
 $\kappa = 0.15 - 0.28$

$$h = 0.003 - 0.04$$

HMC run in standard Φ algorithm, with even-odd preconditioning

- fixed $\tau = 1$ per trajectory,
- acceptance rate > 75..85 %,
- tuned by stepsize $\Delta \tau$;
- no alarming autocorrelation times for $\langle \bar{\psi} i \gamma_5 \tau^3 \psi \rangle_h$,
- autocorrelation times generically bigger for κ above the Aoki phase.
- Parallel tempering swaps strongly suppressed (if $\Delta \tau$ are optimally tuned for each (κ, h) pair).

Observables of interest

1. Order parameter $\langle \bar{\psi} i \gamma_5 \tau^3 \psi \rangle$

Full fermion matrix $M(U,h) = \text{diag} \left(\mathcal{M}(U,h), \mathcal{M}(U,-h) \right)$,

with $\mathcal{M}(U,h) = 1 - \kappa D + ih\gamma_5$ in one-flavor subspace.

Full fermion determinant positive :

$$\operatorname{Det} M(U,h) = \operatorname{det} [\mathcal{M}(U,h)\mathcal{M}(U,-h)] = |\operatorname{det} [\mathcal{M}(U,h)]|^2.$$

The order parameter is then

$$\langle \bar{\psi}i\gamma_5\tau^3\psi\rangle_h \simeq \frac{-1}{12V} \Big\langle \operatorname{Tr}\left[i\gamma_5\tau^3M^{-1}(U,h)\right]\Big\rangle_U$$

Calculated as

$$\langle \bar{\psi} i \gamma_5 \tau^3 \psi \rangle_h \simeq \frac{1}{12V} \Big\langle \Im \mathfrak{m} \operatorname{tr} \left[\gamma_5 \mathcal{M}^{-1}(U,h) \right] \Big\rangle_U$$

with the final tr estimated by a stochastic estimator : tr $[\gamma_5 \mathcal{M}(U,h)^{-1}] \simeq \eta^{\dagger} \gamma_5 \zeta$ with η Gaussian complex vectors and $\zeta = \mathcal{M}(U,h)^{-1} \eta$. Finally, take the limits $h \to 0$ and $V \to \infty$!

Observables of interest

- 1. Order parameter $\langle \bar{\psi} i \gamma_5 \tau^3 \psi \rangle$
- 2. Pion norm (Bitar et al. (1989)

$$||\pi||^{2} = \sum_{x} \pi_{x} \pi_{0} = \sum_{x} (\bar{\psi}_{x} \gamma_{5} \psi_{x}) (\bar{\psi}_{0} \gamma_{5} \psi_{0})$$

with $\mathcal{M}(U,h)^{\dagger} = \gamma_{5} \mathcal{M}(U,-h) \gamma_{5}$
 $||\pi||^{2} = \frac{1}{24V} \operatorname{Tr} \left[M(U,h)^{-1\dagger} M(U,h)^{-1} \right]$
 $||\pi||^{2} = \frac{1}{12V} \operatorname{tr} \left[\mathcal{M}(U,h)^{-1\dagger} \mathcal{M}(U,h)^{-1} \right]$

Hermitean matrix $\gamma_5 \mathcal{M}(U, h = 0)$ has eigenvalues λ_j , the eigenvalues of $\gamma_5 \mathcal{M}(U, h)$ are $\tilde{\lambda}_j = \lambda_j + ih$

$$\langle ||\pi||^2 \rangle_U = \frac{1}{12V} \Big\langle \sum_j \frac{1}{\lambda_j^2 + h^2} \Big\rangle_U$$

The pion norm operator is sensitive to small eigenvalues of $\gamma_5 \mathcal{M}(U, h = 0)$: configurations with zero eigenvalues of $\mathcal{M}(U, h = 0)$ produce poles in $||\pi||^2$.

Observables of interest

- 1. Order parameter $\langle \bar{\psi} i \gamma_5 \tau^3 \psi \rangle$
- 2. Pion norm (Bitar *et al.* (1989)

Actually, the trace is evaluated by a stochastic estimator : $\langle ||\pi||^2 \rangle_U \simeq \frac{1}{12V} \langle \zeta^{\dagger} \zeta \rangle_U$

with η Gaussian complex vectors and $\zeta = \mathcal{M}(U,h)^{-1}\eta$.

