Old and New Physics with Domain Wall Fermion Lattice QCD

6th Workshop of the APS Topical Group on Hadronic Physics
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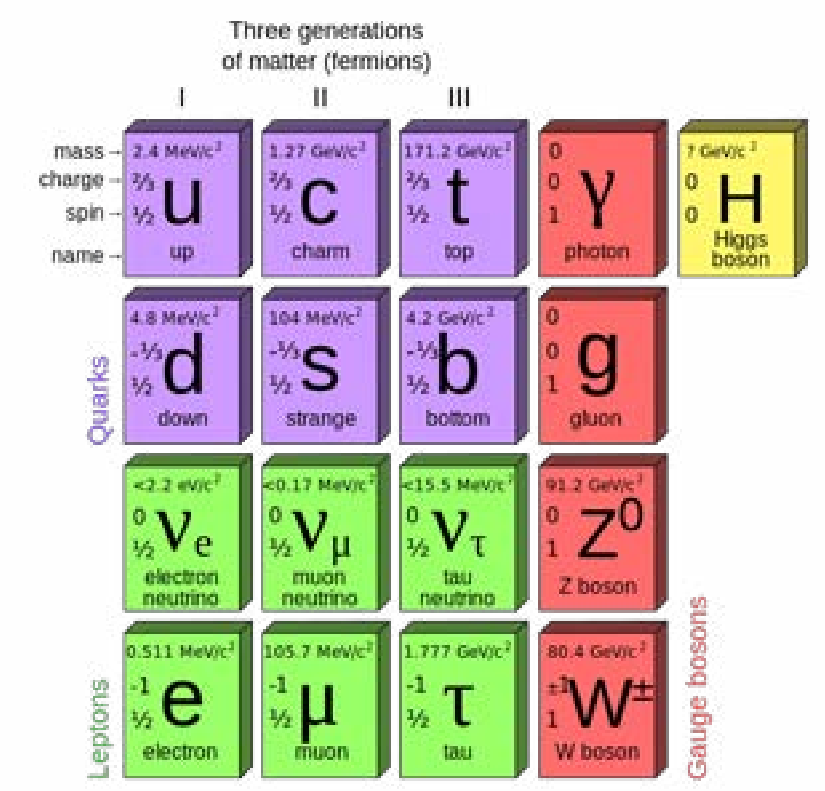
Columbia University
RBC Collaboration

This work done in conjuction with
RBC Collaboration
UKQCD Collaboration
HotQCD Collaboration

Known Elementary Particles



$$m_u = 2.19 \pm 0.15\,\text{MeV}$$

$$m_d = 4.67 \pm 0.20\,\text{MeV}$$

$$m_s = 94 \pm 3\,\text{MeV}$$

$$m_c = 1.275 \pm 0.025\,\text{GeV}$$

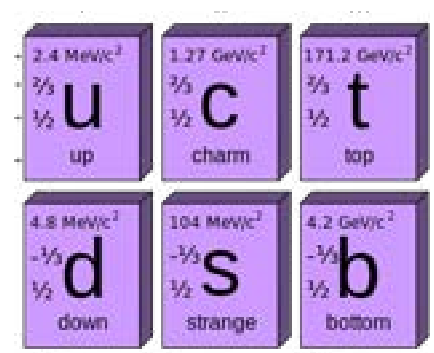
$$m_b = 4.18 \pm 0.03\,\text{GeV}$$

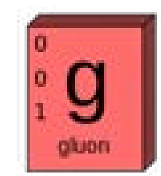
$$m_t = 173.5 \pm 0.6 \pm 0.8\,\text{GeV}$$

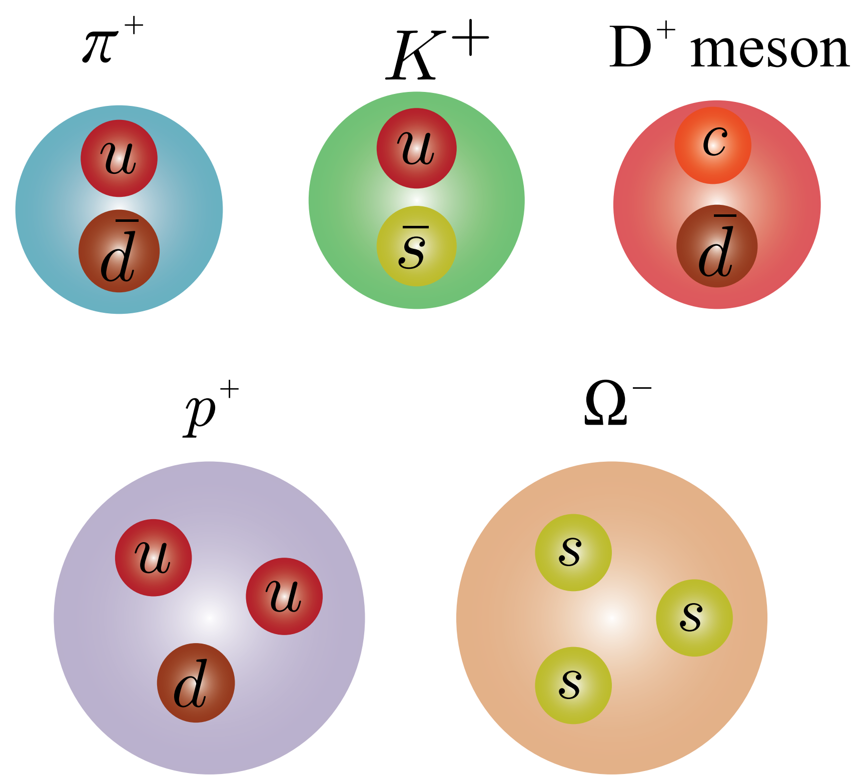
QCD

Theory of interactions of quarks

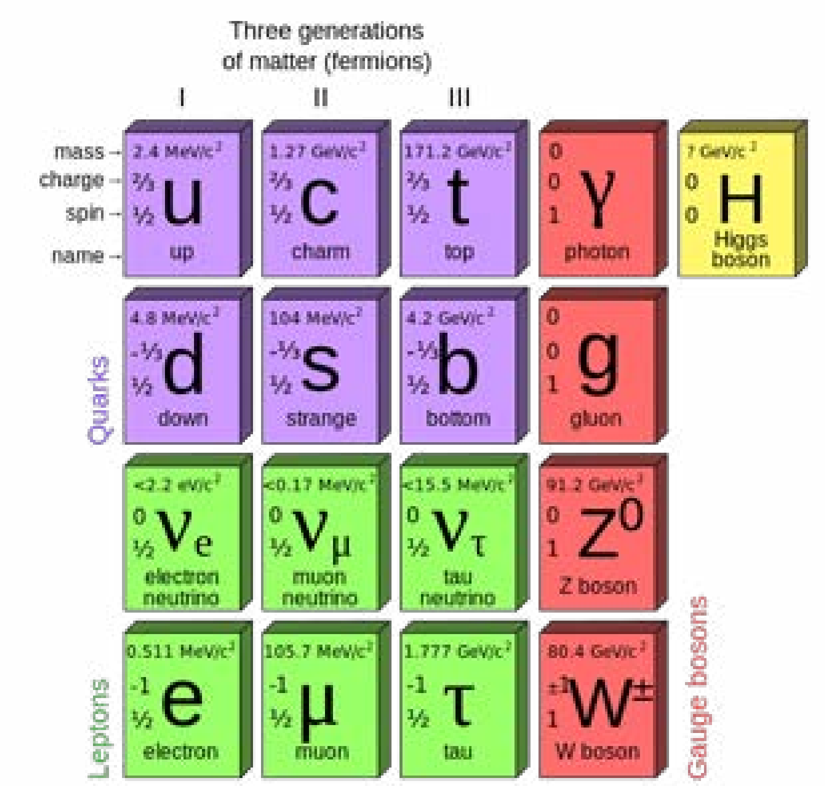
Interactions mediated by gluons







Known Elementary Particles



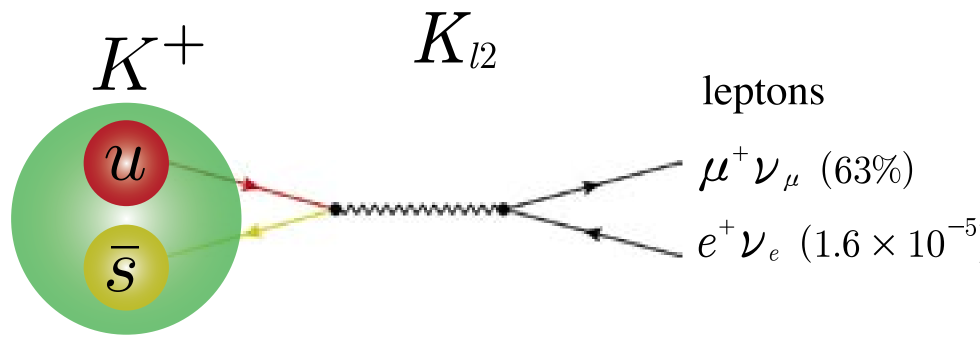
Standard Model quark decays involve elements of a 3 by 3 unitary matrix, the CKM matrix, described by 4 parameters

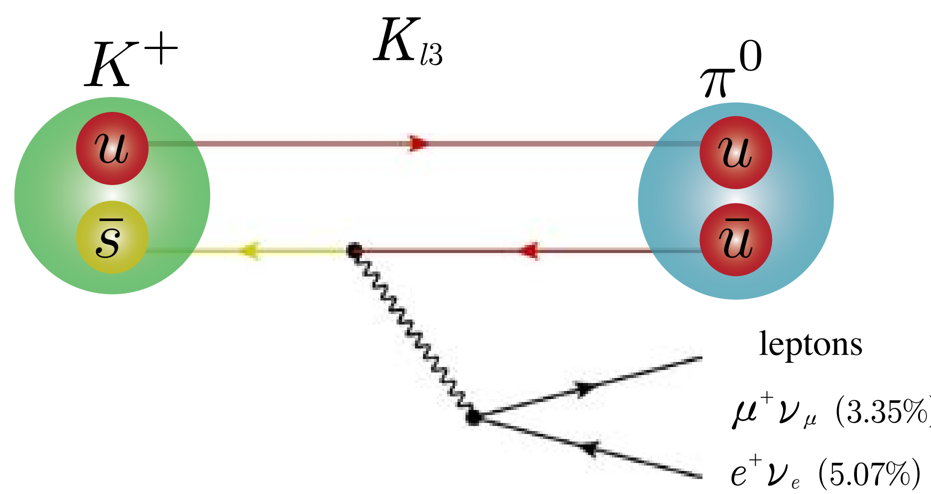
$$\begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix}$$

QCD + Electroweak

Decays of quarks via weak interactions predicted by Standard Model.

