Numerical lattice QCD with light quarks

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"Towards a serious computation of the b-quark mass"

Rainer Sommer, talk given at a recent specialist's meeting

- Numerical lattice QCD still has important deficits
- Achieving reliability and precision remains to be one of the principal goals in this field

Simulations of lattice QCD with light sea quarks turn out to be much less "expensive" than previously estimated

No of operations [in Tflops×year] required for an ensemble of 100 gauge fields*

$$5\left[\frac{20\ \mathrm{MeV}}{m}\right]^3\left[\frac{L}{3\ \mathrm{fm}}\right]^5\left[\frac{0.1\ \mathrm{fm}}{a}\right]^7$$

Ukawa, Berlin 2001

*Two-flavour QCD, O(a) improved Wilson quarks, quark mass m, $2L \times L^3$ lattice, spacing a

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Ukawa, Berlin 2001

$$0.05\left[\frac{20\text{ MeV}}{m}\right]^{1}\left[\frac{L}{3\text{ fm}}\right]^{5}\left[\frac{0.1\text{ fm}}{a}\right]^{6}$$

Giusti, Tucson 2006

*Two-flavour QCD, O(a) improved Wilson quarks, quark mass m, $2L\times L^3$ lattice, spacing a

- ⋆ *The acceleration is due to progress in algorithms*

  Sexton & Weingarten '92, Hasenbusch '01,
  ML '03f, Urbach et al. '05

- ⋆ *Better program efficiency & faster computers speed-up the simulations by another big factor*

- ⋆ *It is now almost compulsory to include light sea quarks in the simulations*

- ⋆ *Many teams around the world, strong competition*

  ALPHA, Bern, CERN-Rome, ETMC, HPQCD, JLQCD, MILC,
  PACS-CS, QCDSF, RBC, UKQCD, ...

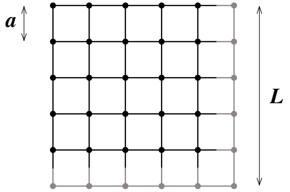
Outline

1. Lattice sizes, etc.
2. Which lattice QCD?
3. Wilson fermions & chiral symmetry
4. Why are QCD simulations so difficult?
5. The DD-HMC algorithm
6. First studies of "QCD light"

Lattice sizes, quark masses, ...

Systematic limitations

- Lattice-spacing and finite-volume effects
- The light-quark mass m is larger than the physical one



Available range of a, L, m must be such that the results can be extrapolated to $a \to 0$, $L \to \infty$ and $m \to 0$

Experience suggests that simulations in the range

$$a = 0.05 - 0.1 \text{ fm}$$

$$M_\pi = 200 - 500 \text{ MeV}$$

$$L \geq 2 \text{ fm}, \quad M_\pi L \geq 3$$

will be required

Example

$a = 0.05$ fm

$L = 3.2$ fm

$M_\pi = 200$ MeV

$\Rightarrow$

128×64^3 lattice $= 33 \times 10^6$ pts

gauge field $= 18$ GB

quark propagator $= 72$ GB

$m \sim \frac{1}{12} m_s \sim 8$ MeV

Which lattice QCD?

The formulation of lattice QCD is not unique

$$S_{\text{lat}} = S_0 + aS_1 + a^2 S_2 + \dots$$

$$\mathcal{O}_{\text{lat}} = \mathcal{O}_0 + a\mathcal{O}_1 + a^2\mathcal{O}_2 + \dots$$

May have different requirements

- Simplicity & conceptual clarity
- Preserve chiral symmetry
- Reduce lattice-spacing effects

Wilson action
Symanzik, LW, Iwasaki actions
O(a) improvement
Improved staggered quarks
Domain-wall fermions
Perfect action
Neuberger fermions
twisted-mass QCD
...

The philosophy adopted here is to

* keep things simple at the fundamental level
  $\Rightarrow$ stick to Wilson's formulation

* develop powerful algorithms and adapted computational strategies

* simulate very large lattices using these

Wilson fermions & chiral symmetry

The Wilson–Dirac operator

$$D_{\rm w} = \frac{1}{2}\{\gamma_\mu(\nabla_\mu^* + \nabla_\mu) - a\nabla_\mu^*\nabla_\mu\} + m_0$$

violates the isovector chiral symmetry

$$\left\langle\left\{\partial_\mu A_\mu^k(x) - 2mP^k(x)\right\}\Phi_1(y_1)\ldots\right\rangle = \text{contact terms} + {\rm O}(a)$$

Wilson '74
Bochicchio, Maiani, Martinelli & Testa '85

Not a fundamental problem, but the effects can be large at the accessible lattice spacings

