Stability of lattice QCD simulations and the thermodynamic limit

Martin Lüscher

CERN — Theory Division

In collaboration with L. Del Debbio, L. Giusti, R. Petronzio, N. Tantalo

"At small quark masses, lattice QCD with Wilson quarks is difficult to simulate, because the massive Wilson–Dirac operator is not protected from arbitrarily low eigenvalues"

Chiral Perturbation Theory confronts Lattice QCD, Valencia, 29–30 November 2005

Spectral gap, asymmetry, . . .

Hermitian Wilson–Dirac operator

$$Q_{\rm m} = \gamma_5 D_{\rm m}$$

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

Spectral gap

$$\mu = \min\{|\lambda| \mid \lambda \text{ is an eigenvalue of } Q_{\rm m}\}$$

Spectral asymmetry

$$\eta = \tfrac{1}{2}\{N_{\lambda\geq 0} - N_{\lambda<0}\} \in \mathbb{Z}$$

With Ginsparg–Wilson quarks we have

$\mu \geq m =$ bare current-quark mass

$\eta = 0 \quad (\text{if } m > 0)$

Wilson quarks break chiral symmetry

$\Rightarrow$ $\mu \ll m$ is not excluded

$\Rightarrow$ there can be fields with $\eta \neq 0$

The distributions of μ and η are properties of the theory, not of a particular simulation algorithm

Stability and the spectral gap

Stable situation

⇒ HMC algorithm works well

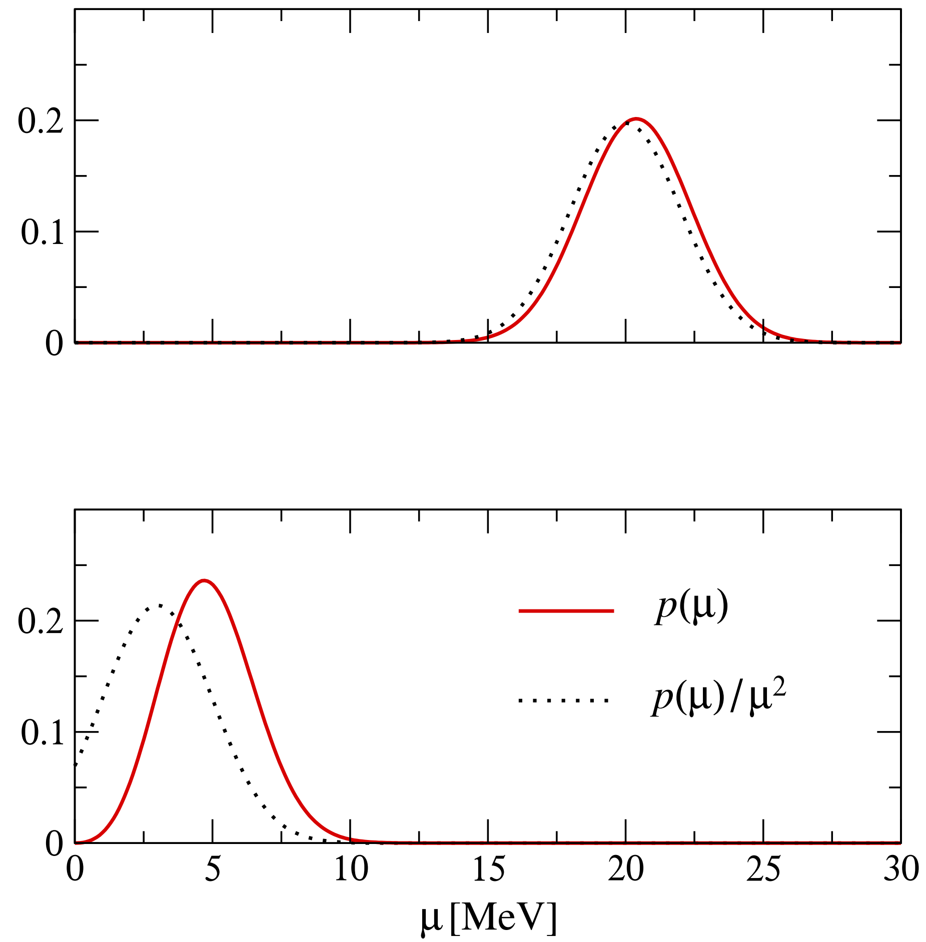
⇒ Small statistical fluctuations

Potentially unstable situation

⇒ HMC becomes inefficient

⇒ Ergodicity problems

$p(\mu)$: distribution of the gap



In unquenched QCD this is not a fundamental problem

Ergodicity?