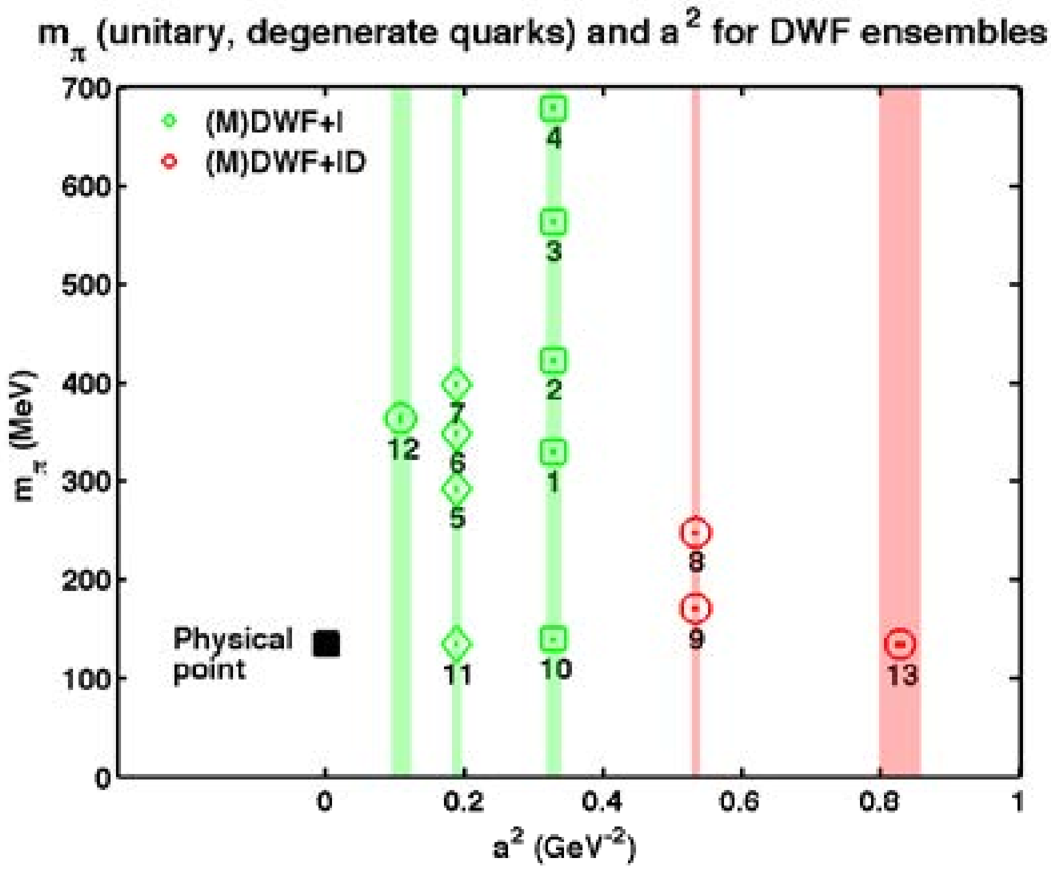
Experiments measure decays of hadrons





For K_{l3} we have: $\Gamma_{K\to\pi l\nu} = C_K^2 \frac{G_F^2 m_K^5}{192\pi^3} I \, S_{EW}\left[1 + 2\Delta_{SU(2)} + 2\Delta_{EM}\right] |V_{us}|^2 |f_+(0)|^2$

Major Development: Ensembles with Physical Quark Masses



2+1 flavors, (M)DWF
RBC and UKQCD Collaborations

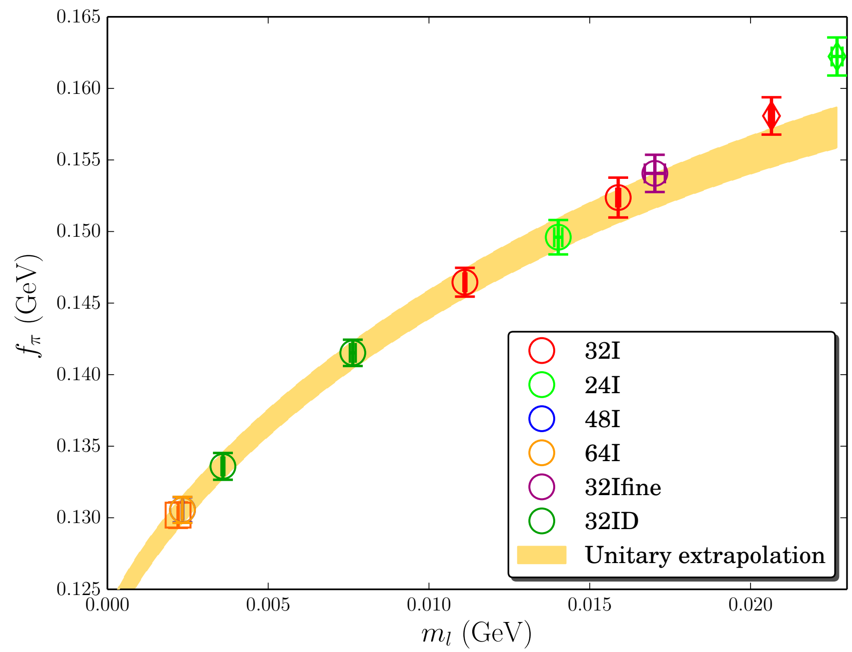
Large volume ensembles with physical quark masses are also being produced and used by the European BMW Collaboration (hex-smeared clover fermions) and the US MILC/FNAL group (HISQ staggered fermions)

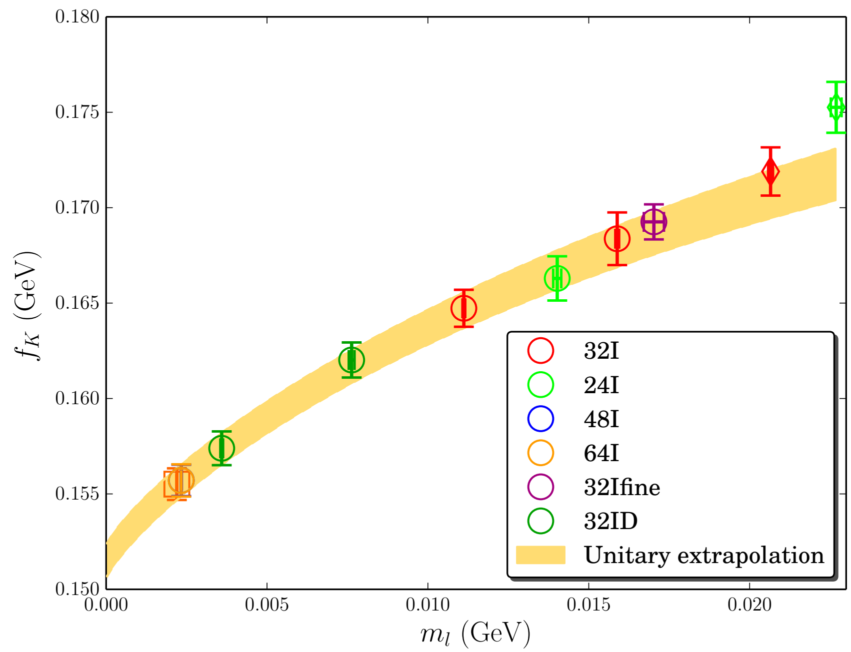
Small Chiral Extrapolation

Input m_l, m_s and a bare coupling. Find measured mass ratios are close to physical

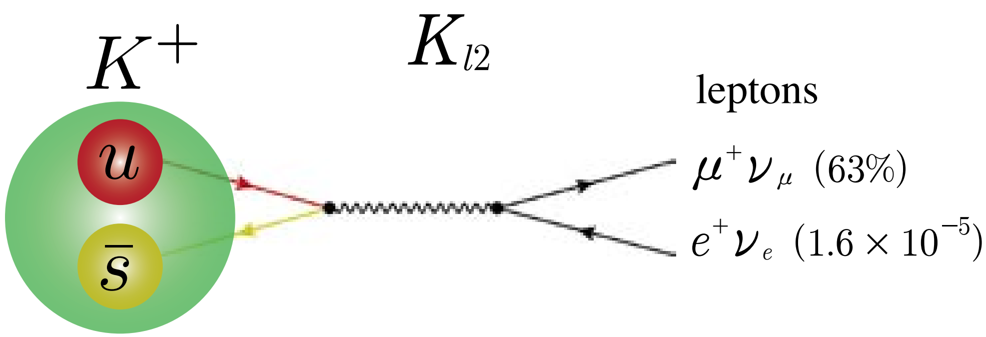
Use SU(2) chiral perturbation theory and reweighting in m_s to make small corrections

Quantity	Physical Value	Ens. 10 Value	Deviation	Ens. 11 Value	Deviation
m_π/m_K	0.2723	0.2790	2.4%	0.2742	0.7%
m_π/m_Ω	0.0807	0.0830	2.8%	0.0822	1.9%
m_K/m_Ω	0.2964	0.2974	0.3%	0.2998	1.2%





