Physical Point Simulation in 2+1 Flavor Lattice QCD

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July 29, 2009
Plan of talk

§1. The PACS-CS project
§2. Reweighting method
§3. Parameters
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1. The PACS-CS project

Parallel Array Computer System for Computational Sciences

operation started on 1 July 2006 at CCS in U.Tsukuba
collaboration members
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Physics plan

aim: 2+1 flavor QCD simulation at the physical point

<table>
<thead>
<tr>
<th></th>
<th>PACS-CS</th>
<th>CP-PACS/JLQCD</th>
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</thead>
<tbody>
<tr>
<td>gauge action</td>
<td>Iwasaki</td>
<td>Iwasaki</td>
</tr>
<tr>
<td>quark action</td>
<td>clover with $c_{NP}^{SW}$ 0.07,0.1,0.122</td>
<td>clover with $c_{NP}^{SW}$ 0.07,0.1,0.122</td>
</tr>
<tr>
<td>$a$ [fm]</td>
<td>$\gtrsim (3\text{fm})^3$</td>
<td>$\sim (2\text{fm})^3$</td>
</tr>
<tr>
<td>volume</td>
<td>physical point</td>
<td>64MeV</td>
</tr>
<tr>
<td>$m_{ud}^{AWI}$</td>
<td>DDHMC with improvements</td>
<td>HMC</td>
</tr>
<tr>
<td>algorithm for ud</td>
<td>UV-filtered exact PHMC</td>
<td>exact PHMC</td>
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<tr>
<td>algorithm for s</td>
<td></td>
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Why is physical point simulation necessary?

- difficult to trace chiral logs for chiral extrapolation
- ChPT is not always a good guiding principle
- need a proper treatment of resonances
- simulations with different up and down quark masses

⇒ there are two types of problems
(1) Computational cost

\[ \frac{m_π}{m_ρ} \]

\[ Tflops \text{ years} \]

\[ N_f=2+1 \]
\[ 10000 \text{ MD} \]
\[ a=0.1\text{fm} \]
\[ L=3\text{fm} \]

successfully solved by (Mass-Preconditioned) DDHMC

PRD79(2009)034503
(2) Fine tuning on physical point

need 3 simulation points within a few MeV differences around the physical point in 2+1 flavor case
⇒ demanding computational cost

try reweighting method both for ud and s quarks
§ 2. Reweighting method

original: \((\kappa_{ud}, \kappa_s) \Rightarrow \text{target: } (\kappa'_{ud}, \kappa'_s)\) assuming \(\rho_q \equiv \kappa'_q / \kappa_q \approx 1\)

\[
\langle \mathcal{O}[U](\kappa'_{ud}, \kappa'_s) \rangle_{(\kappa'_{ud}, \kappa'_s)} = \frac{\langle \mathcal{O}[U](\kappa'_{ud}, \kappa'_s) R_{ud}[U] R_s[U] \rangle_{(\kappa'_{ud}, \kappa'_s)}}{\langle R_{ud}[U] R_s[U] \rangle_{(\kappa_{ud}, \kappa_s)}}
\]

reweighting factors

\[
R_{ud}[U] = |\text{det } [W[U](\rho_{ud})]|^2, \quad R_s[U] = \text{det } [W[U](\rho_s)]
\]

where \(W[U](\rho_q) \equiv \frac{D_{\kappa'_q}[U]}{D_{\kappa_q}[U]}\)
Evaluation of $R_{ud}[U]$

introduce a complex bosonic field $\eta$

$$R_{ud}[U] = |\det [W[U](\rho_{ud})]|^2$$

$$= \langle e^{-|W^{-1}[U](\rho_{ud})\eta|^2+|\eta|^2}\rangle_\eta$$

given a set of $\eta^{(i)}$ ($i = 1, \ldots, N_\eta$) with the Gaussian distribution

$$R_{ud}[U] = \lim_{N_\eta \to \infty} \frac{1}{N_\eta} \sum_{i=1}^{N_\eta} e^{-|W^{-1}[U](\rho_{ud})\eta|^2+|\eta|^2}$$
Evaluation of $R_s[U]$

assume $\det W[U](\rho_s)$ is positive

$$R_s[U] = \det [W[U](\rho_s)]$$
$$= \langle e^{-|W^{-1/2}[U](\rho_s)\eta|^2 + |\eta|^2} \rangle_\eta$$

