Cutoff-effects in the spectrum of dynamical Wilson fermions

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ALPHA Collaboration

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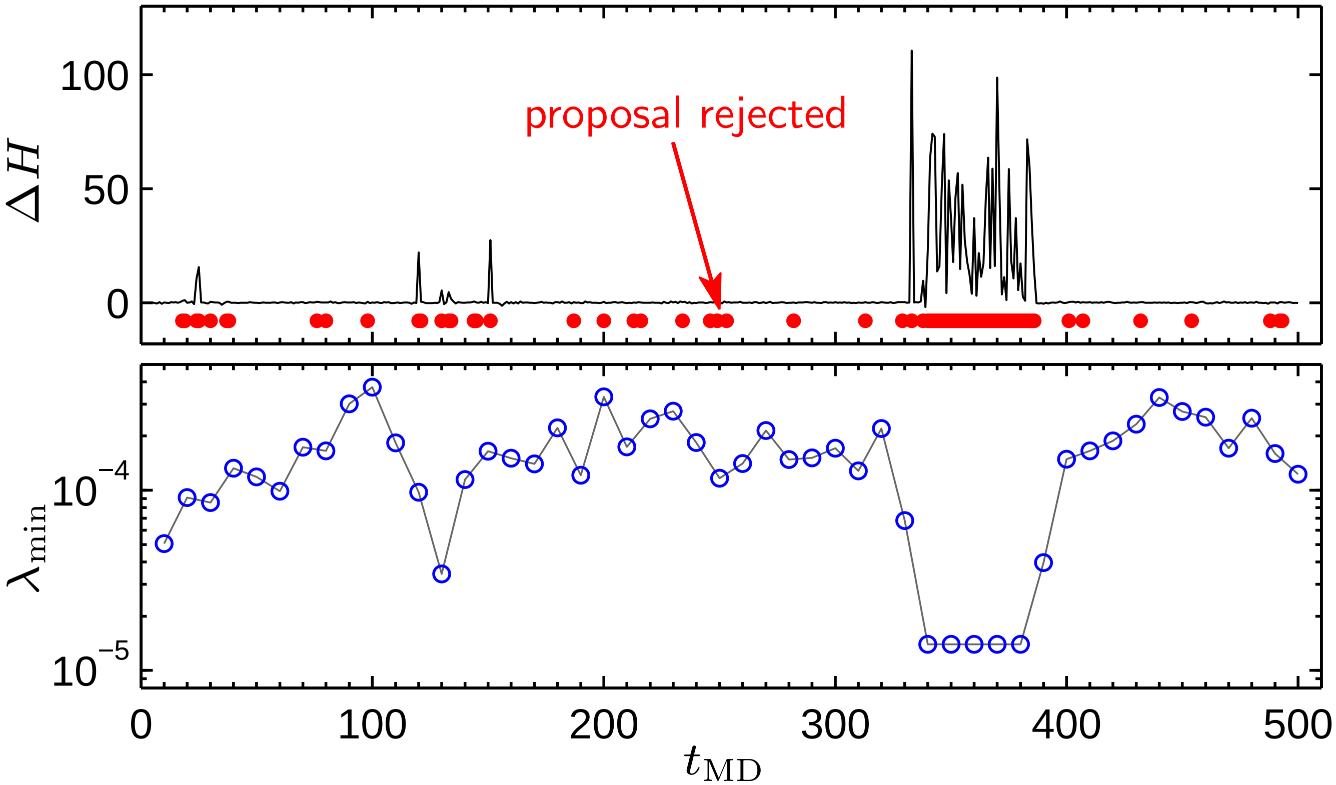
Overview

- Motivation: Algorithmical problems
- Setup and parameters
- Comparison of small eigenvalue distribution: $N_f = 0$ vs. $N_f = 2$
- Finer lattices
- Conclusions

Motivation

HMC, $N_f = 2$
$8^3 \times 18$ lattice
$\beta = 5.2$
$\kappa = 0.1355$



small eigenvalues
$\downarrow$
Large MD forces
$\downarrow$
MD evolution difficult

Joo et.al. 2000

Also: small eigenvalues $\longrightarrow$ large propagators $\longrightarrow$ "spikes" in fermionic observables

Both problems are related to the occurrence of very small eigenvalues of the Dirac operator	$\Longrightarrow$	This is an unexpected problem for our dynamical simulations (IR cutoffs!).