Simplest Matrix Elements: f_π and f_K

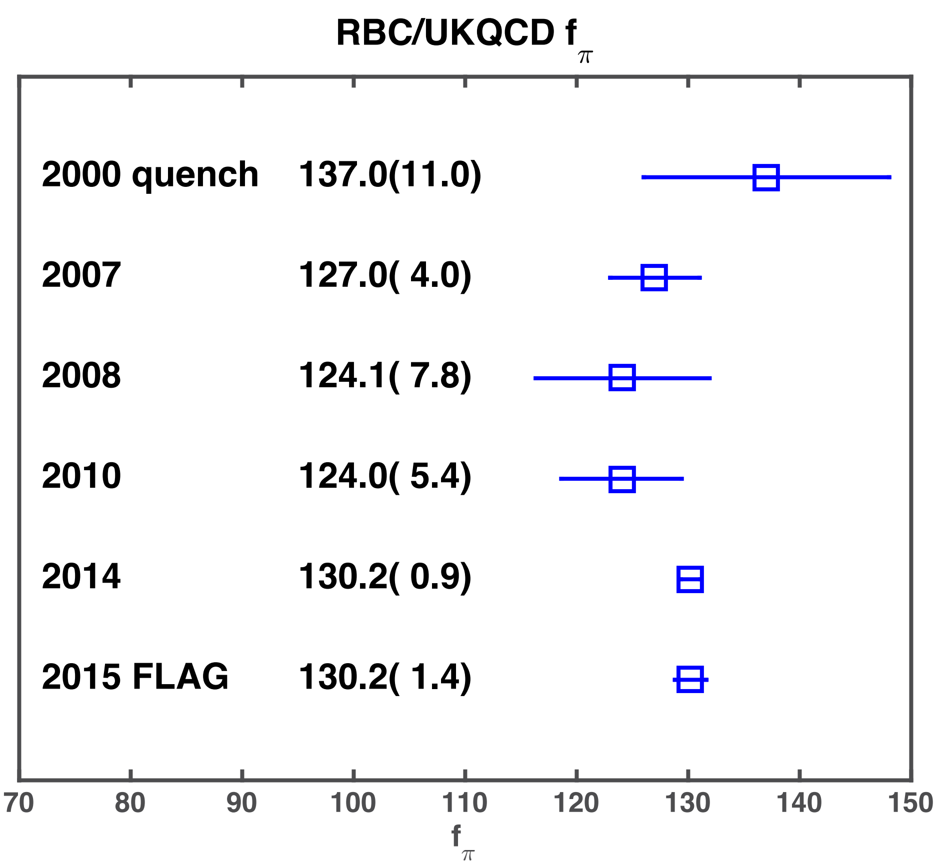


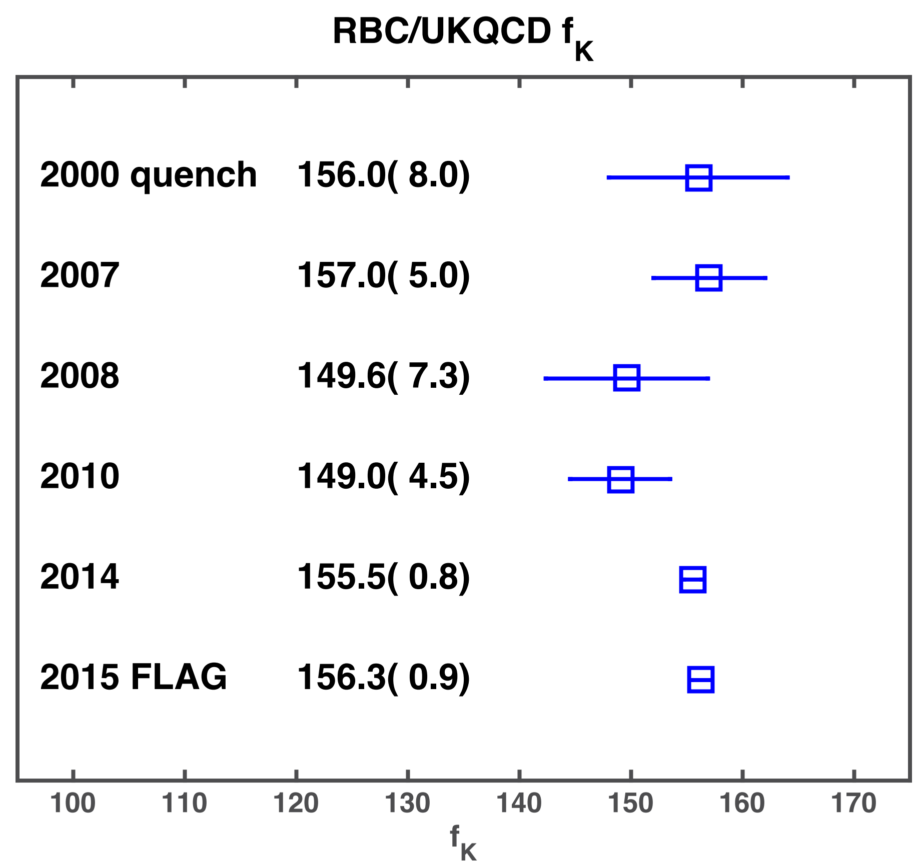
Inputs are m_π, m_K and m_Ω

Use SU(2) ChPT to extrapolate

Now have ensembles with essentially physical quark masses (few percent) arXiv:1411.7017 (RBC-UKQCD)

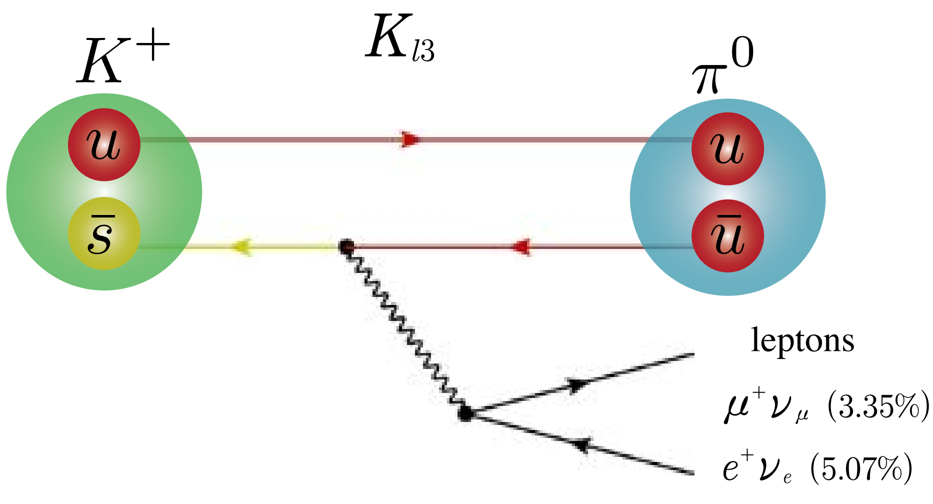
f_π and f_K are predictions

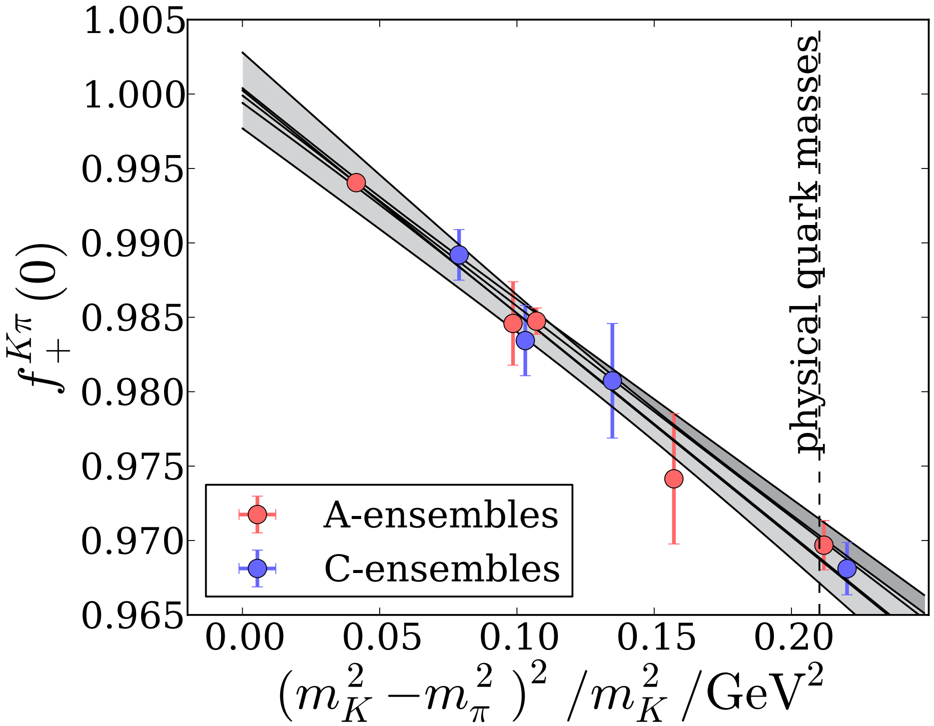




Constraining the CKM Matrix via K_{l3} decays

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





$$f_0(q^2) = f_+(q^2) + \frac{q^2}{m_K^2 - m_\pi^2} f_-(q^2)$$

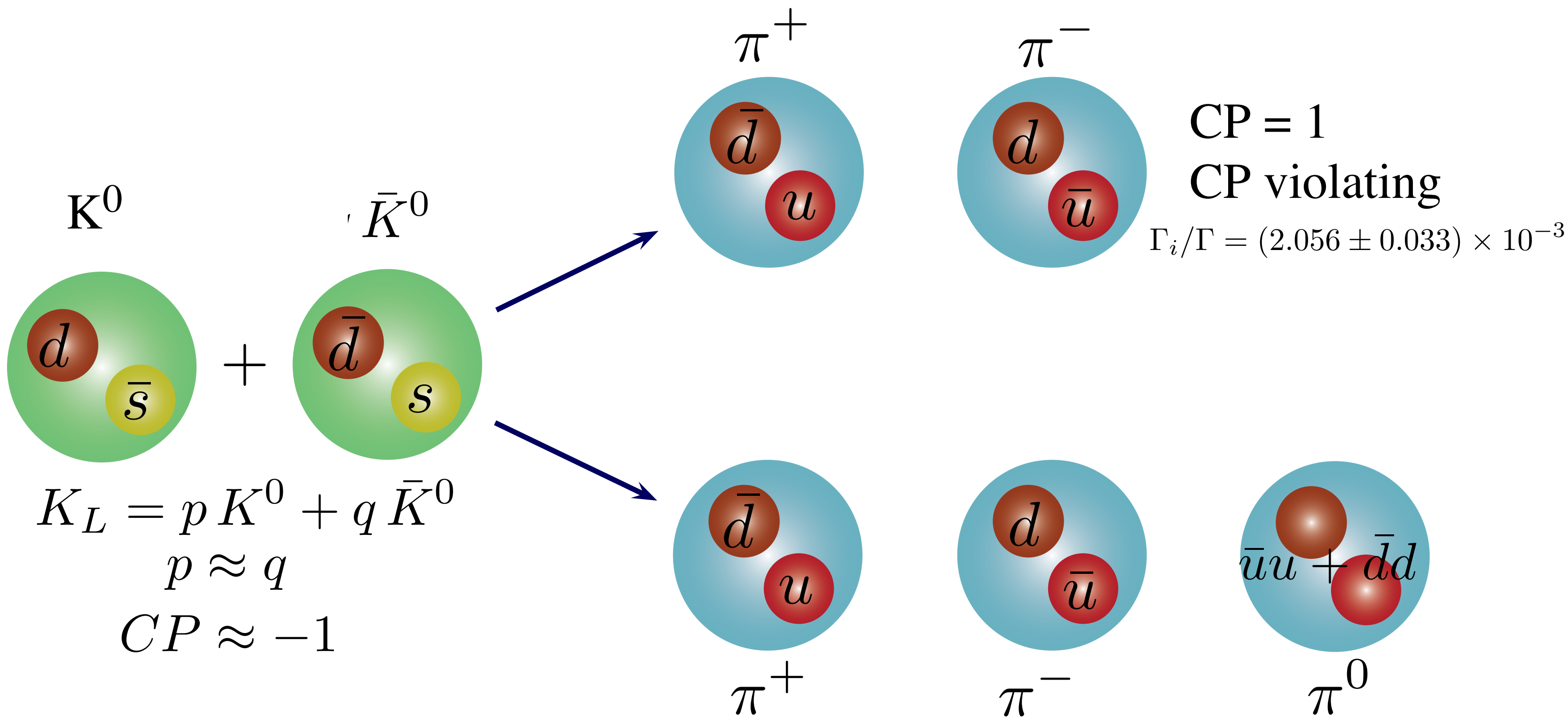
$$\langle \pi(p')|V_\mu|K(p)\rangle = (p_\mu + p'_\mu)f_+(q^2) + (p_\mu + p'_\mu)f_-(q^2)$$