- $\Delta\eta = \pm 1$ if an eigenvalue of Q_{m} crosses 0

- The HMC algorithm tends to preserve η

$\Rightarrow$ an ergodicity problem can arise

- ◇ in the "unstable" situation
- ◇ during thermalization

May lead to long autocorrelation times, incorrect error estimates, fake first-order transitions, ...

Empirical studies of the gap

Simulations using the Schwarz-preconditioned HMC algorithm

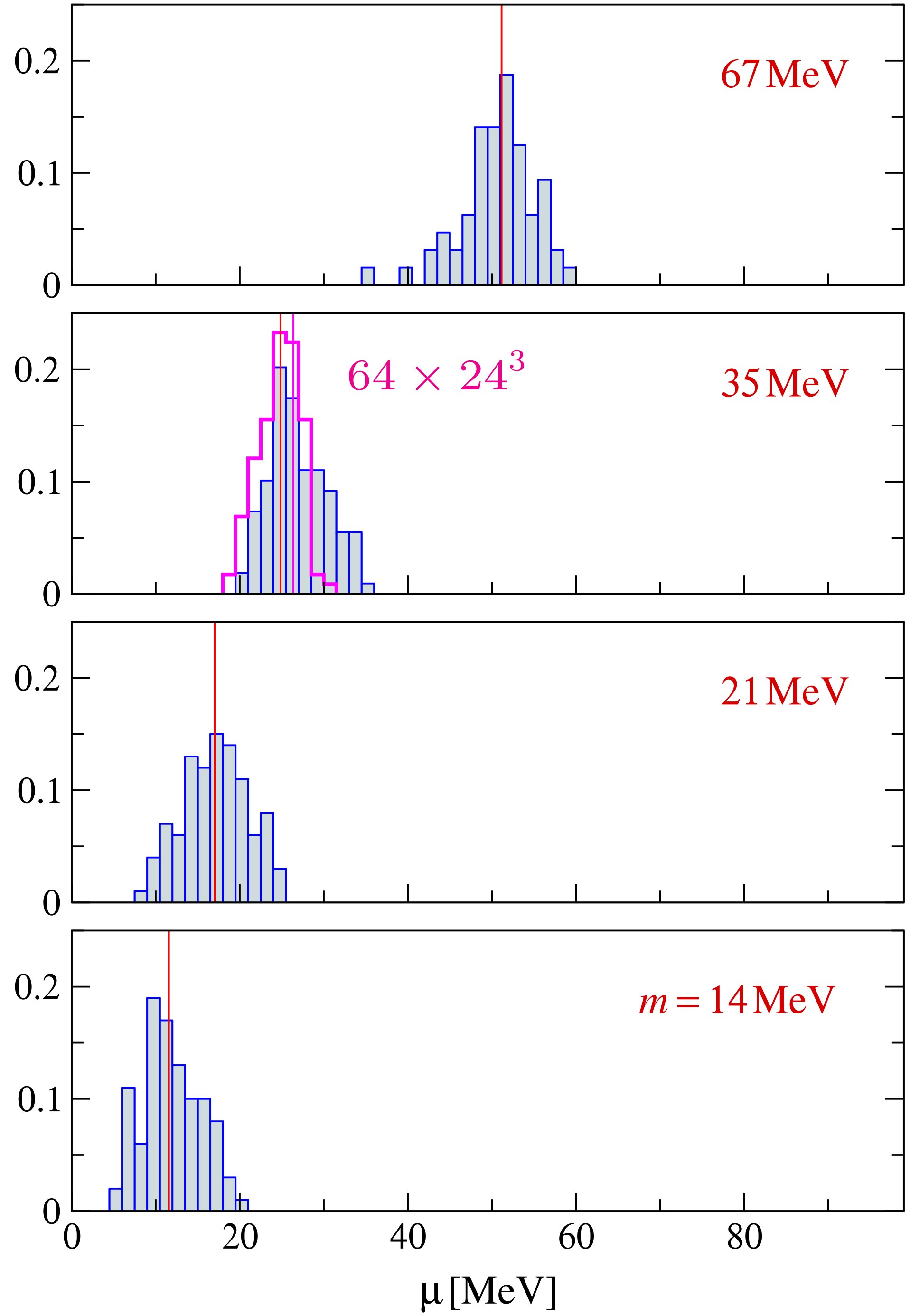
Run Id	Lattice	β	$c_{\rm sw}$	κ	$\sim m/m_{\rm s}$	$N_{\rm cfg}$
A_1	32×24^3	5.6	0	0.15750	0.93	64
A_2				0.15800	0.48	109
A_3				0.15825	0.30	100
A_4				0.15835	0.17	100
B_1	64×32^3	5.8	0	0.15410	0.88	100
B_2				0.15440	0.50	101
C_1	64×24^3	5.6	0	0.15800	0.48	116
D_1	48×24^3	5.3	1.9095	0.13550	1.05	104

