# Lattice QCD for pedestrians (Lattice QCD for physicists) 

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Overview (1): history of "elementary particle physics"


## Overview (2): Standard Model with strong interactions

matter:

| $\nu_{e}$ | $\nu_{\mu}$ | $\nu_{\tau}$ |
| :---: | :---: | :---: |
| $e$ | $\mu$ | $\tau$ |
| $u$ | $c$ | $t$ |
| $d$ | $s$ | $b$ |

forces:

$$
\underbrace{U(1) \times S U(2)}_{\mathrm{EW}} \times \underbrace{S U(3)}_{\mathrm{QCD}}
$$



Relevant parameters for strong interaction: $\alpha_{\mathrm{QCD}}, m_{d, u, s, c, \ldots}$ with basic law

$$
S_{\mathrm{QCD}}=\frac{1}{2} \operatorname{tr}\left(G_{\mu \nu} G^{\mu \nu}\right)+\sum_{q=d, u, s, c \ldots} \bar{q}\left(D+m_{q}\right) q
$$

Phenomenology of QCD with
$1+N_{f}$ parameters

- non-Abelian gauge symmetry $\Longrightarrow$ non-linear
- asymptotic freedom $\Longrightarrow$ perturbation theory at high energy
- confinement $\Longrightarrow$ hadrons $\neq$ fundamental degrees of freedom
- spontaneous breaking of chiral symmetry $\Longrightarrow M_{\pi} \ll 4 \pi F_{\pi}$


## Overview (3): QCD at high energies



Asymptotic freedom
[t'Hooft 1972, Gross-Wilczek/Politzer 1973]

$$
\begin{gathered}
\frac{\beta(\alpha)}{\alpha}=\frac{\mu}{\alpha} \frac{\partial \alpha}{\partial \mu}=\beta_{1} \alpha^{1}+\beta_{2} \alpha^{2}+\ldots \\
\beta_{1}=\left(-11 N_{c}+2 N_{f}\right) /(6 \pi) \\
\text { with } \quad N_{c}=3 \quad \text { gives } \\
\beta_{1}<0 \quad \text { for } \quad N_{f}<33 / 2
\end{gathered}
$$

- virtual gluons anti-screen, i.e. they make a static color source appear stronger at large distance.
- virtual quarks weaken this effect.


## Overview (4): QCD at low energies



- In quenched QCD the $Q Q$ potential keeps growing, $V(r)=\alpha / r+$ const $+\sigma r$.
- In full QCD it is energetically more favorable to pop a light $\bar{q} q$ pair out of the vacuum, $V(r) \leq$ const. Analysis with explicit $\bar{Q} q \bar{q} Q$ state: Bali et al., PRD 71, 114513 (2005).


## Overview (5): QED versus QCD bound state dynamics



Q0: What is the physical meaning of the "wrong sign" of the proton binding energy if current quark masses are used ?
Q1: Do we understand strong dynamics sufficiently well as to postdict the mass of the proton?
Q2: If so, can we turn the calculation around and determine $m_{u d}=\left(m_{u}+m_{d}\right) / 2$ from first principles?

## Overview (6): separating EW from QCD dynamics

Consider $D^{-} \rightarrow K^{0} e^{-} \bar{\nu}_{e}$, mediated through flavor changing weak decay $\bar{c} \rightarrow \bar{s} W^{-}$


Experiment: $\Gamma \propto\left|V_{c s} f_{+}^{D \rightarrow K}\left(q_{*}^{2}\right)\right|^{2}$ and $\Gamma \propto\left|V_{c s} f_{D_{s}}\right|^{2}$ in semileptonic/leptonic decay How do we separate QCD "contamination" from EW "vertex" and extract $V_{c s}$ ?

Would QCD result be precise enough to track BSM physics through inconsistencies ?

## Talk outline

(1) Lattice Basics

- how to put scalars/gluons/quarks on the lattice
(2) Lattice Spectroscopy
- sea versus valence quarks and (partial) quenching
- spectra of stable versus unstable hadrons
(3) Lattice Techniques
- weak and strong coupling expansion
- numerical aspects, parallel architectures
(4) Lattice Phenomenology
- quark masses: $m_{d}, m_{u}, m_{s}, m_{c}$
- decay constants, form factors and CKM-physics
- kaon mixing: $B_{K}, B_{\mathrm{BSM}}, K \rightarrow 2 \pi$ amplitude
(5) Lattice Outreach
- baryon sigma terms, nuclear physics, ...
- QCD thermodynamics at $\mu=0$ and $\mu>0$
- large $N_{c}$, large $N_{f}$, different fermion representations


## Lattice Basics

- path-integral and euclidean spacetime
- spin models and Metropolis algorithm
- how to put scalars on the lattice
- how to put gluons on the lattice
- how to put fermions the lattice
- Wilson versus Susskind/staggered fermions


## Lattice basics (1): path-integral and euclidean spacetime

QFT: $\quad e^{\mathrm{i} S_{\mathrm{M}}}=e^{\mathrm{i} \int L_{\mathrm{M}} d^{4} x_{\mathrm{M}}} \quad x_{\mathrm{M}}=\left(x^{0}, \mathbf{x}\right)=\left(x^{0}, x^{1 / 2 / 3}\right), \quad x^{4} \equiv \mathrm{i} x^{0}$

$$
\begin{gathered}
L_{\mathrm{M}}=\frac{1}{2} \partial_{\mu} \phi \partial^{\mu} \phi-V[\phi], \quad V[\phi(x)] \equiv \frac{m^{2}}{2} \phi^{2}(x)+\frac{\lambda}{4!} \phi^{4}(x) \\
\partial_{\mu} \phi \partial^{\mu} \phi=\left(\partial_{0} \phi\right)^{2}-\left(\partial_{1 / 2 / 3} \phi\right)^{2}=\left(\frac{\partial \phi}{\partial x^{0}}\right)^{2}-\left(\frac{\partial \phi}{\partial x^{1 / 2 / 3}}\right)^{2} \\
L_{\mathrm{E}} \equiv-L_{\mathrm{S}}=\left(\frac{\partial \phi}{\partial x^{1 / 2 / 3}}\right)^{2}+\left(\frac{\partial \phi}{\partial x^{4}}\right)^{2}+\frac{m^{2}}{2} \phi^{2}(x)+\frac{\lambda}{4!} \phi^{4}(x) \quad>0 \quad(\text { for } \lambda>0) \\
\text { i } \int L_{\mathrm{M}} d x^{0} d x^{1} d x^{2} d x^{3}=\int L_{\mathrm{M}} d x^{1} d x^{2} d x^{3} d x^{4}=-\int L_{\mathrm{E}} d x^{1} d x^{2} d x^{3} d x^{4}
\end{gathered}
$$

$\Longrightarrow$ euclidean standard is $e^{-S_{\mathrm{E}}}$ with $S_{\mathrm{E}}=\int L_{\mathrm{E}} d^{4} x_{\mathrm{E}}>0$

| Lorentz symmetry |
| :---: | :---: |
| $\left(x^{0}\right)^{2}-\mathrm{x}^{2}$ invariant |
| $(+---)$ signature |$\quad \longleftrightarrow$| $O(4)$ symmetry |
| :---: |
| $\mathbf{x}^{2}+\left(x^{4}\right)^{2}$ invariant |
| $(++++)$ signature |

[box $L^{3} \times T$ (lattice spacing $a=1$ ) contains $N=L^{3} T$ continuous dofs]

