Lattice calculation of isospin breaking corrections to hadronic observables

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among the questions left open by the standard model there is the origin of flavour

the two lightest quarks, the up and the down, have different masses and different electric charges

nevertheless

\[ \frac{m_d - m_u}{\Lambda_{QCD}} \ll 1 \]

\[ (e_u - e_d)\alpha_{em} \ll 1 \]

for these reasons the group of rotations in this bidimensional (complex) “flavour” space is a good and very useful approximate symmetry of the real world
isospin symmetry

- Rotations in the bidimensional flavour space

\[
\begin{pmatrix}
\bar{u} & \bar{d}
\end{pmatrix}
\begin{pmatrix}
D[U] + m_{ud} & 0 \\
0 & D[U] + m_{ud}
\end{pmatrix}
\begin{pmatrix}
u \\
d
\end{pmatrix}
\]

- The two light quarks are into an \( SU(2) \) doublet and hadrons can be classified according to the representations of the "angular momentum" algebra.

- From isospin symmetry combined with parity we know, for example, that an even number of pseudoscalar mesons cannot scatter (through QCD) into an odd number of pseudoscalar mesons,

\[
\langle \pi\pi | H_{W}^{S=1} | K^{0} \rangle = \begin{cases}
A_0 e^{i\delta_0} \\
A_2 e^{i\delta_2}
\end{cases}
\]

where the strong phases \( \delta_0 \) and \( \delta_2 \) coincide with the scattering phases.

- (Un)explained experimental evidence \( A_0 \gg A_2 \), the so called \( \Delta I = 1/2 \) rule.

\[\text{RBC \& UKQCD arXiv:1212.1474}\]
why isospin breaking?

\[ V^{CKM} = \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \]

except for the ones in the third row, CKM matrix elements can be extracted by (semi)leptonic decay rates, according to

\[ V_{gf} = \frac{\text{experiment}}{\text{theory}} \]
why isospin breaking?

Unitarity of the CKM matrix implies several relations among the different couplings, three of these are the so-called unitarity triangles:

\[ V_{ud}V_{us}^* + V_{cd}V_{cs}^* + V_{td}V_{ts}^* = 0 \]
\[ V_{us}V_{ub}^* + V_{cs}V_{cb}^* + V_{ts}V_{tb}^* = 0 \]
\[ V_{ud}V_{ub}^* + V_{cd}V_{cb}^* + V_{td}V_{tb}^* = 0 \]

The unitarity triangle is the scalar product of the \(d\)-column times the \(b\)-column of the CKM matrix.
why isospin breaking?

we do have a lot of precise experimental measurements in the quark flavour sector of the standard model that, combined with CKM unitarity (first row), allow us to measure hadronic matrix elements

\[
\begin{align*}
\left| \frac{V_{us}}{V_{ud}} \right| F_R & = 0.2758(5) \\
\left| V_{us} F_+^K (0) \right| & = 0.2163(5)
\end{align*}
\]

where \( |V_{ud}| \) comes by combining 20 super-allowed nuclear \( \beta \)-decays and \( |V_{ub}| \) has been neglected because smaller than the uncertainty on the other terms, combine to give

\[
|V_{ud}| = 0.97425(22)
\]

\[
|V_{us}| = 0.22544(95)
\]

\[
F_+^K (0) = 0.9595(46)
\]

\[
\frac{F_+^K}{F_+^\pi} = 1.1919(57)
\]

\[
|V_{ud}|^2 + |V_{us}|^2 = 1
\]

lattice QCD is still needed to postdict these quantities and, in case, to falsify the standard model
concerning theoretical predictions, and lattice QCD in particular, these matrix elements are among the well known quantities

\[
F_{K/F}\pi & F_{\pi}^{K}\pi(0) = 0.956(8) \sim 0.8\%
\]

\[
\frac{F_K}{F_\pi} = 1.193(5) \sim 0.5\%
\]

to do better we should include effects that we have been neglecting up to now...
$F_K/F_\pi$ & $F_{+\pi}^K(q^2)$ beyond the isospin limit

- In practice, it is useful to divide the isospin breaking effects into strong and electromagnetic ones,

$$m_u \neq m_d \quad \text{QCD}$$

$$e_u \neq e_d \quad \text{QED}$$

- In the particular and (lucky) case of these observables, the correction to the isospin symmetric limit due to the difference of the up and down quark masses (QCD) can be estimated in chiral perturbation theory,

$$F_{+\pi}^K(0) = 0.956(8) \quad \sim 0.8\%$$

$$\left( \frac{F_{+\pi}^K 0^+(q^2)}{F_{+\pi}^K 0^-(q^2)} - 1 \right)_{\text{QCD}} = 0.029(4)$$

$$\frac{F_K}{F_\pi} = 1.193(5) \quad \sim 0.5\%$$

$$\left( \frac{F_{+\pi}^K / F_\pi^+}{F_K / F_\pi} - 1 \right)_{\text{QCD}} = -0.0022(6)$$


- We need first principle lattice QCD calculations to avoid uncertainties coming from the effective theory.

- But the home message is: reducing the error on these quantities without taking into account isospin breaking is useless...
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& in preparation

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The gauge configurations

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- Gauge configurations for this study have been taken from the $n_f = 2$ gauge ensembles made publicly available by the ETMC collaboration.

- **Caveat**: the Twisted Mass discretization breaks isospin at finite lattice spacing.

