Towards realistic Simulations of Lattice-QCD: the Approach of Twisted Mass Fermions

Karl Jansen

- Small quark masses and improved scaling quenched
- A surprise for dynamical quarks: the phase structure
Twisted Mass Team

- NIC, Zeuthen
  K. Nagai, M. Papinutto, A. Shindler, C. Urbach, U. Wenger, I. Wetzorke, K.J.

- DESY, Hamburg
  I. Montvay, N. Ukita, E. Scholz

- Münster University
  F. Farchioni, P. Hoffmann, G. Münster

- Humboldt University
  L. Scorzato

- University of Rome II
  R. Frezzotti, G. Rossi
Publications (numerical simulations)

Quenched studies
- Going chiral: *Overlap versus twisted mass fermions*, hep-lat/0411001
- Scaling test for Wilson twisted mass QCD, hep-lat/0312013
- Light quarks with twisted mass fermions, hep-lat/0503031
- Quenched scaling of Wilson twisted mass fermions, hep-lat/0507010
- Flavour breaking effects of Wilson twisted mass fermions, hep-lat/0507032
- Comparing iterative methods for overlap and twisted mass, hep-lat/0409107

Dynamical Quarks
- Exploring the phase structure of lattice QCD with twisted mass quarks, hep-lat/0409098
- Twisted mass quarks and the phase structure of lattice QCD, hep-lat/0406039
- The phase structure of lattice QCD with Wilson quarks and renormalization group improved gluons, hep-lat/0410031
- Lattice spacing dependence of the first order phase transition for dynamical twisted mass fermions, hep-lat/0506025

Overview
- Dynamical twisted mass fermions, hep-lat/0509131
- Plenary talk at Lattice2005, A. Shindler
Wilson (Frezzotti, Rossi) twisted mass QCD (Frezzotti, Grassi, Sint, Weisz)

\[ D_{tm} = m_q + i\mu \tau_3 \gamma_5 + \frac{1}{2} \gamma_\mu \left[ \nabla_\mu + \nabla^*_\mu \right] - a\frac{1}{2} \nabla^*_\mu \nabla_\mu \]

quark mass parameter \( m_q \), twisted mass parameter \( \mu \)

- \( m_q = m_{\text{crit}} \rightarrow O(a) \) improvement for hadron masses, matrix elements, form factors, decay constants

- \( \text{det}[D_{tm}] = \text{det}[D_{\text{Wilson}}^2 + \mu^2] \)
  \( \Rightarrow \) protection against small eigenvalues

- computational cost comparable to staggered talk by C. Urbach

- simplifies mixing problems
twisted mass against overlap fermions: how chiral can we go?

Bietenholz, Capitani, Chiarappa, Hasenbusch, K.J., Nagai, Papinutto, Scorzato, Shcheredin, Shindler, Urbach, Wenger, Wetzorke

$\beta = 5.85$ only

⇒ twisted mass simulations can reach quarks masses as small as overlap substantially smaller than $O(a)$-improved Wilson fermions
Choice of the critical quark mass

relation quark mass \( m_q \) and hopping parameter \( \kappa \), \( \kappa = 1/(2a m_q + 8) \)

- \( \kappa_c (m_{\text{crit}}) \) from vanishing of pion mass
- \( \kappa_c (m_{\text{crit}}) \) from vanishing of PCAC quark mass

→ both lead to \( O(a) \)-improvement (Frezzotti-Rossi)

different but can have substantially \( O(a^2) \)-effects

(Frezzotti, Martinelli, Papinutto, Rossi)
The bending phenomenon

comparison of pion definition and PCAC definition of critical quark mass

\[ \beta = 6.0 \]

\[ f_{PSa} \]

\[ (m_{PSa})^2 \]

→ triggered quite some discussion
(Frezzotti-Rossi, Aoki-Bär, Sharpe-Wu, Sharpe, Frezzotti, Martinelli, Papinutto, Rossi)

→ explanation: pion definition leads to large \( O(a^2) \) cut-off effects \( \propto a^2/m_\pi^4 \)

→ PCAC definition these infrared enhanced cut-off effects are eliminated \( O(a^2) \) cut-off effects \( \propto a^2/m_\pi^4 \)
Scaling of $F_{PS}$
\( \langle x \rangle \) in the pre-twisted mass era

