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Full QCD with dynamical Wilson fermions on a $24^3 \times 40$-lattice – a feasibility study*

TχL-Collaboration:
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The investigation of light sea-quark effects in lattice QCD with dynamical Wilson fermions requires both larger physical volumes and finer lattice resolutions than achieved previously. As high-end supercomputers like the 512-node APE Tower provide the compute power to perform a major step towards the chiral limit (TχL), we have launched a feasibility study on a $24^3 \times 40$ lattice. We approach the chiral limit while refining the resolution , using the standard Wilson fermion action. Following previous work, our Hybrid Monte Carlo simulation runs at $\beta = 5.6$ and two κ-values, 0.1575 and 0.158. From our study, we are confident that, for the APE Tower, a realistic working point has been found corresponding to a volume of 2 fm^3, with chirality characterized by $\frac{1}{m_\pi a} \approx 5.6$.

1. INTRODUCTION

Simulations of full QCD with Wilson fermions at zero temperature so far have been carried out on lattices of size $\leq 16^3 \times 32$, physical volumes < 1.5 (fm)^3 and ratios of $\frac{m_\pi}{m_\rho} > 0.6$ [1]. The latter quantity is a monitor for the closeness to the chiral point. It has been demonstrated [2] that a statistically significant full QCD (reference) sample can be generated in one year's runtime on a 256-node APE computer, at $\frac{m_\pi}{m_\rho} = 0.71$. This however corresponds still to a rather heavy quark mass m_q: by use of chiral perturbation theory we can mock a fictitious "physical" pseudoscalar meson containing two strange quarks, with mass ratio of the size quoted, $\frac{m_{ps}}{m_\phi} \approx \frac{\sqrt{2m_K^2}}{m_\phi} = 0.69$. Thus, in order to quantify light sea quark effects in full QCD, one would rather prefer to work on larger volumes that accommodate a large π-correlation length both in physical and lattice units. This clearly asks for simulations on lattices $> 16^3$ and $\beta \geq 5.6$.

In this note, we describe the TχL project, which is geared to push QCD simulations with standard Wilson fermions further *towards* the *chiral limit*, i.e. beyond $\frac{m_\pi}{m_\rho} < 0.6$ and at appropriate volumes.

The 512-node APE Tower offers sufficient memory to handle a $24^3 \times 40$ lattice. With its CPU-power it can drive an optimized HMC at sufficient speed (*i*) to increase the lattice size by more than a factor of 4 compared to the previous standards described above, (*ii*) to go more chiral, i.e., cope with worse conditioned fermion matrices.

In our exploratory study, we are guided by the experiences described in [1,3], taking advantage of algorithmic achievements such as improved inverters [4] and new parallel preconditioning techniques [5]. We shall report on a Hybrid Monte Carlo simulation on a $24^3 \times 40$ lattice at $\beta = 5.6$ and two κ-values, 0.1575 and 0.158.

2. HOW CHIRAL?

The $24^3 \times 40$ lattice allows to increase ξ_π by a factor of 1.5 compared to Ref. [6], which should suffice to target for $\frac{m_\pi}{m_\rho}$ in the range of .5 – .6.

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Concerning physical volumes and scales we benefit from the increasing $\Delta\beta$-shift [3] as we go to smaller bare quark masses and choose $\beta = 5.6$.

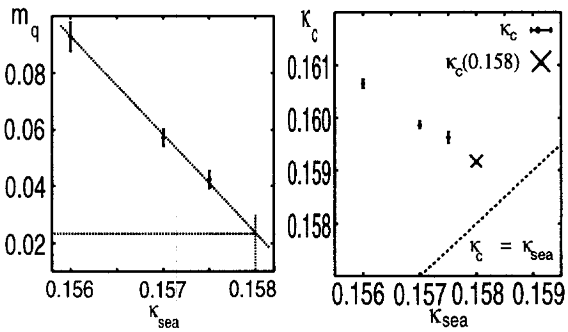

Figure 1. Fixing $\kappa_{\rm sea}$ and estimate for $\kappa_{\rm c,v}$ compared to the results from Ref [6].

For the determination of $\kappa_{\rm sea}$, we extrapolated the relation $m_q a = \frac{1}{2}\left(\frac{1}{\kappa} - \frac{1}{\kappa_c}\right)$ on the data set of Ref. [6] to $m_q a = 0.023$, cf. Fig. 1a, where $\frac{\xi_\pi}{24a}$ is estimated from the mass trajectory to be about .23 of the spatial extension. This value is small enough to protect us from finite size effects. We thus will work at $\kappa = 0.1580$.

