Lattice QCD and ϵ'/ϵ

Peter Boyle
Brookhaven National Laboratory
RBC-UKQCD collaboration
HQL 2021

The RBC & UKQCD collaborations

UC Berkeley/LBNL
Aaron Meyer

BNL and BNL/RBRC
Yasumichi Aoki (KEK)
Peter Boyle (Edinburgh)
Taku Izubuchi
Yong-Chull Jang
Chulwoo Jung
Christopher Kelly
Meifeng Lin
Hiroshi Ohki
Shigemi Ohta (KEK)
Amarjit Soni

CERN
Andreas Jüttner (Southampton)

Columbia University
Norman Christ
Duo Guo
Yikai Huo
Yong-Chull Jang
Joseph Karpie
Bob Mawhinney
Ahmed Sheta
Bigeng Wang
Tianle Wang
Yidi Zhao

University of Connecticut
Tom Blum
Luchang Jin (RBRC)
Michael Riberdy
Masaaki Tomii

Edinburgh University
Matteo Di Carlo
Luigi Del Debbio
Felix Erben
Vera Gülpers
Tim Harris
Raoul Hodgson
Nelson Lachini
Michael Marshall
Fionn Ó hÓgáin
Antonin Portelli
James Richings
Azusa Yamaguchi
Andrew Z.N. Yong

KEK
Julien Frison

University of Liverpool
Nicolas Garron

Michigan State University
Dan Hoying

Milano Bicocca
Mattia Bruno

Peking University
Xu Feng

University of Regensburg
Davide Giusti
Christoph Lehner (BNL)

University of Siegen
Matthew Black
Oliver Witzel

University of Southampton
Nils Asmussen
Alessandro Barone
Jonathan Flynn
Ryan Hill
Rajnandini Mukherjee
Chris Sachrajda

University of Southern Denmark
Tobias Tsang

Stony Brook University
Jun-Sik Yoo
Sergey Syritsyn (RBRC)

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Editors' Suggestion   Featured in Physics

Direct *CP* violation and the $\Delta I = 1/2$ rule in $K \to \pi\pi$ decay from the standard model

R. Abbott,[1] T. Blum,[2,3] P. A. Boyle,[4,5] M. Bruno,[6] N. H. Christ,[1] D. Hoying,[3,2] C. Jung,[4] C. Kelly,[4] C. Lehner,[7,4] R. D. Mawhinney,[1] D. J. Murphy,[8] C. T. Sachrajda,[9] A. Soni,[4] M. Tomii,[2] and T. Wang[1]

(RBC and UKQCD Collaborations)

[1]*Physics Department, Columbia University, New York, New York 10027, USA*
[2]*Physics Department, University of Connecticut, Storrs, Connecticut 06269-3046, USA*
[3]*RIKEN-BNL Research Center, Brookhaven National Laboratory, Upton, New York 11973, USA*
[4]*Brookhaven National Laboratory, Upton, New York 11973, USA*
[5]*SUPA, School of Physics, The University of Edinburgh, Edinburgh EH9 3JZ, United Kingdom*
[6]*Theoretical Physics Department, CERN, 1211 Geneve 23, Switzerland*
[7]*Universität Regensburg, Fakultät für Physik, 93040 Regensburg, Germany*
[8]*Center for Theoretical Physics, Massachusetts Institute of Technology, Boston, Massachusetts 02139, USA*
[9]*School of Physics and Astronomy, University of Southampton, Southampton SO17 1BJ, United Kingdom*