## Lattice basics (2): spin models and Metropolis algorithm



Ising model (in $d=2$ dimensions):
$N=N_{1} N_{2}$ sites
$s_{i}= \pm 1 \quad \forall i \in\{1, \ldots, N\}$
toroidal boundary conditions
spin configuration $s=\left(s_{1}, \ldots, s_{N}\right)$
energy/Hamiltonian $H(s)=-J \sum_{\langle i j\rangle} s_{i} s_{j}-h \sum_{k} s_{k}$
$J>0$, parallel preferred ("ferromagnetic")
$J<0$, antipar. preferred ("antiferromag.")
bounded from below, $H(s)>$ const, as in EQFT
partition function, free energy: $Z=\sum_{s} e^{-\beta H} \equiv e^{-\beta F}$ inverse temperature $\beta=1 /(k T)$ is external parameter overall $2^{N}$ contributions ("proliferation of states")
Task: $\langle O\rangle=\frac{\sum_{s} O(s) e^{-\beta H(s)}}{\sum_{s} e^{-\beta H(s)}}$
Goal: generate sequence of spin configurations in which specific configuration $s$ shows up with probability $p(s)=\frac{1}{Z} e^{-\beta H(s)}, \quad Z \equiv \sum_{s^{\prime}} e^{-\beta H\left(s^{\prime}\right)}$
("Boltzmann distribution", solution MRRTT'53)


## Lattice basics (3): how to put scalars on the lattice

$$
\begin{aligned}
S_{\mathrm{E}}= & a^{4} \sum_{x, \mu}\left\{\frac{1}{2}\left(\nabla_{\mu} \phi\right)(x)\left(\nabla_{\mu} \phi\right)(x)+V[\phi(.)]\right\} \quad \text { [drop "E" henceforth] } \\
& \left(\nabla_{\mu} \phi\right)(x) \equiv \frac{1}{a}[\phi(x+a \hat{\mu})-\phi(x)] \quad \text { ("forward derivative") } \\
& \left(\nabla_{\mu}^{*} \phi\right)(x) \equiv \frac{1}{a}[\phi(x)-\phi(x-a \hat{\mu})] \quad \text { ("backward derivative") } \\
= & a^{4} \sum_{x}\left\{-\frac{1}{2} \phi(x) \triangle \phi(x)+V[\phi(.)]\right\}>0 \quad(\text { for } \lambda>0) \\
& (\triangle \phi)(x)=\left\{\begin{array}{l}
\left(\nabla_{\mu} \nabla_{\mu}^{*} \phi\right)(x) \\
\left(\nabla_{\mu}^{*} \nabla_{\mu} \phi\right)(x)
\end{array}=\sum_{\mu} \frac{\phi(x+a \hat{\mu})-2 \phi(x)+\phi(x-a \hat{\mu})}{a^{2}}\right.
\end{aligned}
$$

EQFT/simulation exploits formal analogy to statistical mechanics:

$$
\begin{gathered}
Z=\int d \phi\left(x_{1}\right) \ldots d \phi\left(x_{N}\right) e^{-S[\phi]} \equiv \int D \phi e^{-S[\phi]} \\
\underbrace{\left\langle\phi\left(x_{1}\right) \ldots \phi\left(x_{n}\right)\right\rangle}_{\substack{\text { means } \\
\text { ordered product of } n=2,3, \ldots \text { fields }}}=\underbrace{\frac{1}{Z} \int D \phi \phi\left(x_{1}\right) \ldots \phi\left(x_{n}\right) e^{-S[\phi]}}_{\begin{array}{c}
\text { finite ratio of two high-dimensional integrals, } \\
\text { each of the } N=L^{3} T \text { fields runs from }-\infty \text { to }+\infty
\end{array}}
\end{gathered}
$$

## Lattice basics (4): how to put gluons on the lattice



Attempts to put gauge fields $A_{\mu}(x)$ on the lattice break gauge invariance by $O(a)$ effects.
Only path-ordered exponentials $\exp \left(\mathrm{i} g \int A(s) d s\right)$ are measurable (Aharonov-Bohm).
Wilson: identify $U_{\mu}(x) \longleftrightarrow e^{\mathrm{i} g \int_{x}^{x+\hat{\mu}} A_{\mu}(\tilde{x}) d \tilde{x}}$ and consider $U_{\mu}(x) \in S U(3)$ fundamental dof.

- $U_{\mu}(x)$ is parallel transporter from $x+\hat{\mu}$ to $x$
- cov. derivative $\left(D_{\mu} \phi\right)(x)=U_{\mu}(x) \phi(x+\hat{\mu})-\phi(x)$
- $U_{\mu}(x)$ transforms into $g(x) U_{\mu}(x+\hat{\mu}) g^{\dagger}(x+\hat{\mu})$
- traced closed loops of links are gauge-invariant

Wilson: simplest gauge action involves $1 \times 1$ loop ("plaquette") $\operatorname{Tr}\left(P_{\mu \nu}\right)=N_{c}-\frac{a^{4} g^{2}}{2} \operatorname{Tr}\left(F_{\mu \nu} F_{\mu \nu}\right)$ $\beta \equiv \frac{2 N_{c}}{g^{2}}$ plays role of $J$ in Ising model $\beta \ll 1 \longleftrightarrow g^{2} \gg 1$ "strong coupling" $\beta \gg 1 \longleftrightarrow g^{2} \ll 1$ "weak coupling"

$$
\begin{aligned}
S & =a^{4} \sum_{x, \mu, \nu} \frac{1}{2} \operatorname{Tr}\left(F_{\mu \nu}(x) F_{\mu \nu}(x)\right) \\
& =\frac{1}{g^{2}} \sum_{x, \mu, \nu}\left\{N_{c}-\operatorname{Tr}\left(P_{\mu \nu}(x)\right)\right\} \\
& =\frac{2 N_{c}}{g^{2}} \sum_{x, \mu<\nu(!)}\left\{1-\frac{1}{N_{c}} \operatorname{Re} \operatorname{Tr}\left(P_{\mu \nu}(x)\right)\right\}
\end{aligned}
$$

## Lattice basics (5): how to put fermions on the lattice

Bosons were handy, because they required second-order operator:

$$
S_{B}=\frac{a^{4}}{2} \sum_{x}\left\{\phi^{\dagger}(x)(-\triangle \phi)(x)+m^{2} \phi^{\dagger}(x) \phi(x)\right\}
$$

Fourier transform $\hat{p}^{2}+m^{2}$ for $m=0$ with $\hat{p} \equiv \frac{2}{a} \sin \left(\frac{a p}{2}\right)$ has only 1 zero in BZ which is (]$\left.\left.-\frac{\pi}{a}, \frac{\pi}{a}\right]\right)^{4}$

Fermions give troubles, since they require first-order operator ("naive fermions"):

$$
S_{F}=a^{4} \sum_{x}\left\{\bar{\psi}(x) \gamma_{\mu} \frac{\nabla_{\mu}+\nabla_{\mu}^{*}}{2} \psi(x)+m \bar{\psi}(x) \psi(x)\right\}
$$

Fourier transform $\mathrm{i} \gamma_{\mu} \bar{p}_{\mu}+m$ for $m=0$ with $\bar{p} \equiv \frac{1}{a} \sin (a p)$
has 16 zeros (one doubling per $\operatorname{dim}$ ) in BZ
$\longrightarrow$ lift 15 of these to $O\left(\frac{1}{a}\right) \quad$ [Wilson]
Simulation as in pure YM, but with Grassmann-valued fermions integrated out:

$$
\langle O\rangle=\frac{\int D U O[U] \operatorname{det}^{N_{f}}(D[U]) e^{-S_{G}[U]}}{\int D U \operatorname{det}^{N_{f}}(D[U]) e^{-S_{G}[U]}} \quad \text { with } \quad D U \equiv \prod_{\mu=1}^{4} \prod_{x}^{N} \underbrace{d U_{\mu}(x)}_{\substack{\text { Haar measure } \\ \text { on SU(3)}}}
$$

## Lattice basics (6): Wilson versus Susskind fermions

Susskind/staggered fermions yield 4 species: $S_{\mathrm{S}}=\sum_{x, y} \bar{\chi}(x) D_{\mathrm{S}}(x, y) \chi(y)$ with

$$
D_{\mathrm{S}}(x, y)=\frac{1}{2} \sum_{\mu} \eta_{\mu}(x)\left\{U_{\mu}(x) \delta_{x+\hat{\mu}, y}-U_{\mu}^{\dagger}(x-\hat{\mu}) \delta_{x-\hat{\mu}, y}\right\}
$$

