Twisted mass QCD at finite temperature

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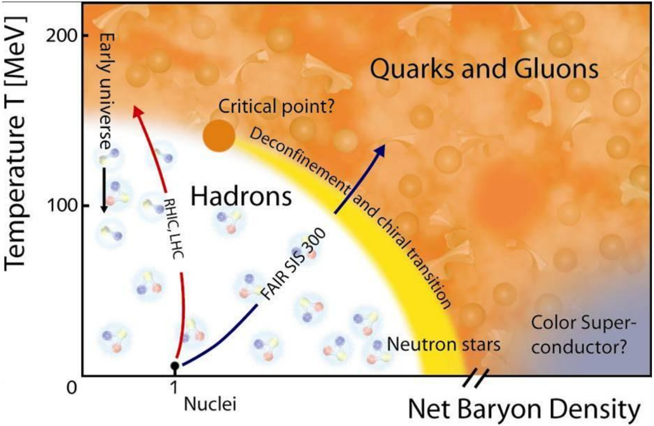
FS QFT Nov 5, 2007

The phase diagram of QCD



- Transition to QGP: crossover or true phase transition?
- $\mu = 0$ (easily) numerically accessible via lattice QCD.
- Results mainly obtained with staggered fermions.

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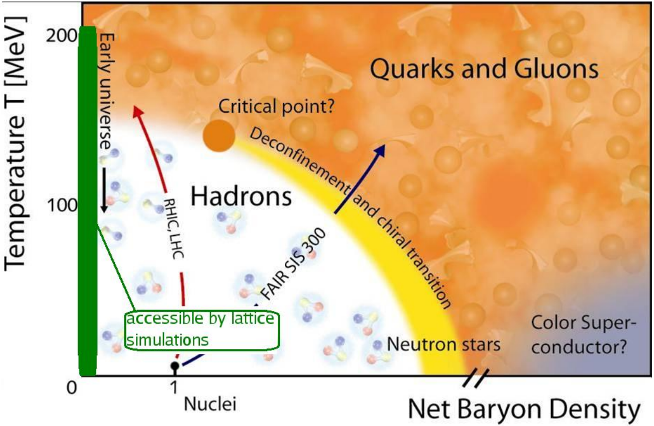

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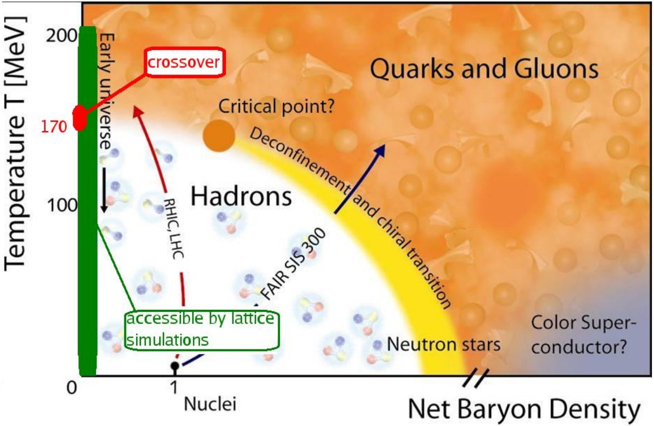

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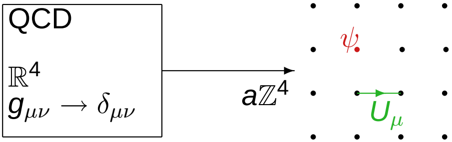
Outline

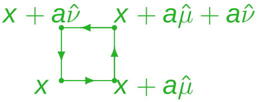
- Short introduction to lattice QCD and Wilson fermions.
  overview for those unfamiliar with lattice QCD, Wilson's fermion discretization
- twisted mass QCD at zero temperature.
  formulation and phase structure
- Thermal expectation values.
  how to calculate thermal equilibrium expectation values in QCD
- Non-interacting theory: Quantification of cutoff effects.
  the free propagator, the Stefan-Boltzmann limit
- Phase structure of finite temperature twisted mass QCD.
  a speculative phase diagram looked at by HMC simulations

Lattice QCD

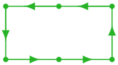


- Fermion fields $\psi(x)$ live on lattice sites.
- Gauge degrees of freedom are represented by the $SU(3)$-valued linkvariables $U_\mu(x) = \exp(iagA^r_\mu(x)T^r)$.
- "Action building": demand that for $a \to 0$ action coincides with continuum version.

