Old and New Physics with Domain Wall Fermion Lattice QCD

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Columbia University
RBC Collaboration

This work done in conjunction with
RBC Collaboration
UKQCD Collaboration
HotQCD Collaboration
Known Elementary Particles

<table>
<thead>
<tr>
<th>Quarks</th>
<th>Mass (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>u</td>
<td>2.19 ± 0.15</td>
</tr>
<tr>
<td>d</td>
<td>4.67 ± 0.20</td>
</tr>
<tr>
<td>s</td>
<td>94 ± 3</td>
</tr>
<tr>
<td>c</td>
<td>1.275 ± 0.025</td>
</tr>
<tr>
<td>b</td>
<td>4.18 ± 0.03</td>
</tr>
<tr>
<td>t</td>
<td>173.5 ± 0.6 ± 0.8</td>
</tr>
</tbody>
</table>

QCD

Interactions mediated by gluons

Theory of interactions of quarks

\[ m_u = 2.19 \pm 0.15 \text{ MeV} \]
\[ m_d = 4.67 \pm 0.20 \text{ MeV} \]
\[ m_s = 94 \pm 3 \text{ MeV} \]
\[ m_c = 1.275 \pm 0.025 \text{ GeV} \]
\[ m_b = 4.18 \pm 0.03 \text{ GeV} \]
\[ m_t = 173.5 \pm 0.6 \pm 0.8 \text{ GeV} \]
11. THE CKM QUARK-MIXING MATRIX

The physical states are obtained by diagonalizing $\rho$ which arises from the Yukawa interactions with the Higgs condensate, this hierarchy using the Wolfenstein parameterization. We define $\delta \equiv \rho - 3 s + c$ where $\lambda \equiv i \epsilon \phi$ is the Higgs field, $Y$ is the charged-current couplings given by $y = \sqrt{\lambda} \times \bar{Q} A L R$, as $(1) \equiv V_{ud} = y_{ud} / \sqrt{\lambda}$, $(2) \equiv V_{us} = y_{us} / \sqrt{\lambda}$, $(3) \equiv V_{ub} = y_{ub} / \sqrt{\lambda}$.

11.1. Introduction

Revised March 2012 by A. Ceccucci (CERN), Z. Ligeti (LBNL), and Y. Sakai (KEK).

The masses and mixings of quarks have a common origin in the Standard Model (SM). The angles $\delta$ and $\theta$ are 3 antisymmetric tensor.

It is known experimentally that $\theta$ is the phase responsible for all approximate results in the literature. For example, $\theta = 90^\circ$.

For $K_{l3}$ we have: $\Gamma_{K \rightarrow \pi l \nu} = C_K^2 \frac{G_F^2 m_K^5}{192 \pi^3} I S_{EW}[1 + 2 \Delta_{SU(2)} + 2 \Delta_{EM}] |V_{us}|^2 |f_+(0)|^2 $
Major Development: Ensembles with Physical Quark Masses

Large volume ensembles with physical quark masses are also being produced and used by the European BMW Collaboration (hex-smeared clover fermions) and the US MILC/FNAL group (HISQ staggered fermions)
Small Chiral Extrapolation

- Input $m_l$, $m_s$ and a bare coupling. Find measured mass ratios are close to physical
- Use SU(2) chiral perturbation theory and reweighting in $m_s$ to make small corrections

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Physical Value</th>
<th>Ens. 10 Value</th>
<th>Deviation</th>
<th>Ens. 11 Value</th>
<th>Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_\pi/m_K$</td>
<td>0.2723</td>
<td>0.2790</td>
<td>2.4%</td>
<td>0.2742</td>
<td>0.7%</td>
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<tr>
<td>$m_\pi/m_\Omega$</td>
<td>0.0807</td>
<td>0.0830</td>
<td>2.8%</td>
<td>0.0822</td>
<td>1.9%</td>
</tr>
<tr>
<td>$m_K/m_\Omega$</td>
<td>0.2964</td>
<td>0.2974</td>
<td>0.3%</td>
<td>0.2998</td>
<td>1.2%</td>
</tr>
</tbody>
</table>
Simplest Matrix Elements: $f_\pi$ and $f_K$