Wilson fermions [slower] yield 1 species: $S_{\mathrm{W}}=\sum_{x, y} \bar{\psi}(x) D_{\mathrm{W}}(x, y) \psi(y)$ with

$$
D_{\mathrm{W}}(x, y)=\frac{1}{2} \sum_{\mu}\left\{\left(\gamma_{\mu}-I\right) U_{\mu}(x) \delta_{x+\hat{\mu}, y}-\left(\gamma_{\mu}+I\right) U_{\mu}^{\dagger}(x-\hat{\mu}) \delta_{x-\hat{\mu}, y}+2 \delta_{x, y}\right\}
$$

Overlap construction, traditionally with $X=D_{\mathrm{W}}-\rho$, makes things even slower:

$$
D_{\mathrm{N}}(x, y)=\frac{\rho}{a}\left(1+X\left(X^{\dagger} X\right)^{-1 / 2}\right)=\frac{\rho}{a}\left(1+\left(X X^{\dagger}\right)^{-1 / 2} X\right)
$$

- main advantage of staggered fermions is their expedience [plus flavored symm.]
- main advantage of Wilson-like fermions is 1-to-1 [latt-cont] flavor identification


## Lattice basics (7): rationale for "smearing+clover"

info: staggered $D_{\mathrm{S}}$ has (for $m=0$ ) EV spectrum on imaginary axis info: overlap $D_{\mathrm{N}}$ has (for $m=0$ ) EV spectrum on unit circle around $(1,0) \in \mathbb{C}$

$\longrightarrow$ link smearing in $D_{\mathrm{W}}$ alone does not help on "horizontal jitter"
$\longrightarrow$ Symanzik improvement $c_{\mathrm{SW}} \simeq 1$ alone does not help much on "mass shift"
$\longrightarrow$ smearing and $c_{\mathrm{SW}} \simeq 1$ cure "mass shift" and "horizontal jitter" in physical branch

## Lattice Spectroscopy

- scale hierarchies in LQCD
- sea quarks versus valence quarks
- terminology: QCD / QQCD / PQQCD
- hadron interpolating fields
- spectroscopy of stable particles
- spectroscopy of scattering states


## Lattice spectroscopy (1): scale hierarchies

typical spacing: $0.05 \mathrm{fm} \leq a \leq 0.20 \mathrm{fm}$ $1 \mathrm{GeV} \leq a^{-1} \leq 4 \mathrm{GeV}$
typical boxsize: $2 \mathrm{fm} \leq L \leq 6 \mathrm{fm}$
require (UV): $\quad a m_{q} \ll 1$
require (IR): $\quad M_{\pi} L \geq 4$


| $u$ <br> Work near <br> $m_{u d} \gtrsim m_{u d}^{\text {phys }}$ | $\overbrace{\text { interpolate to }}^{c}$ | $(t)$ <br> $m_{s}^{\text {phys }}, m_{c}^{\text {phys }}$ |
| :---: | :---: | :---: |
| $\overbrace{\text { extrapolate }}^{c}$ |  |  |
| $m_{b} \rightarrow m_{b}^{\text {phys }}$ |  |  |$|$

For each $\beta$ (a posteriori lattice spacing $a$ ) tune $1 / \kappa_{u d, s, c, \ldots}$ such that $\left\{M_{\pi}^{2}, 2 M_{K}^{2}-M_{\pi}^{2}, M_{\eta_{c}}^{2}, \ldots\right\} / M_{\Omega}^{2}$ assume correct values ("sacrificed observables").

## Lattice spectroscopy (2): sea versus valence quarks

Hadronic correlator in $N_{f} \geq 2$ QCD: $\quad C(t)=\int d^{4} x C(t, \mathbf{x}) e^{\mathrm{ipx}}$ with

$$
C(x)=\left\langle O(x) O(0)^{\dagger}\right\rangle=\frac{1}{Z} \int D U D \bar{q} D q O(x) O(0)^{\dagger} e^{-S_{G}-S_{F}}
$$

where $O(x)=\bar{d}(x) \Gamma u(x)$ and $\Gamma=\gamma_{5}, \gamma_{4} \gamma_{5}$ for $\pi^{ \pm}$and $S_{G}=\beta \sum\left(1-\frac{1}{3} \operatorname{Re} \operatorname{Tr} U_{\mu \nu}(x)\right), S_{F}=\sum \bar{q}(D+m) q$
$\left\langle\bar{d}(x) \Gamma_{1} u(x) \bar{u}(0) \Gamma_{2} d(0)\right\rangle=\frac{1}{Z} \int D U \operatorname{det}(D+m)^{N_{f}} e^{-S_{G}}$

$$
\times \operatorname{Tr}\{\Gamma_{1}(D+m)_{x 0}^{-1} \Gamma_{2} \underbrace{(D+m)_{0 x}^{-1}}_{\gamma_{5}\left[(D+m)_{x 0}^{-1}\right]^{\dagger} \gamma_{5}}\}
$$


(A) Quenched QCD: quark loops neglected

(B) Full QCD

- Choose $m_{u}=m_{d}$ to save CPU time, since isospin $\operatorname{SU}(2)$ is a good symmetry.
- In principle $m_{\text {valence }}=m_{\text {sea }}$, but often additional valence quark masses to broaden data base. Note that "partially quenched QCD" is an extension of "full QCD".
- $(D+m)_{x 0}^{-1}$ for all $x$ amounts to 12 columns (with spinor and color) of the inverse.


## Lattice spectroscopy (3): QCD/QQCD/PQQCD terminology

$N_{f}=0$ "QQCD"
$N_{f}=2$
$N_{f}=2+1$
no dynamical "sea" quarks, only "valence" quarks
$N_{f}=2+1+1$
2 dynamical flavors with common mass $m_{u d}$
3 dynamical flavors with masses $m_{u d}, m_{s}$
$N_{f}=1+1+1+1$
4 dynamical flavors with masses $m_{u d}, m_{s}, m_{c}$

Note: $\quad$ in none of the above cases is $m_{q}=m_{q}^{\text {phys }}$ understood (are to be reached a posteriori through interpolations/extrapolations)
Note: "partially quenched" may mean absent in sea (e.g. $c$ in $N_{f}=2+1$ ) or present in sea with different mass (i.e. $m_{c}^{\text {sea }} \neq m_{c}^{\text {val }}$ )
Note: quenching introduces serious artefacts in theory (non-unitarity, as $\eta^{\prime}$ has double-pole rather than shifted single-pole), but numerically effects seemed to be small [these days QQCD is gone]


## Lattice spectroscopy (4): HQ potential in quenched/full QCD



- asymptotic rise $V(r) \propto \sigma r$ in QQCD ("string tension" $\sigma$ well-defined for $N_{f}=0$ )
- string breaks in (full) QCD, can be seen with better technique (cf. overview)
- short distance part is $V(r) \propto \frac{\alpha}{r}$ or $V(r) \propto \frac{\alpha(r)}{r}$; this can be used to get $\alpha_{V}(r)$


## Lattice spectroscopy (5): meson/baryon interpolating fields

Flavor quantum number is to be kept track of explicitly:

$$
O_{\pi^{+}}(x)=\bar{d}(x) \gamma_{5} u(x), O_{\pi^{0}}(x)=\frac{1}{\sqrt{2}}\left[\bar{u}(x) \gamma_{5} u(x)-\bar{d}(x) \gamma_{5} d(x)\right], O_{\pi^{-}}(x)=\bar{u}(x) \gamma_{5} d(x)
$$

$$
\left\langle O_{\pi^{+}}(x) \bar{O}_{\pi^{+}}(y)\right\rangle=\left\langle\underline{\bar{d}(x) \gamma_{5} u \underline{(x) \bar{u}}(y)\left|\gamma_{5} d(y)\right\rangle, ~}\right.
$$

$$
=\left\langle\operatorname{Tr}\left\{\gamma_{5} D_{m_{d}}^{-1}(y, x) \gamma_{5} D_{m_{u}}^{-1}(x, y)\right\}\right\rangle
$$

$$
=\left\langle\operatorname{Tr}\left\{\left[D_{m_{d}}^{-1}(x, y)\right]^{\dagger} D_{m_{u}}^{-1}(x, y)\right\}\right\rangle
$$