Performed at Bern (8 nodes), CERN (32 nodes) and the Fermi Institute (64 nodes)

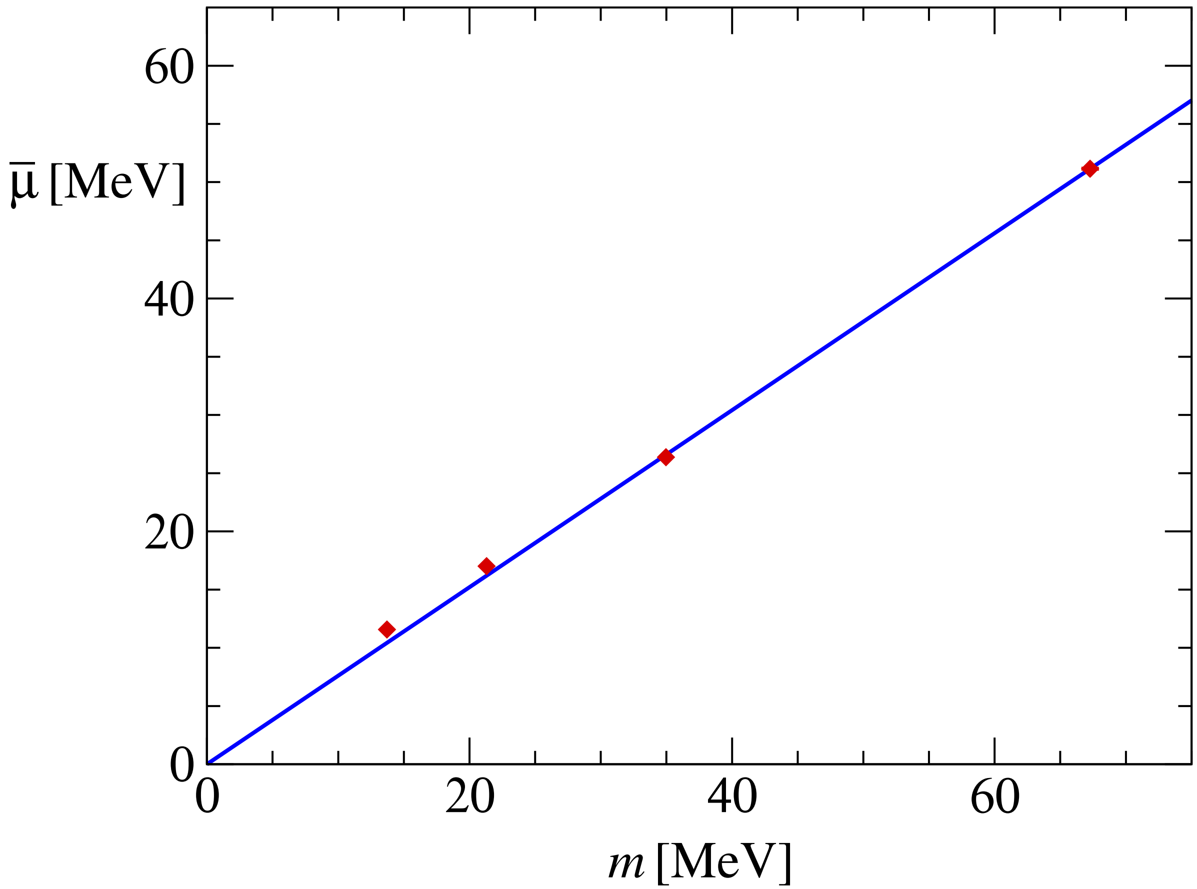
32×24^3 lattice (A_1–A_4)