- Inputs are $m_\pi$, $m_K$ and $m_\Omega$
- Use SU(2) ChPT to extrapolate
- Now have ensembles with essentially physical quark masses (few percent)
arXiv:1411.7017 (RBC-UKQCD)
- $f_\pi$ and $f_K$ are predictions

### RBC/UKQCD $f_\pi$

<table>
<thead>
<tr>
<th>Year</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2000 quench</td>
<td>137.0(11.0)</td>
</tr>
<tr>
<td>2007</td>
<td>127.0(4.0)</td>
</tr>
<tr>
<td>2008</td>
<td>124.1(7.8)</td>
</tr>
<tr>
<td>2010</td>
<td>124.0(5.4)</td>
</tr>
<tr>
<td>2014</td>
<td>130.2(0.9)</td>
</tr>
<tr>
<td>2015 FLAG</td>
<td>130.2(1.4)</td>
</tr>
</tbody>
</table>

### RBC/UKQCD $f_K$

<table>
<thead>
<tr>
<th>Year</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>2000 quench</td>
<td>156.0(8.0)</td>
</tr>
<tr>
<td>2007</td>
<td>157.0(5.0)</td>
</tr>
<tr>
<td>2008</td>
<td>149.6(7.3)</td>
</tr>
<tr>
<td>2010</td>
<td>149.0(4.5)</td>
</tr>
<tr>
<td>2014</td>
<td>155.5(0.8)</td>
</tr>
<tr>
<td>2015 FLAG</td>
<td>156.3(0.9)</td>
</tr>
</tbody>
</table>
Constraining the CKM Matrix via $K_{13}$ decays

$$
\Gamma_{K \to \pi l v} = C_K^2 \frac{G_F^2 m_K^5}{192 \pi^3} I S_{EW} \left[ 1 + 2 \Delta_{SU(2)} + 2 \Delta_{EM} \right] V_{us}^2 |f_+(0)|^2
$$

Small interpolation to the physical point (arXiv:1504.01692 RBC/UKQCD)

$$
f_+^{K\pi}(0) = 0.9685(34)(14), \quad |V_{us}| = 0.2233(5)(9),
\quad 1 - |V_{ud}|^2 - |V_{us}|^2 = 0.0010(4)V_{ud}(2)V_{us}^{\text{exp}}(4)V_{us}^{\text{lat}} = 0.0010(6),
$$
K -> ππ Decays and CP Violation

\[ K^0 = p K^0 + q \bar{K}^0 \]

\[ K_L = p K^0 + q \bar{K}^0 \]

\[ p \approx q \]

\[ CP \approx -1 \]

\[ \eta_{+-} = |\eta_{+-}| e^{i\phi_{+-}} = \frac{A(K_L \rightarrow \pi^+\pi^-)}{A(K_S \rightarrow \pi^+\pi^-)} \]

\[ \eta_{00} = |\eta_{00}| e^{i\phi_{00}} = \frac{A(K_L \rightarrow \pi^0\pi^0)}{A(K_S \rightarrow \pi^0\pi^0)} \]
\[ \varepsilon = \frac{e^{i\pi/4}}{\sqrt{2} \Delta M_K} \left( \text{Im}(M_{12}) + 2 \frac{\text{Im}(A_0)}{\text{Re}(A_0)} \text{Re}(M_{12}) \right) = \kappa \varepsilon \frac{e^{i\phi}}{\sqrt{2}} \left[ \frac{\text{Im}(M_{12}^{\Delta S=2})}{\Delta m_K} \right] \]

\[ \varepsilon_K = \kappa \varepsilon \ C_\varepsilon \ \hat{B}_K \ \text{Im}(\lambda_t) \ \{ \text{Re}(\lambda_c)[\eta_1 S_0(x_c) - \eta_3 S_0(x_c, x_t)] - \text{Re}(\lambda_t) \eta_2 S_0(x_t) \} \ e^{i\pi/4} \]
energy interactions can be accurately captured by a low energy scale far above those accessible to experiments.

