Fluctuations and Reweighting of the Quark Determinant

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in collaboration with

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College of William and Mary - July 16^{th}, 2008 the idea of reweighting the quark determinant is not novel

- A. Duncan, E. Eichten, H. Thacker,
  An Efficient Algorithm for QCD with Light Dynamical Quarks,
  Phys. Rev. D59 (1999) 014505
- A. Duncan, E. Eichten, Y. Yoo,
  Unquenched QCD with light quarks,
  Phys. Rev. D68 (2003) 054505
- M. Della Morte, R. Hoffmann, F. Knechtli, U. Wolff,
  Impact of large cutoff-effects on algorithms for improved Wilson fermions,
  Comput. Phys. Commun. 165 (2005) 49
- K. Jansen, A. Nube, A. Shindler, C. Urbach, U. Wenger,
  Exploring the epsilon regime with twisted mass fermions,
  PoS (LATTICE2007) 084
- A. Hasenfratz, R. Hoffmann, S. Schaefer,
  Reweighting towards the chiral limit
  arXiv:0805.2369v1 (hep-lat)

- numerical simulations of the wilson theory are stable if the distribution of the spectral gap is well separated from the origin,

$$m_\pi L \geq \begin{cases} 2.8 & \text{at } a = 0.08 \text{ fm} \\ 2.3 & \text{at } a = 0.06 \text{ fm} \end{cases}$$

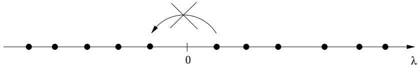
stability bounds for $N_\mathrm{f} = 2$

L. Del Debbio, L. Giusti, M. Luscher, R. Petronzio, N. Tantalo
Stability of lattice QCD simulations and the thermodynamic limit
JHEP 0602:011,2006

- the HMC is not protected against very low eigenvalues (spikes in δH)

- potential ergodicity problems near the stability bound

$$\mathrm{index}(\gamma_5 D_\mathrm{m}) = \tfrac{1}{2}[\#\,\text{pos. eigenvalues} - \#\,\text{neg. eigenvalues}]$$



positive ↔ negative jump unlikely

sectors may not be correctly sampled!

$$\det(D_{\rm m}^\dagger D_{\rm m}) = \det(\mathcal{R}) \times \det(\tilde{D}_{\rm m}^\dagger \tilde{D}_{\rm m}), \qquad D_{\rm m} = D + m$$

$\det(\mathcal{R}) \swarrow$ reweighting factor; $\det(\tilde{D}_{\rm m}^\dagger \tilde{D}_{\rm m}) \searrow$ HMC

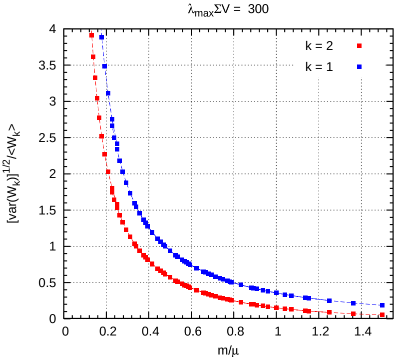
- two proposals for the reweighting factor $\mathcal{W} = \det(\mathcal{R})$

$\tilde{D}_{\rm m}$	$\mathcal{R}$	$\mathcal{R}\Big\vert_{\mu^2 \ll (D_{\rm m}^\dagger D_{\rm m})}$
$D_{\rm m} + i\mu\gamma_5$	$\dfrac{D_{\rm m}^\dagger D_{\rm m}}{D_{\rm m}^\dagger D_{\rm m} + \mu^2}$	$1 - \dfrac{\mu^2}{D_{\rm m}^\dagger D_{\rm m}} + {\rm O}(\mu^4)$
$(D_{\rm m} + i\mu\gamma_5)(D_{\rm m} + i\sqrt{2}\mu\gamma_5)^{-1}(D_{\rm m} + i\mu\gamma_5)$	$\dfrac{(D_{\rm m}^\dagger D_{\rm m})(D_{\rm m}^\dagger D_{\rm m} + 2\mu^2)}{(D_{\rm m}^\dagger D_{\rm m} + \mu^2)^2}$	$1 - \dfrac{\mu^4}{(D_{\rm m}^\dagger D_{\rm m})^2} + {\rm O}(\mu^6)$

- since the high-modes are damped in the reweighting factor, fluctuations are exclusively determined by the low-modes of the Dirac spectrum