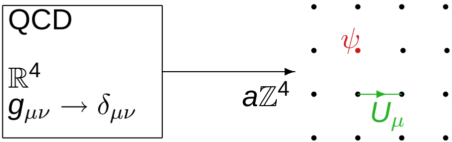
Plaquette $U^P_{\mu\nu}(x)$:



Rectangles $U^{(1\times 2)}_{\mu\nu}(x)$:



Lattice QCD



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Plaquette action ($\beta = \frac{6}{g^2}$)

$$\beta \sum_{x,\mu<\nu} a^4 \left(1 - \frac{1}{3}\mathrm{ReTr}U^P_{\mu\nu}(x)\right)$$

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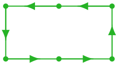
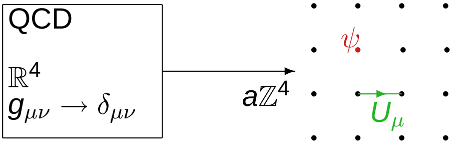


Lattice QCD



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Improved action:

tree-level Symanzik improved gauge action (tlSym)
(uses plaquette and rectangles)

Naive discretization

Fermion matrix

- Replace derivatives by suitable discretization, e. g. the symmetric difference:

$$\nabla_\mu \psi(x) = \frac{1}{2a}\left(\psi(x + a\hat{\mu}) - \psi(x - a\hat{\mu})\right)$$

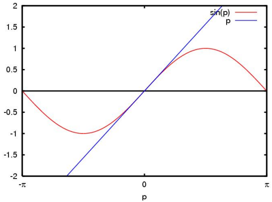
- Then the kernel of the free fermion action $S_F = (\psi, M_F \psi)$ reads:

$$(M_F)_{xy} = \frac{1}{2a}\sum_{\mu=1}^{4} \gamma_\mu \left(\delta_{y,x+a\hat{\mu}} - \delta_{y,x-a\hat{\mu}}\right) + am$$

- The propagator is given by $\Delta_F = M_F^{-1}$:

$$\Delta_F^{-1} = \frac{1}{a} i \sum_{\mu=1}^{4} \gamma_\mu \sin(ap_\mu) + am = i \sum_{\mu=1}^{4} \gamma_\mu \bar{p}_\mu + am$$

Naive discretization
The doubler problem



- Additional zeros of the lattice momentum $\overline{p}$ lead to 15 additional fermion states.
- These doublers have to be removed for interacting theories.

Naive discretization

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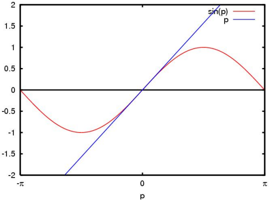

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Wilson term

- Use a "higher derivative" in the fermion Matrix that is irrelevant for $a \to 0$:

$$\frac{r}{2a}\overline{\psi}(x)\left(2\psi(x) - \psi(x + a\hat{\mu}) - \overline{\psi}(x - a\hat{\mu})\right)$$

- Additional mass renders doublers dynamically irrelevant: $\frac{2r}{a}\sum_{\mu=1}^{4}\sin^2(ap_\mu/2)$

Wilson's fermion action

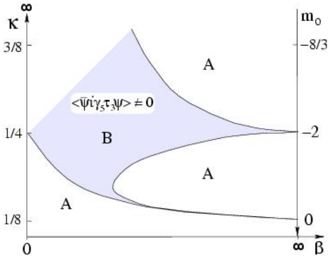
$$S_F(\overline{\psi}, \psi, U) = \sum_x a^4 \Bigg(\overline{\psi}(x)\psi(x) - \kappa \sum_{\mu=\pm 1}^{\pm 4} \overline{\psi}(x + a\hat{\mu})(r + \gamma_\mu) U_\mu(x) \psi(x) \Bigg)$$

with $a^{3/2}(am + 4r)^{1/2}\psi(x) \to \psi(x)$ and $\kappa = \frac{1}{2am+8r}$

Problems:

- Additive mass renormalization, i. e. massless theory for some $m = m_c(\beta)$ (or $\kappa_c(\beta)$).
- Chiral symmetry is explicitly broken by the Wilson term.