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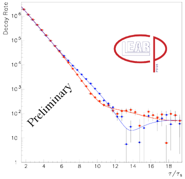
We present a lattice QCD calculation of the $\Delta I = 1/2$, $K \to \pi\pi$ decay amplitude A_0 and ε', the measure of direct *CP* violation in $K \to \pi\pi$ decay, improving our 2015 calculation [1] of these quantities. Both calculations were performed with physical kinematics on a $32^3 \times 64$ lattice with an inverse lattice spacing of $a^{-1} = 1.3784(68)$ GeV. However, the current calculation includes nearly 4 times the statistics and numerous technical improvements allowing us to more reliably isolate the $\pi\pi$ ground state and more accurately relate the lattice operators to those defined in the standard model. We find $\mathrm{Re}(A_0) = 2.99(0.32)(0.59) \times 10^{-7}$ GeV and $\mathrm{Im}(A_0) = -6.98(0.62)(1.44) \times 10^{-11}$ GeV, where the errors are statistical and systematic, respectively. The former agrees well with the experimental result $\mathrm{Re}(A_0) = 3.3201(18) \times 10^{-7}$ GeV. These results for A_0 can be combined with our earlier lattice calculation of A_2 [2] to obtain $\mathrm{Re}(\varepsilon'/\varepsilon) = 21.7(2.6)(6.2)(5.0) \times 10^{-4}$, where the third error represents omitted isospin breaking effects, and $\mathrm{Re}(A_0)/\mathrm{Re}(A_2) = 19.9(2.3)(4.4)$. The first agrees well with the experimental result of $\mathrm{Re}(\varepsilon'/\varepsilon) = 16.6(2.3) \times 10^{-4}$. A comparison of the second with the observed ratio $\mathrm{Re}(A_0)/\mathrm{Re}(A_2) = 22.45(6)$, demonstrates the standard model origin of this "$\Delta I = 1/2$ rule" enhancement.

Motivation

- Baryogenesis: CP violation (CPv) required to generate excess of matter
- Electroweak Phase transition: Standard Model CPv insufficient $\Rightarrow$ new physics if probe CPv?
- (Indirect) Cronin & Fitch PRL 13, 138 (1964), Nobel Prize 1980.



- (Direct) NA48@CERN (PLB 544, 97 (2002)), and KTeV@FNAL (PRD 092001 (2011))

HEP experiment observes magnitude (and infers phases) of amplitude ratios η_{00}, η_{+-}

$$\eta_{00} = \epsilon - 2\epsilon' = \frac{\langle \pi^0\pi^0 | H_W | K_L \rangle}{\langle \pi^0\pi^0 | H_W | K_S \rangle} = \frac{A(K_L \to \pi^0\pi^0)}{A(K_S \to \pi^0\pi^0)}$$

$$\eta_{+-} = \epsilon + \epsilon' = \frac{\langle \pi^+\pi^- | H_W | K_L \rangle}{\langle \pi^+\pi^- | H_W | K_S \rangle} = \frac{A(K_L \to \pi^+\pi^-)}{A(K_S \to \pi^+\pi^-)}$$

CP violation in $K \to \pi\pi$

- K_L has *both* CP even and CP odd components: indirect CPv parametrised by ϵ
- Complex decay amplitudes give rise to direct CPv parametrised by ϵ'

$$
\begin{aligned}
|\epsilon| &= (2.228 \pm 0.011) \times 10^{-3} \\
\mathrm{Re}(\epsilon'/\epsilon) &= \frac{1}{6}\left(1 - \left|\frac{\eta_{00}}{\eta_{+-}}\right|\right) = (16.5 \pm 2.6) \times 10^{-4}
\end{aligned}
$$

Decompose into definite isospin states

$$
\begin{aligned}
|(\pi\pi)_{I=2}\rangle &= \frac{1}{\sqrt{6}}\left(2|\pi^0\pi^0\rangle - |\pi^+\pi^-\rangle - |\pi^-\pi^+\rangle\right) \\
|(\pi\pi)_{I=0}\rangle &= \frac{1}{\sqrt{3}}\left(|\pi^0\pi^0\rangle + |\pi^+\pi^-\rangle + |\pi^-\pi^+\rangle\right) \\
A(K^0 \to (\pi\pi)_{I=0,2}) &= |A_{0,2}|e^{i(\delta_{0,2}+\phi_{0,2})}
\end{aligned}
$$

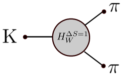
Need standard model calculation of complex amplitudes to draw conclusions from direct CPv

$$
\begin{aligned}
A(K^0 \to \pi^+\pi^-) &= \sqrt{\frac{2}{3}}A_0 e^{i\delta_0} + \sqrt{\frac{1}{3}}A_2 e^{i\delta_2} \\
A(K^0 \to \pi^0\pi^0) &= \sqrt{\frac{2}{3}}A_0 e^{i\delta_0} - 2\sqrt{\frac{1}{3}}A_2 e^{i\delta_2}
\end{aligned}
$$

$$
\epsilon' = \frac{i\omega e^{i(\delta_2-\delta_0)}}{\sqrt{2}}\left(\frac{\mathrm{Im}A_2}{\mathrm{Re}A_2} - \frac{\mathrm{Im}A_0}{\mathrm{Re}A_0}\right)
\qquad
\omega = \mathrm{Re}A_2/\mathrm{Re}A_0
$$