Setup

Action, parameters, geometry:

$\longrightarrow$ Two dynamical flavors of non–perturbatively improved Wilson fermions

$\longrightarrow$ Schrödinger functional (SF): Dirichlet boundary conditions in time,
periodic b.c.'s in space.

$\longrightarrow$ bare gauge coupling $\beta = 5.2$ & 5.5,
corresponding to $a \simeq 0.1$ & $0.07\,\mathrm{fm}$

$\longrightarrow$ lattice volume $L^3 \times T \simeq 1\,\mathrm{fm}^4$

$\Rightarrow$ **Two IR cutoffs: quark mass & SF cutoff**

Algorithms:

$\longrightarrow$ HMC with two pseudo–fermion fields — Hasenbusch 01

$\longrightarrow$ Polynomial HMC (PHMC) — Frezzotti, Jansen 97

- correct ensemble averrage is given by:

$$\langle O \rangle = \frac{\langle O W \rangle_P}{\langle W \rangle_P}$$

denotes average over PHMC ensemble

reweighting factor

- more efficient sampling of configurations carrying small eigenvalues

Error analysis

Autocorrelated data:

$\longrightarrow$ numerical integration of the autocorrelation function for primary and derived observables

Madras & Sokal 88, Wolff 03

Histograms for PHMC:

$\longrightarrow$ observable $f = \langle \phi[U] \rangle$

$\longrightarrow$ probability that ϕ is in interval $I_n = [i_n, i_{n+1}]$:

$$P_n = \langle \chi_n(\phi) \rangle, \quad \text{where} \quad \chi_n(x) = \begin{cases} 1 & x \in I_n \\ 0 & x \notin I_n \end{cases}$$

$\Rightarrow$ for PHMC: $P_n = \langle \chi_n(\phi) \rangle = \dfrac{\langle \chi_n(\phi) W \rangle_P}{\langle W \rangle_P}$

$\Rightarrow$ error analysis of this ratio gives a "reweighted histogram with errorbars"

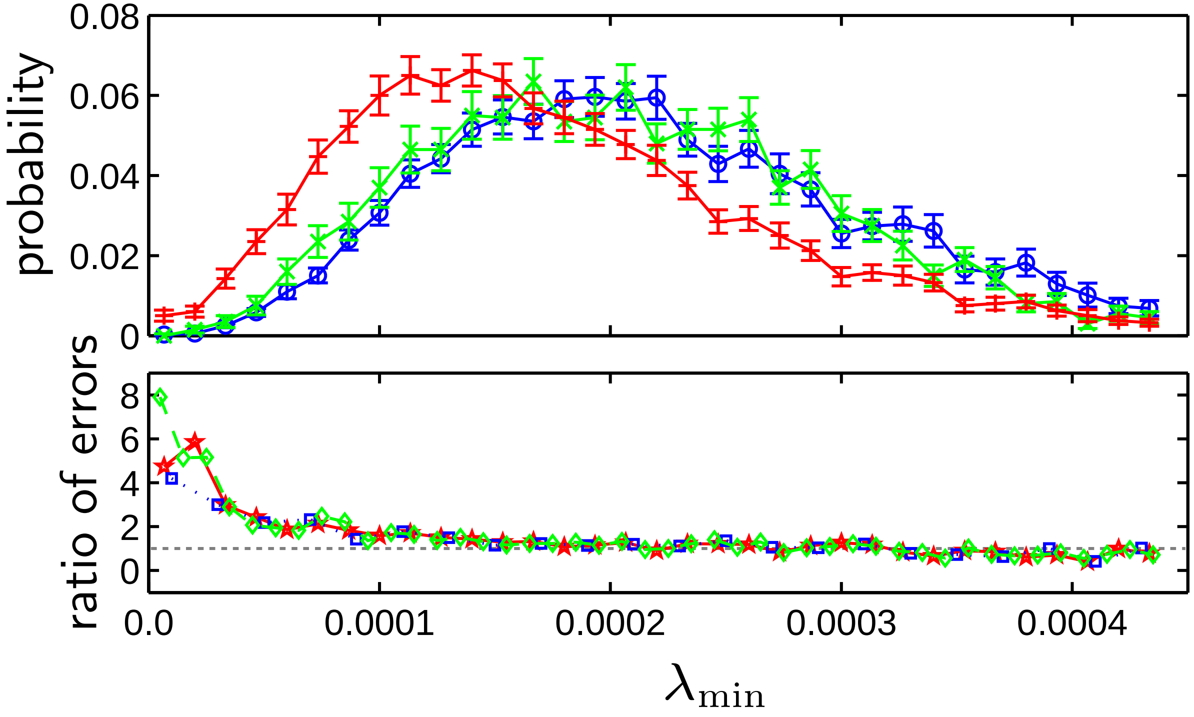
Hermitian, even-odd preconditioned Dirac operator