Aoki phase: (κ, β)-phasediagram



[hep-lat/0309059]

- Parity-flavour broken phase (for $N_f = 2$).
- Two pions are massless Goldstone bosons.
- The third pion acquires a non-vanishing mass.

The order parameter for the Aoki phase is given by:

$$\left\langle \overline{\psi} i \gamma_5 \tau^3 \psi \right\rangle$$

twisted mass QCD

Continuum

QCD in twisted basis

$$S_F = \int d^4x\, \overline{\chi}(x) \left(\gamma_\mu D_\mu + m + i\mu\gamma_5\tau^3\right) \chi(x)$$

- Aoki order parameter as new mass term.
- Connection to physical basis by chiral/flavour rotation:

$$\psi = e^{\frac{i}{2}\omega\gamma_5\tau^3}\chi \qquad \overline{\psi} = \overline{\chi}e^{\frac{i}{2}\omega\gamma_5\tau^3}$$

$$m = M\cos\omega \qquad \mu = M\sin\omega \qquad \Rightarrow M = \sqrt{m^2 + \mu^2}$$

- The twist angle gives the direction of the chiral symmetry breaking mass (interpreted as an external field).

Frezzotti, Grassi, Sint, Weisz 1999/2000

twisted mass QCD
Lattice

- The Wilson term is not invariant under the chiral/flavour rotations.
- For every value of the twist angle, there is a different regularization of continuum QCD.

Lattice fermion matrix with twisted mass term

$$M_{\rm tm} = M_W^c + m + i\mu\gamma_5\tau^3$$

or

$$M_{\rm tm} = M_W(\kappa) + 2i\kappa\mu\gamma_5\tau^3$$

Benefits:

- No exceptional configurations as $\mathrm{Det}_f M_{\rm tm} = M_W M_W^\dagger + \mu^2$.
- Lattice artefacts become dependent of twist angle.

Automatic improvement

- For $\omega = \frac{\pi}{2}$ there is automatic $\mathcal{O}(a)$ improvement: Any observable with non-vanishing expectation value does not contain $\mathcal{O}(a)$ cutoff effects.
- At full twist the mass is completely determined by the twisted mass parameter μ.
- The untwisted mass must be tuned to its critical value $m_c(\beta)$.
- A practical definition for full twist is given by the PCAC relation:

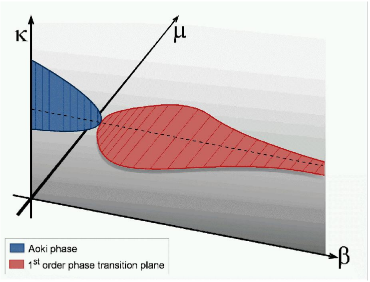
$$m_{\mathrm{PCAC}} = \frac{\sum_{\mathbf{x}} \langle \partial_0 A_0^r(x) P^r(0) \rangle}{2 \sum_{\mathbf{x}} \langle P^r(x) P^r(0) \rangle}$$

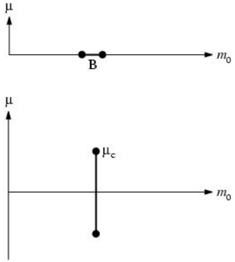
With:

$$P^r(x) = \overline{\chi}(x) \gamma_5 \frac{\tau^r}{2} \chi(x) \qquad A_\mu^r(x) = \overline{\chi}(x) \gamma_\mu \gamma_5 \frac{\tau^r}{2} \chi(x)$$

Frezzotti, Rossi: JHEP 08:007(2004)

Extended phase structure





- Phase diagram for tmQCD in three dimensions: (κ, β, μ).
- Aoki phase in $(\mu = 0)$-plane for strong coupling.
- For weak coupling there is the "normal scenario" realized: first order transition plane intersecting the $(\mu = 0)$-plane perpendicularly.

cf. PoS(Lat2005)072 (left figure) and JHEP 09:035(2004) (right figures)

Now let's turn on the heat:

Lattice QCD at Finite Temperature

- Partition function and free energy density.
- Thermal continuum expectation values.
- QCD at finite temperature.