Hadronic processes are intrinsically non-perturbative: calculating strong dynamics $\Rightarrow$ LQCD

Overview



$$\epsilon' = \frac{i\omega e^{i(\delta_2-\delta_0)}}{\sqrt{2}}\left(\frac{\mathrm{Im}A_2}{\mathrm{Re}A_2} - \frac{\mathrm{Im}A_0}{\mathrm{Re}A_0}\right)$$

$$A_I = F\frac{G_F}{\sqrt{2}}V_{ud}^* V_{us}\sum_{i=1}^{10}\sum_{j=1}^{7}\left[(z_i(\mu) + \tau y_i(\mu))Z_{ij}^{\mathrm{lat}\to\overline{\mathrm{MS}}}M_j^{I,lat}\right]$$

- CKM phase leads to CPV via imaginary part

$$\tau = -\frac{V_{ts}^* V_{td}}{V_{us}^* V_{ud}} = 0.0014606 + 0.00060408i$$

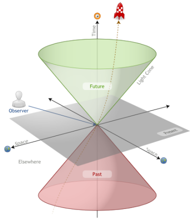
- $M_j^{I,lat}$ Lattice determines QCD hadronic matrix element of four quark operators
- F Lellouch-Luscher Finite volume correction
- $z_i(\mu)$ and $y_i(\mu)$ are perturbative Wilson coefficient
- Z_{ij} Nonperturbative QCD running to scale μ; perturbative matching to $\overline{MS}$ at μ

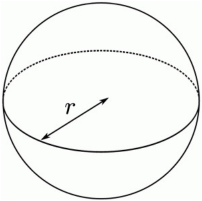
Euclidean space correlation functions

Importance sampled numerical path integration: must Wick rotate to Euclidean space

$$\int \mathcal{D}U\mathcal{D}\bar{\psi}\mathcal{D}\psi e^{iS_G^M} e^{iS_F^M} \rightarrow \int \mathcal{D}U\mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-S_G^E} e^{-S_F^E}$$

so that probability amplitude becomes a *partition function probability measure*.





$$G^M(\vec{r}, t) = \frac{1}{4\pi r}\delta(r - t),$$

$$G^M(\vec{p}, t) = \frac{ie^{i\omega_p t}}{2\omega_p}.$$

$$G^E(\vec{r}, t) = \frac{1}{4\pi^2(r^2 + t^2)},$$

$$G^E(\vec{p}, t) = \frac{e^{-\omega_p t}}{2\omega_p}.$$

- Interpolating operators: use *uud* operator in color singlet, get proton *eventually*

Weak Hamiltonian

Underlying weak processes $\Rightarrow$ low energy effective four quark operators

$$H_W = \frac{G_F}{\sqrt{2}} V_{us}^* V_{ud} \sum_{i=1}^{10} \left[z_i(\mu) - \frac{V_{ts}^* V_{td}}{V_{us}^* V_{ud}} y_i(\mu) \right] Q_i(\mu)$$

where z_i and y_i are NLO perturbative Wilson coefficients.
The scale μ should be large to minimise QCD perturbative errors.

$$Q_1 = (\bar{s}_i u_j)_{\mathrm{V-A}} (\bar{u}_j d_i)_{\mathrm{V-A}} \qquad Q_2 = (\bar{s}u)_{\mathrm{V-A}} (\bar{u}d)_{\mathrm{V-A}}$$

$$Q_3 = (\bar{s}d)_{\mathrm{V-A}} \sum_q (\bar{q}q)_{\mathrm{V-A}} \qquad Q_4 = (\bar{s}_i d_j)_{\mathrm{V-A}} \sum_q (\bar{q}_j q_i)_{\mathrm{V-A}}$$

$$Q_5 = (\bar{s}d)_{\mathrm{V-A}} \sum_q (\bar{q}q)_{\mathrm{V+A}} \qquad Q_6 = (\bar{s}_i d_j)_{\mathrm{V-A}} \sum_q (\bar{q}_j q_i)_{\mathrm{V+A}}$$