$\left\langle O_{\pi^{0}}(x) \bar{O}_{\pi^{0}}(y)\right\rangle=6$ terms, 2 connected and 4 disconnected, latter cancel for $m_{u}=m_{d}$

$$
\left\langle O_{N}(x) O_{\bar{N}}(y)\right\rangle=\langle(\text { contractions }) u(x) u(x) d(x) \bar{u}(y) \bar{u}(y) \bar{d}(y)\rangle
$$

$$
t=t_{f}
$$



$$
t=0
$$



(A) Local Interpolating operators

(B) Extended Interpolating operators

$\left\langle N\left(\vec{q}, t_{f}\right) \quad \sum_{\vec{x}} e^{i \vec{q} \cdot \vec{x}} \bar{s}\left(\vec{x}, t^{\prime}\right) \Gamma s\left(\vec{x}, t^{\prime}\right) \quad N(\overrightarrow{0}, 0)\right\rangle$

## Lattice spectroscopy (6): pseudoscalar meson correlators

Excellent data quality even on our lightest ensemble ( $M_{\pi} \simeq 190 \mathrm{MeV}$ and $L \simeq 4.0 \mathrm{fm}$ ):

Point_[from]_Gauss, 3.57_m0.0483_m0.007_48x64


Gauss_[from]_Gauss, 3.57_m0.0483_m0.007_48x64
 $\cosh (.) / \sinh ($.$) for -P P,\left|P A_{0}\right|,\left|A_{0} P\right|, A_{0} A_{0}$ with Gauss source and local/Gauss sink $C_{X x, Y y}(t)=c_{0} e^{-M_{0} t} \pm c_{0} e^{-M_{0}(T-t)}+\ldots$ with $X, Y \in\left\{P, A_{0}\right\}$ and $x, y \in\{$ loc, gau $\}$
$\longrightarrow c_{0}=G \tilde{G} / M_{0}, G \tilde{F}, F \tilde{G}, F \tilde{F} M_{0}$ (left) and $c_{0}=\tilde{G} \tilde{G} / M_{0}, \tilde{G} \tilde{F}, \tilde{F} \tilde{G}, \tilde{F} \tilde{F} M_{0}$ (right)
$\longrightarrow$ combined 1-state fit of 8 correlators with 5 parameters yields $M_{\pi}, F_{\pi}, m_{\mathrm{PCAC}}$

## Lattice spectroscopy (7): spectroscopy of stable states

stable states: meaning is under strong interactions (example: $\pi, N, \ldots$ )

$$
\begin{aligned}
\langle A(x) B(y)\rangle & =\sum_{n \geq 0} \frac{1}{2 E_{n}}\langle 0| A(\mathbf{x}, 0) e^{-E_{n} x_{4}}|n\rangle\langle n| e^{+E_{n} y_{4}} B(\mathbf{y}, 0)|0\rangle \\
& =\sum_{n \geq 0} \frac{1}{2 E_{n}}\langle 0| A(\mathbf{x}, 0)|n\rangle\langle n| B(\mathbf{y}, 0)|0\rangle e^{-E_{n}\left(x_{4}-y_{4}\right)}
\end{aligned}
$$

Consider local effective mass $M_{\mathrm{eff}}(t)=\frac{1}{2} \log \left(\frac{C(t-1)}{C(t+1)}\right)$ and determine plateau value:



## Lattice spectroscopy (8): spectroscopy of unstable/mixing states

unstable states: meaning is under strong interactions (example: $\rho, \Delta, \ldots$ )


2-particle ( $\pi \pi, \pi K, K K, \pi N, N N$ ) states:
Scattering length and phase-shift can be determined in Euclidean space from tower of states in finite volume [Lüscher 1991].

Example: $L$-dependence of states with $\pi \pi$ or $\rho$ quantum numbers is different for small (dashed blue) versus large (full red) $g_{\pi \pi \rho}$.

Original framework by Lüscher refined in many respects [Rummukainen and Gottlieb, Rusetsky et al] and successfully applied to a variety of systems.

Method in practice rather demanding, since limited number of $L$ values available, and extraction of high-lying states remains a challenge.

Results on $\pi \pi, \pi K, K K, \pi D, \pi N, N N, \ldots$ from various groups, e.g. Beane/Savage et al [NPLQCD], Dudek et al [HSC], Lang et al, Mohler et al, Aoki et al [HAL-QCD], ...

## Lattice Techniques

- strong coupling expansion
- weak coupling expansion
- iterative solvers
- CPUs in parallel mode
- GPUs in farming mode
- postprocess: $a \rightarrow 0, V \rightarrow \infty, m_{q} \rightarrow m_{q}^{\text {phys }}$


## Lattice techniques (1): strong-coupling perturbation theory


(A) Minimum tiling of a $6 \times 6$ Wilson loop.

(B) Tiling of one face of a plaquette-plaquette correlation function


Strong coupling PT: expansion in $\beta=6 / g_{0}^{2}$; expansion about "disorder", i.e. about rough configurations.
Rather large $O(20)$ orders can be reached by massive amount of computer algebra.

$$
W_{1 \times 1}(r, t)=\left(\frac{\beta}{2 N_{c}^{2}}\right)^{r t}(1+O(\beta))
$$

$\longrightarrow$ confinement proven to leading order in SCPT

Weak coupling PT: expansion in $g_{0}^{2}=6 / \beta$; expansion about "order", i.e. about smooth configurations.
Already 2-loop computations extremely tedious due to broken Lorentz invariance.
$\longrightarrow$ most successful are "mixed schemes" in which $W_{2 \times 2}, W_{3 \times 3}, W_{4 \times 4}$ are analytically linked to $W_{1 \times 1}$ and the latter is measured in simulation

## Lattice techniques (2): weak-coupling perturbation theory

$Z$-factors ("renormalization") needed/useful for lattice-to-continum matching; distinguish operators with/without anomalous dimension, beware of mixing:

$$
\begin{gathered}
\langle.| O_{i}^{\mathrm{cont}}(\mu)|.\rangle=\sum_{j} Z_{i j}(a \mu)\langle\cdot| O_{j}^{\mathrm{latt}}(a)|\cdot\rangle \\
Z_{i j}(a \mu)=\delta_{i j}-\frac{g_{0}^{2}}{16 \pi^{2}}\left(\Delta_{i j}^{\mathrm{latt}}-\Delta_{i j}^{\mathrm{cont}}\right)=\delta_{i j}-\frac{g_{0}^{2}}{16 \pi^{2}} C_{F} z_{i j} \\
Z_{S}(a \mu)=1-\frac{g_{0}^{2}}{4 \pi^{2}}\left[\frac{z_{S}}{3}-\log \left(a^{2} \mu^{2}\right)\right] \quad Z_{V}=1-\frac{g_{0}^{2}}{12 \pi^{2}} z_{V} \\
Z_{P}(a \mu)=1-\frac{g_{0}^{2}}{4 \pi^{2}}\left[\frac{z_{P}}{3}-\log \left(a^{2} \mu^{2}\right)\right] \quad Z_{A}=1-\frac{g_{0}^{2}}{12 \pi^{2}} z_{A}
\end{gathered}
$$

Generically $\left[z_{P}-z_{S}\right] / 2=z_{V}-z_{A}$, and for a chiral action either side vanishes.
Typically $n$-loop LPT yields results with leading cut-off effects $O\left(\alpha^{n} a\right)$; usual hope/ belief is that with non-perturbative improvement Symanzik scaling window is larger.