Partition function

- Grand canonical ensemble: (V, T, μ) are fixed.
- All possible ensembles are equivalent in the thermodynamic limit $N, V \to \infty$ with a constant density N/V.
- Here we always consider zero chemical potential $\mu = 0$ which is equivalent to $\langle n \rangle = 0$ (in the thermodynamic limit).

Grand canonical partition function

$$Z(T, V, \mu) = \mathrm{Tr}\, e^{-\beta(H - \mu_j N_j)}$$

- Free energy density: $f = -\frac{T}{V} \ln Z$
- Pressure: $p = -f = \frac{T}{V} \ln Z$

Thermal expectation values

- Equilibrium expectation value:

$$\langle F \rangle = \frac{1}{Z} \mathrm{Tr}\, F e^{-\beta H}$$

- For the trace evaluation use set of orthonormal states $|\phi\rangle$:

$$Z = \mathrm{Tr}\, e^{-\beta H} = \int \mathrm{d}\phi \left\langle \phi | e^{-\beta H} | \phi \right\rangle$$

- Interpreting $\exp(-\beta H)$ as time evolution in the imaginary time $\tau = it$, the functional integral is introduced in the well-known way for zero-temperature transition amplitudes:

$$Z = \int_{\text{period.}} \mathcal{D}\phi \; \exp\left[- \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3 x \, \mathcal{L} \right]$$

- The periodicity in the fields is due to the trace evaluation.

QCD at finite temperature

- For QCD with fields $\overline{\psi}, \psi, A$:

$$\langle F \rangle = \int \mathcal{D}\left[\overline{\psi}, \psi, A\right] \; F(\overline{\psi}, \psi, A) e^{-S(\beta)}$$

- The fermion fields obey antiperiodic boundary conditions:

$$\psi(\mathbf{x}, 0) = -\psi(\mathbf{x}, \beta)$$

- Finite time extension leads to discrete Matsubara modes ($n \in \mathbb{Z}$):

$$\omega_n = 2\pi n T \quad \text{(bosons)} \qquad \omega_n = (2n+1)\pi T \quad \text{(fermions)}$$

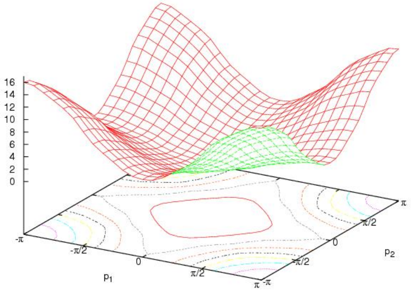
- Finite temperature on the lattice: $T = (aN_t)^{-1}$

Quantifying Cutoff Effects:

Non-Interacting Theory

- The free propagator.
- Stefan-Boltzmann limit: continuum.
- Stefan-Boltzmann limit on the lattice.

The free propagator



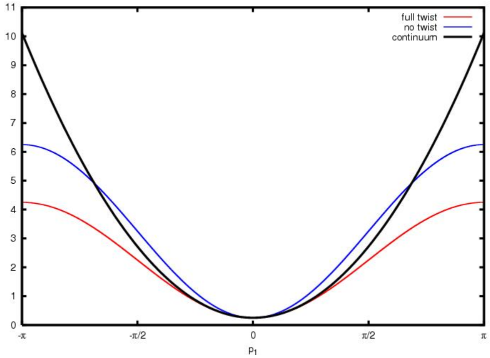
Free twisted mass propagator

$$\Delta_{\text{tm}}(p) = \frac{-i \sum_\nu \gamma_\nu \overline{p}_\nu + \frac{1}{2}\hat{p}^2 + m_0 - i\mu\gamma_5\tau^3}{\overline{p}^2 + \left(\frac{1}{2}\hat{p}^2 + m\right)^2 + \mu^2}$$

with $\hat{p}_\nu = \frac{1}{2}\sin\left(\frac{p_\nu}{2}\right)$ and $\overline{p}_\nu = \sin(p_\nu)$