- We have been working in a mixed-action setup by introducing $O(a^2)$ errors coming from violations of unitarity...
the calculation of QED isospin breaking effects on the lattice it has been done for the first time in Duncan, Eichten, Thacker, Phys. Rev. Lett. 76 (1996)

QED is treated in the quenched approximation in its “non-compact” formulation

because the photons are massless and unconfined this approach may introduce large finite volume effects...

the calculation of isospin breaking effects on the lattice poses a theoretical problem

\[
Z = \int DADUD\psi e^{-Se[A]-\beta Sg[U]+Sf[A,U;m_u,m_d]}
\]

\[
= \int DADU e^{-Se[A]-\beta Sg[U]} \left\{ \det(D_u[U,A] + m_u) \det(D_d[U,A] + m_d) \right\}
\]

must be real and >0

if \(m_u \neq m_d\) and \(e_u \neq e_d\), this can be only achieved by recurring to non (ultra) local and, consequently, very expensive fermion formulations or to reweighting

furthermore, the effect is very small and it can be extremely difficult to see it with limited statistical accuracy
our QCD isospin breaking on the lattice

- our idea is to calculate QCD isospin corrections at first order in

\[
\frac{m_d - m_u}{\Lambda_{QCD}} \sim \alpha_{em} \sim O(\varepsilon)
\]

- in order to calculate QED corrections to a given correlator \( \mathcal{O}(x) \) we have to cope with

\[
T\langle \mathcal{O}(x_i) \rangle \quad \rightarrow \quad T \int d^4y d^4z \ D_{\mu\nu}(y - z) \ \langle \mathcal{O}(x_i) J^\mu(y) J^\nu(z) \rangle
\]

- and solve the infrared problem associated with a proper definition of the finite volume lattice photon propagator

- and solve the ultraviolet problem associated with the divergences coming from the contact interactions of the two electromagnetic currents of the quarks. in the continuum one would get

\[
J^\mu(x) J_\mu(0) \sim c_1(x) + \sum_f c_f^m(x) m_f \bar{\psi}_f \psi_f + c_g(x) G_{\mu\nu} G^{\mu\nu} + \cdots
\]

- where the \( c_f^m \) coefficients correspond to the separate renormalization of the quark masses, \( c_g \) to the renormalization of the strong coupling constant and \( c_1 \) to the vacuum polarization, all induced by QED
in order to perform combined QCD+QED lattice simulations one can use the non-compact formulation of QED:

\[
S_{QED} = \frac{1}{4} \sum_{x; \mu, \nu} \left( \nabla^+_{\mu} A_{\nu}(x) - \nabla^+_{\nu} A_{\mu}(x) \right)^2
\]

\[
= -\frac{1}{4} \sum_{x; \mu, \nu} \left\{ A_{\nu}(x) \nabla^-_{\mu} \left[ \nabla^+_{\mu} A_{\nu}(x) - \nabla^+_{\nu} A_{\mu}(x) \right] - A_{\mu}(x) \nabla^-_{\nu} \left[ \nabla^+_{\mu} A_{\nu}(x) - \nabla^+_{\nu} A_{\mu}(x) \right] \right\}
\]

by using a covariant gauge fixing, one gets:

\[
\nabla^-_{\mu} A_{\mu}(x) = 0 \quad \longrightarrow \quad S_{QED} = \frac{1}{2} \sum_x A_{\mu}(x) \left[ -\nabla^-_{\nu} \nabla^+_{\nu} \right] A_{\mu}(x)
\]

\[
= \frac{1}{2} \sum_k A^*_\mu(k) \left[ 2 \sin(k_{\nu}/2) \right] A_{\mu}(k)
\]

note that the zero momentum mode, the infrared problem, is not constrained by any “derivative” gauge fixing, and there is a residual gauge ambiguity

\[
\nabla^-_{\mu} \left[ A_{\mu}(x) + c \right] = \nabla^-_{\mu} A_{\mu}(x)
\]
by assuming that one is able to sample properly the QED gauge potential $A_\mu(x)$ (we shall discuss this point in the next few slides), gauge invariance works as follows:

- the QED links are defined by

$$A_\mu(x) \rightarrow E_\mu(x) = e^{-i e A_\mu(x)}$$

- QCD+QED covariant lattice derivatives are defined according to

$$\bar{\psi}(x) D^+_{\mu} \psi(x) = \bar{\psi}(x) E_\mu(x) U_\mu(x) \psi(x + \mu) - \bar{\psi}(x) \psi(x)$$

- the “exact” gauge invariance is

$$\begin{align*}
\psi(x) & \rightarrow e^{i e \lambda(x)} \psi(x) \\
\bar{\psi}(x) & \rightarrow \bar{\psi}(x) e^{-i e \lambda(x)} \\
A_\mu(x) & \rightarrow A_\mu(x) + \nabla^+_\mu \lambda(x)
\end{align*}$$
in order to sample the QED gauge potential, the strategy followed by other groups is the following

\[ A_\mu(x + L \nu) = A_\mu(x) \rightarrow k_\mu = \frac{2\pi n_\mu}{L} \rightarrow S_{QED} = \frac{1}{2} \sum_{k \neq 0} A_\mu(k)^* [2 \sin(k_\nu/2)]^2 A_\mu(k) \]

the action is quadratic and diagonal in momentum space so, by excluding the zero momentum mode, \( A_\mu(k) \) can be obtained by an heat-bath algorithm (actually they choose a different gauge, diagonalize the action and perform a gaussian sampling... ) and the gauge potential in coordinate space is obtained by (fast) fourier transform