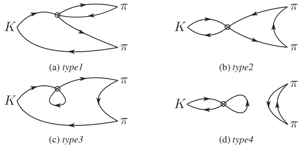
$$Q_7 = \frac{3}{2} (\bar{s}d)_{\mathrm{V-A}} \sum_q e_q (\bar{q}q)_{\mathrm{V+A}} \qquad Q_8 = \frac{3}{2} (\bar{s}_i d_j)_{\mathrm{V-A}} \sum_q e_q (\bar{q}_j q_i)_{\mathrm{V+A}}$$

$$Q_9 = \frac{3}{2} (\bar{s}d)_{\mathrm{V-A}} \sum_q e_q (\bar{q}q)_{\mathrm{V-A}} \qquad Q_{10} = \frac{3}{2} (\bar{s}_i d_j)_{\mathrm{V-A}} \sum_q e_q (\bar{q}_j q_i)_{\mathrm{V-A}}$$

- Operators mix under renormalisation
- Renormalise via intermediate non-perturbative off-shell momentum scheme
  - momentum scheme step scaling used to match at 4 GeV from coarse simulation
- Use Domain wall fermions to preserve continuum chiral and flavor symmetries
  - no additional unphysical operator mixing - V-A current “does what it says”
  - off-shell improved: reduces discretisation effects in renormalisation

Lattice calculation

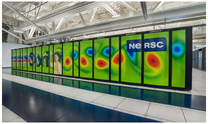
Four classes of Wick contraction:



- G-parity boundary conditions give pions relative momentum; volume tuned to give (near) physical kinematics
- I=0 final state all four contribute ⇒ “disconnected” (gluonic connection)
- I=2 final state only connected

Gluonic correlation randomly sampled: disconnected graphs are noisy!

Calculation started 216 configurations on BlueGene/Q at BNL (2015)
Calculation finished using Cori/KNL at NERSC 741 configurations (2020)



I=2 amplitudes

2015 Phys. Rev. Lett. 115 (2015) 21, 212001

- A_2 connected and measured relatively precisely PRD 92 (2015) no.7, 074502
- $(5.5\mathrm{fm})^3$, physical pion mass, continuum limit w/ 2 lattice spacings (1.73, 2.36 GeV).
- Perturbative truncation in scheme change Z, Wilson coefficients at $\mu = 3$GeV dominates sys error

$$\mathrm{Re}\, A_2 = 1.50(4)_{\mathrm{stat}}(14)_{\mathrm{sys}} \times 10^{-8}\mathrm{Ge}V$$
$$\mathrm{Im}\, A_2 = -6.99(20)_{\mathrm{stat}}(84)_{\mathrm{sys}} \times 10^{-13}\mathrm{Ge}V$$

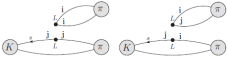
$\Delta I = 1/2$ rule

- Kaons 450x more likely to decay to $I = 0$ $\pi\pi$ states
- arXiv:1212.1474, arXiv:1502.00263
- $\Delta_I = 1/2$ rule is now a quantitative prediction with only QCD as input

Gell-Mann & Pais (1954): decay amplitude to $|(\pi\pi)_{I=0}\rangle$ state is dominant

$$\frac{\mathrm{Re}(A_0)}{\mathrm{Re}(A_2)}(\text{experiment}) = 22.45(6)$$

$$\frac{\mathrm{Re}(A_0)}{\mathrm{Re}(A_2)}(\text{Lattice}) = 19.9(2.3)(4.4)$$

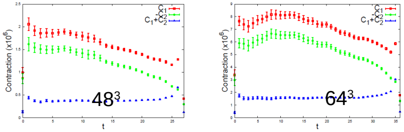


Contraction ①. Contraction ②.

$\mathrm{Re}(A_2) \sim ① + ②$

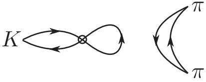
find ② $\approx -0.7$①

[Phys.Rev. D91 (2015) no.7, 074502]



I=0 amplitudes

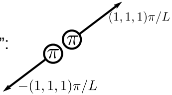
- Substantially more challenging
- $I = 0$ $\pi\pi$ state has vacuum quantum numbers: disconnected graphs



(d) *type4*

PhysRevLett 115 (2015) 21, 212001

- Physical quark masses; coarse $a^{-1} = 1.38$ GeV; $(4.6\text{fm})^3$ volume controls FV errors
- Gparity BC's eliminate at rest $\pi\pi$ state



- Single "$\pi\pi$ operator" - back to back momenta:
- Single "$\pi\pi$ operator" - back to back momenta:
- 21% & 65% statistical errors on $\mathrm{Re}(A_0)$ and $\mathrm{Im}(A_0)$ (disconn.)
  Strong cancellation between Q_4 and Q_6
- 15% sys error due to perturbative truncation