$\longrightarrow$ example: $\lambda_{\min}$, the smallest eigenvalue of $\hat{Q}^2$

Error analysis: Example

The smallest eigenvalue $\lambda_{\min}$:

PHMC unreweighted
HMC
PHMC



$$\frac{\text{bin-error from HMC}}{\text{bin-error from PHMC}}$$

(same # of independent measurements)

PHMC produces more configurations with small eigenvalues
→ smaller error on the distribution at the infrared end.

$N_f = 2$ versus $N_f = 0$ at matched physics

Naïve expectation: Determinant suppresses small eigenvalues

$$\langle O \rangle = \int_{\text{fields}} O\, e^{-S_g} \det(D+m)^{N_f}$$

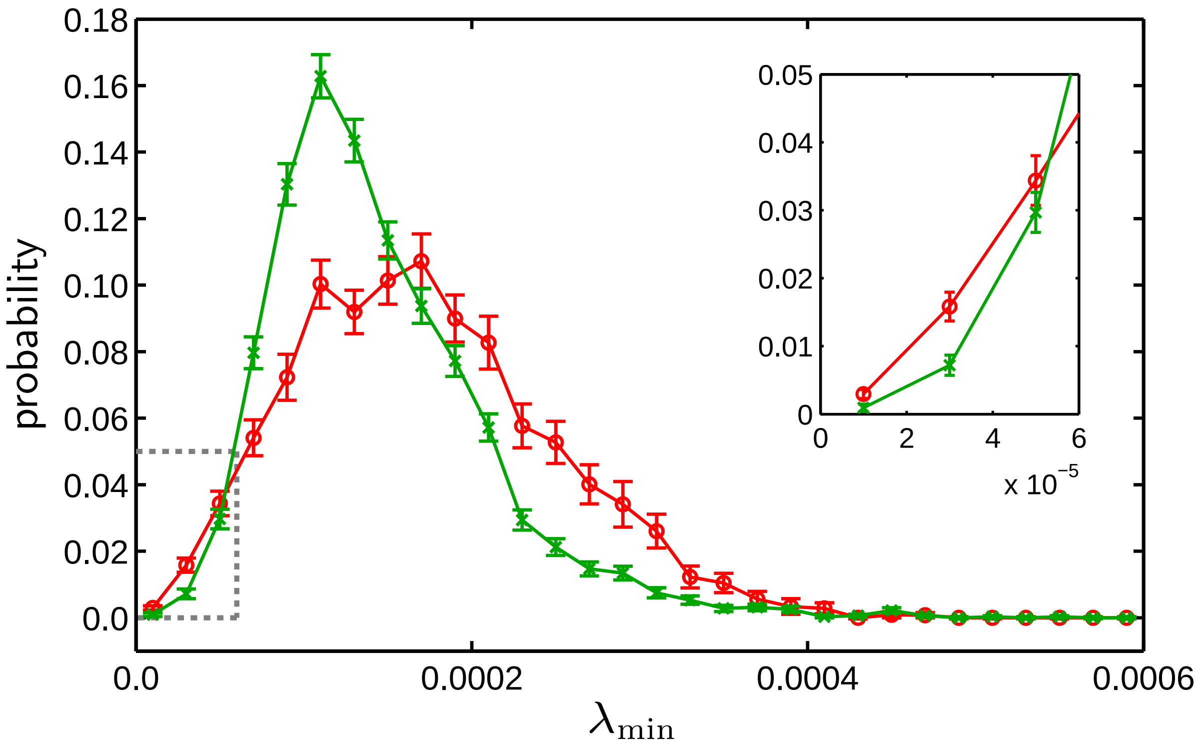
Lattice size: $8^3 \times 18$

Lattice spacing: $\simeq 0.1\text{fm}$

Lm_{PS} fixed UKQCD 02

$N_f = 0 \quad (\beta = 6.0)$:
$\langle \lambda_{\min} \rangle = 1.44(1) \cdot 10^{-4}$
$P(\lambda_{\min} < 4 \cdot 10^{-5}) = 0.81(16)\%$

$N_f = 2 \quad (\beta = 5.2)$:
$\langle \lambda_{\min} \rangle = 1.72(5) \cdot 10^{-4}$
$P(\lambda_{\min} < 4 \cdot 10^{-5}) = 1.88(26)\%$



The determinant increases the average smallest eigenvalue, but: we now find more very small eigenvalues. . . → cutoff–effect?