Can do better by including O(a) counterterms

$$D_{\rm w} \to D_{\rm w} + ac_{\rm sw}\,\frac{i}{4}\,\sigma_{\mu\nu}F_{\mu\nu}$$

$$A_\mu^k \to A_\mu^k + ac_{\rm A}\partial_\mu P^k$$

With properly tuned $c_{\rm sw}$ and $c_{\rm A}$

$$\left\langle \left\{ \partial_\mu A_\mu^k(x) - 2mP^k(x) \right\} \Phi_1(y_1) \ldots \right\rangle = \text{contact terms} + \mathrm{O}(a^2)$$

Symanzik '80

Sheikholeslami & Wohlert '85, ML, Sint, Sommer & Weisz '96, . . .

The residual symmetry violations tend to be small at $a \leq 0.1\,\mathrm{fm}$

Deep in the chiral regime, O(a) improvement is automatic

Sharpe & Singleton '98

Effective chiral theory

$$\mathcal{L}_{\text{eff}} = \tfrac{1}{4}F^2\,\mathrm{tr}\{\partial_\mu U^\dagger \partial_\mu U\} - \tfrac{1}{2}F^2 B\,\mathrm{tr}\{U^\dagger M + M^\dagger U\}$$

$$\overline{\psi}\sigma_{\mu\nu}F_{\mu\nu}\psi \;\longrightarrow\; \Lambda^5\,\mathrm{tr}\{U^\dagger + U\}$$

$\Rightarrow$ counterterm has no physical effect

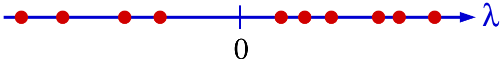
Moreover, on the pion pole,

$$\partial_\mu P^k = B A_\mu^k$$

$\Rightarrow$ counterterm is cancelled by the current normalization

In practice, however, the quark masses cannot be made arbitrarily small

Eigenvalues of the massive hermitian Dirac operator $\gamma_5 D_{\rm w}$



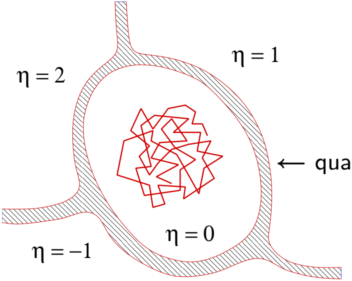
$\mu = \min|\lambda|$ (spectral gap)

$\eta = \frac{1}{2}\{N_{\lambda>0} - N_{\lambda<0}\} \in \mathbb{Z}$ (spectral asymmetry)

$\mu \geq m$ and $\eta = 0$ if chiral symmetry is preserved

Otherwise may have arbitrarily low eigenvalues and non-zero asymmetry

Again not a fundamental problem, but simulations may be trapped



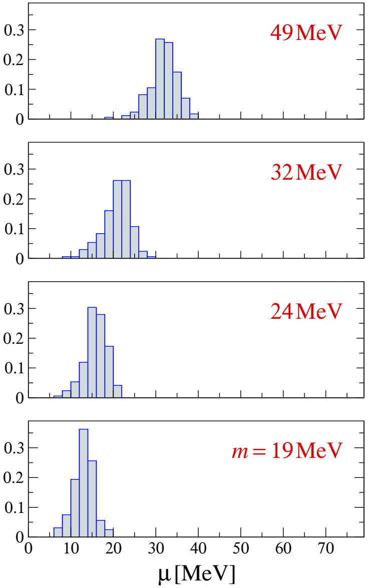
May lead to large statistical fluctuations, incorrect error estimates, fake first-order transitions, . . .

Probability distribution of the gap

$a \simeq 0.08\,\mathrm{fm},\ L \simeq 1.9\,\mathrm{fm}$

$\mathrm{O}(a)$ counterterms included

Del Debbio, Giusti, ML, Tantalo, Petronzio '06



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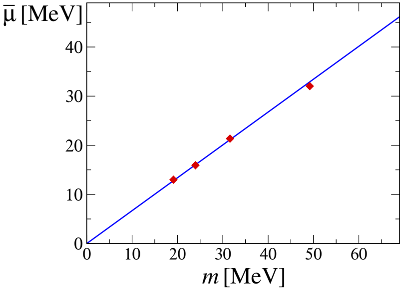
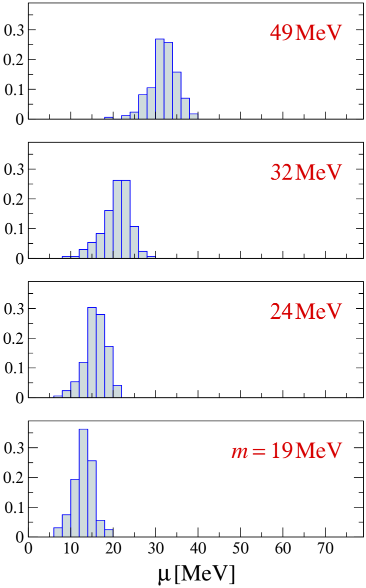
Median of the gap vs quark mass