To put this parameter choice into perspective, we sketched in Fig. 1b the approach of the critical κ at fixed $\kappa_{\rm sea}$, $\kappa_{\rm c,v}$, [6], towards κ_c, the locus of which is $\kappa_{\rm sea} = \kappa_c$ (the diagonal line). The cross marks the current estimate for our working point. Notice that our parameter choice, $\kappa_{\rm sea} = 0.158$, appears to be reasonably positioned within the 'chirality gap'.

In the lattice discretization of the fermionic action, we switched from the usual o/e representation to the full representation of $M = \mathbf{1} - \kappa D$, employing a new SSOR preconditioning scheme [5,7,8]. In particular on the APE machine, this method offers an overall gain of 100 % in execution time, as seen from Tab. 1.

Algo		$\kappa = 0.1575$	$\kappa = 0.1580$
o/e	t/s	8200	–
SSOR	t/s	3800	9100

Table 1
Average time to generate 1 trajectory on the APE100 Tower.

3. SIMULATION

We have tuned the HMC timestep to achieve acceptance rates larger than 60 %. For the SSOR scheme with twice as many degrees of freedom as in the o/e case, we chose $T = 0.5$. For this trajectory length, in the production runs, the 32 bit machine precision induces a reversibility error $\delta(\Delta S)$ in the range of just 2 % of the average ΔS for an inversion residue of $r = 10^{-8}$. This is due to *local* computations, *global* summations being carried out in emulated double precision arithmetic. It should be said that the impact of this error of ΔS onto the canonical distribution deserves further attention. The chosen HMC run parameters are given in Tab. 2.

Algo	κ	T	dt	acc/%	r
o/e	0.1575	1	0.008	70	10^{-8}
SSOR	0.1575	0.5	0.004	72	10^{-8}
SSOR	0.1580	0.5	0.004	66	10^{-8}

Table 2
Parameters of the HMC simulation.

During the thermalization phase we carefully approached the lowest quark mass in a near adiabatic fashion, to protect the system from oscillating through the shielding transition. We forked the run into two κ-branches after an initial thermalization of 480 trajectories. The production status reported is given by 830 trajectories (out of which 350 are thermalized) for $\kappa = 0.1575$ and 1500 trajectories (out of which 750 are thermalized) for $\kappa = 0.1580$.

4. PRELIMINARY RESULTS

We have performed first tentative measurements of the autocorrelation $C(t)$ of the plaquette. In Fig. 2, we plot the autocorrelation function for the plaquette at $\kappa = 0.158$. On the large lattice volume we can profit from a substantial self averaging effect suppressing the fluctuations of the plaquette as well as of other intensive quantities. The plot indicates that the autocorrelation times come out surprisingly small and might settle well below $\tau_{\text{int}} = 50$ for the plaquette. We mention that the autocorrelation function for

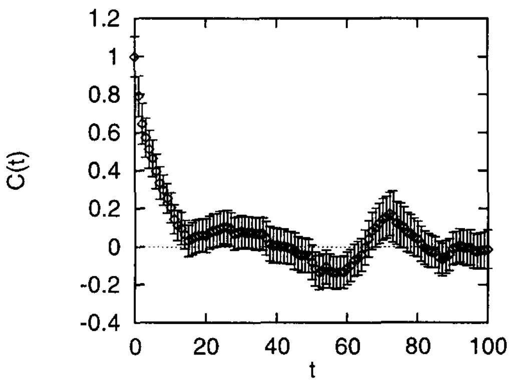

Figure 2. Autocorrelation function of plaquette.

light meson masses looks similar.

Using 22 configurations drawn from a sample of 600 trajectories we have computed the potential following Ref. [3]. We performed a 30 step APE smearing and evaluated the potential for a time extension of 5 where a plateau in the local mass is emerging. We have fitted for a "string tension" in the range up to 1 fm. In Tab. 3 we quote a preliminary estimate for the ensueing scale and physical lattice volume V_s.

We monitored local meson masses to position the run with respect to chirality: on a sample of 19 configurations we retrieve a rough first guesstimate of $m_\pi a$ and $m_\rho a$, see Tab. 3. Our findings suggest $\frac{m_\pi}{m_\rho}$ to be 0.56(4).

a^{-1}	V_s	m_π SL	m_ρ SL	$\frac{m_\pi}{m_\rho}$
2.37(1) GeV	2 fm	0.178(5)	0.32(2)	0.56(4)

Table 3
Results for the lattice scale from potential, and masses in lattice units.

5. CONCLUSIONS AND OUTLOOK

In the TχL-feasibility study, we find that $\frac{m_\pi}{m_\rho}$-ratio appears to reach the target region indeed, where $\frac{\xi_\pi}{a} = 5.6 < 0.25 \times V_s^{\frac{1}{3}}$. The lattice resolution is increased (with respect to the small lattice results) to $a^{-1} = 2.37$ GeV. We are encouraged by the observed autocorelation times and expect > 50 independent configurations from 8 months future runtime on APE Towers.

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