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

$$f_+^{K\pi}(0) = 0.9685(34)(14)\,, \qquad |V_{us}| = 0.2233(5)(9)\,,$$

$$1 - |V_{ud}|^2 - |V_{us}|^2 = 0.0010(4)_{V_{ud}}(2)_{V_{us}^{\rm exp}}(4)_{V_{us}^{\rm lat}} = 0.0010(6)\,,$$

K -> ππ Decays and CP Violation

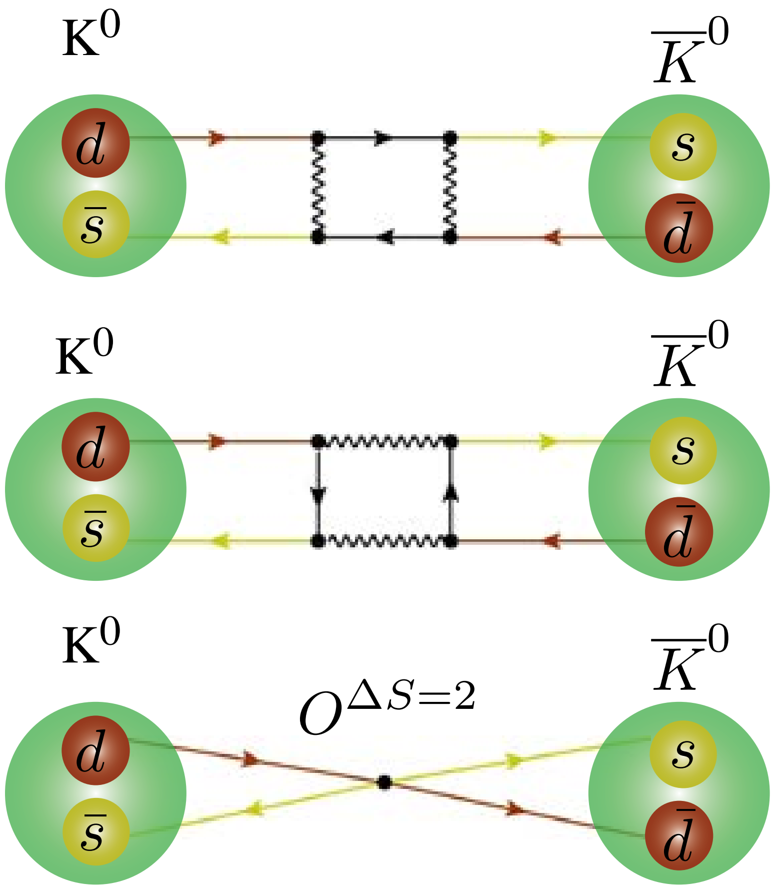


$$\eta_{+-} = |\eta_{+-}|e^{i\phi_{+-}} = \frac{A(K_L \to \pi^+\pi^-)}{A(K_S \to \pi^+\pi^-)}$$

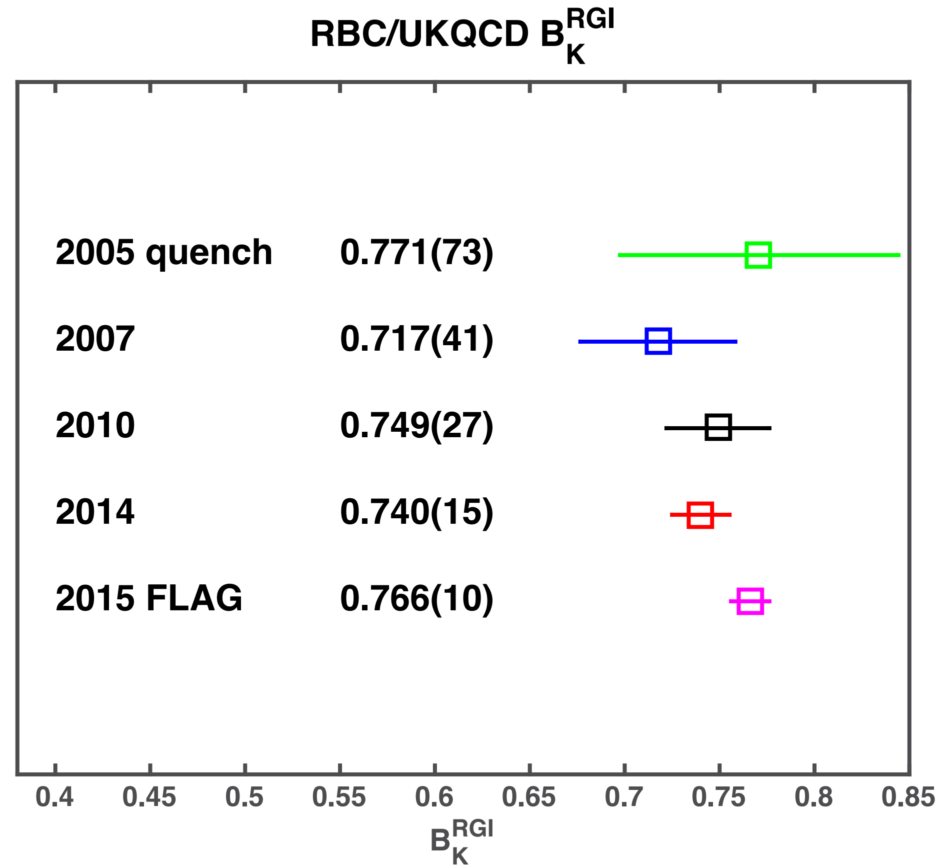
$$\eta_{00} = |\eta_{00}|e^{i\phi_{00}} = \frac{A(K_L \to \pi^0\pi^0)}{A(K_S \to \pi^0\pi^0)}$$

CP Violation in Mixing

$$K^0 \leftrightarrow \overline{K}^0$$



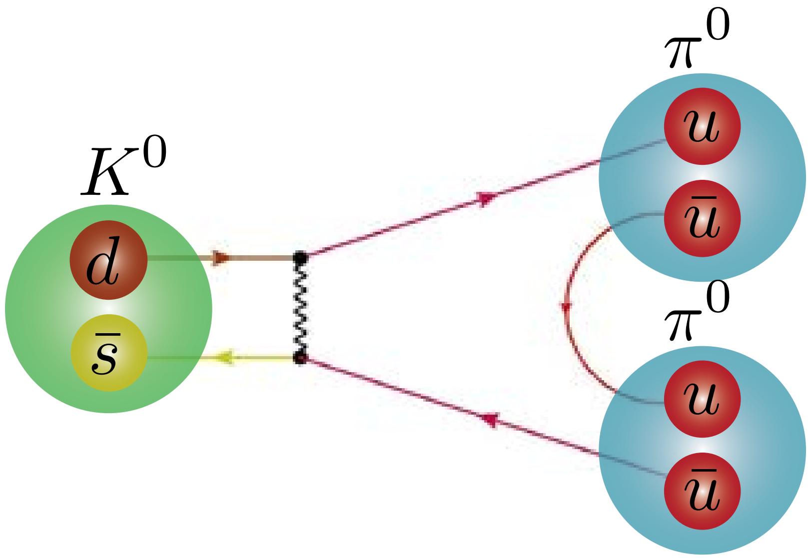
arXiv:1411.7017 RBC-UKQCD

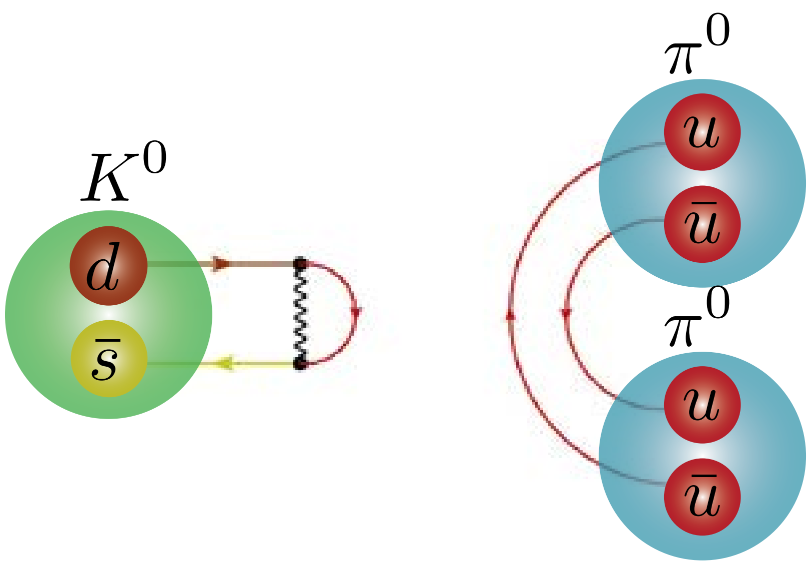


$$\varepsilon = \frac{e^{i\pi/4}}{\sqrt{2}\,\Delta M_K}\left(\mathrm{Im}(M_{12}) + 2\,\frac{\mathrm{Im}(A_0)}{\mathrm{Re}(A_0)}\,\mathrm{Re}(M_{12})\right) = \kappa_\varepsilon\,\frac{e^{i\phi_\varepsilon}}{\sqrt{2}}\left[\frac{\mathrm{Im}\left(M_{12}^{O^{\Delta S=2}}\right)}{\Delta m_K}\right]$$