I=0 amplitudes

- Re(A_0) and Re(A_2) from expt.
- Lattice values for Im(A_0), Im(A_2) and the phase shifts,

$$\mathrm{Re}\left(\frac{\varepsilon'}{\varepsilon}\right) = \mathrm{Re}\left\{\frac{i\omega e^{i(\delta_2-\delta_0)}}{\sqrt{2}\varepsilon}\left[\frac{\mathrm{Im}A_2}{\mathrm{Re}A_2} - \frac{\mathrm{Im}A_0}{\mathrm{Re}A_0}\right]\right\}$$

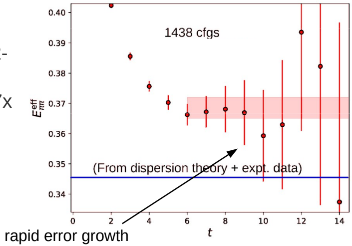
$$= \begin{cases} 1.38(5.15)(4.43)\times 10^{-4}, & \text{(our result)} \\ 16.6(2.3)\times 10^{-4} & \text{(experiment)} \end{cases}$$

- Result is 2.1σ below experimental value.
- Total error on Re(ε'/ε) is ~3x the experimental error
- "This is now a quantity accessible to lattice QCD"!
- Focus since has been to improve statistics and reduce / improve understanding of systematic errors.

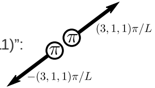
$\pi\pi$ phase shift puzzle

- Essential to understand ππ system:
  - Energy needed to extract ground-state matrix element
  - Energy also needed to compute phase-shift (Luscher)
  - Derivative of phase-shift w.r.t. energy is required for Lellouch-Luscher finite-volume correction (F)
- 2015 calculation phase shift $\delta_0(E_{\pi\pi} \approx m_K) = 23.8(5.0)^\circ$ substantially smaller than prediction obtained by combining dispersion theory with experimental input, 36°.

- Result was very stable under varying fit range and also with 2-state fits.
- Increasing statistics by almost 7x did not resolve ($\delta_0 = 19.1(2.5)^\circ$)
- Nevertheless, most likely explanation is excited-state contamination hidden by rapid reduction in signal/noise.



$\pi\pi$ phase shift Resolution!

"ππ(311)": 

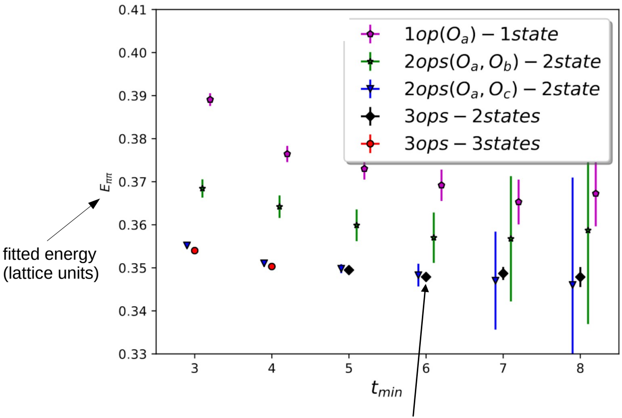
$\sigma = \frac{1}{\sqrt{2}}(\bar{u}u + \bar{d}d)$

- Introduce two more $\pi\pi$ operators
- More powerful than just increasing statistics (from 230 to 741)
- Why? Sensitivity to near degenerate states

$$C_{ij}(t) = \langle O_i^\dagger(t) O_j(t) \rangle = \sum_\alpha A^*_{i,\alpha} A_{j,\alpha} e^{-m_\alpha t}$$

- If we have excess operators and a single state amplitude matrix: $\begin{pmatrix} AA & AB \\ BA & BB \end{pmatrix}$ is determined by *two* variables. *Not the case* if two nearby states.
- Enable fit to resolve this.