The free propagator
Inverse absolute value

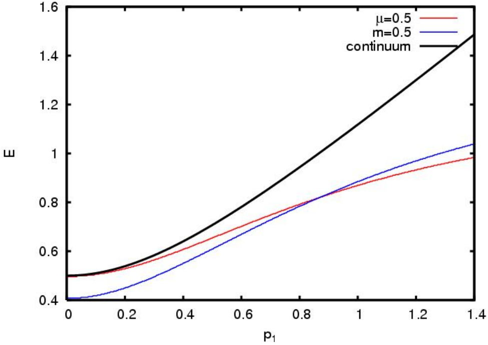
- Inverse absolute value squared:
  $|\Delta_{\text{tm}}|^{-2} = \left(\Delta_{\text{tm}}\Delta_{\text{tm}}^{\dagger}\right)^{-1} \sim \mathbf{1}$
- Continuum value: $p^2 + m^2$



Dispersion relation

- Dispersion relation $E(\mathbf{p})$ is defined by zeros of the propagator's denomenator using $E = ip_4$:

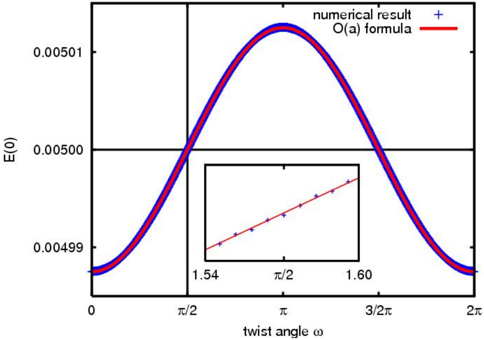
$$\sum_{j=1}^{3} \bar{p}_j^2 - \sinh^2(E) + \left(\frac{1}{2} \sum_{j=1}^{3} \hat{p}_j^2 - 2\sinh^2\left(\frac{E}{2}\right) + m_0 \right)^2 + \mu^2 = 0$$



Dispersion relation
$\mathcal{O}(a)$ effects

- $E(0)$ can be used to quantify cutoff effects.
- Expanding the denominator of the propagator in powers of a leads to the following approximation:

$$E(0) = M\left(1 - \frac{1}{2}aM\cos(\omega)\right) + \mathcal{O}(a^2)$$



Stefan-Boltzmann-Limit

What is the pressure of an ideal gas of bosons and/or fermions?

$$Z = \mathrm{Tr}\, e^{-\beta H} = \sum_{\{n_{\mathbf{p},\lambda}\}} e^{-\beta \sum_{\mathbf{p}} n_{\mathbf{p},\lambda} \varepsilon_{n_{\mathbf{p}}}} = \left(\prod_{\mathbf{p}} \sum_{n_{\mathbf{p}}} e^{-\beta n_{\mathbf{p}} \varepsilon_{\mathbf{p}}} \right)^g$$

Energy states $\varepsilon_{\mathbf{p}}^2 = \mathbf{p}^2 + m^2$ with degeneracy g; $n_{\mathbf{p}} \in \mathbb{N}$ for bosons and $n_{\mathbf{p}} \in \{0, 1\}$ for fermions.

$$p = T \frac{\partial \ln Z}{\partial V} = \frac{T}{V} \ln Z$$

SB-Limit

Continuum results

QCD Gluons

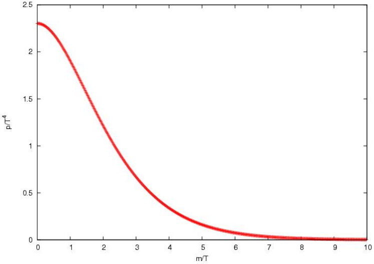
$$\frac{p_{SB}}{T^4} = 16\frac{\pi^2}{90}$$

Massless fermions

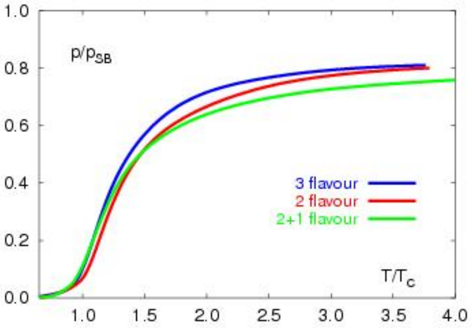
$$\frac{p_{SB}}{T^4} = \frac{21}{2} n_f \frac{\pi^2}{90}$$