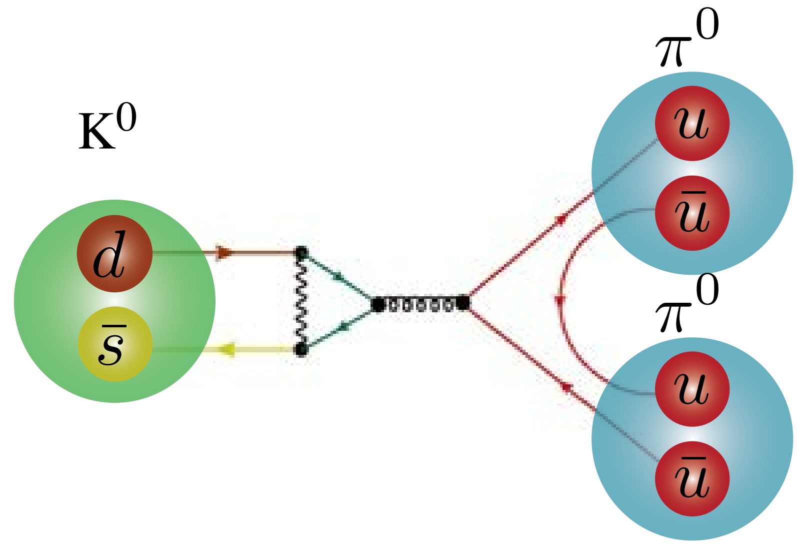
$$\varepsilon_K = \kappa_\varepsilon\, C_\varepsilon\, \hat{B}_K\, \mathrm{Im}(\lambda_t)\,\{\mathrm{Re}(\lambda_c)[\eta_1\, S_0(x_c) - \eta_3\, S_0(x_c, x_t)] - \mathrm{Re}(\lambda_t)\,\eta_2\, S_0(x_t)\}\, e^{i\pi/4}$$

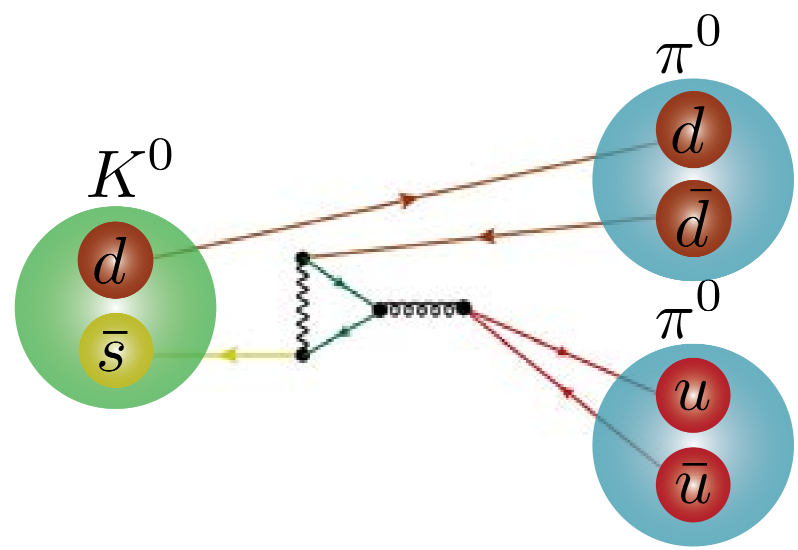
Kaon Decays Via Exchange
CP Conserving





Kaon Decays Via "Penguin" Diagrams
Give Indirect CP violation

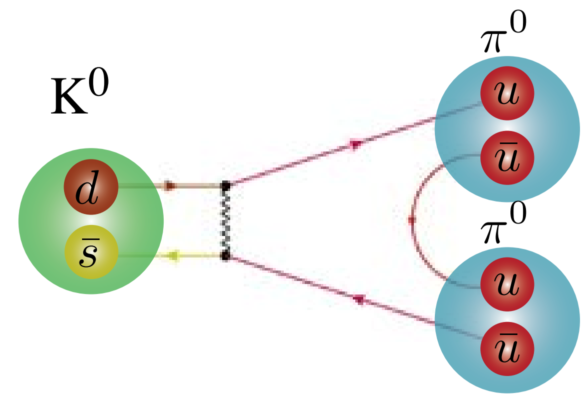




Described by effective weak Hamiltonian:

$$H_W = \frac{G}{\sqrt{2}} V_{us}^* V_{ud} \sum_{i=1}^{10} \left[z_i(\mu) + \tau y_i(\mu) \right] Q_i(\mu).$$

K -> $(\pi\pi)_{I=2}$ 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.

Re(A_2) from experiment is (1.4787   0.0031) 10^{-8} GeV. Im(A_2) is unknown.

First result for a single lattice spacing (PRL 108 (2012) 141601 RBC-UKQCD)

$$\mathrm{Re}(A_2) = (1.3861 \quad 0.046_{stat} \quad 0.258_{sys}) \quad 10^{-8}\ \mathrm{GeV}$$

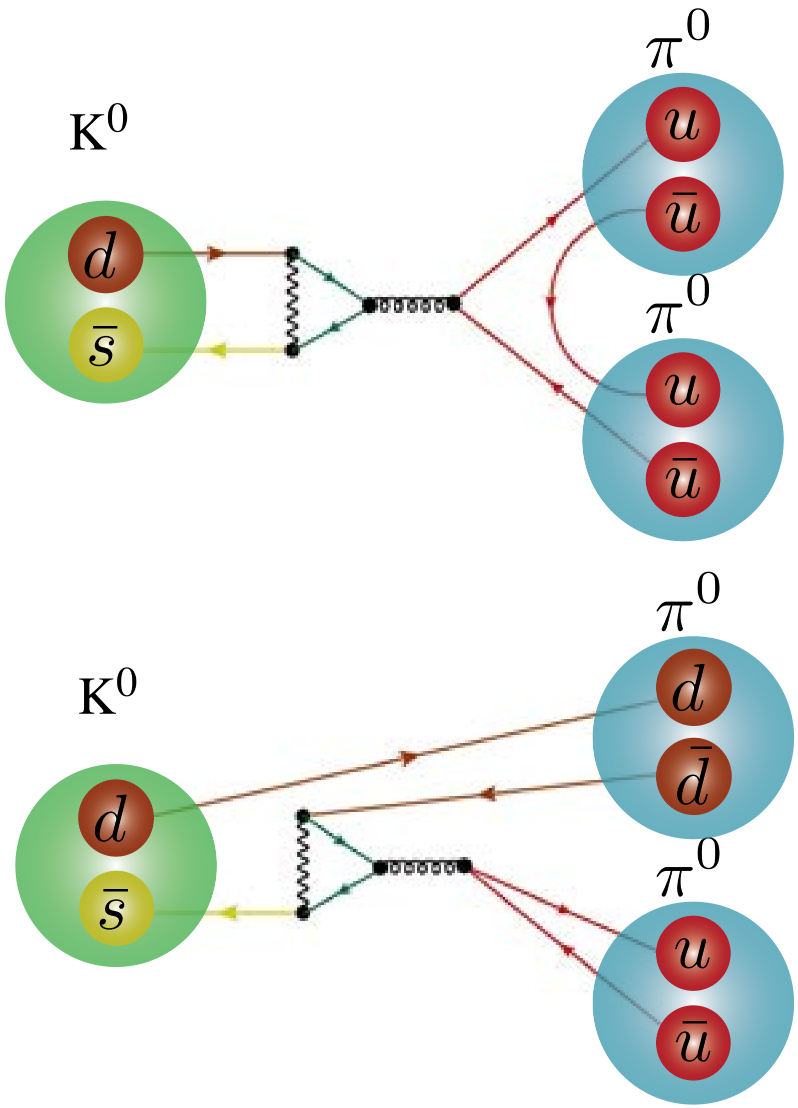
$$\mathrm{Im}(A_2) = (-6.54 \quad 0.46_{stat} \quad 1.20_{sys}) \quad 10^{-13}\ \mathrm{GeV}$$

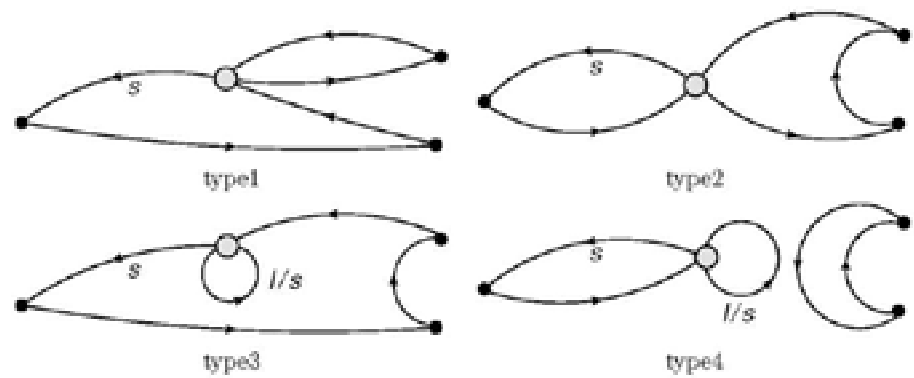
Now have finished ensemble 10 and 11 calculations, with smaller statistical errors and an extrapolation to the continuum limit (PRD91 (2015) 7, 0704502 RBC-UKQCD)

$$\mathrm{Re}(A_2) = (1.50 \quad 0.04_{stat} \quad 0.14_{sys}) \quad 10^{-8}\ \mathrm{GeV}$$

$$\mathrm{Im}(A_2) = (-6.99 \quad 0.20_{stat} \quad 0.84_{sys}) \quad 10^{-13}\ \mathrm{GeV}$$

K -> $(\pi\pi)_{I=0}$ Amplitudes





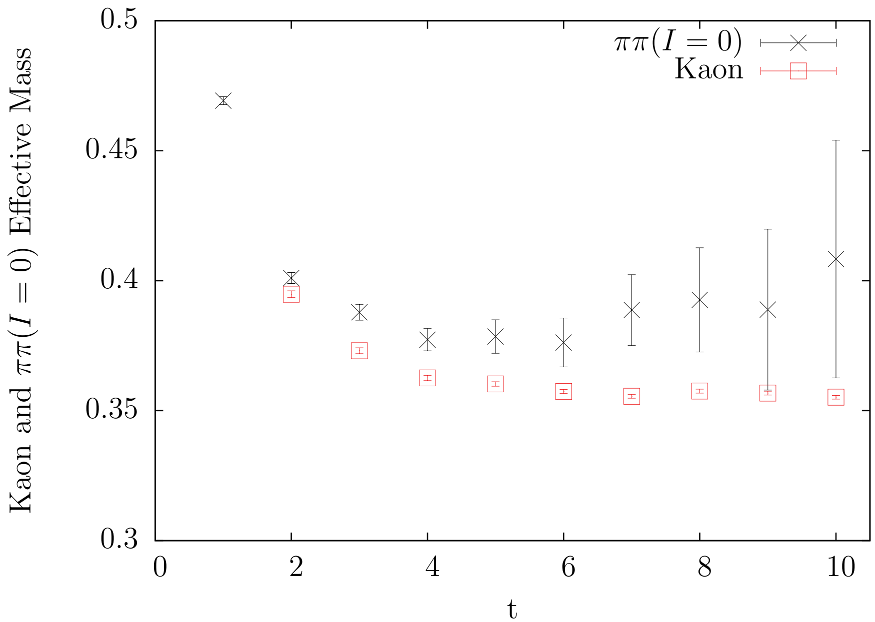
Disconnected quark diagrams enter - noisy