Width of the distribution

$$\sigma \simeq \frac{a}{\sqrt{V}}, \qquad V \equiv TL^3/a^4$$

Require $\bar{\mu} \geq 3\sigma$ to be safe of accidental zero modes

-
-
-

$\Rightarrow$ *if* $a \leq 0.1\,\mathrm{fm}$, *the condition is fulfilled at any* m *where* $M_\pi L \geq 3$

$\Rightarrow$ *the large-volume regime of QCD is safe*

Summary

- Wilson fermions are simple, conceptually clean and preserve many symmetries of QCD
- Chiral symmetry violations can be reduced to $O(a^2)$
- In the large-volume regime, the Wilson–Dirac operator has a safe spectral gap proportional to m

For most applications of LQCD, Wilson fermions are a good choice

Why are QCD simulations so difficult?

MC methods require $\mathbb{C}$-number fields & non-negative measures
$\Rightarrow$ use pseudo-fermions

$$(\det D_{\mathrm{w}})^2 = \int \mathrm{D}[\phi]\, \mathrm{e}^{-S_{\mathrm{pf}}[\phi]}$$

$$S_{\mathrm{pf}}[\phi] = a^4 \sum_x \phi(x)^\dagger (D_{\mathrm{w}}^\dagger D_{\mathrm{w}})^{-1} \phi(x)$$

The total action is now real and bounded from below but non-local

There is a hierarchy of scales

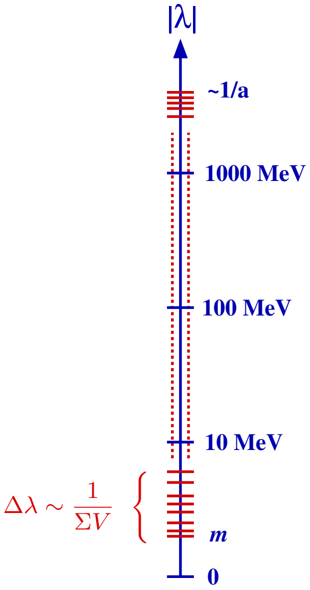
$$m \ll M_\pi \ll 4\pi F_\pi$$

linked to the spontaneous breaking of chiral symmetry

Leutwyler '74; Leutwyler & Smilga '92

$\Rightarrow$ condition number $\lambda_{\max}/\lambda_{\min}$ is large

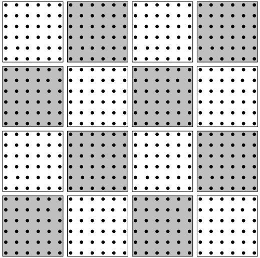
$\Rightarrow$ computation of $D_{\rm w}^{-1}\phi$ is expensive



The DD-HMC algorithm

Uses of domain-decomposition ideas in lattice QCD

- ⋆ Computation of $D_{\mathrm{w}}^{-1}\phi$ using a "Schwarz preconditioner"
- ⋆ Simulation algorithm including a doublet of light sea quarks



ML CPC 156 (2004) 209; CPC 165 (2005) 199

Domain decompositions provide an opportunity to separate low- and high-frequency modes

Let's go into some details ...

The quark determinant factorizes

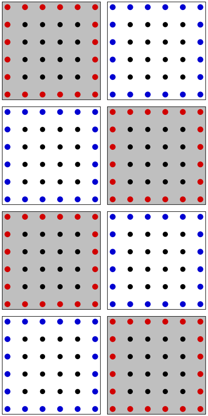
$$\det D_{\rm w} = \prod_{\text{blocks } \Lambda} \det D_\Lambda \times \det R$$

$\uparrow$

$D_{\rm w}$ with Dirichlet b.c.

where the block interaction is given by

$$R = 1 - \sum_{\text{pairs } \Lambda,\Lambda^*} D_\Lambda^{-1} D_{\partial\Lambda} D_{\Lambda^*}^{-1} D_{\partial\Lambda^*}$$