## Lattice techniques (3): sparse iterative solvers

$$
\begin{aligned}
D_{\mathrm{st}}(x, y) & =\frac{1}{2} \sum_{\mu} \eta_{\mu}(x)\left\{U_{\mu}(x) \delta_{x+\hat{\mu}, y}-U_{\mu}^{\dagger}(x-\hat{\mu}) \delta_{x-\hat{\mu}, y}\right\}+m \delta_{x, y} \\
D_{\mathrm{W}}(x, y) & =\frac{1}{2} \sum_{\mu}\left\{\left(\gamma_{\mu}-I\right) U_{\mu}(x) \delta_{x+\hat{\mu}, y}-\left(\gamma_{\mu}+I\right) U_{\mu}^{\dagger}(x-\hat{\mu}) \delta_{x-\hat{\mu}, y}\right\}+\left(4+m_{0}\right) \delta_{x, y}
\end{aligned}
$$

staggered:


Wilson:

overlap:


- $D$ is $12 N \times 12 N$ complex sparse matrix, for $N=64^{3} \times 128$ this is $40210^{6} \times 40210^{6}$
- each line/column contains only $1+3 \cdot 2 \cdot 8=49$ non-zero entries
- inverse is full [non-sparse], example above would require $2.410^{6} \mathrm{~TB}$ of memory
- CG solver yields $D^{-1} \eta \simeq c_{0} \eta+c_{1} D \eta+\ldots+c_{n} D^{n} \eta$ with $n^{2} \propto \operatorname{cond}\left(D^{\dagger} D\right)=\frac{\lambda_{\text {max }}}{\lambda_{\text {min }}}$


## Lattice techniques (4): new CPU packing strategies

SMP versus SIMD:


JUQUEEN [IBM BG/Q] 06/2012-10/2012


02/2013-...
processor type compute node racks, nodes, cores memory performance (double) power consumption network topology network bandwidth network latency

64-bit PowerPC A2 1.6 GHz (205 Gflops each) 16-way SMP processor (water cooled) 8, 8'192, 131'072 28, 28'672, 458'752 16 GB per node, aggregate 131 TB 1678/1380 Teraflops peak/Linpack $<100 \mathrm{~kW} /$ rack, aggregate 0.8 MW
5D torus among compute nodes (incl. global barriers) 40 Gigabyte/s
$2.5 \mu \mathrm{sec}$ (light travels 750 meters)

## Lattice techniques (5): new GPU programming models

GPUs originally designed for tasks in computer
 graphics (e.g. rendering).

GPUs nowadays frequently used for OpenMPparallelizable scientific computations.

Hardware connection via PCl bus (overhead from data transfer before/after computation).

```
void transform_10000by10000grid(float in[10000][10000], float *out[10000][10000]){
    for(int x=0; x<10000; x++){
        for(int y=0; y<10000; y++){
            *out[x][y] = do_something(in[x][y]); // local operation !!!
        }
    }
}
```

Popular programming languages: CUDA, OpenCL, ...
Issues of single (32bit) versus double (64bit) precision ...
Excellent price/performance ratio paid for by human work ...

## Lattice techniques (6): theory for $a \rightarrow 0, L \rightarrow \infty, m_{q} \rightarrow m_{q}^{\text {phys }}$

Lattice breaks Lorentz symmetry (softly, i.e. recovered in observables under $a \rightarrow 0, V \rightarrow \infty$ ) but maintains gauge-invariance.
Lattice spacing $a$ and quark masses $m_{u d, s, . .}^{\text {scheme }}$ are quantities that emerge from the parameters $\beta$ and $1 / \kappa_{u d, s, \ldots}$ of the simulations; hence a suitable number of observables must be "sacrificed" to set the lattice spacing and to adjust the quark masses.

$a \rightarrow 0 \quad$ Symanzik effective theory of cut-off effects has simple consequence: plot data versus correct power of $a$ (e.g. $\alpha a$, depends on action used) and extrapolate linearly.
$V \rightarrow \infty \quad$ Chiral perturbation theory predicts that every quantity has asymptotic finite-volume effects which scale exponentially in $M_{\pi} L$; in relative shift $\left[f_{B}(L)-f_{B}(\infty)\right] / f_{B}(\infty)=$ const $e^{-M_{\pi} L}$ often "const" from ChPT.
$m_{q} \rightarrow m_{q}^{\text {phys }} \quad$ Traditionally extrapolation $M_{\pi}^{2} \rightarrow(134.8 \mathrm{MeV})^{2}$ via ChPT, modern simulations often bracket $m_{u d}^{\text {phys }}$ by those in the simulation (in such case linear interpolation seems sufficient).

Almost all lattice computations concern quantities (masses, decay constants, form factors) for which no backrotation to Minkowski spacetime is required.

Final result: S. Dürr et al, Science 322, 1224 (2008)


## Lattice Phenomenology

- light quark masses from spectroscopy
- decay-constants and form-factors for CKM physics
- light flavor $(d, u, s)$ physics: $f_{\pi}, f_{K}, \ldots$
- heavy flavor $(c, b)$ physics: $f_{D}, f_{D_{s}}, f_{B}, f_{B_{s}}, \ldots$
- indirect CP violation: $B_{K}, B_{\mathrm{BSM}}, B_{D}, B_{B}, \ldots$
- $K \rightarrow 2 \pi$ amplitudes and $\Delta I=1 / 2, \epsilon^{\prime} / \epsilon$


## Quark masses (1): anatomy of $N_{f}=2+1$ computation

1. Choose observables to be "sacrificed", e.g. $M_{\pi}, M_{K}, M_{\Omega}$ in $N_{f}=2+1$ QCD, and get "polished" experimental values, e.g. $M_{\pi}=134.8(3) \mathrm{MeV}, M_{K}=494.2(5) \mathrm{MeV}$ in a world without isospin splitting and without electromagnetism [arXiv:1011.4408].
2. For a given bare coupling $\beta$ (yields $a$ ) tune bare masses $1 / \kappa_{u d, s}$ such that the ratios $M_{\pi} / M_{\Omega}, M_{K} / M_{\Omega}$ assume their physical values (in practice: inter-/extrapolation).

$$
M_{\pi, K, \Omega} \longleftrightarrow m_{q}^{\text {bare }}
$$

3. Read off $1 / \kappa_{u d, s}$ or determine bare $a m_{u d, s}$ via AWI and convert them (perturbatively or non-perturbatively) to the scheme of your choice (e.g. MS at $\mu=3 \mathrm{GeV}$ ).

$$
m_{q}^{\mathrm{bare}} \longleftrightarrow m_{q}^{\mathrm{SF} / \mathrm{RI}} \longleftrightarrow m_{q}^{\overline{\mathrm{MS}}}
$$

4. Repeat steps 2 and 3 for at least 3 different lattice spacings and extrapolate the (finite-volume corrected) result to the continuum via Symanzik scaling.

Depending on details, step 3 can be rather demanding [ $\mathrm{RI} / \mathrm{MOM}$, SF renormalization]. Below, guided tour using plots from BMW-collaboration [arXiv:1011.2403,1011.2711].

## Quark masses (2): Final result for ratio $m_{s} / m_{u d}$

In QCD ratios like $m_{s} / m_{u d}$ are renormalization group invariant (RGI), hence step 3 in this list is skipped (detail: we invoke $\alpha a$ and $a^{2}$ scaling).


Final result $m_{s} / m_{u d}=27.53(20)(08)$ amounts to $0.78 \%$ precision.