Massive fermions

$$\frac{p_{SB}}{T^4} = \frac{21}{2} \sum_f g(m_f/T) \frac{\pi^2}{90}$$



Counting degrees of freedom



[hep-lat/0002003]

Pion gas:

$$\frac{p}{T^4} = 3\frac{\pi^2}{90}$$

QGP:

$$\frac{p}{T^4} = \left(\frac{21}{2}n_f + 16\right)\frac{\pi^2}{90}$$

Lattice calculations

Fermions

Pressure for fermions

$$\frac{p}{T^4} = 12N_t^4 \int_p \ln\left(|M_W|^2 + \mu^2\right)$$

- Evaluation of the partition function:

$$\ln Z = \ln \mathrm{Det} M_{\mathrm{tm}} = 4N_c \ln\left(M_W M_W^\dagger + \mu^2\right)$$

  (reading $M_W M_W^\dagger$ as a scalar)
- Normalization to $p(T=0) = 0$:

$$\int_p f(p) = \int_{[0,2\pi)^3} \frac{\mathrm{d}^3 p}{(2\pi)^3} \frac{1}{N_t} \sum_{n=1}^{N_t} f(\mathbf{p}, -\omega_n) - \int_{[0,2\pi)^4} \frac{\mathrm{d}^4 p}{(2\pi)^4} f(\mathbf{p}, p_4)$$

- Pressure has no $\mathcal{O}(a)$ artefacts.

Lattice calculations

Gauge bosons

Pressure for gauge bosons

$$\frac{p}{T^4} = -8N_t^4 \int_k \ln\left(4\sum_{\mu=1}^{4}\sin^2(k_\mu/2)\right) \text{ (plaquette)}$$

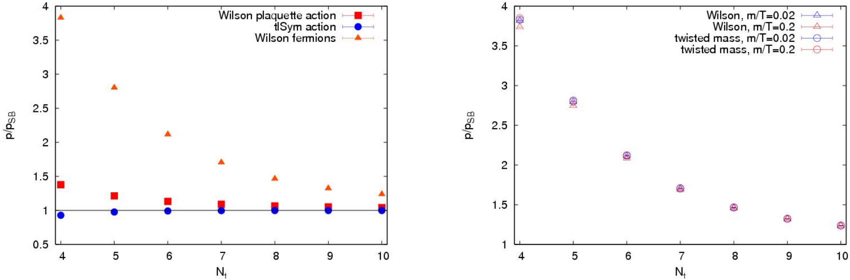
$$\frac{p}{T^4} = -4N_t^4 \int_k \left(\ln\left(\mathrm{Det}(\Delta_G)^{-1}_{\mu\nu}(k)\right) - 2\ln\left(4\sum_{\mu=1}^{4}\sin^2(k_\mu/2)\right)\right)$$
(tlSym)

- Partition function:

$$\ln Z = \frac{1}{2}\ln \mathrm{Det}\Delta_G$$

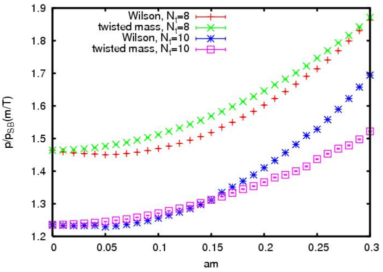
- Subtract ghost contribution.
- Determinant evaluation for tlSym done automatically by a computer program.

Continuum limit for p/p_{SB}

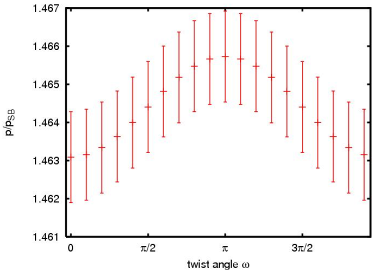


$$T = \frac{1}{aN_t} \quad \text{and} \quad \frac{m}{T} = (am)N_t$$

Lattice artefacts



Increasing mass parameter for fixed N_t.