it can be shown that the effect of this **infrared regularization** is a **finite volume effect**. classically:

\[ S_{QED} \rightarrow \frac{1}{2} \sum_x A_\mu(x) \left[ -\nabla^-_\nu \nabla^+_\nu \right] A_\mu(x) + \frac{1}{L^3} \sum_x \xi_\mu A_\mu(x) \rightarrow A_\mu(k = 0) = \frac{\partial S}{\partial \xi_\mu} = 0 \]

at quantum level: this prescription does not affect short distance physics (no new divergences)

the prescription solves the “inconsistency” with the finite volume Gauss’s law because the following equation is valid for \( k \neq 0 \) only:

\[ \nabla^-_\mu F_{\mu\nu}(x) = j_\nu(x) \rightarrow 0 = \sum_\vec{x} \nabla^-_i E_i(t, \vec{x}) = e \sum_\vec{x} \delta^3(t, \vec{x}) = 1 \]
non-compact QED on the lattice: our approach

- we want to deal with QED on the lattice at fixed order in the expansion with respect to $\hat{\alpha}_{em}$

- to this end, we need to expand the lattice action with respect to the electric charge

\[
\sum_x \bar{\psi}(x) \{ D[U, E] - D[U, 1] \} \psi(x) = \\
+ \sum_{x, \mu} e A_\mu(x) i \left\{ \bar{\psi}(x) U_\mu(x) \frac{W - \gamma^\mu}{2} \psi(x + \mu) - \bar{\psi}(x + \mu) U_\mu^\dagger(x) \frac{W + \gamma^\mu}{2} \psi(x) \right\} \\
+ \sum_{x, \mu} \frac{e^2}{2} A_\mu(x) A_\mu(x) \left\{ \bar{\psi}(x) U_\mu(x) \frac{W - \gamma^\mu}{2} \psi(x + \mu) + \bar{\psi}(x + \mu) U_\mu^\dagger(x) \frac{W + \gamma^\mu}{2} \psi(x) \right\} \\
+ \ldots \\
= \sum_{x, \mu} \left\{ e A_\mu(x) V^\mu(x) + \frac{e^2}{2} A_\mu(x) A_\mu(x) T^\mu(x) + \ldots \right\}
\]

the "Wilson" contribution is $W = \{ 1, i \gamma_5 \tau^3 \}$ in clover and twisted mass QCD respectively

note: tadpole currents $T^\mu(x)$ are required to have gauge invariance at order $e^2$

note: the point split vector current is exactly conserved: $\nabla_\mu V^\mu(x) = 0$
let us consider, for example, the following contribution to the mass splittings of the kaons:

\[-\text{disc.} = \frac{e_s e_u e^2}{2} \sum_{x,y} D_{\mu\nu}(x - y) T\langle 0 | \bar{s}(t) \gamma_5 u(t) V_s^\mu(x) V_u^\nu(y) \bar{u}(0) \gamma_5 s(0) | 0 \rangle\]

where \(D_{\mu\nu}(x - y)\) is the propagator of the gauge potential \(A_\mu\): this means that we are also using the QED in its non-compact lattice formulation. now, in order to properly define the lattice propagator of \(A_\mu\) we must

- fix the QED gauge; we have used

\[\nabla^-_\mu A_\mu(x) = 0 \quad \longrightarrow \quad S_{QED} = \frac{1}{2} \sum_x A_\mu(x) \left[ -\nabla^-_\nu \nabla^+_\nu \right] A_\mu(x) = \frac{1}{2} \sum_k A_\mu(k) \left[ 2 \sin(k_\nu / 2) \right]^2 A_\mu(k)\]

- introduce the infrared regulated photon propagator,

\[P^\perp \phi(x) = \phi(x) - \frac{1}{V} \sum_y \phi(y)\]

\[D^\perp_{\mu\nu}(x - y) = \left[ \frac{\delta_{\mu\nu}}{-\nabla^\rho \nabla^\rho} P^\perp \right] (x - y) = \sum_{k \neq 0} \frac{e^{ik(x - y)}}{[2 \sin(k_\nu / 2)]^2}\]
we have decided to work directly in coordinate space, thus avoiding fourier transforms, by applying the following stochastic technique:

- we extract a set of four independent real fields distributed according to a real $\mathbb{Z}_2$ distribution,

$$
\sum_B B_\mu(x)B_\nu(y) = \delta_{\mu\nu} \delta(x - y)
$$

- for each field we solve numerically the equation

$$
\left[-\nabla_\nu \nabla_\nu^+\right]C_\mu[B; x] = P_\perp B_\mu(x) \quad \rightarrow \quad C_\mu[B; x] = \left[\frac{1}{-\nabla_\nu \nabla_\nu^+} P_\perp\right] B_\mu(x) \nonumber \\
= \left[ P_\perp \frac{1}{-\nabla_\nu \nabla_\nu^+} P_\perp\right] B_\mu(x) \nonumber \\
= \sum_z D_\perp(x - z)B_\mu(z)
$$