Guagnelli, K.J., Palombi, Petronzio, Shindler, Wetzorke

- Schrödinger Functional
- combined Wilson and \( O(a) \)-improved Wilson
- controlled
  - non-perturbative renormalization
  - continuum limit
  - finite volume effects
  - statistical errors

![Graph showing \( \langle x \rangle^{MS} \) vs. \( m_{\pi}^2 \) for \( \mu = 2 \, \text{GeV} \)](image-url)
\[ \langle x \rangle \text{ with twisted mass} \]

\[ \langle x \rangle_{\overline{\text{MS}}} (\mu=2 \text{ GeV}) \]

\[ m_{\text{PS}}^2 [\text{GeV}^2] \]

- Wilson tmQCD at \( \pi/2 \)
- Combined Wilson-Clover
- Experimental value
$F_{PS}$ and $m_{\rho}$ in the continuum
Flavour breaking effects

\begin{align*}
\frac{m^2 - 1}{m^2} & \quad (a/r_0)^2 \\
\frac{m^2 - 1}{m^2} & \quad (a/r_0)^2
\end{align*}

- $m_{\pi^-} = 297$ MeV
- $m_{\pi^-} = 382$ MeV
Summary of quenched situation for maximally twisted mass QCD

- $O(a)$-improvement verified

- with PCAC definition of critical quark mass: also $O(a^2)$ effects small

- pion masses of $O(250)$MeV perfectly possible

- flavour breaking effects are $O(a^2)$ size comparable with staggered fermions

With available improved dynamical algorithms

$\Rightarrow$ nothing between us and dynamical simulations of maximally twisted mass QCD
Let me describe a typical computer simulation: [...] the first thing to do is to look for phase transitions (G. Parisi)

lattice simulations are done under the assumption that the transition is continuum like

- first order, jump in \( < \bar{\Psi} \Psi > \) when quark mass \( m \) changes sign
- pion mass vanishes at phase transition point

\( \rightarrow \) twisted mass fermions offer a tool to check this
Metastabilities in plaquette expectation value

cold (high plaquette) and hot (low plaquette) starts: long-living states

non-vanishing $\mu$

pure Wilson case
Lattice spacing dependence of the phase transition

Plaquette expectation value

PCAC quark mass
Earlier signs of phase diagram

- **Earlier signs of first order phase transitions**
  Blum, PRD 50 3377 ('94)
  my own little experiments

- **Aoki Phase**
  Bitar, hep-lat/9602027
  Sternbeck, Ilgenfritz, Kerler, Müller-Preussker, Stüben, hep-lat/0309059, hep-lat/0309057
Phase structure anticipated from M. Creutz
Taken from talk A. Ukawa, ILFTN workshop in Izu, Japan

Putting things together……

Perhaps, the tip simply stops moving and turns into a line of 1st order transition at some value of beta near 4.0…..

Cf M. Creutz, hep-lat/9608024
Interpretation in the framework of chiral perturbation theory

Sharpe, Singleton; Münster; Sharpe, Wu; Scorzato

Chiral lagrangian uncluding $O(a)$ lattice artefacts

\[
\mathcal{L}_2 = \frac{F_0^2}{4} \text{Tr} \left( \partial_\mu U^\dagger \partial_\mu U \right) - \frac{F_0^2}{4} \text{Tr} \left( \chi U^\dagger + U \chi^\dagger \right) - \frac{F_0^2}{4} \text{Tr} \left( \rho U^\dagger + U \rho^\dagger \right),
\]

\[
U(x) = \exp \left( \frac{i}{F_0} \pi_b(x) \tau_b \right), \quad \chi = 2B_0(\bar{m} 1 - i \mu \tau_3), \quad \rho = 2W_0 a 1
\]

Writing $U = u_0 1 + i u_a \tau_a, \quad a = 1, 2, 3, \quad u \equiv (u_0, u_1, u_2, u_3), \quad u \cdot u = 1$

physical significance of $u_0$

\[
\langle \bar{q} q \rangle = -2F_0^2 B_0 \langle u_0 \rangle
\]
effective potential (at $\mu = 0$)
\[ V = -c_1 u_0 + c_2 u_0^2, \]
where
\[ c_1 = 2F_0^2(B_0 m_q + W_0 a) \]
Including $\mu$ potential up to $O(a^2)$
\[ V = -c_1 u_0 + c_2 u_0^2 + c_3 u_3, \]
\[ c_3 = 2F_0^2 B_0 \mu. \]
First order phase transition for $c_2 < 0$ (case $c_2 > 0$: Aoki phase)
$c_1 = 0 \Rightarrow$ first order phase transition, where $u_0$ changes sign discontinuously.
Properties of phase transition