Improved analysis resolves phase shift puzzle



Result compatible with dispersive value: $\delta_0(479.5 \text{ MeV}) = 32.3(1.0)(1.4)^\circ$

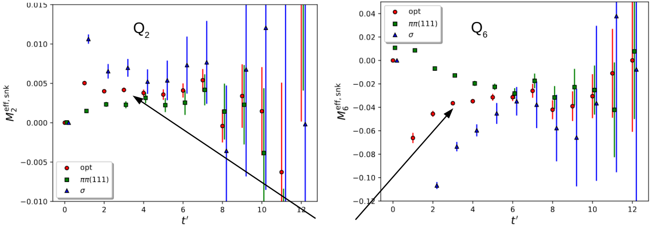
I=0 amplitudes

- Convenient to visualize data by taking "optimal" linear combination of the two most important operators that best projects onto ground-state.

$$\mathcal{O}_{\rm opt} = r_1 \mathcal{O}_{\pi\pi(111)} + r_2 \mathcal{O}_\sigma$$

$$r_1 = 5.24(18) \times 10^{-7}$$
$$r_2 = -2.86(17) \times 10^{-4}$$

using ππ fits



strong, clear plateau + improved precision

Systematic error budget

- Primary systematic errors of 2015 work:
  - Finite lattice spacing: 12%
  - Wilson coefficients: 12%
  - Renormalization (mostly PT matching): 15%
  - Excited-state: $\leq$ 5% but now known to be significantly underestimated
  - Lellouch-Luscher factor (derivative of $\pi\pi$ phase shift wrt. energy): 11%
- In our new work we have used step-scaling to raise the renormalization scale from 1.53 → 4.00 GeV: 15% → 5%
- 3 operators have dramatically improved understanding of $\pi\pi$ system: Lellouch-Luscher factor 11% → 1.5%
- Detailed analysis shows no evidence of remaining excited-state contamination: Excited state error now negligible!
- Still single lattice spacing: Discretization error unchanged.
- Evidence that Wilson coefficient systematics are driven by using PT for 3-4f matching, not improved by higher μ:
  Wilson coeff error unchanged.

Systematic error budget

- Our simulation does not include effects of isospin breaking or EM effects.
- While these effects are typically small O(1%), heavy suppression of A_2 (ΔI=1/2 rule) means relative effect on A_2 and ε' could be O(20%).
- Current best determination of effect uses NLO χPT and $1/N_c$ expansion predicts 23% correction to our result:

  Include as separate systematic error.

[Cirigliano *et al*, JHEP 02 (2020) 032]

- Combining our new result for Im(A_0) and our 2015 result for Im(A_2), and again using expt. for the real parts, we find

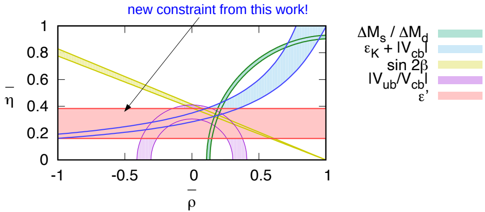
$$\mathrm{Re}\left(\frac{\varepsilon'}{\varepsilon}\right) = \mathrm{Re}\left\{\frac{i\omega e^{i(\delta_2-\delta_0)}}{\sqrt{2}\varepsilon}\left[\frac{\mathrm{Im}A_2}{\mathrm{Re}A_2} - \frac{\mathrm{Im}A_0}{\mathrm{Re}A_0}\right]\right\}$$

$$= 0.00217(26)(62)(50)$$

(26): stat; (62): sys; (50): IB + EM

Consistent with experimental result:

$$\mathrm{Re}(\epsilon'/\epsilon)_{\mathrm{expt}} = 0.00166(23)$$



Other calculations

Not covered in detail:

- Need independent calculations:
- Ishizuka, Ishikawa, Ukawa, Yoshie: Phys.Rev.D 98 (2018) 11, 114512
- $m_\pi = 260$ MeV, improved Wilson
- Unphysical masses, harder renormalisation problem

$$\epsilon'/\epsilon = 0.0019(57)$$

- Calculation at the physical quark masses planned

Summary and Outlook

- Massively improved calculation of A_0
- Only the QCD Lagrangian and CKM as input
- Statistics helped, better measurements methods helped
- Reproduce $\Delta I = 1/2$ rule
- SM ϵ' is consistent with experimental observation
- Reproduce $\pi\pi$ phase shifts
- Total error 3.6x experiment
- Promising avenue for new physics in CP, aim to improve with....

Next steps:

- Biggest pure lattice sys-error is discretisation.
- Use Perlmutter supercomputer: 30x per node over Cori computer (after network upgrade)
- Add $40^3 \times 64$ and $48^3 \times 64$ at 1.7 and 2.1 GeV.