- by using the properties of the $\mathbb{Z}_2$ noise we thus obtain

$$
\sum_B B_\mu(y)C_\nu[B; x] = D_\perp(x - z) \sum_B B_\mu(y)B_\nu(z) = D_\perp^{\mu\nu}(x - y)
$$
coming back to our example, we get

\[- \begin{array}{c}
\frac{e_se_u e^2}{2} \sum_{x,y} D^\perp_{\mu\nu}(x - y) \ T\langle 0 | \bar{s}(t)\gamma_5 u(t) \ V_s^\mu(x) \ V_u^\nu(y) \ \bar{u}(0)\gamma_5 s(0) | 0 \rangle \\
= \frac{e_se_u e^2}{2} \sum_B \sum_{x,y} B_{\mu}(y)C_{\nu}[B; x] \ T\langle 0 | \bar{s}(t)\gamma_5 u(t) \ V_s^\mu(x) \ V_u^\nu(y) \ \bar{u}(0)\gamma_5 s(0) | 0 \rangle
\end{array} \]

the problem is thus reduced to the calculation of two sequential propagators

\[D_f[U, 1]\Psi_B^f(x) = \sum_{\mu} B_{\mu}(x)\Gamma^\mu_{V} S_f[U; x] \]
\[D_f[U, 1]\Psi_C^f(x) = \sum_{\mu} C_{\mu}[B; x]\Gamma^\mu_{V} S_f[U; x] \]

for different values of the \(B_{\mu}(x)\) and \(C_{\mu}[B; x]\) fields (we have used 3 electromagnetic stochastic sources per QCD gauge configuration) and then calculate the corrected correlator according to

\[- \begin{array}{c}
\begin{array}{c}
\frac{e_se_u e^2}{2} \left\langle \begin{array}{c}
\text{Tr} \{ [\Psi_B^s]^\dagger(t) \ \Psi_C^u(t) \} \end{array} \right\rangle_{B, U}
\end{array}
\end{array} \]
non-compact QED on the lattice: our approach

\[- \begin{array}{l}
\frac{e_u e e^2}{2} \left\langle \text{Tr} \left\{ [\Psi^s_B]^\dagger(t) \Psi^u_C(t) \right\} \right\rangle^{B,U}
\end{array}\]

\[= - \frac{e_s e_u e^2}{2} \left\langle \sum_{x,y} B_\mu(x) C_\nu[B; y] \text{Tr} \left\{ \gamma_5 S_s[U; t-x] \Gamma^\mu V S_s[U; x] \gamma_5 S_{ud}[U; -y] \Gamma^\nu V S_{ud}[U; y-t] \right\} \right\rangle^{B,U}\]

does it work?

\[R^{\text{exch}}_K(t) = \frac{\partial}{\partial e^2} \left( \frac{G^2}{M_K} e^{-t M_K} \right) \approx \frac{G^2}{M_K} e^{-t M_K}\]

well, from the numerical point of view it seems to work. ok, what about the physics?
the ultraviolet problem

- on the lattice, the short distance expansion of two electromagnetic currents is

\[ J^\mu(x)J_\mu(0) + T^\mu(x) \sim c_1(x)1 + \sum_f c^f_k(x)\bar{\psi}_f i\gamma_5 \tau^3 \psi_f + \sum_f c^f_m(x)m_f \bar{\psi}_f \psi_f + c_g(x)G_{\mu\nu}G^{\mu\nu} + \cdots \]

- on the left we have the (non Lorentz–invariant) tadpole contribution required for gauge invariance

- on the right, with Wilson fermions, we have the linear divergent contributions associated with the electromagnetic shifts of the critical masses of the quarks

- our perturbative expansion is defined as follows

\[
\mathcal{O}(e^2, g_s, m_u, m_d, m_s, k_u, k_d, k_s) = \left[ \mathcal{O} + \Delta \mathcal{O} \right] (0, g^0_s, m^0_{ud}, m^0_{ud}, m^0_s, k_0, k_0, k_0) + \Delta \mathcal{O} \bigg|_{\bar{g} = \bar{g}_0}
\]

\[
\Delta \mathcal{O} = \left\{ \frac{e^2}{2} \frac{\partial^2}{\partial e^2} + \frac{1}{2} \left( g_s - g^0_s \right)^2 \frac{\partial^2}{\partial g^2_s} + (m_f - m^0_f) \frac{\partial}{\partial m_f} + (k_f - k^0) \frac{\partial}{\partial k_f} \right\} \mathcal{O}(\bar{g}) \bigg|_{\bar{g} = \bar{g}_0}
\]
matching QCD+QED with isosymmetric QCD

\[
\mathcal{O}(\bar{g}) = \mathcal{O}(\bar{g}_0) + \left\{ \frac{e^2}{2} \frac{\partial^2}{\partial \bar{e}^2} + \frac{1}{2} \left( g_s - g_s^0 \right)^2 \frac{\partial^2}{\partial g_s^2} + (m_f - m_f^0) \frac{\partial}{\partial m_f} + (k_f - k_0) \frac{\partial}{\partial k_f} \right\} \mathcal{O}(\bar{g}_0)
\]

the parameters \( \bar{g}_0 \) can eventually be fixed independently from \( \bar{g} \) by performing “standard” QCD simulations, by neglecting isospin breaking effects and by using external hadronic inputs to calibrate the isosymmetric lattice.