## Quark masses (3): $N_{f}=3$ RI-running extrapolation for $Z_{S}$

Evolution $Z_{S}^{\mathrm{RI}}(\mu) / Z_{S}^{\mathrm{RI}}(4 \mathrm{GeV})$ has no visible cut-off effects among three finest lattices:

$\longrightarrow$ separate continuum limit with $R_{S}^{\mathrm{RI}}(\mu, 4 \mathrm{GeV})=\lim _{\beta \rightarrow \infty} Z_{S, \beta}^{\mathrm{RI}}(4 \mathrm{GeV}) / Z_{S, \beta}^{\mathrm{RI}}(\mu)$

## Quark masses (4): $N_{f}=3 \mathrm{RI}$-scheme-running ratio for $Z_{S}$

On the finest lattice we make contact within errors to 4-loop PT for $\mu \geq 4 \mathrm{GeV}$ :


## Quark masses (5): $N_{f}=3 \mathbf{R I}$ and $\overline{\mathrm{MS}}$ perturbative series for $Z_{S}$




- RI series (left) converges less convincingly than $\overline{\mathrm{MS}}$ series (right)
- difference "4-loop" to "4-loop/ana" indicates size of 5-loop effects
- ratio suggests that higher-loop effects in RI are $<1 \%$ at $\mu=4 \mathrm{GeV}$
- ratio suggests that higher-loop effects in $\overline{\mathrm{MS}}$ are negligible down to $\mu=2 \mathrm{GeV}$


## Quark masses (6): Final results for $m_{s}$ and $m_{u d}$

Good scaling of $m_{u d, s}^{\mathrm{RI}}(4 \mathrm{GeV})$ out to the coarsest lattice ( $a \sim 0.116 \mathrm{fm}$ ):



Conversion with analytical 4-loop formula at 4 GeV and downwards running in $\overline{\mathrm{MS}}$ :

|  | $m_{u d}$ | $m_{s}$ |
| :--- | :--- | ---: |
| $\mathrm{RI}(4 \mathrm{GeV})$ | $3.503(48)(49)$ | $96.4(1.1)(1.5)$ |
| RGI | $4.624(63)(64)$ | $127.3(1.5)(1.9)$ |
| $\overline{\mathrm{MS}}(2 \mathrm{GeV})$ | $3.469(47)(48)$ | $95.5(1.1)(1.5)$ |

$\mathrm{RGI} / \overline{\mathrm{MS}}$ results (table $1.9 \%$ prec.) need to be augmented by a $\sim 1 \%$ conversion error.

## Quark masses (7): splitting $m_{u d}$ with information from $\eta \rightarrow 3 \pi$

The process $\eta \rightarrow 3 \pi$ is highly sensitive to QCD isospin breaking (from $m_{u} \neq m_{d}$ ) but rather insensitive to QED isospin breaking (from $q_{u} \neq q_{d}$ ), and this is captured in $Q$.

Rewrite the Leutwyler ellipse in the form

$$
\frac{1}{Q^{2}}=4\left(\frac{m_{u d}}{m_{s}}\right)^{2} \frac{m_{d}-m_{u}}{m_{d}+m_{u}}
$$

and use the conservative estimate $Q=22.3(8)$ of [Leutwyler, Chiral Dynamics 09] together with our result $m_{s} / m_{u d}=27.53(20)(08)$ to get the asymmetry parameter

$$
\frac{m_{d}-m_{u}}{m_{d}+m_{u}}=0.381(05)(27) \quad \longleftrightarrow \quad m_{u} / m_{d}=0.448(06)(29)
$$

from which we then obtain individual $m_{u}, m_{d}$ values (note: $m_{u}=0$ strongly disfavored)

|  | $m_{u}$ | $m_{d}$ | $m_{s}$ |
| :--- | :---: | :---: | ---: |
| $\mathrm{RI}(4 \mathrm{GeV})$ | $2.17(04)(10)$ | $4.84(07)(12)$ | $96.4(1.1)(1.5)$ |
| RGI | $2.86(05)(13)$ | $6.39(09)(15)$ | $127.3(1.5)(1.9)$ |
| $\overline{\mathrm{MS}}(2 \mathrm{GeV})$ | $2.15(03)(10)$ | $4.79(07)(12)$ | $95.5(1.1)(1.5)$ |

## Lattice phenomenology (1): CKM physics ...



## Lattice phenomenology (2): ... via external currents

Pion decay


$$
\pi^{-}(\mathrm{d} \overline{\mathrm{u}}) \rightarrow \mu^{-}+\overline{\mathrm{v}}_{\mu}
$$

Kaon decay


$$
\mathrm{K}-(\mathrm{s} \bar{u}) \rightarrow \mu^{-}+\overline{\mathrm{v}}_{\mu}
$$

$$
\begin{aligned}
& J_{\mu}^{\mathrm{CC}}=(\bar{u}, \bar{c}, \bar{t}) \gamma_{\mu} \frac{1}{2}\left[1-\gamma_{5}\right] V_{\mathrm{CKM}}\left(\begin{array}{c}
d \\
s \\
b
\end{array}\right) \\
& \langle 0|\left(\bar{u} \gamma_{\mu} \gamma_{5} d\right)(x)\left|\pi^{-}(p)\right\rangle=\mathrm{i} f_{\pi} p_{\mu} e^{\mathrm{i} p x} \\
& \langle 0|\left(\bar{u} \gamma_{\mu} \gamma_{5} s\right)(x)\left|K^{-}(p)\right\rangle=\mathrm{i} f_{K} p_{\mu} e^{\mathrm{i} p x}
\end{aligned}
$$

$$
\left(\begin{array}{c}
d^{\prime} \\
s^{\prime} \\
b^{\prime}
\end{array}\right)=\underbrace{\left(\begin{array}{ccc}
V_{u d} & V_{u s} & V_{u b} \\
V_{c d} & V_{c s} & V_{c b} \\
V_{t d} & V_{t s} & V_{t b}
\end{array}\right)}_{V_{\mathrm{CKM}}}\left(\begin{array}{c}
d \\
s \\
b
\end{array}\right)
$$

$\Longrightarrow$ strong dynamics restricted to matrix elements $\langle 0| A_{\mu}|\pi\rangle,\langle 0| A_{\mu}|K\rangle$ and form factors $\langle\pi| V_{\mu}|K\rangle$ etc.

## $f_{K} / f_{\pi}$ calculation (1): Marciano's observation

- $\left|V_{u d}\right|$ is known, from super-allowed nuclear $\beta$-decays, with $0.03 \%$ precision [HT].
- $\left|V_{u s}\right|$ is much less precisely known, but can be linked to $\left|V_{u d}\right|$ via a relation involving $f_{K} / f_{\pi}$, with everything else known rather accurately:

$$
\frac{\Gamma\left(K \rightarrow l \bar{\nu}_{l}\right)}{\Gamma\left(\pi \rightarrow l \bar{\nu}_{l}\right)}=\frac{\left|V_{u s}\right|^{2}}{\left|V_{u d}\right|^{2}} \frac{f_{K}^{2}}{f_{\pi}^{2}} \frac{M_{K}\left(1-m_{l}^{2} / M_{K}^{2}\right)^{2}}{M_{\pi}\left(1-m_{l}^{2} / M_{\pi}^{2}\right)^{2}}\left\{1+\frac{\alpha}{\pi}\left(C_{K}-C_{\pi}\right)\right\}
$$

- CKM unitarity $\left|V_{u d}\right|^{2}+\left|V_{u s}\right|^{2}+\left|V_{u b}\right|^{2}=1$ (with $\left|V_{u b}\right|$ being negligibly small) is genuine to the SM ; any deviation is a unambiguous signal of BSM physics.
$\Longrightarrow$ calculate $f_{K} / f_{\pi}$ in $N_{f}=2+1$ QCD (with quark masses extrapolated to the physical point) on the lattice; the precision attained gives the precision of $\left|V_{u s}\right|$.