$a \simeq 0.08$ fm

$m_\pi = 294$–676 MeV



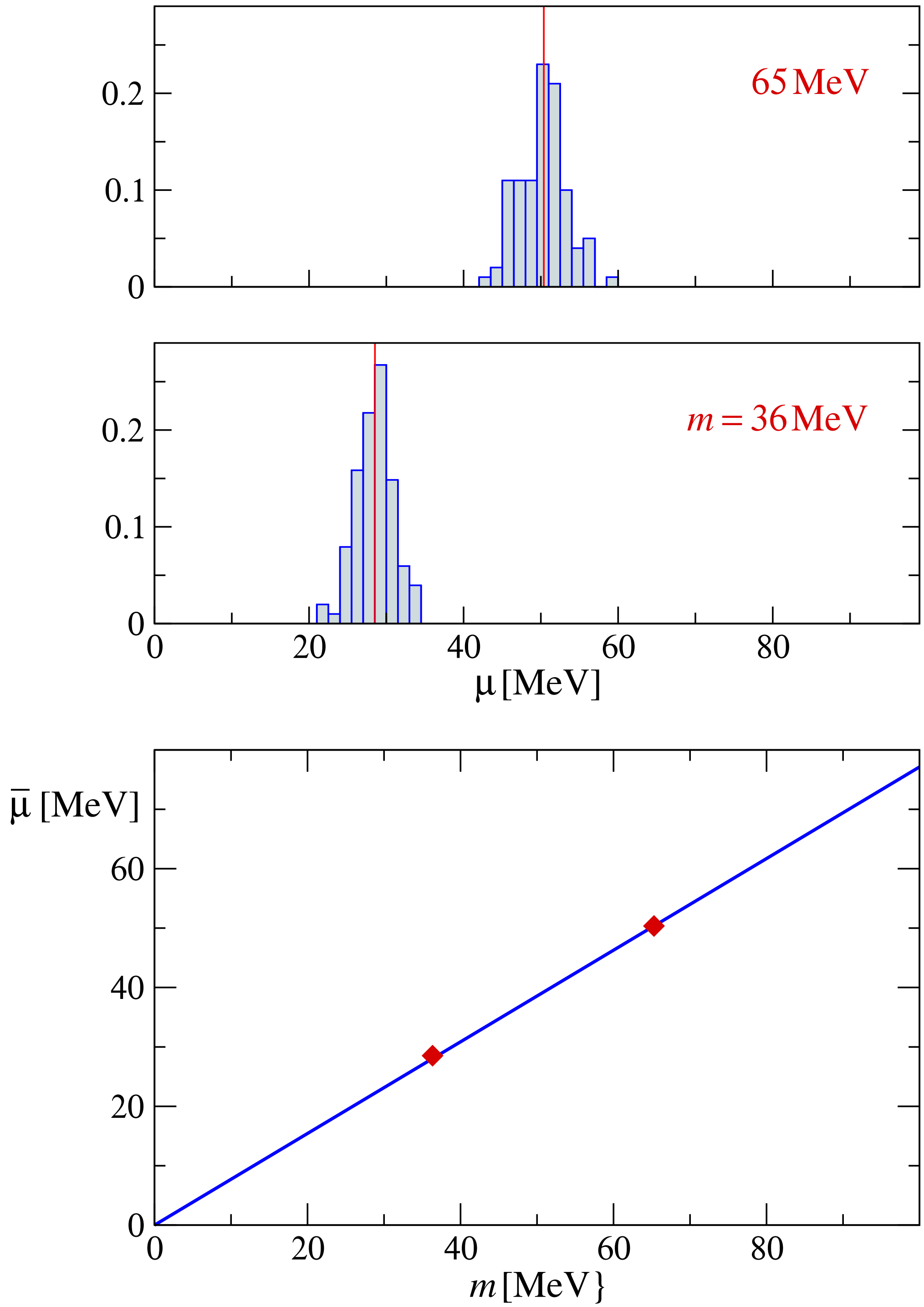
Mass-dependence of the median $\bar{\mu}$ $(32 \times 24^3$ lattice, A_1–$A_4)$