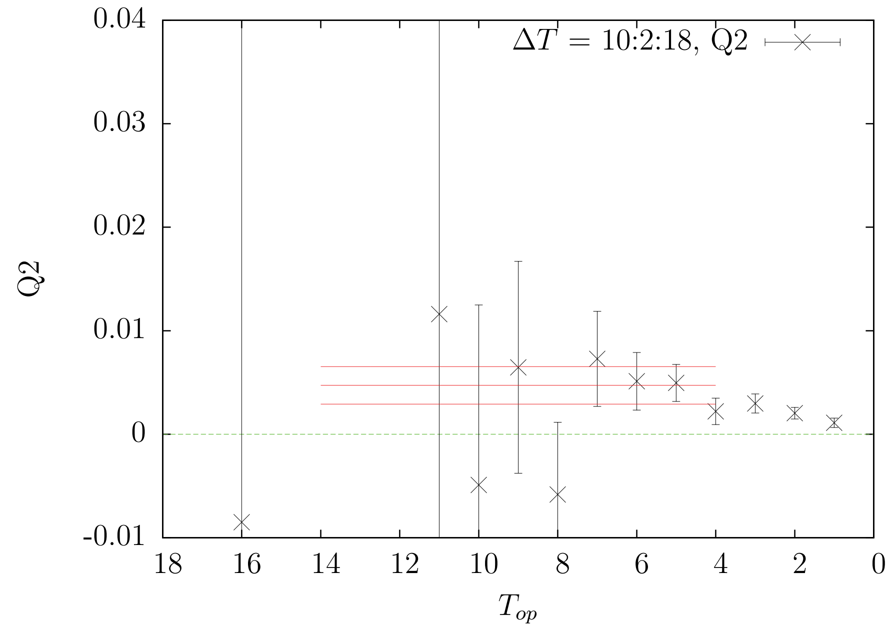
Need more than antiperiodic boundary conditions on one quark to ensure the have relative momenta: G parity boundary conditions used

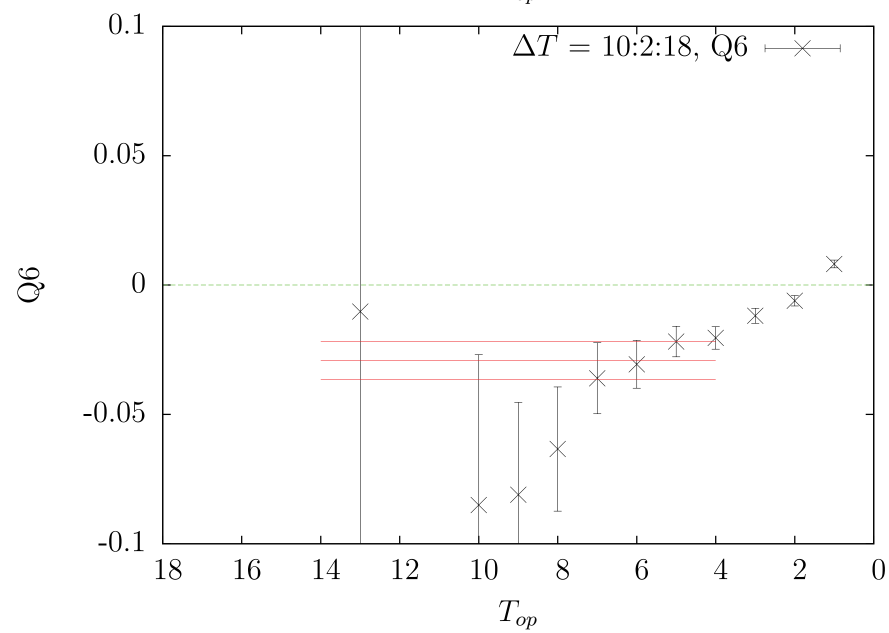
Need to generate G parity ensembles, since see and valence sectors require same boundary conditions.

G parity evolution by Chris Kelly. Operator code by Daiqian Zhang.

K -> $(\pi\pi)_{I=0}$ Amplitudes







Have to match K and $\pi\pi$ energies

Q2 is most important matrix element for Re(A_0) and Q6 for Im(A_0)

Plateaus visible, but more data planned

Results from ~200 measurements expected very soon!

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

Generic Process	Examples	Experiment	LQCD calculates
$Kl2$	$K^+ \to \mu^+ \nu_\mu$ $K^+ \to e^+ \nu_e$	f_K	f_K (also f_π)
$Kl3$	$K^+ \to \pi^0 \, l^+ \, \nu_l$ $K^0 \to \pi^- \, l^+ \, \nu_l$	$\lvert V_{us} f^+(0) \rvert^2$	$f^+(0)$
$Kl4$	$K \to \pi \, \pi \, l \, \bar{\nu}_l$		??
$K \to \pi\pi$ (CP conserving)	$K^0 \to \pi^+ \, \pi^-$ $K^+ \to \pi^+ \, \pi^0$	$\lvert A_0 \rvert$ $\lvert A_2 \rvert$	$\lvert A_0 \rvert \; \lvert A_2 \rvert$ (SM_{cpc} inputs)
Δm_K (CP conserving)	$K^0 \leftrightarrow \pi \, \pi \leftrightarrow \overline{K}^0$ (LD) $K^0 \leftrightarrow O_{\Delta S=2} \leftrightarrow \overline{K}^0$ (SD)	Δm_K	Δm_K (SM_{cpc} inputs)
$K^0 \to \pi \; \pi$ (indirect CP violation)	$K_L \to \pi \, \pi$ $\left(K^0 \leftrightarrow \overline{K}^0\right) \to \pi \, \pi$ independent of π π isospin	$\epsilon = \dfrac{\hat{B}_K F_K^2 \, \mathrm{SM}}{\Delta m_K}$	$B_K, \dfrac{\mathrm{Im}(A_0)}{\mathrm{Re}(A_0)}$
$K^0 \to \pi \; \pi$ (direct CP violation)	$K_L \to \pi \, \pi$ depends on π π isospin	$\mathrm{Re}(\epsilon'/\epsilon)$ $= f(A_0, A_2, \mathrm{SM})$	$A_0 \;\; A_2$ (SM_{cpc} inputs)
$K \to \pi l l$	$K_L \to \pi^0 l^+ l^-$ $K_S \to \pi^0 l^+ l^-$		??

SM_{cpc} = Standard Model CP-conserving parameters

Computers

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

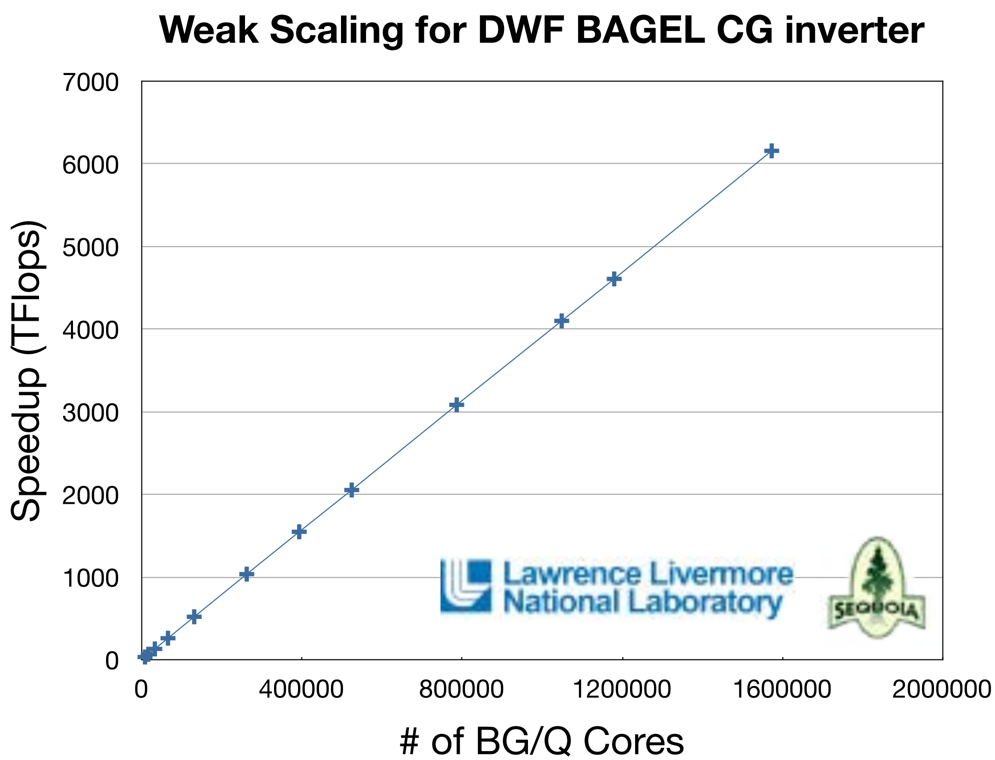
IBM BGQ 2012-
200 GFlops/node

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

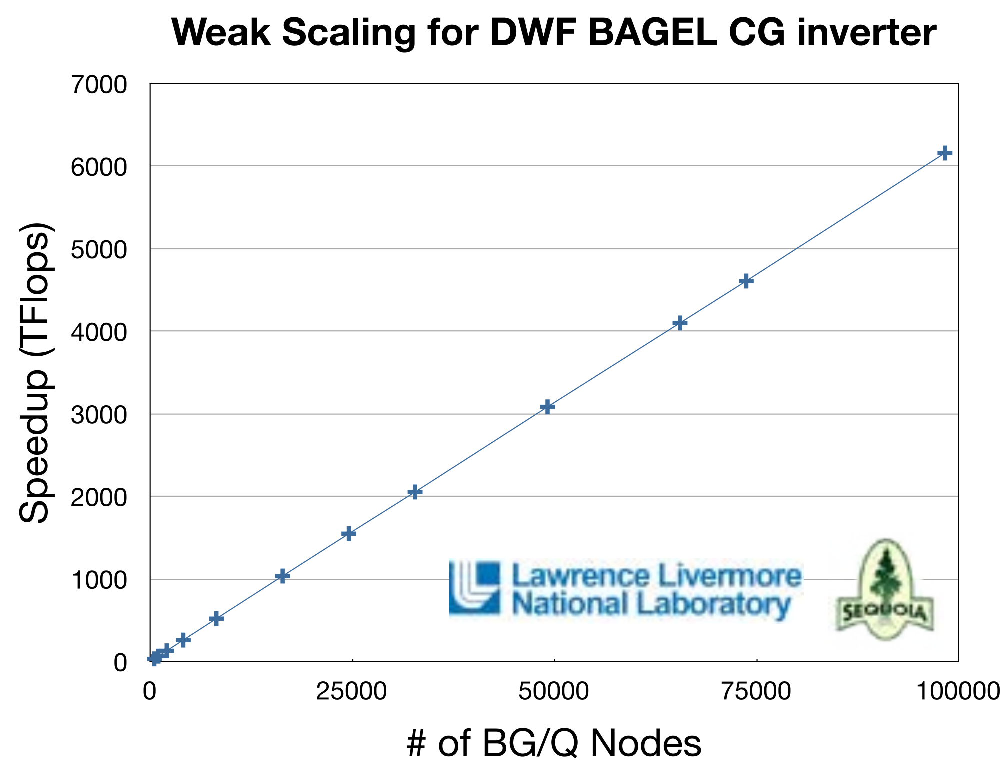
RBC/UKQCD have production jobs on the Argonne ALCF BGQ that sustain 1 PFlops on 32 racks = 32k nodes = 0.5 M cores.