- 3. Polyakov loop $\Omega_{\vec{x}}$
 - exclude quasi-deconfinement (small volume) at T = 0
 - localize the thermal transition at finite T relative to the Aoki phase signal

Numerical results

A typical data set for the order parameter



- Projection over $\kappa \implies \kappa^*$ (maximum for $h \neq 0$)
- Projection over $h \Rightarrow \langle \bar{\psi} i \gamma_5 \tau^3 \psi \rangle$, limit $h \to 0$ along κ^*



Figure 5.6: The order parameter $\langle \bar{\psi}i\gamma_5\tau^3\psi\rangle$ measured on a 6⁴ lattice as a function of h at $\beta = 4.0$. On the left hand side at the values of $\kappa \leq \kappa^*$, whereas at $\kappa \geq \kappa^*$ on the right hand side. The lines are spline interpolations to guide the eye.



Figure 5.7: The order parameter $\langle \bar{\psi}i\gamma_5\tau^3\psi\rangle$ measured on a 6⁴ lattice as a function of h at $\beta = 4.3$. Again on the left hand side at values $\kappa \leq \kappa^*$, whereas at $\kappa \geq \kappa^*$ on the right hand side. The lines are spline interpolations to guide the eye.

Typical behavior of the pion norm



Pion norm at $\beta = 4.0$



Order parameter at $\beta = 4.0$



ansatz

$$f(h) = A + Bh^{C} + \dots$$
 [Bitar $C \equiv 1/3$]

Fisher plot : test of the mean-field behavior

plot all data points in the

 $h/\langle \bar{\psi}i\gamma_5\tau^3\psi\rangle - \langle \bar{\psi}i\gamma_5\tau^3\psi\rangle^2$ plane :

- mean-field behavior : straight parallel lines
- lines for κ_c^{lower} and κ_c^{upper} go through the origin
- positive intercept \Rightarrow non-vanishing order parameter



Figure 5.11: The squared order parameter $\langle \bar{\psi}i\gamma_5\tau^3\psi \rangle^2$ is shown as a function of $h/\langle \bar{\psi}i\gamma_5\tau^3\psi \rangle$ at $\kappa \leq \kappa^*$ on the left hand side and at $\kappa \geq \kappa^*$ on the right hand side. The data are taken from simulations on a 6⁴ lattice at $\beta = 4.0$. The dotted lines are lines of constant *h*. The values are h = 0.003, 0.005, 0.01, 0.02, 0.03, 0.04, from left to right.



Figure 5.12: The squared order parameter $\langle \bar{\psi}i\gamma_5\tau^3\psi \rangle^2$ is shown as a function of $h/\langle \bar{\psi}i\gamma_5\tau^3\psi \rangle$ at $\kappa \leq \kappa^*$ on the left hand side and at $\kappa \geq \kappa^*$ on the right hand side. The data are taken from simulations on a 6⁴ lattice at $\beta = 4.3$. The dotted lines are lines of constant *h*. The values are h = 0.003, 0.005, 0.01, 0.02, from left to right.

Order parameter at $\beta = 4.3$



using the same ansatz

$$f(h) = A + Bh^C + \dots$$

robust against correction terms

fit parameter at $\beta = 4.0$ and $\beta = 4.3$:

A > 0 B = 1.00(4) C = 0.65(2)

Pion norm at $\beta = 4.3$, $\beta = 4.6$, $\beta = 5.0$



 κ



Figure 5.13: The squared order parameter $\langle \bar{\psi}i\gamma_5\tau^3\psi\rangle^2$ is shown as a function of $h/\langle \bar{\psi}i\gamma_5\tau^3\psi\rangle$ at $\kappa \leq \kappa^*$ on the left hand side and at $\kappa \geq \kappa^*$ on the right hand side. The data are taken from simulations on a 6⁴ lattice at $\beta = 4.6$. The dotted lines are lines of constant *h*. The values are h = 0.005, 0.01, 0.02, from left to right.

at the present time, since they require a large amount of computing resources. Thus the limit of infinite lattice size can only insufficiently be extrapolated. Looking at the Figures 5.14 and 5.15 where the order parameter $\langle \bar{\psi}i\gamma_5\tau^3\psi\rangle$ is shown as a function of h, it can be verified that the more h is decreased the more finite lattice size effects are relevant. Nevertheless, they neither increase nor decrease substantially if measured on a 8^4 and a 10^4 and thus are almost negligible. Only the results at $\beta = 4.0$ from simulations on a 4^4 lattice differ from the remaining ones. From the Fisher plots it also turns out that the finite-size corrections go into the right direction as the lattice size is increased, *i.e.* they extrapolate rather to a finite value on the ordinate.