Finer lattices

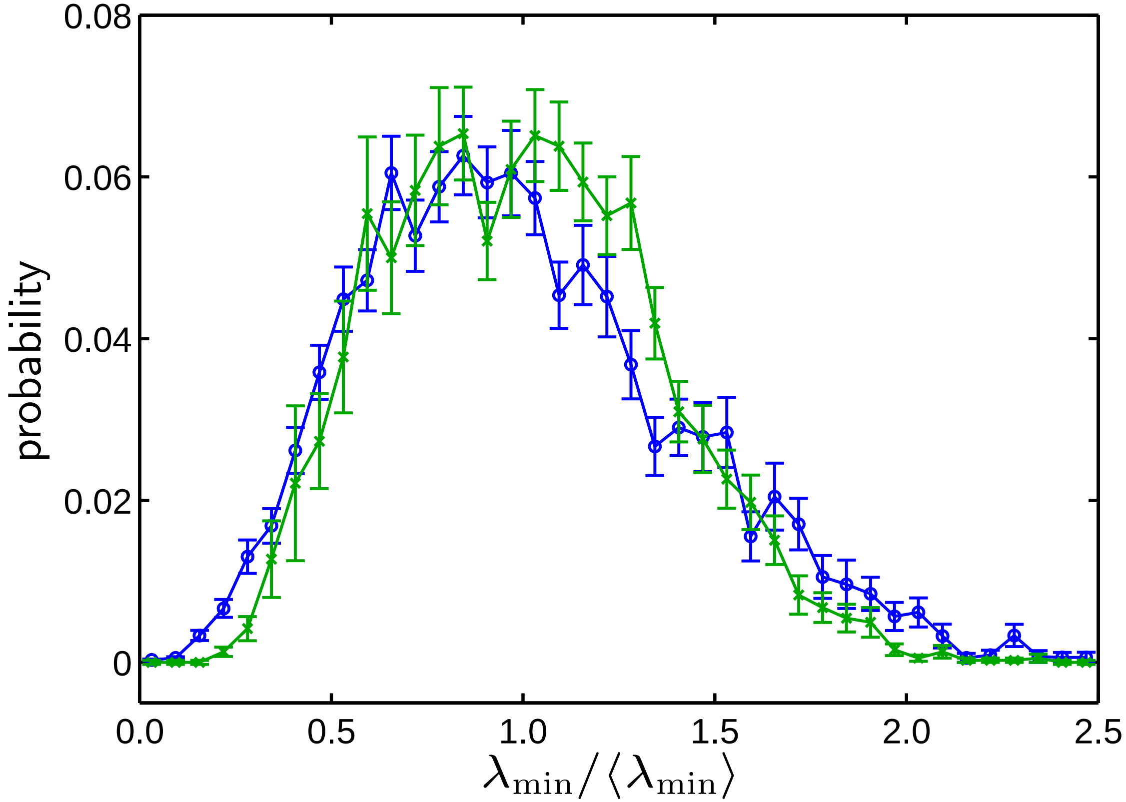
Through matching using the SF coupling $\bar{g}^2$ find β' such that

the lattice spacing a' is: $$\frac{a(\beta = 5.2)}{a(\beta = \beta')} = \frac{12}{8} \qquad \Rightarrow \quad \beta' \simeq 5.5$$

algo.	PHMC	HMC
size	$8^3 \times 18$	$12^3 \times 27$
β	5.2	5.5

— Lm_{PCAC} fixed —

Only on the finer lattice the spectrum is well separated from zero!



The tail of the distribution of λ_{min} is interpreted as a cutoff–effect.