on the other hand, when simulations of the full theory are performed, one can use the following matching condition

\[
\begin{align*}
\text{experiment} & \quad \longrightarrow \quad g_i & \longrightarrow \quad \hat{g}_i(\mu) = Z_i(\mu) g_i & \longrightarrow \quad \hat{g}_i^0(\mu^*) = \hat{g}_i(\mu^*) \\
& \quad \longrightarrow \quad g_i^0 = \frac{\hat{g}_i^0(\mu^*)}{Z_i^0(\mu^*)}
\end{align*}
\]

note that, once the critical masses have been adjusted the two theories are continuum–like and that a physical observable is RGI invariant:

\[
\mathcal{O}(\hat{g}_i) = \mathcal{O} \left( \hat{g}_i^0 \right) + \left\{ \hat{e}^2 \frac{\partial^2}{\partial \hat{e}^2} + \frac{1}{2} \left( \hat{g}_s - \frac{Z_{gs}}{Z_{gs}^0} \hat{g}_s^0 \right)^2 \frac{\partial^2}{\partial \hat{g}_s^2} + \left( \hat{m}_f - \frac{Z_{mf}}{Z_{mf}^0} \hat{m}_f^0 \right) \frac{\partial}{\partial \hat{m}_f} + \Delta k_f \frac{\partial}{\partial k_f} \right\} \mathcal{O}(\hat{g}_i^0)
\]

in other words, the counter–terms do arise because the renormalization constants (the bare parameters) of the two theories are different.
The expansion of the lattice path–integral

- Let us consider the path–integral representation of a generic observable $O(\vec{g})$

$$O(\vec{g}) = \frac{\int dA e^{-\text{SQED}[A]} dU e^{-\beta \text{SQCD}[U]} \prod_{f=1}^{n_f} \det (D_f[U, E]) \, O[U, E]}{\int dA e^{-\text{SQED}[A]} dU e^{-\beta \text{SQCD}[U]} \prod_{f=1}^{n_f} \det (D_f[U, E])}$$

$$= \frac{\int dA e^{-\text{SQED}[A]} dU e^{-\beta^0 \text{SQCD}[U]} \prod_{f=1}^{n_f} \det (D_f[U, 1]) \, R[U, E] \, O[U, E]}{\int dA e^{-\text{SQED}[A]} dU e^{-\beta^0 \text{SQCD}[U]} \prod_{f=1}^{n_f} \det (D_f[U, 1]) \, R[U, E]}$$

$$= \frac{\langle R[U, E] \, O[U, E] \rangle}{\langle R[U, E] \rangle}, \quad R[U, E] = e^{-(\beta - \beta^0) \text{SQCD}[U]} \prod_{f=1}^{n_f} \frac{\det (D_f[U, E])}{\det (D_f[U, 1])}$$

- The corrections are obtained by applying the differential operator $\Delta$ to the previous expression

$$\Delta O = \langle \Delta O[U, 1] \rangle + \left\{ \langle \Delta R[U, 1] \, O[U, 1] \rangle - \langle \Delta R[U, 1] \rangle \langle O[U, 1] \rangle \right\}_{\text{VP}[O]}$$
by using the explicit expression of the lattice Dirac operator

\[
D^\pm_f[U, E] \psi(x) = (m_f \pm i\gamma_5 k_f) \psi(x) - \sum_\mu \frac{\mp i\gamma_5 - \gamma_\mu}{2} U_\mu(x)[E_\mu(x)]^e f \psi(x + \mu)
- \sum_\mu \frac{\mp i\gamma_5 + \gamma_\mu}{2} U_\mu^\dagger(x - \mu)[E_\mu^\dagger(x - \mu)]^e f \psi(x - \mu)
\]

together with the following formulae and the associated graphical notation

\[
\frac{\partial S_f}{\partial e} = -S_f \frac{\partial D_f}{\partial e} S_f = e_f \\
\frac{1}{2} \frac{\partial^2 S_f}{\partial e^2} = S_f \frac{\partial D_f}{\partial e} S_f \frac{\partial D_f}{\partial e} S_f - \frac{1}{2} S_f \frac{\partial^2 D_f}{\partial e^2} S_f = e_f^2 + e_f^2 \\
\frac{\partial S_f}{\partial m_f} = -S_f \frac{\partial D_f}{\partial m_f} S_f = - \\
\frac{\partial S^\pm_f}{\partial k_f} = -S^\pm_f \frac{\partial D^\pm_f}{\partial k_f} S^\pm_f = \mp
\]
by using the explicit expression of the lattice Dirac operator
\[ D_f^\pm [U, E] \psi(x) = (m_f \pm i\gamma_5 k_f) \psi(x) - \sum_\mu \frac{\mp i\gamma_5 - \gamma_\mu}{2} U_{\mu}(x)[E_{\mu}(x)]^{e_f} \psi(x + \mu) - \sum_\mu \frac{\mp i\gamma_5 + \gamma_\mu}{2} U_{\mu}^\dagger(x - \mu)[E_{\mu}^\dagger(x - \mu)]^{e_f} \psi(x - \mu) \]

together with the following formulae and the associated graphical notation
\[ \frac{\partial R}{\partial \beta} = \frac{3}{(g_0^2)^4} S_{QCD} D[U] = G_{\mu \nu} G^{\mu \nu} \]
\[ \frac{\partial r_f}{\partial e} = \text{Tr} \left( S_f \frac{\partial D_f}{\partial e} \right) = -e_f \]
\[ \frac{1}{2} \frac{\partial^2 r_f}{\partial e^2} = \frac{1}{2} \text{Tr} \left( S_f \frac{\partial^2 D_f}{\partial e^2} \right) - \frac{1}{2} \text{Tr} \left( S_f \frac{\partial D_f}{\partial e} S_f \frac{\partial D_f}{\partial e} \right) + \frac{1}{2} \text{Tr} \left( S_f \frac{\partial D_f}{\partial e} \right) \text{Tr} \left( S_f \frac{\partial D_f}{\partial e} \right) \]
\[ = -e_f^2 - e_f^2 + e_f^2 \]
the corrections to the quark propagator in a fixed QCD gauge are given by

\[
\Delta \rightarrow \pm = (e_f e_e)^2 \rightarrow + (e_f e_e)^2 \rightarrow \mp \Delta k_f \rightarrow