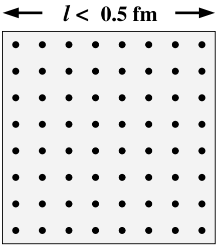
On the blocks an infrared cutoff

$$q \geq \pi/l > 1\,\mathrm{GeV}$$

is implied by the boundary conditions

$\Rightarrow$ *theory is weakly coupled*

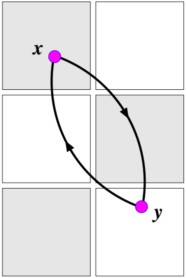
$\Rightarrow$ *easy to simulate at all quark masses*



In other words

$$\det D_{\mathrm{w}} = \underbrace{\prod_{\text{blocks } \Lambda} \det D_{\Lambda}}_{\text{easy}} \times \underbrace{\det R}_{\text{long range}}$$

The block-interactions are actually weak



$$\frac{\delta^2\,(\ln\det D_{\rm w})}{\delta A_\mu^a(x)\delta A_\nu^b(y)} =$$

$$\mathrm{tr}\{T^a\gamma_\mu S(x,y)T^b\gamma_\nu S(y,x)\} \sim |x-y|^{-6}$$

$\Rightarrow$ $\det R$ is a small correction

The DD-HMC algorithm

- builds on these properties
- is exact and scales like m^{-1}
- is well suited for parallel processing

First studies of "QCD light"

Del Debbio, Giusti, ML, Petronzio, Tantalo [CERN – Tor Vergata]

Simulations of two-flavour QCD, including a valence s-quark

- $32 \times 24^3, \ldots, 64 \times 32^3$ lattices
- $a = 0.052, \ldots, 0.079\,\mathrm{fm}$
- $m_{\mathrm{sea}} \equiv m = \frac{1}{4} m_s, \ldots, m_s$
- 100–170 field configurations at each mass

Performed on PC clusters at Bern, CERN, Rome and on a CRAY-XT3 at CSCS Manno

Physical sea-quark effects?

0^- meson propagator at $\vec{p} = 0$

$$\langle PP \rangle \sim \mathrm{e}^{-Mt} + c\,\mathrm{e}^{-M't} + \ldots$$

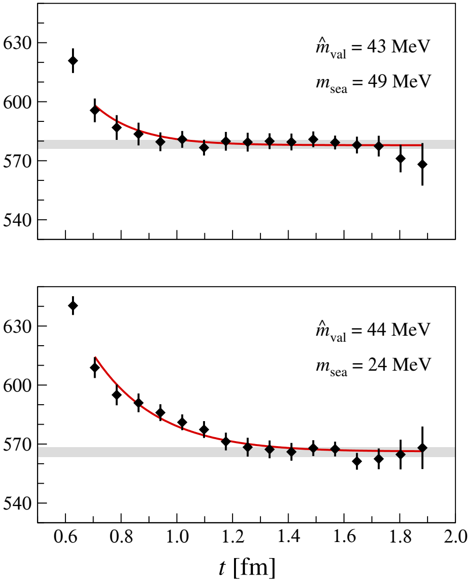
Expect

$$M' = M + 2M_\pi$$

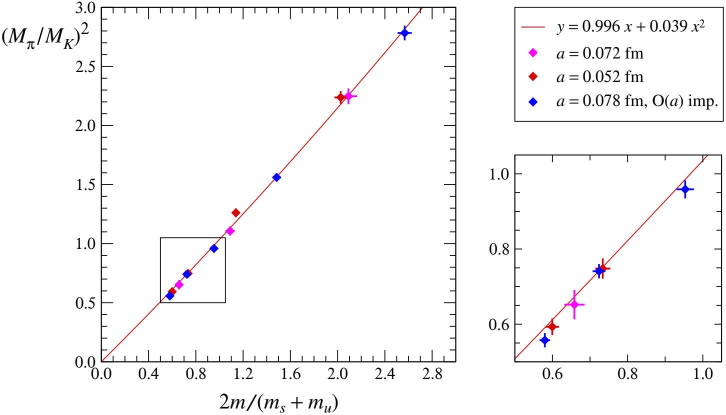
Plots of the effective mass

$$M_{\mathrm{eff}}(t) = -\frac{\mathrm{d}}{\mathrm{d}t} \ln\langle PP \rangle$$

confirm this



Chiral behaviour of the pion mass



Statistical errors are weakly correlated. Surprisingly small cutoff effects!