## $f_{K} / f_{\pi}$ calculation (2): adjusting quark masses

$N_{f}=2+1$ lattice QCD: set $m_{u d}, m_{s}$ by adjusting $M_{\pi}, M_{K}$ to their physical values

$\longrightarrow$ extract $f_{K} / f_{\pi}$ on unitary ensembles and extrapolate to the physical mass point $\longrightarrow f_{K} / f_{\pi}=1$ at $m_{u d}=m_{s}$ means that $f_{K} / f_{\pi}-1$ is calculated with $\sim 5 \%$ accuracy

## $f_{K} / f_{\pi}$ calculation (3): chiral extrapolation

- chiral $S U(3)$ formula:

$$
\begin{aligned}
\frac{F_{K}}{F_{\pi}}=1 & +\frac{1}{32 \pi^{2} F_{0}^{2}}\left\{\frac{5}{4} M_{\pi}^{2} \log \left(\frac{M_{\pi}^{2}}{\mu^{2}}\right)-\frac{1}{2} M_{K}^{2} \log \left(\frac{M_{K}^{2}}{\mu^{2}}\right)\right. \\
& \left.-\left[M_{K}^{2}-\frac{1}{4} M_{\pi}^{2}\right] \log \left(\frac{4 M_{K}^{2}-M_{\pi}^{2}}{3 \mu^{2}}\right)\right\}+\frac{4}{F_{0}^{2}}\left[M_{K}^{2}-M_{\pi}^{2}\right] L_{5}
\end{aligned}
$$

- chiral $S U(2)$ _plus_strange formula [RBC/UKQCD 08], simplified form:

$$
\frac{F_{K}}{F_{\pi}}=\left.\frac{F_{K}}{F_{\pi}}\right|_{m_{u d}=0}\left\{1+\frac{5}{8} \frac{M_{\pi}^{2}}{(4 \pi F)^{2}} \log \left(\frac{M_{\pi}^{2}}{\Lambda^{2}}\right)\right\}
$$

- polynomial expansion $F_{\pi} / F_{K}=d_{0}+d_{1}\left(M_{\pi}-M_{\pi}^{\mathrm{ref}}\right)+d_{2}\left(M_{\pi}-M_{\pi}^{\mathrm{ref}}\right)^{2}$, e.g. around $M_{\pi}^{\mathrm{ref}}=300 \mathrm{MeV}$, at fixed physical $m_{s}$, with $\Delta_{\pi, K} \equiv\left(M_{\pi, K}^{2}-M_{\pi, K}^{\mathrm{ref} 2}\right) / M_{\Omega}^{2}$ suggests:

$$
\frac{F_{K}}{F_{\pi}}=c_{0}+c_{1} \Delta_{\pi}+c_{2} \Delta_{\pi}^{2}+c_{3} \Delta_{K}
$$

$\longrightarrow$ use all of them and count spread towards systematic uncertainty

## $f_{K} / f_{\pi}$ calculation (4): infinite volume extrapolation

- finite volume effects on $F_{K}, F_{\pi}$ are known at the 2-loop level [CDH 05]

$$
\begin{aligned}
\frac{F_{\pi}(L)}{F_{\pi}} & =1+\sum_{n=1}^{\infty} \frac{m(n)}{\sqrt{n}} \frac{1}{M_{\pi} L} 1 \frac{M_{\pi}^{2}}{\left(4 \pi F_{\pi}\right)^{2}}\left[I_{F_{\pi}}^{(2)}+\frac{M_{\pi}^{2}}{\left(4 \pi F_{\pi}\right)^{2}} I_{F_{\pi}}^{(4)}+\ldots\right] \\
\frac{F_{K}(L)}{F_{K}} & =1+\sum_{n=1}^{\infty} \frac{m(n)}{\sqrt{n}} \frac{1}{M_{\pi} L} \frac{F_{\pi}}{F_{K}} \frac{M_{\pi}^{2}}{\left(4 \pi F_{\pi}\right)^{2}}\left[I_{F_{K}}^{(2)}+\frac{M_{K}^{2}}{\left(4 \pi F_{\pi}\right)^{2}} I_{F_{K}}^{(4)}+\ldots\right]
\end{aligned}
$$

with $I_{F_{\pi}}^{(2)}=-4 K_{1}\left(\sqrt{n} M_{\pi} L\right)$ and $I_{F_{K}}^{(2)}=-\frac{3}{2} K_{1}\left(\sqrt{n} M_{\pi} L\right)$, where $K_{1}($.$) is a Bessel$ function of the second kind, and lengthy expressions for $I_{F_{\pi}}^{(4)}, I_{F_{K}}^{(4)}$

- finite volume effects cancel partly in the ratio, as evident from the 1-loop formula

$$
\frac{F_{K}(L)}{F_{\pi}(L)}=\frac{F_{K}}{F_{\pi}}\left\{1+\sum_{n=1}^{\infty} \frac{m(n)}{\sqrt{n}} \frac{1}{M_{\pi} L} \frac{M_{\pi}^{2}}{\left(4 \pi F_{\pi}\right)^{2}}\left[\frac{F_{\pi}}{F_{K}} I_{F_{K}}^{(2)}-I_{F_{\pi}}^{(2)}\right]\right\}
$$

- BMW uses $\frac{F_{K}(L)}{F_{\pi}(L)} / \frac{F_{K}}{F_{\pi}}$ at 1-loop and 2-loop level, and $F_{\pi}(L) / F_{\pi}$ at 2-loop level

$\longrightarrow$ plot shows data $\left(M_{\pi}^{2}, 2 M_{K}^{2}-M_{\pi}^{2}\right)-\operatorname{fit}\left(M_{\pi}^{2}, 2 M_{K}^{2}-M_{\pi}^{2}\right)+\operatorname{fit}\left(M_{\pi}^{2},\left[2 M_{K}^{2}-M_{\pi}^{2}\right]_{\mathrm{phys}}\right)$
$\longrightarrow f_{K} / f_{\pi}$ scales rather nicely [note $a^{2} / \mathrm{fm}^{2}=0.0042,0.0072,0.0156$ ]
$\Longrightarrow f_{K} / f_{\pi}=1.192(7)(6)$ at physical $m_{u d}$ and $m_{s}$, in continuum, in infinite volume


## $f_{K} / f_{\pi}$ calculation (6): update on $\left|V_{u s}\right|$ and CKM unitarity

- Latest nuclear structure calculations [Hardy Towner'09] give

$$
\left|V_{u d}\right|=0.97425(22) .
$$

- Plug experimental information $\Gamma(K \rightarrow \mu \bar{\nu}) / \Gamma(\pi \rightarrow \mu \bar{\nu})=1.3363(37)$ [PDG'08] and $C_{K}-C_{\pi}=-3.0 \pm 1.5$ [Marciano] into Marciano's equation; this yields

$$
\frac{\left|V_{u s}\right|}{\left|V_{u d}\right|} \frac{f_{K}}{f_{\pi}}=0.27599(59) .
$$

- Upon combining the previous one/two points and our value for $f_{K} / f_{\pi}$ we obtain

$$
\frac{\left|V_{u s}\right|}{\left|V_{u d}\right|}=0.2315(19) \quad \text { and } \quad\left|V_{u s}\right|=0.2256(17) .
$$

- Upon including $\left|V_{u b}\right|=3.39(36) 10^{-3}$ [PDG'08] we end up with [BMW, 1001.4692]

$$
\left|V_{u d}\right|^{2}+\left|V_{u s}\right|^{2}+\left|V_{u b}\right|^{2}=1.0001(9) .
$$

## $f_{K} / f_{\pi}$ calculation (7): FLAG summary



## Lattice Outreach

- baryon sigma terms and dark matter
- nuclear physics from first principles
- QCD thermodynamics at $\mu=0$
- QCD thermodynamics at $\mu>0$
- hadronic contributions to muon $g-2$
- isospin splitting and electromagnetism
- large $N_{c}$, larger $N_{f}$, different representations


## Lattice outreach (1): WIMPS via nucleon sigma terms



Traditionally large uncertainty from matrix elements
$\sigma_{u d}=m_{u d}\langle N| \bar{u} u+\bar{d} d|N\rangle$
$\sigma_{s}=m_{s}\langle N| \bar{s} s|N\rangle$
(RGI, dimension of mass)

Universe: 73\% dark energy 23\% dark matter 4\% baryons

Dark matter stays dark, unless WIMP-Nucleon scattering can be probed down to tiny cross-sections.