The admixture of the CP-even combination of $K^0$ decay into a two-pion state with isotopic spin 0 and 2 involves massive quark fields whose magnitude is determined from experiment to be $2\times10^{-8}$.

The violation of CP symmetry was discovered as a subleading effect to phase mixing which can only be introduced if there are three generations of quarks in Nature. This CP-violating mixing is the indirect effect connecting the quarks $u$ and $d$ and $s$

Described by effective weak Hamiltonian:

$$H_W = \frac{G}{\sqrt{2}} V_{us}^* V_{ud} \sum_{i=1}^{10} [z_i(\mu) + \tau y_i(\mu)] Q_i(\mu).$$
**K -> (ππ)_{I=2} Amplitudes**

- Need moving pions and correct kinematics. Use tuned lattice volume and antiperiodic spatial boundary conditions for one quark.
- Only connected diagrams enter.
- Finite volume matrix element corrected by Lelloch-Luscher factor to get infinite volume amplitude.
- \( \text{Re}(A_2) \) from experiment is \((1.4787 \pm 0.0031) \times 10^{-8} \text{ GeV} \). \( \text{Im}(A_2) \) is unknown.
- First result for a single lattice spacing (PRL 108 (2012) 141601 RBC-UKQCD)
  \[
  \text{Re}(A_2) = (1.3861 \pm 0.046_{\text{stat}} \pm 0.258_{\text{sys}}) \times 10^{-8} \text{ GeV}
  \]
  \[
  \text{Im}(A_2) = (-6.54 \pm 0.46_{\text{stat}} \pm 1.20_{\text{sys}}) \times 10^{-13} \text{ GeV}
  \]
- Now have finished ensemble 10 and 11 calculations, with smaller statistical errors and an extrapolation to the continuum limit (PRD91 (2015) 7, 0704502 RBC-UKQCD)
  \[
  \text{Re}(A_2) = (1.50 \pm 0.04_{\text{stat}} \pm 0.14_{\text{sys}}) \times 10^{-8} \text{ GeV}
  \]
  \[
  \text{Im}(A_2) = (-6.99 \pm 0.20_{\text{stat}} \pm 0.84_{\text{sys}}) \times 10^{-13} \text{ GeV}
  \]
Calculating the two-pion decay and mixing of neutral K mesons

Table 1: Estimates of the major systematic errors in this calculation of \( \text{Re} A_2 \) and \( \text{Im} A_2 \).

- Disconnected quark diagrams enter - noisy
- Need more than antiperiodic boundary conditions on one quark to ensure the have relative momenta: G parity boundary conditions used
- Need to generate G parity ensembles, since sea and valence sectors require same boundary conditions.
K -> (ππ)_{I=0} Amplitudes

- Have to match K and ππ energies
- Q2 is most important matrix element for Re(A₀) and Q6 for Im(A₀)
- Plateaus visible, but more data planned
- Results from ~200 measurements expected very soon!

\[
\text{Re} \left( \frac{\varepsilon'}{\varepsilon} \right) = \frac{i \omega e^{\delta_2 - \delta_0}}{\sqrt{2} \varepsilon} \left[ \frac{\text{Im} A_2}{\text{Re} A_2} - \frac{\text{Im} A_0}{\text{Re} A_0} \right]
\]
<table>
<thead>
<tr>
<th>Generic Process</th>
<th>Examples</th>
<th>Experiment</th>
<th>LQCD calculates</th>
</tr>
</thead>
</table>
| Kl2             | $K^+ \to \mu^+\nu_\mu$  
$K^+ \to e^+\nu_e$  | $f_K$               | $f_K$ (also $f_\pi$) |
| Kl3             | $K^+ \to \pi^0 l^+\nu_l$  
$K^0 \to \pi^- l^+\nu_l$  | $|V_{us}f^+(0)|^2$  | $f^+(0)$          |
| Kl4             | $K \to \pi \pi l \bar{\nu}_l$  |                     | ??               |
| $K \to \pi\pi$ (CP conserving) | $K^0 \to \pi^+\pi^-$  
$K^+ \to \pi^+\pi^0$  | $|A_0|$             | $|A_0|\ |A_2|$ (SM_{cpc} inputs) |
| $\Delta m_K$ (CP conserving) | $K^0 \leftrightarrow \pi\pi \leftrightarrow \bar{K}^0$ (LD)  
$K^0 \leftrightarrow O_{\Delta S=2} \leftrightarrow \bar{K}^0$ (SD)  | $\Delta m_K$         | $\Delta m_K$ (SM_{cpc} inputs) |
| $K^0 \to \pi\pi$ (indirect CP violation) | $K_L \to \pi\pi$  
$\left(K^0 \leftrightarrow \bar{K}^0\right) \to \pi\pi$ independent of $\pi\pi$ isospin | $\epsilon = \frac{\hat{B}_K F_K^2 \text{SM}}{\Delta m_K}$  | $B_K, \frac{\text{Im}(A_0)}{\text{Re}(A_0)}$ |
| $K^0 \to \pi\pi$ (direct CP violation) | $K_L \to \pi\pi$ depends on $\pi\pi$ isospin | $\text{Re}(\epsilon'/\epsilon) = f(A_0, A_2, \text{SM})$  | $A_0, A_2$ (SM_{cpc} inputs) |
| $K \to \pi ll$ | $K_L \to \pi^0 l^+ l^-$  
$K_S \to \pi^0 l^+ l^-$  |                     | ??               |