- [m_f - m_0] \rightarrow - e^2 e_f \sum_{f_1} e_{f_1} \rightarrow - e^2 \sum_{f_1} e_{f_1}^2 \rightarrow

+ (g_s - g_0^2) \rightarrow + e^2 \sum_{f_1 f_2} e_{f_1} e_{f_2} \rightarrow + \sum_{f_1} \mp \Delta k_{f_1} \rightarrow

+ \sum_{f_1} [m_{f_1} - m_0] \rightarrow - e^2 \sum_{f_1} e_{f_1}^2 \rightarrow
the corrections to the quark propagator in a fixed QCD gauge are given by

$$\Delta \pm = (e_f e)^2 \pm (e_f e)^2 \pm \Delta k_f$$

$$- [m_f - m_f^0] - e^2 e_f \sum_{f_1} e_{f_1}$$

$$+ \text{[isosym. vac. pol.]}$$

all isosymmetric vacuum polarization effects will cancel in the calculation of genuine isospin breaking effects, i.e. $M_{\pi^+} - M_{\pi^0}$ and $M_{K^+} - M_{K^0}$ in our case
hadron masses

- Let's consider a two-point correlator in the full theory ($m_u \neq m_d$ and $e_q \neq 0$)

$$C_{HH}(t; \vec{g}) = \langle \mathcal{O}_H(t) \mathcal{O}_H^\dagger(0) \rangle_{\vec{g}} \quad \rightarrow \quad e^{M_H} = \frac{C_{HH}(t-1; \vec{g})}{C_{HH}(t; \vec{g})} + \text{non leading exps.}$$

where $\mathcal{O}_H$ is an interpolating operator having the quantum numbers of a given hadron $H$.

- If $H$ is a charged particle, the correlator $C_{HH}(t; \vec{g})$ is not QED gauge invariant. For this reason it is not possible, in general, to extract physical informations directly from the residues of the different poles.

- On the other hand, the mass of the hadron is gauge invariant and finite in the continuum limit, provided that the parameters of the actions have been properly renormalized. It follows that, at any given order in a perturbative expansion with respect to any of the parameters of the action, the ratio $C_{HH}(t-1; \vec{g})/C_{HH}(t; \vec{g})$ is both gauge and renormalization group (RGI) invariant.

- By applying the differential operator $\Delta$ to full theory correlators, we shall find expressions of the form

$$C_{HH}(t; \vec{g}) = C_{HH}(t; \vec{g}^0) \left[ 1 + \frac{\Delta C_{HH}(t; \vec{g}^0)}{C_{HH}(t; \vec{g}^0)} + \ldots \right]$$

$$M_H - M_H^0 = -\partial_t \frac{\Delta C_{HH}(t; \vec{g}^0)}{C_{HH}(t; \vec{g}^0)} + \ldots$$

where we have defined $\partial_t f(t) = f(t) - f(t - 1)$.
the physics: pions mass difference

\[ \Delta M_{\pi^0} = - \frac{e_u^2 + e_d^2}{2} e^2 \partial_t + \frac{(e_u - e_d)^2}{2} e^2 \partial_t - (e_u^2 + e_d^2)e^2 \partial_t + 2[m_{ud} - m_{ud}^0] \partial_t + \sum_{f=sea} (e_u + e_d)e^2 \partial_t - (\Delta k_u + \Delta k_d) \partial_t + [\text{isosym. vac. pol.}] \]

In practice, our mixed action approach consists in neglecting all the contributions that are not present in the continuum and that are cutoff effects. To the (non-unitary) lattice theory it can be given a local formulation by using a suitable number of valence fields.
by expanding the two-point function of an interpolating operator having the quantum numbers of the charged pions, we get

\[
\Delta M_{\pi^+} = - e_u e_d e^2 \partial_t
\]

\[
- (e_u^2 + e_d^2) e^2 \partial_t + 2[m_{ud} - m_{ud}^0] \partial_t
\]

\[
+ (e_u + e_d) e^2 \sum_{f=sea} e_f \partial_t - (\Delta k_u + \Delta k_d) \partial_t + [\text{isosym. vac. pol.}]
\]
the physics: pions mass difference

\[ M_{\pi}^{\text{eff}}(t) \]

\[ R_{\text{exch}}(t) \]

\[ M_{\pi^+} - M_{\pi^0} = \frac{(e_u - e_d)^2}{2} e^2 \partial_t \]

In order to take into account the effect of periodic boundary conditions along the time direction

\[ \Delta \left( \frac{R_P e^{-tM_P}}{R_P e^{-tM_P}} \right) = \text{const.} - t\Delta M_P \quad \rightarrow \quad \text{const.} + \Delta M_P (t - T/2) \tanh \left[ M_P^0 (t - T/2) \right] \]
the physics: pions mass difference

the pions mass difference at first order is a very “clean” theoretical prediction!