SU(2) ChPT predicts

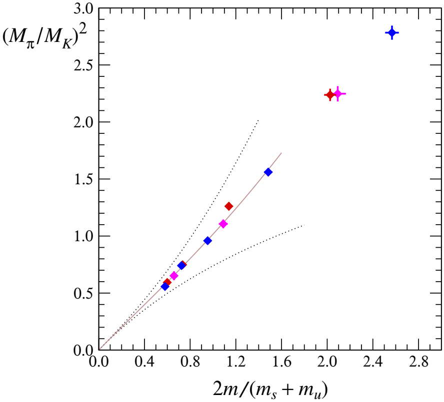
$$M_\pi^2 = M^2 R_\pi, \quad M^2 = 2Bm$$

$$R_\pi = 1 + \frac{M^2}{32\pi^2 F^2} \ln(M^2/\Lambda_3^2) + \ldots$$

where, in real-world QCD,

$$F = 86.2 \pm 0.5\,\mathrm{MeV}$$

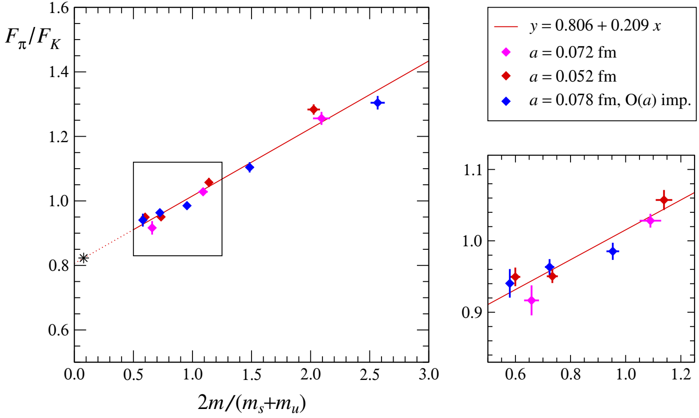
$$\ln(\Lambda_3^2/M^2)\big|_{M=139\,\mathrm{MeV}} = 2.9 \pm 2.4$$



Gasser & Leutwyler '84

⇒ *NLO ChPT is compatible with the data up to $M_\pi \simeq 600$ MeV*

Pseudo-scalar decay constant

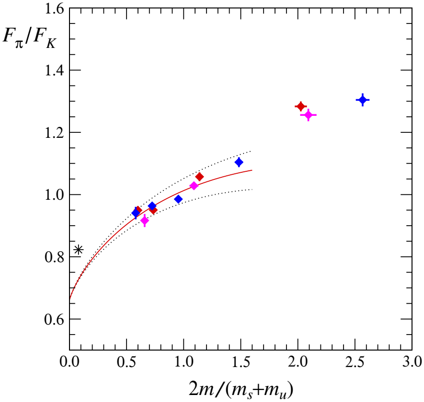


From ChPT one expects

$$F_\pi = F - \frac{M^2}{16\pi^2 F} \ln(M^2/\Lambda_4^2) + \ldots$$

$$\ln(\Lambda_4^2/M^2)\big|_{M=139\,\mathrm{MeV}} = 4.4 \pm 0.2$$

Colangelo, Gasser & Leutwyler '01



Not sure what to conclude

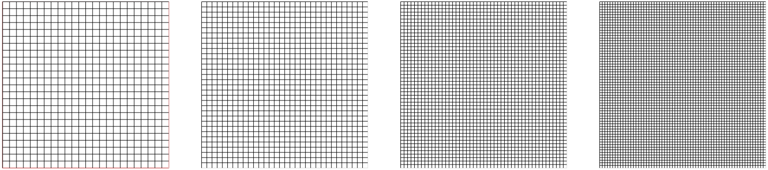
- Finite-volume and lattice effects must be understood
- Will need more data at smaller quark masses

Concluding remarks & perspectives

In the last few years, there has been important technical progress in numerical lattice QCD

$\Rightarrow$ *the principal obstacle (inclusion of the sea quarks) is practically gone*

48×24^3 | 64×32^3 | 96×48^3 | 128×64^3

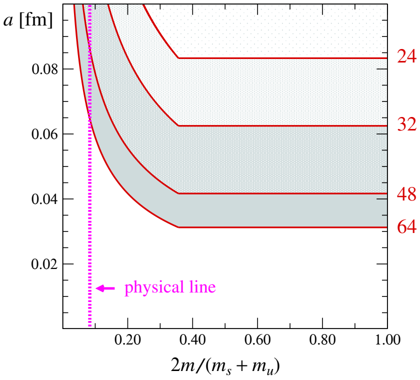


1997 | 2005 | 2007 | 2011?

On a given lattice, the bounds

$$L \geq 2\,\mathrm{fm} \quad \text{and} \quad M_\pi L \geq 3$$

set a limit on the range of a and m



How about including the strange quark? Not so difficult . . . PACS-CS '06

Now look forward to studying light-quark physics!