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



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



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

Quantum Chromodynamics

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

$$Z = \int [dA] \prod_{i=1}^{3} \det\left[D(A, g_0, m_0^i)\right] \exp\left\{-\frac{i}{4}(\partial_\mu A_\nu - \partial_\nu A_\mu + g_0 f^{abc} A_\mu^b A_\nu^c)^2\right\}$$

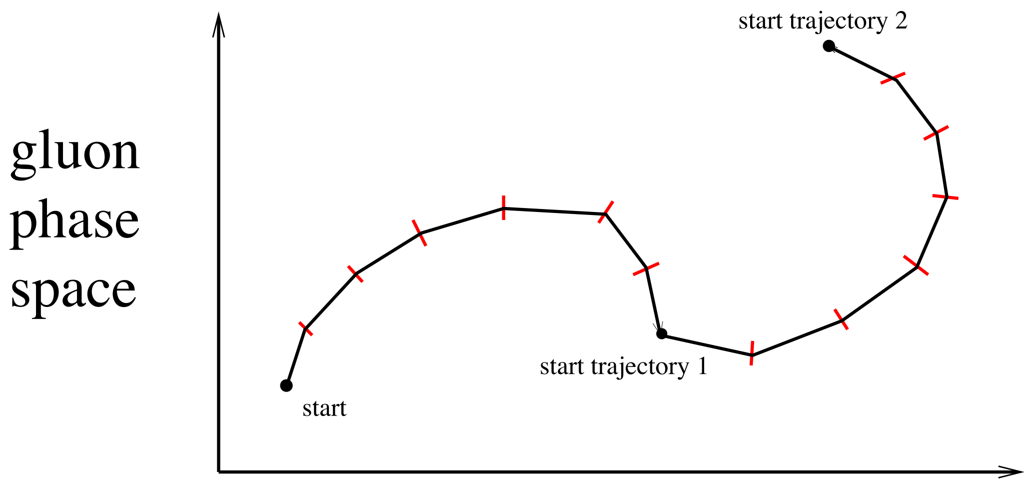
$$D(A, g_0, m_0^i) \equiv i\gamma^\mu(\partial_\mu - igA_\mu^a t^a/2) - m_0^i$$

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

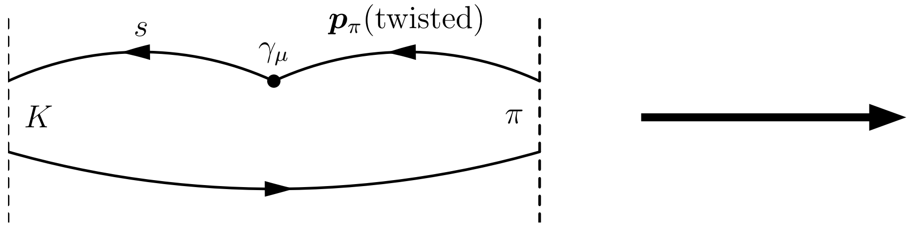
$$\det[D(m)] = \underbrace{\frac{\det[D(m)]}{\det[D(m_1)]}}_{\substack{\text{For } m \approx m_1 \text{ gives} \\ \text{small force but} \\ \text{expensive to calculate}}} \times \underbrace{\frac{\det[D(m_1)]}{\det[D(m_2)]}}_{\substack{\text{Control force size from} \\ m_1 \text{ and } m_2\text{, less} \\ \text{expensive to calculate}}} \cdots \det[D(m_n)]$$

* 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, $O(dt^4)$

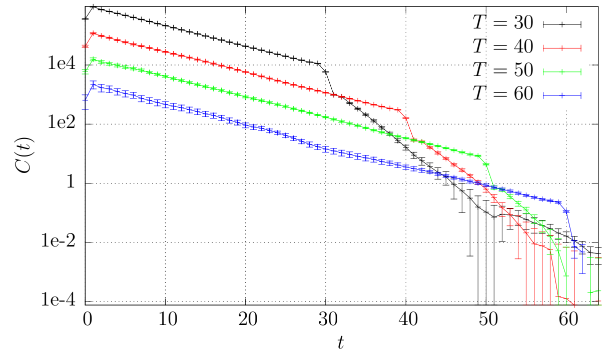
These are giving 10-100   speed-up over a decade ago.

* 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]ψ = s for fixed U

Calculating eigenvectors of D[U] 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 $f_\pi, f_K, B_K, m_{ud}, m_s, f^+_{K\pi}(0), K \to (\pi\pi)_{I=2}$ 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

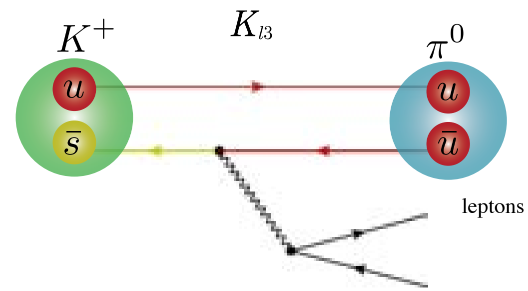
	Ensemble 10	Ensemble 11
EigCG setup time	29.5	66
Exact light quark time	18.7	13
Sloppy light quark time	64	55
Exact strange quark time	8	17
Contraction time	3	16
Total time	123	167
Total time on partition	5.2 days	5.3 hrs

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 $f^{+}_{K\pi}(0)$

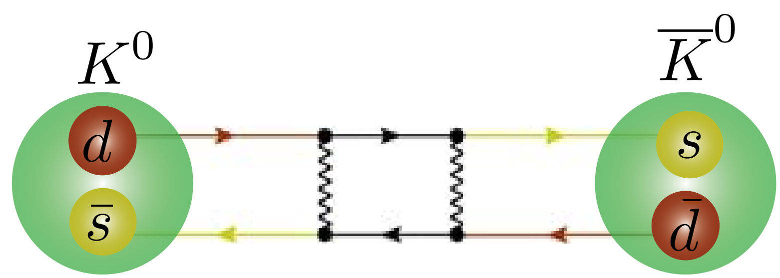
$K-\pi$ sep	AMA?	$f^{+}_{K\pi}(0)$	$f^{-}_{K\pi}(0)$	Z_V
20:24	AMA	0.9672(45)	-0.1327(123)	0.7123(13)
20:28	AMA	0.9602(52)	-0.1254(97)	0.7089(17)
20:32	AMA	0.9639(49)	-0.1318(96)	0.7093(16)
24:28	AMA	0.9598(59)	-0.1230(112)	0.7087(18)
24:32	AMA	0.9646(52)	-0.1322(106)	0.7092(17)
20:24	exact	1.0018(253)	-0.1206(320)	0.7315(150)
20:28	exact	0.9552(227)	-0.0850(205)	0.7016(157)
20:32	exact	0.9537(246)	-0.1004(215)	0.6971(162)
$m_{\rm res}$		0.0006148(59)		



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

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

$K-K$ sep	AMA?	B_K
20:4:24	AMA	0.5836(11)
20:4:28	AMA	0.5844(12)
20:4:32	AMA	0.5839(12)
20:4:24	exact	0.5712(109)
20:4:28	exact	0.5870(110)
20:4:32	exact	0.5845(116)



More work can reduce perturbative matching errors

QCD Thermodynamics with DWF

The HotQCD Collaboration has done simulations on 32^3 8 and 64^3 8 lattices with physical pions
(PRL 113 (2014) 8, 082001 HotQCD)

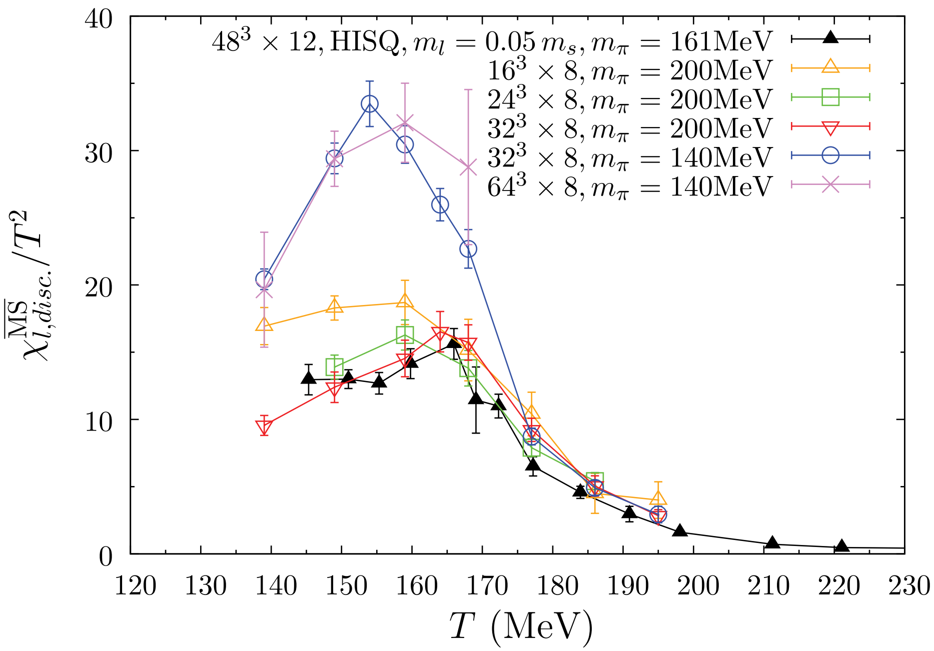
Susceptibilities show larger peaks than for HISQ ensembles