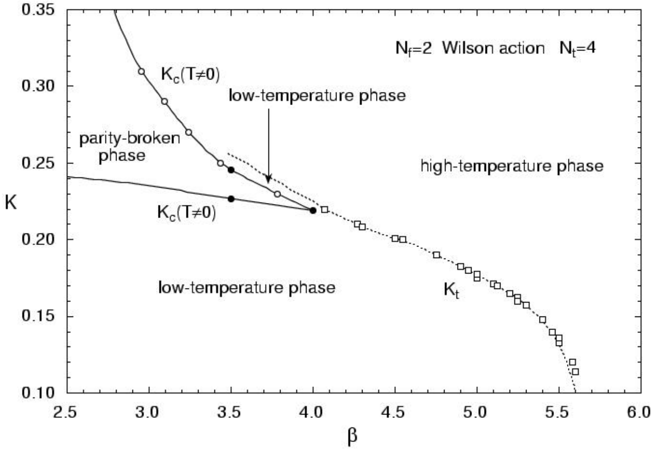
Pressure normalized to continuum value as a function of the twist angle.

Interacting tmQCD on the Lattice: Finite Temperature Phase Structure

- Speculative phase structure at finite temperature.
- Observables for simulations.
- Results.

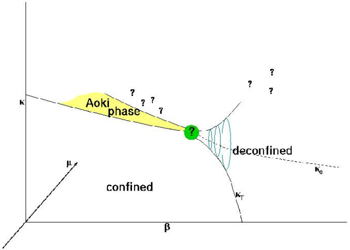
Wilson fermions at finite temperature

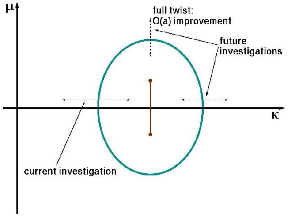
Aoki phase and finite temperature transition



[hep-lat/9508008]

Speculative phase diagram for tmQCD





- Speculative phase diagram.
  Creutz: `Phys. Rev. D76 054501 (2007)`
- Based on the relation of the bare parameters:

$$M = \sqrt{\frac{1}{4}\left(\frac{1}{\kappa} - \frac{1}{\kappa_c(\beta)}\right)^2 + \mu^2}$$

Lattice Observables

Plaquette expectation value

$$\langle P \rangle = \left\langle \mathrm{Tr}\, U_{\mu\nu}^{P}(x) \right\rangle$$

- Interpreted as internal energy of the gauge sector.
- A rise in $\langle P \rangle$ indicates the deconfinement transition.

Lattice Observables

Polyakov loop

$$L(\mathbf{x}) = \frac{1}{N_c} \mathrm{Tr} \prod_{n_4=0}^{N_t-1} U_4(\mathbf{x}, x_4)$$

- The Polyakov loop expectation value is related to the free energy of a single static quark in pure gauge theory:

$$\langle L \rangle = e^{-\beta F}$$

- In pure gauge theory $\langle L \rangle$ is also the order parameter for the breaking of the Z_3 symmetry.
- A rise in $\langle L \rangle$ indicates the deconfinement transition.

Lattice Observables

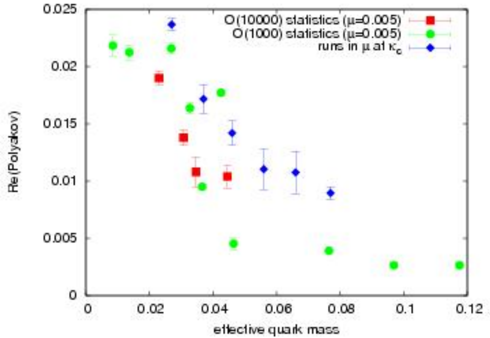
Pionnorm

$$\|\pi\|^2 = \sum_x \left\langle \overline{d}(x)\gamma_5 u(x)\overline{u}(0)\gamma_5 d(0) \right\rangle$$

- Pionnorm is the zero momentum pion correlator.
- The pion correlator peaks at the phase transition or crossover.
- The advantage of this fermionic observable is its invariance under the chiral-flavour transformations of the flavour doublets $\psi = (u, d)$:

$$\psi \to e^{\frac{i}{2}\omega\gamma_5\tau^3}\psi \qquad \overline{\psi} \to \overline{\psi}e^{\frac{i}{2}\omega\gamma_5\tau^3}$$

Conical structure



- $\beta = 3.9$, $16^3 \times 8$
- Runs in κ at $\mu = 0.005$.
- Run in μ at $\kappa = \kappa_c = 0.160856$.