Therefore it can be assumed that at each h the result from the largest lattice lies within errors on the envelope in the limit of infinite lattice size, apart from the ones at h = 0.003. These were obtained only from simulations on a 6⁴ lattice and thus larger finite-size effects cannot be excluded at this small value of h.

Consequently, for the following fits⁴ only the data for h > 0.003 — each taken from the largest lattice — were used and are referred to as the data in the infinite volume limit.

In [26] it is pointed out that in this limit the data are expected to behave as

$$f(h) = A + Bh^{\frac{1}{3}} + \dots$$
(5.3)

in the presence of a parity-flavour-breaking phase which corresponds to a mean-field like *ansatz*. Following [26] the data were fitted to (5.3) with linear and/or quadratic

⁴ In this study the data were fitted using an implementation of the nonlinear least-squares (NLLS) Marquardt-Levenberg algorithm provided by gnuplot 3.7.2.

Order parameter at $\beta = 4.6$



A > 0 B = 1.00(4) C = 0.65(2)

Some problems at $\beta = 4.6$

- asymmetric peak
- displacement with increasing volume

Order parameter at $\beta = 5.0$



There is obviously no finite value of the order parameter at h = 0on lattice sizes up to 12^4 .

Conclusion : Phase diagram at T=0



Conclusion : Phase diagram at T=0



 $\beta = 4.0: \quad 0.215 \simeq \kappa_c^{(1)} < 0.220 \qquad 0.220 < \kappa_c^{(2)} < 0.225$ $\beta = 4.3: \quad 0.205 < \kappa_c^{(1)} < 0.210 \qquad 0.210 < \kappa_c^{(2)} < 0.215.$

3 The finite-temperature case

Proposal for T > 0 (Aoki *et al.* 97/98)

The Aoki phase forms a cusp surrounded by the confined phase



Results for $8^3 \times 4$ and $10^3 \times 4$ at $\beta = 4.6$ and fixed h = 0.005

(few preliminary results also presented at Lattice 2003 by A. Sternbeck)



After Lattice 2003, as long as the Cray T3E was running,

 \Rightarrow continuing data taking on a finer κ grid for $\beta = 4.6$

Polyakov loop L, susceptibility χ_L , $\bar{\psi}\psi$, $||\pi||^2$ and $\langle\bar{\psi}i\gamma_5\tau^3\psi\rangle$ vs. κ



Finer structure in $||\pi||^2$, L, $\langle \bar{\psi}i\gamma_5\tau^3\psi\rangle$ and $\bar{\psi}\psi$ near κ_c



Extrapolation to h = 0 for $8^3 \times 4$ and $10^3 \times 4$ at $\beta = 4.6$



 \Rightarrow a non-vanishing condensate

established over the interval 0.19690 $\leq \kappa \leq 0.19710$

Fisher plot for $8^3 \times 4$ and $10^3 \times 4$ at $\beta = 4.6$



- \Rightarrow result above corroborated by Fisher plot
- \Rightarrow the finite T transition is located at $\kappa = 0.1971$

Warning: strong autocorrelations seen at $\kappa = 0.19710$



4 Conclusion

- For the zero temperature case the Aoki phase can only be confirmed at strong coupling, i.e. β < 4.6
 - Does the result change on larger lattices ? ($\gg 10^4$)
 - Does a broken phase exist with improved Wilson action ?
- For the non-zero temperature case an Aoki phase can be confirmed even at $\beta = 4.6$ κ
 - the phase is shifted to lower κ $\kappa_{T>0} = 0.19705 \leftrightarrow \kappa_{T=0} = 0.1983$
 - the Aoki phase seems to pass into the
 finite temperature transition line (not separable so far)