64×32^3 lattice (B_1, B_2)

$a \simeq 0.06$ fm

$m_\pi = 496, 658$ MeV



Statistical fluctuations of the gap

Consider a random fluctuation of the gauge field

$$\delta U(x,\mu) = \omega(x,\mu) U(x,\mu)$$

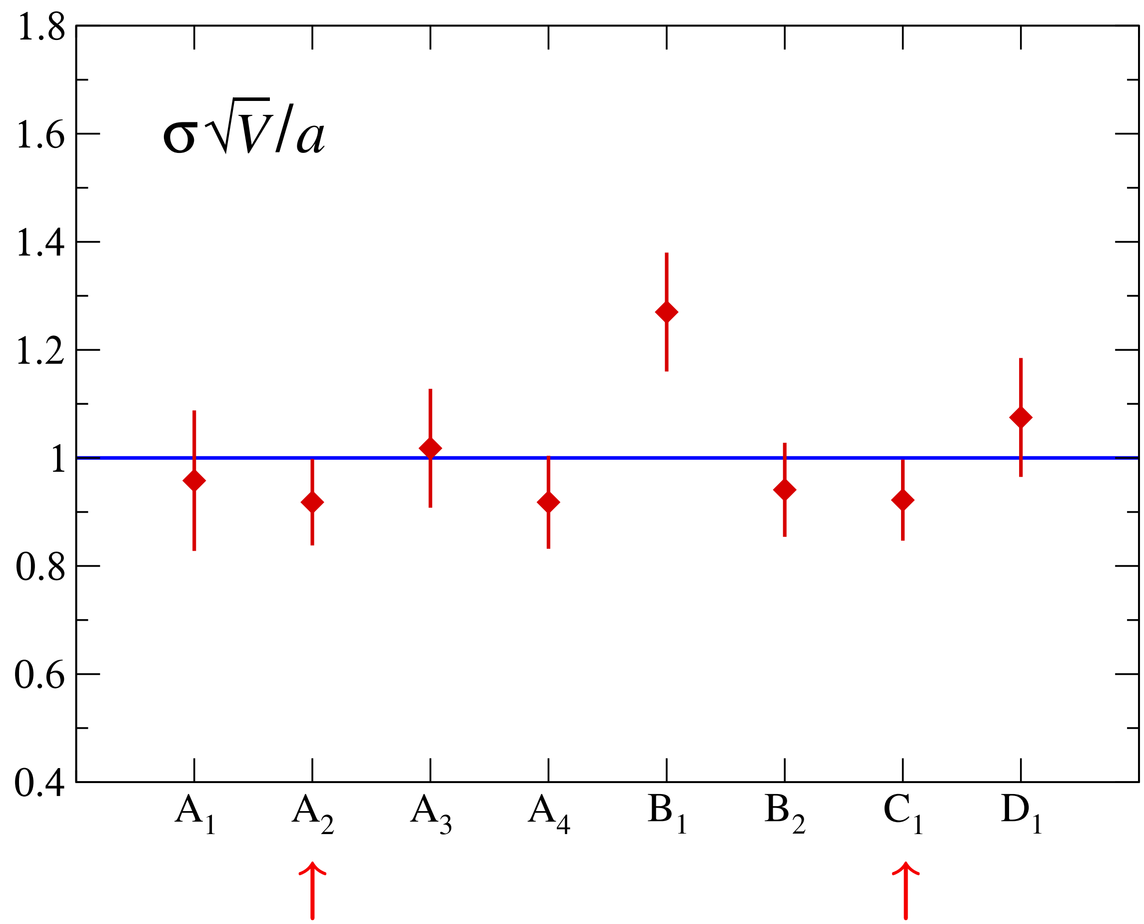
To first order we have

$$\delta\mu = a^4 \sum_x \psi(x)^\dagger \delta Q_{\mathrm{m}} \psi(x), \qquad a^4 \sum_x |\psi(x)|^2 = 1$$