$\text{SM}_{cpc} = \text{Standard Model CP-conserving parameters}$
Columbia/RBRC
QCDSP 1998-2005
0.050 GFlops/node

Columbia/RBRC/
UKQCD
QCDOC 2005-2011
0.8 GFlops/node

IBM BGL 2005-2013
2.8 GFlops/node

IBM BGP 2007-
13.6 GFlops/node

IBM BGQ 2012-
200 GFlops/node

~ 4,000× speed-up per node in 15 years, for QCD
~ 700× speed-up in Flops/$ in 15 years (no inflation)
~ 1,000× speed-up in Flops/(inflation adjusted $)

RBC/UKQCD have production jobs on the Argonne ALCF BGQ that sustain 1 PFlops on
32 racks = 32k nodes = 0.5 M cores.

This performance comes from very carefully tuned assembly code on BGQ, produced by
Peter Boyle (University of Edinburgh), using his BAGEL code generator
Scaling for Dirac Equation Solver

Weak Scaling for DWF BAGEL CG inverter

Code developed by Peter Boyle at the STFC funded DiRAC facility at Edinburgh
Quantum Chromodynamics

- Like QED, but with SU(3) local gauge symmetry

\[ Z = \int [dA] \prod_{i=1}^{3} \det \left[ D(A, g_0, m_i^0) \right] \exp \left\{ -\frac{i}{4} (\partial_\mu A_\nu - \partial_\nu A_\mu + g_0 f^{abc} A^b_\mu A^c_\nu)^2 \right\} \]

\[ D(A, g_0, m_i^0) \equiv i\gamma^\mu (\partial_\mu - igA^a_\mu t^a / 2) - m_i^0 \]

- Good approximation: Only include three (or four) light quarks in path integral
- Gluon self-interaction yields a very non-linear system.
- Chiral symmetry of system broken by vacuum state
- Quarks bound in hadrons
Algorithms for Gauge Field Production

- Producing gauge fields:
  * Use classical molecular dynamics to move through gauge field space
  * Quark loops give back reaction on gauge fields by solving Dirac equation
  * Hasenbusch mass preconditioning allows tuning back reaction

\[
\det[D(m)] = \frac{\det[D(m)]}{\det[D(m_1)]} \times \frac{\det[D(m_1)]}{\det[D(m_2)]} \cdots \det[D(m_n)]
\]

For \( m \approx m_1 \) gives small force but expensive to calculate
Control force size from \( m_1 \) and \( m_2 \), less expensive to calculate

- RBC/UKQCD uses 7 levels of intermediate masses
- Integrate different d.o.f on different time scales (Sexton-Weingarten integrators)
- Use higher order integrators, currently RBC/UKQCD use force gradient, \( O(dt^4) \)

- These are giving 10-100\( \times \) speed-up over a decade ago.