Strong quark mass dependence

Pseudocritical temperature with physical pions:

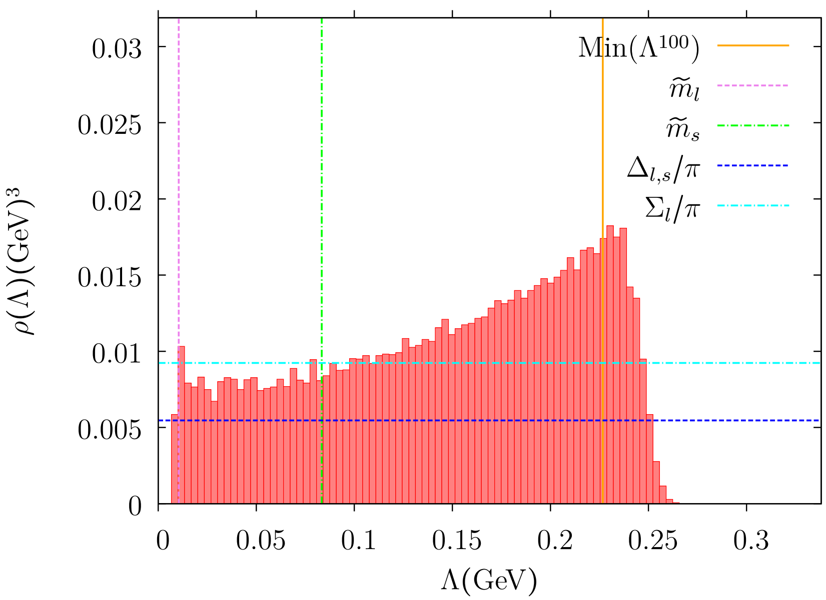
T_c = 155(1)(8) MeV

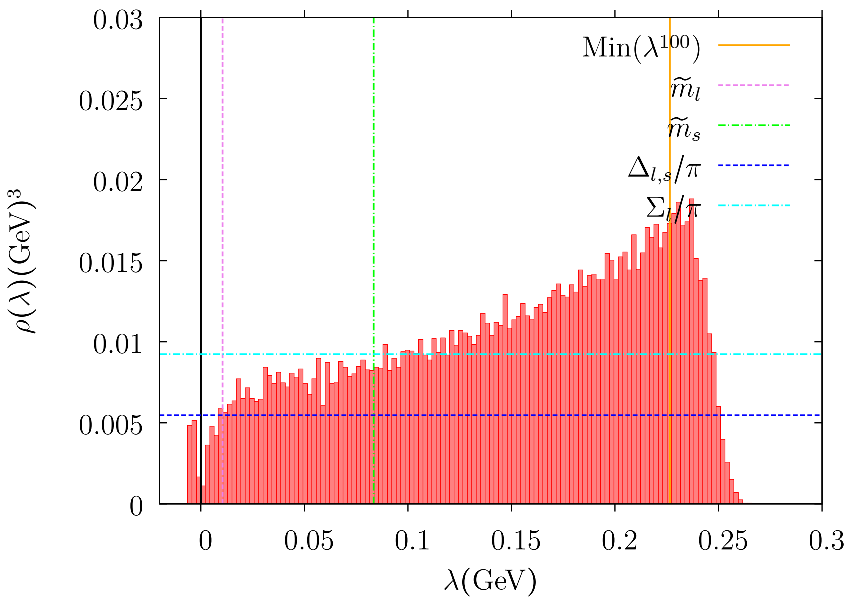
This T_c changes to about 165 MeV when m_π = 200 MeV



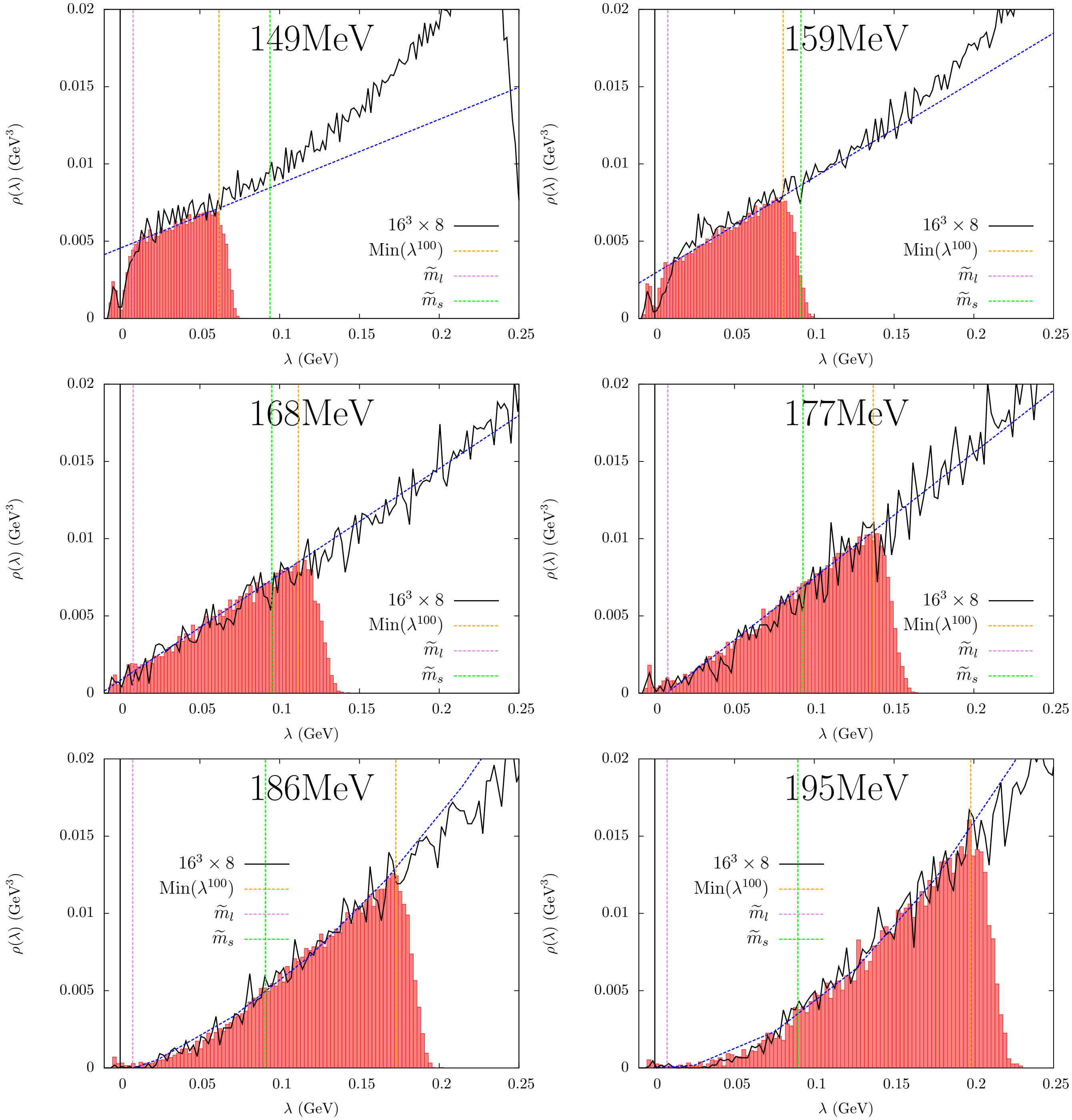
Eigenvalue Density of Dirac Operator, T = 0

Jasper Lin, Columbia PhD Thesis





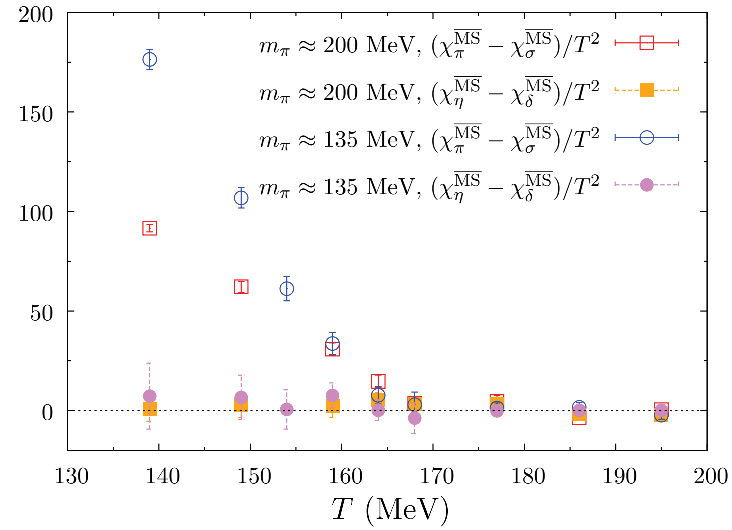
Eigenvalue Density of Dirac Operator, T ≠ 0



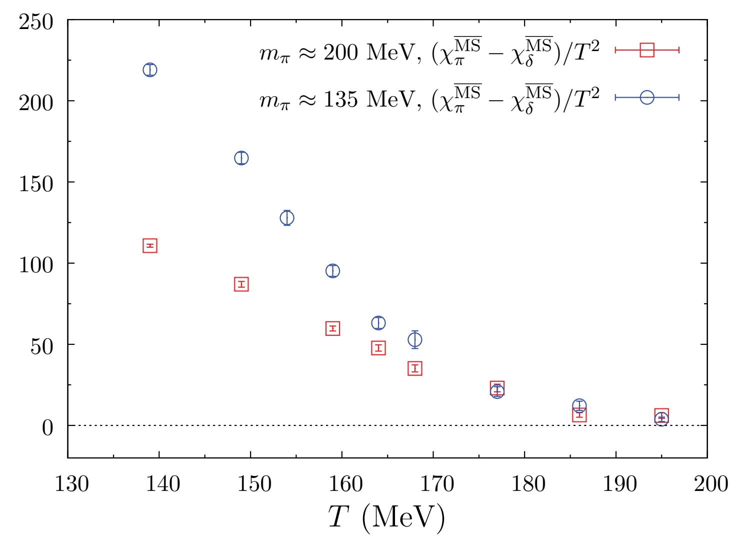
PRD86 (2012) 094503
HotQCD

Symmetries for T ≠ 0

Difference of susceptibilities related by $SU(2)_L$ $SU(2)_R$, showing breaking for low temperatures and accurate chiral symmetry for T 164 MeV



Difference of susceptibilities related by $U(1)_A$ 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 improvement in computer power in 15 years.

Evolution algorithms to produce gauge fields are 10-100 faster

Measurement algorithms are > 10 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 precison comparisons of theory and experiment and, hopefully, new physics.