endpoint of the transition $\mu_c$

$$\mu_c = \frac{|c_2|}{F_0^2 B_0} \sim a^2$$

neutral pion mass

$$m_{\pi 3}^2 = \frac{1}{2F_0^2 |c_2|} (4c_2^2 - c_3^2) \sim a^2$$

ccharged pion mass

$$m_{\pi 1}^2 = m_{\pi 2}^2 = \frac{2 |c_2|}{F_0^2} \sim a^2.$$ 

condensate

$$\Delta < \bar{\chi} \chi > = -4F_0^2 B_0 \sqrt{1 - \frac{c_3^2}{4c_2^2}} = -\frac{4F_0^3 B_0}{\sqrt{2 |c_2|}} m_{\pi 3},$$
Revealing the generic phase structure of lattice QCD
Phase structure of 2-dimensional Wilson twisted mass Gross-Neveu model in large-N

Kei-ichi Nagai, K.J.

extension to twisted mass of old work by
Aoki, PRD 30,2653 ('84), Aoki&Higashijima, Prog. Theor. Phys. 76 521 ('86),
Izubuchi,Noaki,Ukawa, hep-lat/9805019
Dependence of first transition on the gauge action

- plaquette gauge action
- add rectangular loop with coefficient
  - $c_2 = -1.4088$ DBW2 action
  - $c_2 = -1/12$ Tree level Symanzik improved action (tlSym)
Chiral perturbation theory for the phase transition

In the regime \( m/\Lambda_{QCD} \gtrsim a\Lambda_{QCD} \)

\[
M = 2B_0/Z_P \sqrt{m_{PCAC,\chi}^2 + \mu^2} \quad \Lambda_R = 4\pi F_0 \quad \cos \omega = \frac{m_{PCAC,\chi}}{\sqrt{m_{PCAC,\chi}^2 + \mu^2}}
\]

\[
m^2_\pi = M + \frac{8}{F_0^2} \left\{ M^2(2L_{86} - L_{54}) + 4aM \cos \omega(w - \tilde{w}) \right\} + \frac{M^2}{32F_0^2\pi^2} \log \left( \frac{M}{\Lambda_R^2} \right)
\]

\[
f_\pi = F_0 + \frac{4}{F_0} \left\{ ML_{54} + 4a \cos \omega \tilde{w} \right\} - \frac{M}{16F_0\pi^2} \log \left( \frac{M}{\Lambda_R^2} \right)
\]

\[
g_\pi = B_0/Z_P \left[ F_0 + \frac{4}{F_0} \left\{ M(4L_{86} - L_{54}) + 4a \cos \omega(2w_s - \tilde{w}) \right\} - \frac{M}{32F_0\pi^2} \log \left( \frac{M}{\Lambda_R^2} \right) \right]
\]

parameters to fit: \( B_0/Z_P, F_0, L_{86}, L_{54}, w, \tilde{w} \)
Confronting $\chi$PT with simulation data

![Graph 1](am$^2$ vs $\chi$)

![Graph 2](af vs $\chi$)
Where we stand

• tlSym action:
  \[ \beta = 3.75 \ (a = 0.12\text{fm}) \] minimal pion mass of \( m_{\pi}^{\text{min}} > 400\text{MeV} \)
difficult to run, large correlations in plaquette time history
  \[ \beta = 3.9 \ (a = 0.09\text{fm}) \] minimal pion mass of \( m_{\pi}^{\text{min}} = 280\text{MeV} \) on \( 16^3 \cdot 32 \)
smooth runs, no metastabilities

• \( N_f = 2 + 1 + 1 \)
  - Algorithm (PHMC) is working fine
  - first results available
  - tuning not very difficult
Conclusion

★ Wilson twisted mass fermions at maximal twist

→ are $O(a)$-improved

→ with PCAC definition: also $O(a^2)$ effects are small at small quark masses

→ pseudo scalar masses $O(250)\text{MeV}$ can be reached, quenched and dynamical

→ with existing algorithmic improvements performance costs are comparable to (in-exact) staggered fermion simulations

→ $N_f = 2 + 1 + 1$ simulations seem to go smooth (PHMC algorithm, tuning)

⇒ a combination of tlSym gauge and maximally twisted mass fermions defines an action that is ready to go