## Lattice outreach (2): sigma terms via Feynman-Hellmann

Lattice can compute $\sigma_{u d}$ and $\sigma_{s}$ directly or via Feynman-Hellmann theorem:
$\sigma_{u d}=m_{u d} \frac{\partial M_{N}}{\partial m_{u d}}=M_{\pi}^{2} \frac{\partial M_{N}}{\partial M_{\pi}^{2}} \quad$ and $\quad \sigma_{s}=m_{s} \frac{\partial M_{N}}{\partial m_{s}}=\left(2 M_{K}^{2}-M_{\pi}^{2}\right) \frac{\partial M_{N}}{\partial\left(2 M_{K}^{2}-M_{\pi}^{2}\right)}$


$\Longrightarrow$ we find $\quad \sigma_{u d}=39(4)\binom{+18}{-7} \mathrm{MeV}$ and $\sigma_{s}=34(14)\left(\begin{array}{c}\binom{24}{-24} \mathrm{MeV}\end{array}\right.$
$\longrightarrow$ in consequence $\quad m_{u d}\langle N| \bar{u} u+\bar{d} d|N\rangle \simeq m_{s}\langle N| \bar{s} s|N\rangle$

## Lattice outreach (3): nuclear physics from first principles



## Lattice outreach (4): QCD thermodynamics at $\mu=0$

Established: QCD with physical $m_{u d}, m_{s}$ at zero chemical potential (as relevant in early universe) shows crossover.

Different definitions of "transition temperature" $T_{c}$ yield different values [ $\left.P,\langle\bar{\psi} \psi\rangle, \ldots\right]$, but for one definition everyone should agree in the continuum.

Long standing discrepancy between WuppertalBudapest (left) and HotQCD (right) now resolved.




## Lattice outreach (5): QCD thermodynamics at $\mu>0$

At non-zero baryon density (equivalent: chemical potential $\mu \neq 0$ ) the fermion determinant becomes complex, which creates a major difficulty to the concept of importance sampling.

A clear establishment of a second-order endpoint would be a major leap forward.


In QCD many approaches to solve the sign problem have been tried:

- absorb phase in observable [ancient]
- two-parameter reweighting from $\mu=0$ [Fodor Katz]
- work at imaginary $\mu$ and continue [Philipsen deForcrand]
- compute Taylor coefficients at $\mu=0$

In QCD-inspired models many tricks/reformulations become possible.

## Lattice outreach (6): hadronic contributions to muon $g-2$

Hadronic contributions to vacuum polarization provide one of the major sources of systematic uncertainty in the computation of $a_{\mu}=\left(g_{\mu}-2\right) / 2$. Can the lattice help ?

$$
a_{\ell}^{\mathrm{HVP}}=\left(\frac{\alpha}{\pi}\right)^{2} \int_{0}^{\infty} d Q^{2} f\left(Q^{2}\right) \bar{\Pi}\left(Q^{2}\right)
$$

with known $f$ and $\bar{\Pi}\left(Q^{2}\right)=\Pi\left(Q^{2}\right)-\Pi(0)$ and $\Pi_{\mu \nu}(q)=\left(q^{2} g_{\mu \nu}-q_{\mu} q_{\nu}\right) \Pi\left(q^{2}\right)$ can be computed as the Fourier transformed 2-point function of the electromagnetic current.


Recent computations include:
Feng et al, Phys.Rev.Lett. 107 (2011) 081802 [arXiv:1103.4818]
Della Morte et al, JHEP 1203 (2012) 055 [arXiv:1112.2894]
Kerrane et al, Phys.Rev. D85 (2012) 074504 [arXiv:1107.1497]

## Lattice outreach (7): isospin splittings and electromagnetism

In standard $N_{f}=2+1$ lattice studies two sources of isospin breaking are ignored (updown mass difference, electromagnetic). Since they are both small, it would appear reasonable to include both of them a posteriori, by reweighting the configurations.

PACS-CS has long experience with reweighting in the quark mass; they used reweighting in $m_{u d}$ to shift $M_{\pi}$ from 156 MeV to 135 MeV .

In arXiv:1205.2961 they extend this approach to account for QED effects and the up-down quark mass difference. They find $M_{K^{0}}>M_{K}^{ \pm}$.


Pioneering publication for QCD+QED on the lattice is Duncan et al, Phys. Rev. Lett. 76 (1996) 3894-3897 [hep-lat/9602005].
Continuation by RBC/UKQCD Phys.Rev. D76 (2007), Phys.Rev. D82 (2010) 094508.
Still, there remain issues relating to finite-volume corrections, see e.g. Hayakawa Uno, Prog.Theor.Phys. 120 (2008) 413 and Portelli et al, PoS LATTICE2011 (2011) 136.

## Lattice outreach (8): $N_{f}=1+1+1+1$ plus QED simulations

- 2002-20??:
$N_{f}=2+1$ QCD requires 3 polished input values [e.g. $M_{\pi}, M_{K}, M_{\Omega}$ in theory with $m_{u}, m_{d} \rightarrow\left(m_{u}+m_{d}\right) / 2$ and $e \rightarrow 0$ ]
$\longrightarrow$ analysis suggests $M_{\pi}=134.8(3) \mathrm{MeV}, M_{K}=494.2(5) \mathrm{MeV}$ [see FLAG report]
- 2010-????:
$N_{f}=2+1+1$ QCD requires 4 polished input values [ditto and $M_{D_{s}}$ in theory with $m_{u}, m_{d} \rightarrow\left(m_{u}+m_{d}\right) / 2$ and $\left.e \rightarrow 0\right]$
$\longrightarrow$ charm unquenched, but no conceptual change on isospin issue
- 2014-????:
$N_{f}=1+1+1+1$ QCD requires 5 input variables [e.g. $M_{\pi^{ \pm}}, M_{K^{ \pm}}, M_{K^{0}}, M_{D_{s}}, M_{\Omega}$ ]
$\longrightarrow$ requires disconnected contribution to flavor-singlet quantities
$\longrightarrow$ analysis of $\pi^{0}-\eta-\eta^{\prime}-\gamma$ mixing mandatory to extract physical masses
$\longrightarrow$ QED and QCD renormalization intertwined ( $m_{s} / m_{d}$ is RGI, $m_{u} / m_{d}$ is not)
$\longrightarrow$ final word on $m_{u} \stackrel{?}{=} 0$ [in QCD+QED] will be possible


## Lattice outreach (9): Large $N_{c}$, larger $N_{f}$, higher representations

QCD with $N_{c} \rightarrow \infty$ and fixed $\lambda=g^{2} N_{c}$ gets much simpler [weakly coupled hadrons, OZI exact, chiral loops $\sim 1 / N$, axial anomaly $\sim 1 / N]$; lattice is almost unnecessary ;-)

$T_{c} / \sqrt{\sigma}$ for $N_{c} \rightarrow \infty$
Lucini, Rago, Rinaldi, 1202.6684


Anomalous mass dimension 2-index symm-representation, $N_{f}=2$ DeGrand, Shamir, Svetitsky, 1202.2675

## Summary



- Lattice solves QCD from first principles: euclidean QFT, analytical and numerical methods
- Remnants of lattice formulation to be removed:
$\diamond$ continuum extrapolation: $a \rightarrow 0$
$\diamond$ infinite volume extrapolation: $L \rightarrow \infty$
$\diamond$ chiral inter/extrapolation: $m_{q} \rightarrow m_{q}^{\text {phys }}$


## Lattice'90, Tallahassee

- Hadron spectroscopy with one stable particle on in and out side is simple
- Hadron spectroscopy with multiparticle states on in or our side is challenging
- Wealth of applications in flavor physics, nuclear physics, (perhaps) BSM physics
- Formulation useful for addressing conceptual issues in euclidean QFT


## Epilogue: lattice literature

- G. Colangelo et al. [FLAG], Eur. Phys. Jour. C 71, 1695 (2011) [arXiv:1011.4408].
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- J. Smit, Introduction to Quantum Fields on a Lattice, Cambridge University Press, 2002.
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