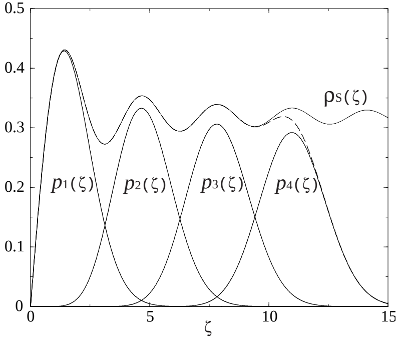
$$\frac{\sqrt{\mathrm{var}(\mathcal{W})}}{\langle \mathcal{W} \rangle} \equiv \frac{\sqrt{\langle \mathcal{W}^2 \rangle - \langle \mathcal{W} \rangle^2}}{\langle \mathcal{W} \rangle}$$

- Random Matrix Theory may be used for illustration purposes:



Fluctuations:

- do not depend on the volume V!!
- depend only upon the ratio $\frac{m}{\mu}$
- are modest if $\frac{m}{\mu} > \frac{1}{2}$



P. H. Damgaard, S. M. Nishigaki

Phys. Rev. D63 (2001) 045012

- $\mathcal{W} = \det(\mathcal{R}) = \mathrm{e}^{\mathrm{tr}\log\mathcal{R}} = \exp\left\{\sum_i \log \mathcal{R}_i\right\}$
- $\mathrm{O}(V)$ eigenvalues contribute to the sum
- each eigenvalue fluctuates by $\mathrm{O}(\frac{1}{V})$

$\Rightarrow$ **fluctuations are $\mathrm{O}(1)$!**

- stochastic representation with $N_{\rm pf}$ gaussian pseudofermions

$$\mathcal{W} = \frac{1}{N_{\rm pf}} \sum_{i=1}^{N_{\rm pf}} \frac{\int \mathcal{D}\phi_i^* \mathcal{D}\phi_i \mathrm{e}^{-\phi_i^* \mathcal{R}[U]^{-1} \phi_i}}{\int \mathcal{D}\phi_i^* \mathcal{D}\phi_i \mathrm{e}^{-\phi_i^* \phi_i}} = \left\langle \frac{1}{N_{\rm pf}} \sum_{i=1}^{N_{\rm pf}} \mathrm{e}^{-\phi_i^* (\mathcal{R}[U]^{-1} - 1) \phi_i} \right\rangle_{\{\phi_i\}}$$

- pseudofermions increase fluctuations of the reweighting factor

$$\mathcal{O}_{\mathcal{R}}[U, \{\phi_i\}] \equiv \tfrac{1}{N_{\rm pf}} \sum_{i=1}^{N_{\rm pf}} \mathrm{e}^{-\phi_i^* (\mathcal{R}[U]^{-1} - 1) \phi_i}$$

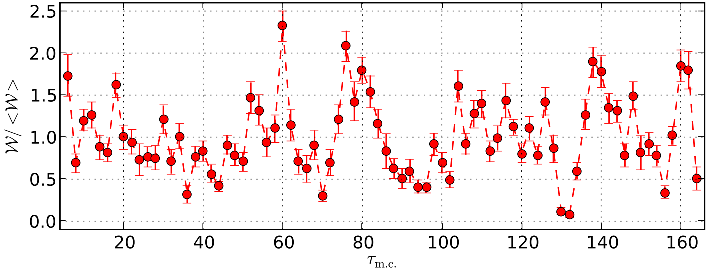
$$\begin{aligned} \mathrm{var}[\mathcal{O}_{\mathcal{R}}] &= \langle\!\langle \mathcal{O}_{\mathcal{R}}[U, \{\phi_i\}]^2 \rangle\!\rangle - \langle\!\langle \mathcal{O}_{\mathcal{R}}[U, \{\phi_i\}] \rangle\!\rangle^2 \\ &= \mathrm{var}[\mathcal{W}] + \tfrac{1}{N_{\rm pf}} \left\langle (\det \mathcal{R}^2) \left[\det[\mathcal{R}(2 - \mathcal{R})]^{-1} - 1 \right] \right\rangle \end{aligned}$$

- numerical tests on existing $N_{\mathrm{f}} = 2$ gauge confs. from **CLS**
- algorithm: **DD-HMC**
- lattice parameters:

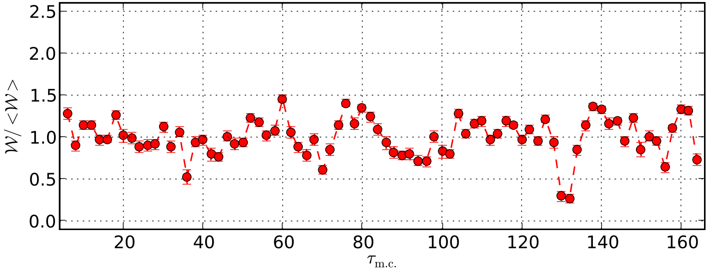
$$V = 64 \times 32^3\,, \qquad \beta = 5.30\,, \qquad c_{\mathrm{sw}} = 1.90952\,,$$

$$N_{\mathrm{pf}} = 24\,, \qquad \frac{m_{\mathrm{sea}}}{\mu} = \left\{\sqrt{2},\, 1,\, \frac{2}{3},\, \frac{1}{2}\right\}$$

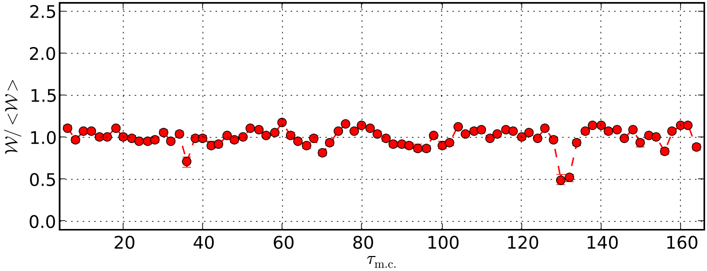
$$\mu = \frac{3}{2} m_{\rm sea} = 23 \text{ MeV } (\overline{\rm MS} \text{ @ } 2 \text{ GeV}) \qquad \mathcal{R} = \frac{(D_{\rm m}^\dagger D_{\rm m})(D_{\rm m}^\dagger D_{\rm m} + 2\mu^2)}{(D_{\rm m}^\dagger D_{\rm m} + \mu^2)^2}$$



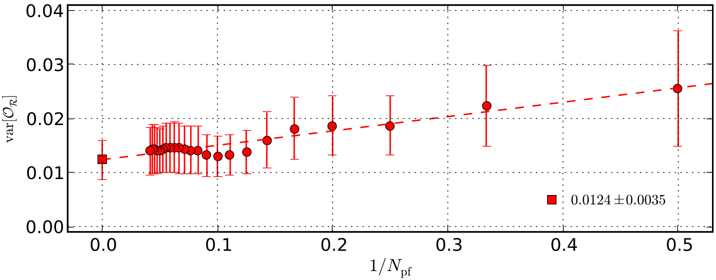
$\mu = m_{\rm sea} = 15$ MeV ($\overline{\rm MS}$ @ 2 GeV)



$$\mu = \frac{1}{\sqrt{2}} m_{\rm sea} = 11 \text{ MeV } (\overline{\rm MS} \text{ @ } 2 \text{ GeV})$$



$$\mu = \frac{1}{\sqrt{2}} m_{\mathrm{sea}} = 11 \text{ MeV } (\overline{\mathrm{MS}} \text{ @ } 2 \text{ GeV})$$



- comparison RMT vs. numerical simulations

$\frac{m_{\rm sea}}{\mu}$	$\left.\frac{\sqrt{\mathrm{var}(\mathcal{W}_1)}}{\langle\mathcal{W}_1\rangle}\right\|_{\rm RMT}$	$\left.\frac{\sqrt{\mathrm{var}(\mathcal{W}_1)}}{\langle\mathcal{W}_1\rangle}\right\|_{\rm M.C.}$	$\left.\frac{\sqrt{\mathrm{var}(\mathcal{W}_2)}}{\langle\mathcal{W}_2\rangle}\right\|_{\rm RMT}$	$\left.\frac{\sqrt{\mathrm{var}(\mathcal{W}_2)}}{\langle\mathcal{W}_2\rangle}\right\|_{\rm M.C.}$
$\sqrt{2}$	0.186	0.419	0.0527	0.111
1	0.357	0.641	0.153	0.216
$2/3$	0.640	1.458	0.353	0.418
$1/2$	0.942	3.533	0.575	0.579

conclusions

- reweighting looks feasible
- high-modes damped, fluctuations produced only by low-modes
- fluctuations independent of the volume, RMT suggests
- numerical results on existing CLS configurations in the ball-park of RMT

outlook

- improved evaluation of $\mathcal{W}$ (eigenvalues, ...)
- implementation of the DD-HMC with reweighted fermion determinants