Taylor expansion for $W^{-1/2}[U](\rho_s)\eta$

$$W^{-1}[U](\rho_s) = \frac{D_{\kappa_s}[U]}{D_{\kappa_s'}[U]}$$
$$= 1 - (1 - \rho_s) \left(1 - (D_{\kappa_s'}[U])^{-1}\right)$$
$$= 1 - X[U](\rho_s)$$

where $|1 - \rho_s| \ll 1$

⇒ expansion of $W^{-1/2}[U](\rho_s)\eta$ in terms of $X[U](\rho_s)$
Additional technique

Hasenfratz-Hoffmann-Schaefer

determinant breakup: divide \((\kappa_q' - \kappa_q)\) into \(N_B\) subintervals

\[
\kappa_q \Rightarrow \kappa_q + \Delta_q \Rightarrow \ldots \Rightarrow \kappa_q + (N_B - 1)\Delta_q \Rightarrow \kappa_q',
\]

with \(\Delta_q = (\kappa_q' - \kappa_q)/N_B\)

\[
\det \left[ W^{-1}[U](\rho_q) \right] = \det \left[ W^{-1}[U] \left( \frac{\kappa_q + \Delta_q}{\kappa_q} \right) \right] \times \det \left[ W^{-1}[U] \left( \frac{\kappa_q + 2\Delta_q}{\kappa_q + \Delta_q} \right) \right] \times \ldots \times \det \left[ W^{-1}[U] \left( \frac{\kappa_q'}{\kappa_q + (N_B - 1)\Delta_q} \right) \right],
\]

reduce fluctuations of the reweighting factors
3. Parameters

simulation parameters

- original: $(\kappa_{ud}, \kappa_s) = (0.137785, 0.136600)$
- 1000 MD time, still increasing
- MP$^2$DDHMC for ud quark with $8^4$ block, $\rho_1 = 0.9995$, $\rho_2 = 0.99$
- UV-filtered PHMC for s quark with $N_{\text{poly}} = 220$

reweighting parameters

- target: $(\kappa'_{ud}, \kappa'_s) = (0.137800, 0.136645), (0.137800, 0.136690)$
- breakup intervals: $\Delta_{ud} = (0.137800 - 0.137785)/2$
- $\Delta_s = (0.136690 - 0.136600)/4$
- $N_\eta = 10$ for stochastic estimation of $R_{ud, s}$
4. Preliminary Results

concentrate on \((\kappa'_{ud}, \kappa'_{s}) = (0.137800, 0.136645)\)

- results for \(R_{ud,s}\)
- Reweighting for plaquette
- Reweighting for \(m_\pi, m_K, m_\Omega\)
  (physical inputs for \(m_{ud}, m_{s}, a^{-1}\))
- hadron spectrum
- locate the physical point
Reweighting factors on each configuration

normalized with $\langle R_{ud,s} \rangle = 1$
Reweighting factors vs. plaquette value

![Graph showing reweighting factors vs. plaquette value with clear dependence](image)

**clear dependence**
Plaquette histogram w/ and w/o $R_{ud}$

distribution is slightly moved toward larger values
Plaquette histogram w/ and w/o $R_s$

Distribution is slightly moved toward larger values.
\textbf{\pi} effective mass

\[ \pi \text{ effective mass} \]

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure.png}
\caption{\textbf{\pi} effective mass}
\end{figure}

rewighting effects are observed
$K$ effective mass

K effective mass

similar to $\pi$ case
$\Omega$ effective mass

$m_\Omega$ is slightly decreased.
Hadron spectrum in comparison with experiment

\[ \frac{(m_h/m_\Omega)_{\text{lat}}}{(m_h/m_\Omega)_{\text{exp}}} - 1 \]

\[ m_\pi/m_\Omega, m_K/m_\Omega \] are properly tuned
Locate the physical point

confirmed with three data point analysis

$$\Delta m_{ud} \sim 1\text{MeV}, \Delta m_s \lesssim 3\text{MeV}$$
5. Summary

- Chiral extrapolation is not necessary anymore
- $(6\text{fm})^3$ box simulation is under way
- starting point for precision measurements