If the lowest mode extends over the whole lattice, this implies

$$\left\langle (\delta\mu)^2 \right\rangle \propto \frac{a^2}{V}$$

Suggests that the width σ of the gap distribution scales like $a/\sqrt{V}$



$\sigma\sqrt{V}/a$
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
A_1
A_2
A_3
A_4
B_1
B_2
C_1
D_1

Stability range

Define the stability range through $\bar{\mu} \geq 3\sigma$

$$m \geq \frac{3a}{Z\sqrt{V}} = \frac{3a}{Z\sqrt{2}L^2} \quad \text{(on } 2L \times L^3 \text{ lattices)}$$

$$\bar{\mu} \simeq Zm$$

$$\sigma \simeq a/\sqrt{V}$$

Substituting $m_\pi^2 = 2Bm$, this becomes

$$m_\pi L \geq \sqrt{3\sqrt{2}aB/Z}$$

$$m_\pi L \geq \begin{cases} \mathbf{2.8} & \text{at } a = 0.08 \text{ fm} \\ \mathbf{2.3} & \text{at } a = 0.06 \text{ fm} \\ \mathbf{3.2} & \text{at } a = 0.09 \text{ fm, O}(a) \text{ improved} \end{cases}$$

$\Rightarrow$ *constraint is irrelevant in the large-volume regime of QCD*

Theoretical issues

- What is the precise relation between $\bar{\mu}$ and m?
- Are the lowest modes extended over the whole lattice?
- Can the eigenvalue distributions be computed in ChPT or RMT?

Spectral density in infinite volume

Let $\alpha_1 \leq \alpha_2 \leq \ldots$ be the eigenvalues of Q_{m}^2

$$\rho(\alpha) = \lim_{V\to\infty} \frac{1}{V} \sum_{k\geq 1} \langle \delta(\alpha - \alpha_k) \rangle$$

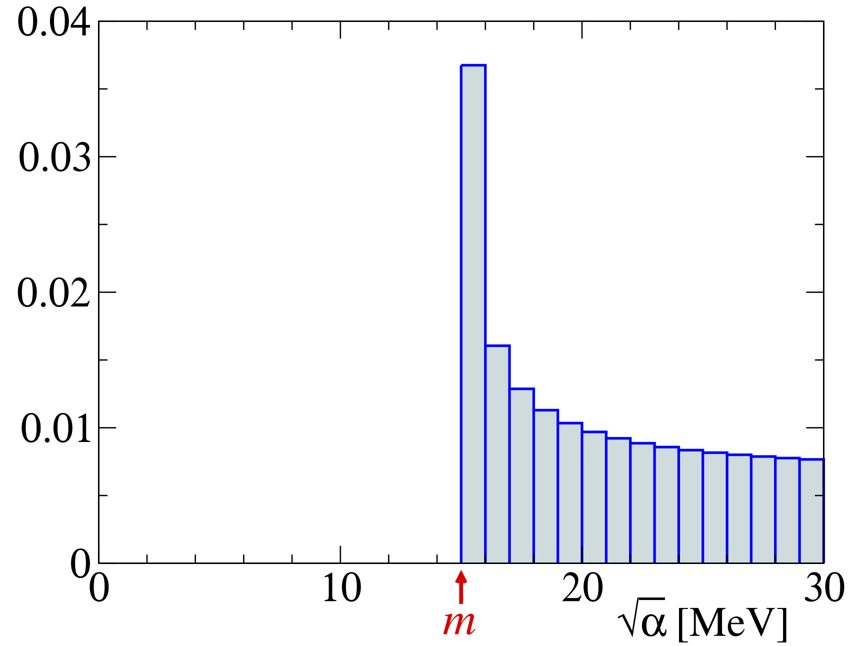
⋆ Limit exists   van Hemmen '82

⋆ Single eigenvalues don't count

⋆ With GW quarks

$$\rho(\alpha) \underset{\alpha\downarrow m^2}{=} \frac{\Sigma}{\pi\sqrt{\alpha - m^2}}$$

Number of modes per bin and fm^4



Working hypothesis

The spectral density $\rho(\alpha)$ *vanishes below some* $\bar{\alpha} > 0$*,*
and it is non-zero at or immediately above this value

It is then possible to show that

⋆ $\rho(\alpha)$ is multiplicatively renormalizable

⋆ $\sqrt{\bar{\alpha}} = Z_{\mathrm{A}} m$ up to $\mathrm{O}(a)$ corrections

Renormalization (abbreviated)