\[ M_{\pi^+}^2 - M_{\pi^0}^2 = (e_u - e_d)^2 e^2 M_\pi \partial_t - e^2 = 4\pi \hat{\alpha}_{em} = \frac{4\pi}{137} \]

the neglected contribution vanishes in the chiral limit, it is \( O(\hat{\alpha}_{em} \hat{m}_{ud}) \).
the physics: pions mass difference

- our data need to be extrapolated with respect to the simulated quark masses, to the continuum and to the infinite volume limits

- chiral formulae and finite volume effects have been calculated in chiral perturbation theory coupled to electromagnetism by using the same infrared regularization of our work (removal of the zero momentum mode)

  \[ \left[ M_{\pi^+}^2 - M_{\pi^0}^2 \right] = 2\hat{e}^2 F_0^2 \left\{ C - (3 + 4C) \frac{M_{\pi}^2}{32\pi^2 F_0^2} \left[ \log \left( \frac{M_{\pi}^2}{\mu^2} \right) + K(\mu) \right] \right\} \]

  \[ \left[ M_{\pi^+}^2 - M_{\pi^0}^2 \right] (\infty) - \left[ M_{\pi^+}^2 - M_{\pi^0}^2 \right] (L) = -\frac{\hat{e}^2}{4\pi L^2} [H_2(M_{\pi} L) - 4C H_1(M_{\pi} L)] \]

  \[ \sim \hat{e}^2 \frac{2.8373}{4\pi} \left( \frac{M_{\pi}}{L} + \frac{2}{L^2} \right) \]

- finite volume effects are predicted to be large. these are not peculiar of our method, QED is a long–range interaction and any lattice calculation comes with power–law fve...
we have considered different fitting functions. in particular

\[ f_1^\pi [C, K, A_{\pi}] = f_{\chi_\pi} [C, K] + f_{\chi_\pi}^{\pi} C + A_{\pi} [a^0]^2 \]

\[ f_2^\pi [C, K, A_{\pi}, B_{\pi}] = C + K \hat{m}_{ud} + \frac{B_{\pi}}{L} + A_{\pi} [a^0]^2 \]

\[ f_3^\pi [C, K, A_{\pi}, B_{\pi}] = C + K \hat{m}_{ud} + \frac{B_{\pi}^2}{L^2} + A_{\pi} [a^0]^2 \]

- extrapolated results are compatible and all the fits have \( \chi^2 / dof \sim 1 \)
- fitted finite volume effects are much smaller than the \( \chi_{\text{pt}} \) prediction
- lighter pions and larger volumes will be required in order to make a definite statement concerning this point...
by expanding the two-point functions of the kaons we get

\[ M_{K^+} - M_{K^0} = -2\Delta m_{ud} \partial t - (\Delta k_u - \Delta k_d) \partial t + (e_u^2 - e_d^2) e^2 \partial t + \sum_f e_f \partial t \]

in order to use this formula for physical applications we first need to discuss the numerical determination of the electromagnetic critical masses \( \Delta k_u \) and \( \Delta k_d \)

afterwards, the kaons mass difference can be used in order to extract \( \Delta m_{ud} \) and/or to define a renormalization prescription in order to separate QCD from QED isospin breaking corrections

the OZI violating “sea–tadpole” contributions will be neglected in the following by relying on what we call the \textit{electroquenched} approximation
according to Dashen’s theorem, in the $SU(3)$ chiral limit, also in presence of electromagnetic interactions, the neutral pion and the neutral kaons are Goldstone’s bosons

$$\lim_{m_f \to 0} M_{\pi 0} = \lim_{m_f \to 0} M_{K 0} = 0$$

by using the formulae for the corrections to $M_{\pi 0}$ and to $M_{K 0}$ in the electroquenched approximation and by noting that for the exact vector symmetries of the chiral theory $\Delta k_d = \Delta k_s$, we get

$$\Delta k_f = -\frac{e_f^2}{2} e^2 \lim_{m_f \to 0}$$
an alternative determination of the electromagnetic critical masses, that does not require chiral extrapolations, can be obtained by using the following Ward identity of the twisted theory

\[
\langle \nabla_\mu \left[ \bar{\psi}_f \gamma^\mu \tau^1 \psi_f \right] (x) \left[ \bar{\psi}_f \gamma^5 \tau^2 \psi_f \right] (0) \rangle \bar{g} = 0
\]

by working as in the case of the pions and kaons masses and by expanding the previous relation, we get

\[
\Delta k_f = -\frac{e_f^2 e^2}{2}
\]
the physics: kaons mass difference
the physics: kaons mass difference

\[ R_{K}(t) \]

\[ R_{\text{self}}(t) \]
by using the numerical determinations of the critical masses counter terms, the formulae for $M_{K^+} - M_{K^0}$ can be used in order to separate QCD from QED isospin breaking contributions.
to this end we need to observe that the bare parameters of the full theory $\Delta m_{ud}$ and $m_{ud}$ mix under renormalization

$$\Delta m_{ud} = \frac{1}{2} \left( \frac{\hat{m}_d}{Z_{m_d}} - \frac{\hat{m}_u}{Z_{m_u}} \right) = \frac{\Delta \hat{m}_{ud}}{Z_{ud}} + \frac{\hat{m}_{ud}}{Z_{ud}}$$