* Hard to be completely quantitative here, since without these algorithmic speed-ups, we could not even try current simulations
Algorithms for Measurements

\[ T = |t_K - t_\pi| \]

- Time translated the n-point function, on a fixed background gauge field, are sufficiently decorrelated (independent enough) to make them worth calculating.
- This means many solutions of the Dirac equation \( D[U_\mu]\psi = s \) for fixed \( U_\mu \)
- Calculating eigenvectors of \( D[U_\mu] \) with small eigenvalues (low-modes) speeds up subsequent solves. Can be done with EigCG or Lanczos algorithms.
- Alternatives for Wilson fermions are domain decomposition and multigrid, giving similar speed-up with smaller memory requirements.
- Further improvement from all-mode-averaging of Blum, Izubuchi and Shintani
  * Separates measurements into expensive parts, with small statistical errors after a few measurements, and inexpensive parts, where many measurements are needed.
Measurement Times

- RBC/UKQCD has measurements of $f_\pi, f_K, B_K, m_{ud}, m_s, f_{K\pi}^+(0), K \rightarrow (\pi\pi)_{I=2}$ all in a single executable, using EigCG deflation and all mode averaging,

- In production on ensemble 10, using RBRC/BNL and Edinburgh BGQ's. In production on ensemble 11 on Mira at the ALCF

- Ensemble 10 runs on 1 rack, ensemble 11 on 32 racks. Number of EigCG low modes is 600 for ensemble 10, 1500 for ensemble 11

<table>
<thead>
<tr>
<th></th>
<th>Ensemble 10</th>
<th>Ensemble 11</th>
</tr>
</thead>
<tbody>
<tr>
<td>EigCG setup time</td>
<td>29.5</td>
<td>66</td>
</tr>
<tr>
<td>Exact light quark time</td>
<td>18.7</td>
<td>13</td>
</tr>
<tr>
<td>Sloppy light quark time</td>
<td>64</td>
<td>55</td>
</tr>
<tr>
<td>Exact strange quark time</td>
<td>8</td>
<td>17</td>
</tr>
<tr>
<td>Contraction time</td>
<td>3</td>
<td>16</td>
</tr>
<tr>
<td>Total time</td>
<td>123</td>
<td>167</td>
</tr>
<tr>
<td>Total time on partition</td>
<td>5.2 days</td>
<td>5.3 hrs</td>
</tr>
</tbody>
</table>

- With more deflation, the ensemble 11 calculation is only 1.3× ensemble 10
Improvement from All Mode Averaging

- For $f_{K\pi}(0)$ RBC/UKQCD statistical errors are 5× smaller with AMA than exact only. With 26 configurations, have 0.5% statistical error for $f_{K\pi}(0)$

<table>
<thead>
<tr>
<th>$K - \pi$ sep</th>
<th>AMA?</th>
<th>$f_{K\pi}^+(0)$</th>
<th>$f_{K\pi}^-(0)$</th>
<th>$Z_V$</th>
</tr>
</thead>
<tbody>
<tr>
<td>20:24</td>
<td>AMA</td>
<td>0.9672(45)</td>
<td>-0.1327(123)</td>
<td>0.7123(13)</td>
</tr>
<tr>
<td>20:28</td>
<td>AMA</td>
<td>0.9602(52)</td>
<td>-0.1254(97)</td>
<td>0.7089(17)</td>
</tr>
<tr>
<td>20:32</td>
<td>AMA</td>
<td>0.9639(49)</td>
<td>-0.1318(96)</td>
<td>0.7093(16)</td>
</tr>
<tr>
<td>24:28</td>
<td>AMA</td>
<td>0.9598(59)</td>
<td>-0.1230(112)</td>
<td>0.7087(18)</td>
</tr>
<tr>
<td>24:32</td>
<td>AMA</td>
<td>0.9646(52)</td>
<td>-0.1322(106)</td>
<td>0.7082(17)</td>
</tr>
<tr>
<td>20:24</td>
<td>exact</td>
<td>1.0018(253)</td>
<td>-0.1206(320)</td>
<td>0.7315(150)</td>
</tr>
<tr>
<td>20:28</td>
<td>exact</td>
<td>0.9552(227)</td>
<td>-0.0850(205)</td>
<td>0.7016(157)</td>
</tr>
<tr>
<td>20:32</td>
<td>exact</td>
<td>0.9537(246)</td>
<td>-0.1004(215)</td>
<td>0.6971(162)</td>
</tr>
<tr>
<td>$m_{\text{res}}$</td>
<td></td>
<td>0.0006148(59)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- FNAL/MILC (arXiv:1212.4993) has $f_{K\pi}(0) = 0.9667 \pm 0.0023_{\text{stat}} \pm 0.0033_{\text{sys}}$