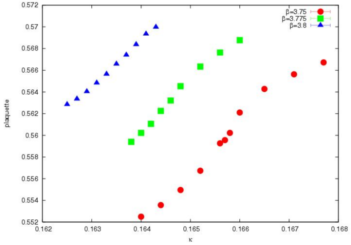
Mapping to effective bare quark mass using:

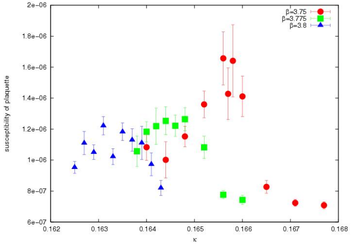
$$M = \sqrt{\frac{1}{4}\left(\frac{1}{\kappa} - \frac{1}{\kappa_c(\beta)}\right)^2 + \mu^2}$$

Thermal transition line

$\mu = 0.005$

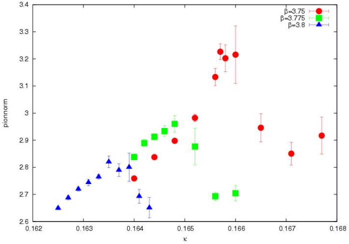
Plaquette





- $16^3 \times 8$, $\mu = 0.005$
- 10-20k HMC sweeps.

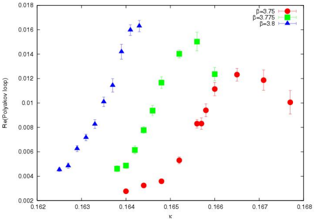
Pionnorm

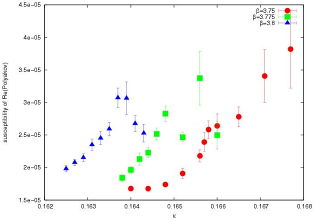


Thermal transition line

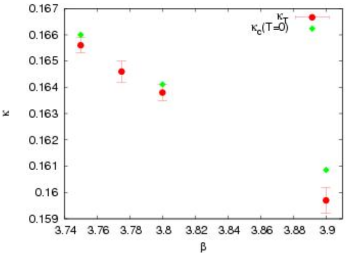
$\mu = 0.005$

Polyakov loop





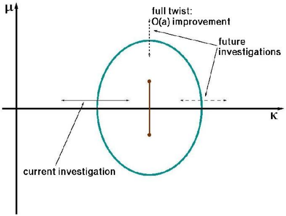
- Plaquette signal broadens with increasing β.
- Polyakov loop signal becomes better.
- κ_T is decreasing with growing β.

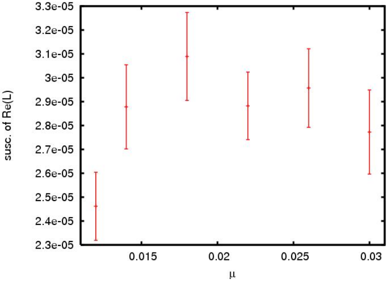


Thermal transition line

What's next. . .

- Check of the cone structure.
- Investigation of the phase diagram at full twist.





Conclusions

- Quantification of cutoff effects:
  - The dispersion relation obtained from the free propagator shows a minimization of cutoff effects for full twist
  - The pressure compared to the continuum Stefan-Boltzmann limit shows that $\mathcal{O}(a^2)$ effects vary only slightly with the twist angle.
  - What about the weak coupling expansion in $\mathcal{O}(g^2)$?
- Phase structure of tmQCD at non-zero temperature: PoS(Lat2007)238
  - The thermal transition line at vanishing twist is possibly part of a transition surface in the (κ, β, μ) space.
  - Some evidence for the existence of this conical surface has been found.
  - At $\mu = 0.005$ there is a thermal transition line; an investigation for maximal twist is ongoing.