this happens because the up and the down have different electric charge and

$$\frac{1}{Z_{ud}} = \frac{1}{2} \left( \frac{1}{Z_{m_d}} + \frac{1}{Z_{m_u}} \right) \quad \frac{1}{Z_{ud}} = \frac{1}{2} \left( \frac{1}{Z_{m_d}} - \frac{1}{Z_{m_u}} \right) \neq 0$$

the mixing does not happen in isosymmetric QCD and we have

$$\frac{1}{Z^0_{ud}} = Z^0_P \quad \frac{1}{Z^0_{ud}} = 0 \quad \implies \quad \Delta m_{ud} = Z^0_P \Delta \hat{m}_{ud} + \frac{\hat{m}_{ud}}{Z_{ud}}$$

note that by neglecting all the contributions of $O(\alpha em \Delta m_{ud})$ also the divergent contributions of this order appearing in the $\Delta m_{ud}$ formula above have to be neglected
QCD and QED isospin breaking corrections to $M_{K^+} - M_{K^0}$ can be now conveniently separated according to

\[
\left[ M_{K^+} - M_{K^0} \right]^{QED} (\mu) = -\frac{2\hat{m}_{ud}}{Z_{ud}} \partial_t - (\Delta k_u - \Delta k_d)\partial_t + (e_u^2 - e_d^2)e^2 \partial_t
\]

\[
\left[ M_{K^+} - M_{K^0} \right]^{QCD} (\mu) = -2\Delta \hat{m}_{ud} Z_P^0 \partial_t
\]
in what we call the \textit{electroquenched} approximation, we have computed the Dashen’s theorem breaking parameter

\[ \varepsilon_{\gamma}(\mu) = \frac{\left[ M_{K^+}^2 - M_{K^0}^2 \right]_{QED}(\mu)}{M_{\pi^+}^2 - M_{\pi^0}^2} - 1, \quad \varepsilon_{\gamma} \sim 0.7 \text{ from FLAG} \]

in our previous work on the calculation of QCD isospin breaking corrections we had used \( \varepsilon_{\gamma} = 0.7(5) \) to calculated the QCD corrections to the \( K\ell2 \) decay rate
we have considered different fitting functions. In particular

\[ f_1^\epsilon[E, A_\epsilon] = E + A_\epsilon [a^0]^2 \]

\[ f_2^\epsilon[E, A_\epsilon, B_\epsilon] = E + A_\epsilon [a^0]^2 + \frac{B_\epsilon}{L} \]

\[ f_3^\epsilon[E, A_\epsilon, B_\epsilon] = E + A_\epsilon [a^0]^2 + \frac{B_\epsilon^2}{L^2} \]

All the fits have \( \chi^2/dof \sim 1 \)

The data are flat within the quoted errors and we have not attempted a complicated \( SU(3) \) chiral extrapolation. We get

\[ \epsilon_{\gamma}(\overline{MS}, 2GeV) = 0.79(18)(20) \rightarrow [M_{K+}^2 - M_{K^0}^2]^{QCD}(\overline{MS}, 2GeV) = -6.16(23)(25) \times 10^3 \text{ MeV}^2 \]
summary of the results

\[ M^2_{\pi^+} - M^2_{\pi^0} = 1.44(13)(16) \times 10^3 \text{ MeV}^2 \]

\[ [M^2_{K^+} - M^2_{K^0}]^{QED}(\overline{MS}, 2\text{GeV}) = 2.26(23)(25) \times 10^3 \text{ MeV}^2 \]

\[ [M^2_{K^+} - M^2_{K^0}]^{QCD}(\overline{MS}, 2\text{GeV}) = -6.16(23)(25) \times 10^3 \text{ MeV}^2 \]

\[ \varepsilon_{\gamma}(\overline{MS}, 2\text{GeV}) = 0.79(18)(20) \]

\[ [\hat{m}_d - \hat{m}_u](\overline{MS}, 2\text{GeV}) = 2.39(8)(18) \text{ MeV} \]

\[ \frac{\hat{m}_u}{\hat{m}_d}(\overline{MS}, 2\text{GeV}) = 0.66(2)(8) \]

\[ \hat{m}_u(\overline{MS}, 2\text{GeV}) = 2.4(2)(3) \text{ MeV} \]

\[ \hat{m}_d(\overline{MS}, 2\text{GeV}) = 4.8(2)(3) \text{ MeV} \]

\[ \left[ \frac{F_{K^+}/F_{\pi^+}}{F_{K}/F_{\pi}} - 1 \right]^{QCD}(\overline{MS}, 2\text{GeV}) = -0.0040(3)(3) \]

\[ [M_n - M_p]^{QCD}(\overline{MS}, 2\text{GeV}) = 2.9(6)(3) \text{ MeV} \]
we have a method to calculate both QED and QCD leading isospin breaking effects on the lattice, and in general to handle with QED+QCD lattice simulations

we have shown that the ultraviolet divergences associated with a double insertion of the quarks electromagnetic currents can be removed, also with Wilson quarks, by a redefinition of the parameters of the full theory with respect to the corresponding isosymmetric quantities

we have provided a theoretically well defined prescription in order to separate QED from QCD isospin breaking corrections to hadron masses

first results are encouraging, though...

our results are affected by systematic errors: particularly important are the ones associated with chiral extrapolations and finite volume effects

finite volume effects may be large! this is not because of our method, this is physics: QED is a long-range interaction!

more work required for electromagnetic corrections to decay rates...