- $B_K$ has 0.2% statistical errors as well, 10× smaller than without AMA

<table>
<thead>
<tr>
<th>$K - K$ sep</th>
<th>AMA?</th>
<th>$B_K$</th>
</tr>
</thead>
<tbody>
<tr>
<td>20:4:24</td>
<td>AMA</td>
<td>0.5836(11)</td>
</tr>
<tr>
<td>20:4:28</td>
<td>AMA</td>
<td>0.5844(12)</td>
</tr>
<tr>
<td>20:4:32</td>
<td>AMA</td>
<td>0.5839(12)</td>
</tr>
<tr>
<td>20:4:24</td>
<td>exact</td>
<td>0.5712(109)</td>
</tr>
<tr>
<td>20:4:28</td>
<td>exact</td>
<td>0.5870(110)</td>
</tr>
<tr>
<td>20:4:32</td>
<td>exact</td>
<td>0.5845(116)</td>
</tr>
</tbody>
</table>

- More work can reduce perturbative matching errors
QCD Thermodynamics with DWF

- The HotQCD Collaboration has done simulations on $32^3 \times 8$ and $64^3 \times 8$ lattices with physical pions (PRL 113 (2014) 8, 082001 HotQCD)
- Susceptibilities show larger peaks than for HISQ ensembles
- Strong quark mass dependence
- Pseudocritical temperature with physical pions:
  \[ T_c = 155(1)(8) \text{ MeV} \]
- This $T_c$ changes to about 165 MeV when $m_\pi = 200$ MeV
Eigenvalue Density of Dirac Operator, $T = 0$

Jasper Lin, Columbia PhD Thesis
Eigenvalue Density of Dirac Operator, $T \neq 0$

FIG. 7. The eigenvalue spectrum for $T = 149 - 195$ MeV, expressed in the MS scheme at the scale $\mu = 2$ GeV. The imaginary, “unphysical” eigenvalues are plotted as $-\frac{q^2}{\lambda} - m_l^2$.

The spectra from the $32^3 \times 8$ ensembles are plotted as histograms and fit with a linear ($T = 149 - 178$ MeV) or a quadratic ($T = 186 - 195$ MeV) function (blue dashed line).

The spectrum from each of the $16^3 \times 8$ ensembles [9] is plotted as a black solid line.
Symmetries for $T \neq 0$

- Difference of susceptibilities related by $\text{SU}(2)_L \times \text{SU}(2)_R$, showing breaking for low temperatures and accurate chiral symmetry for $T > 164$ MeV

- Difference of susceptibilities related by $\text{U}(1)_A$ showing breaking for $T > 164$ MeV
Conclusions

- After 30 years of QCD simulations, large volume, physical 2+1 flavor ensembles are begin produced by a number of collaborations, including DWF fermions, with continuum chiral symmetries at finite lattice spacing.
- Many technical improvements are being used: twisted b.c. for particle states, NPR, RI-SMOM renormalization, EigCG, deflation, Lellouch-Luscher relation
- We can now do quite sophisticated field theory numerically
- 4,000\times improvement in computer power in 15 years.
- Evolution algorithms to produce gauge fields are 10-100\times faster
- Measurement algorithms are > 10\times faster
- Our most refined measurements have total errors in the 0.2 - 1% range
- 5 - 10% errors for much more complicated observables are now possible
- 2+1+1 flavor DWF ensembles with 1/a = 3 GeV being generated. Accurate inclusion of charm and charm loops
- Enormous opportunity for precision comparisons of theory and experiment and, hopefully, new physics.