$N_f = 2$ versus $N_f = 0$ at a finer lattice spacing

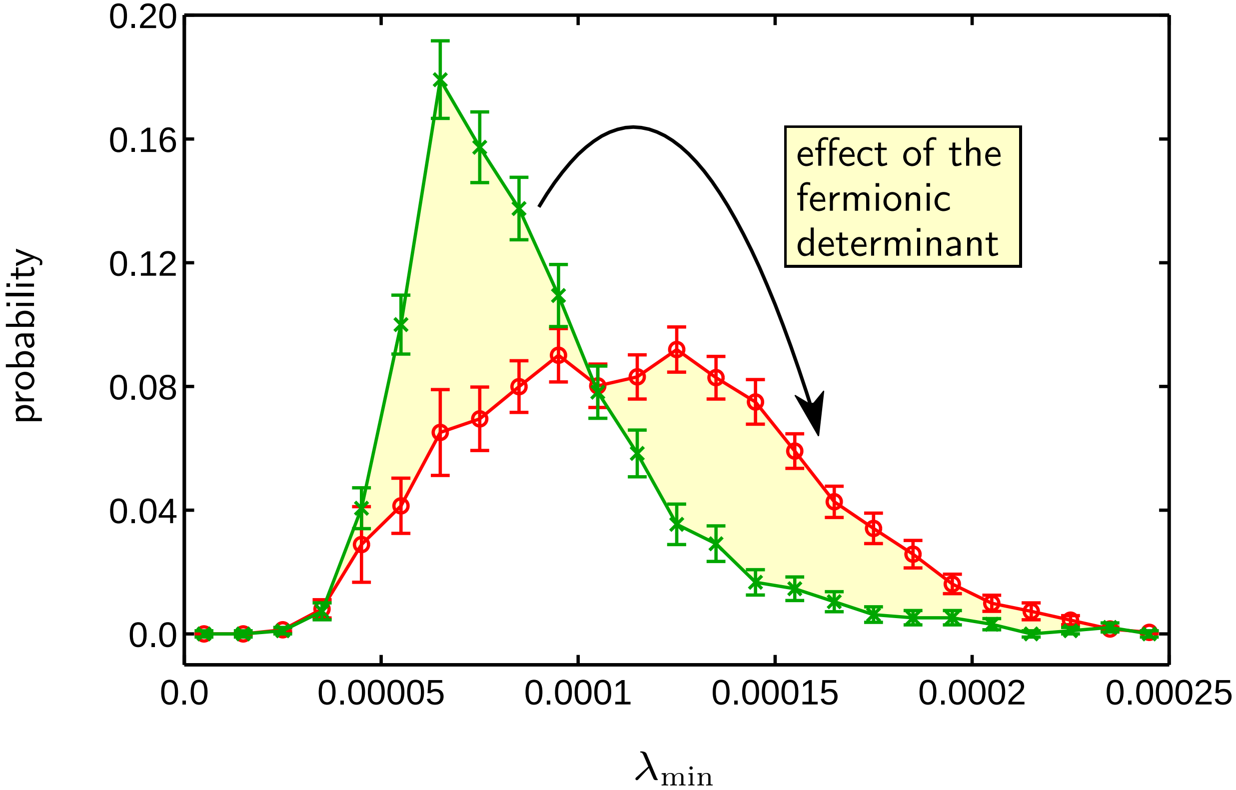
Lattice size: $12^3 \times 27$

Lattice spacing: $\simeq 0.07\mathrm{fm}$

— Lm_{PCAC} fixed —

$N_f = 0 \quad (\beta = 6.26)$:
$\langle \lambda_{\min} \rangle = 0.88(1) \cdot 10^{-4}$

$N_f = 2 \quad (\beta = 5.5)$:
$\langle \lambda_{\min} \rangle = 1.16(6) \cdot 10^{-4}$



The excess of very small eigenvalues in the dynamical case has disappeared, which supports our interpretation as a cutoff–effect.

Conclusions

→ Problems in simulating dynamical Wilson fermions at a lattice spacing of $\simeq 0.1\mathrm{fm}$ are due to the occurrence of very small eigenvalues

→ HMC (with two pseudo–fermions) and PHMC show comparabel performance, but PHMC is well adapted to sample this part of the spectrum

At (approximately) matched physical parameters we find

$a \simeq 0.1\mathrm{fm}$ → compared to the quenched case $\langle \lambda_{\mathrm{min}} \rangle$ is larger with two dynamical fermions, but the distribution has a much longer tail towards zero

$a \simeq 0.07\mathrm{fm}$ → again $\langle \lambda_{\mathrm{min}} \rangle$ is larger for $N_f = 2$ and for both the spectrum is well separated from zero

At $\beta = 5.2$ the spectrum of the Wilson–Dirac operator is strongly distorted. This is a cutoff–effect and disappears rapidly with increasing β.