Resolvent

$$R(z) = \int_{\bar{\alpha}}^{\infty} \mathrm{d}\alpha \, \frac{\rho(\alpha)}{\alpha^2(z-\alpha)}$$

Expansion for $|z| < \bar{\alpha}$

$$R(z) = \sum_{k=0}^{\infty} M_k z^k, \qquad M_k = -\int_{\bar{\alpha}}^{\infty} \mathrm{d}\alpha \, \frac{\rho(\alpha)}{\alpha^{k+3}}$$

$$M_k = a^{4n-4} \sum_{x_1,\ldots,x_{n-1}} \langle P_{12}(x_1) P_{23}(x_2) \ldots P_{n1}(0) \rangle \,, \quad n = 2k+6$$

$\Rightarrow$ the moments M_k renormalize multiplicatively with $(Z_{\mathrm{P}})^n$

The renormalized quantities

$$\rho_{\mathrm{R}}(\alpha) = Z_{\mathrm{P}}^2 \rho\big(Z_{\mathrm{P}}^2 \alpha\big)\,, \qquad \bar{\alpha}_{\mathrm{R}} = Z_{\mathrm{P}}^{-2} \bar{\alpha}$$

are thus expected to have a well-defined continuum limit

Relation to the current-quark mass m

Renormalization & universality

$$m_{\mathrm{R}} = Z_{\mathrm{A}} Z_{\mathrm{P}}^{-1} m \quad \Rightarrow \quad \frac{\sqrt{\bar{\alpha}_{\mathrm{R}}}}{m_{\mathrm{R}}} = \text{independent of } Z_{\mathrm{P}} = \text{universal} = 1$$

The bare quantities thus satisfy $\sqrt{\bar{\alpha}} = Z_{\mathrm{A}} m$, up to $\mathrm{O}(a)$ corrections

Run Id	Z_{A}	$\bar{\mu}/m$	$\bar{\mu} - Z_{\mathrm{A}} m$ [MeV]	N_{lower}
A_1	$0.78(2)^a$	$0.76(1)$	-1.4	1
A_2	$0.78(1)^a$	$0.75(1)$	-1.1	1
A_3	$0.79(*)^b$	$0.80(3)$	0.2	0
A_4	$0.79(*)^b$	$0.85(4)$	0.8	0
B_1	$0.78(2)^a$	$0.77(1)$	-0.6	1
B_2	$0.80(*)^b$	$0.78(1)$	-0.6	1
C_1	$0.78(1)^a$	$0.72(1)$	-2.1	1
D_1	$0.75(1)^c$	$0.68(1)$	-5.3	2

[a] RI-MOM, Bećirević et al. ($\mathrm{SPQ_{CD}R}$ collab.) '05

[b] Tadpole-improved boosted perturbation theory

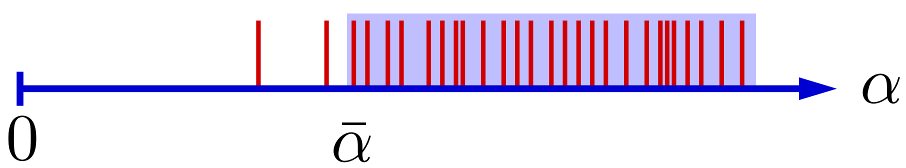
[c] SF chiral Ward identity, Della Morte et al. (ALPHA collab.) '05

$\Rightarrow$ $\bar{\mu} \simeq Z_{\mathrm{A}} m$ on all lattices

$\Rightarrow$ data support working hypothesis

However, the detailed behaviour of $\bar{\mu}$ may be complicated

- It is possible that $\lim_{V\to\infty} \bar{\mu} \neq \sqrt{\bar{\alpha}}$



- There could be important O(a) corrections

Conclusion

In the large-volume regime, the massive Wilson–Dirac operator is, effectively, protected from arbitrarily low eigenvalues

On $2L \times L^3$ lattices with $a \leq 0.1$ fm, there is a safe spectral gap if $m_\pi L \geq 3$

Simulations in this regime are feasible using current technologies

⋆ No ergodicity problems, stability, efficiency

⋆ Small statistical errors

⋆ Anyway required for the baryons, pion phase shifts, ...