Leading isospin breaking effects on the lattice





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ISOSPIN BREAKING EFFECTS Isospin symmetry is an almost exact property down up +2/3 -1/3 of the strong interactions **Isospin breaking effects are induced by:** $m_u \neq m_d$: $O[(m_d - m_u)/\Lambda_{QCD}] \approx 1/100$ "<u>Strong</u>" $Q_u \neq Q_d$: $O(\alpha_{em}) \approx 1/100$ "Electromagnetic"

Since electromagnetic interactions renormalize quark masses the two corrections are intrinsically related

Though small, IB effects can play a very important role



Theoretical motivations



But the knowledge of m_u and m_d separately is important

- Accurate knowledge of quark masses is important for our understanding of flavor physics at the fundamental level

 $m_u \simeq 2.5 \text{ MeV}$ $m_d \simeq 5 \text{ MeV}$

 $m_t \simeq 175 \text{ GeV}$ $m_b \simeq 4.3 \text{ GeV}$

 $m_c \simeq 1.2 \text{ GeV}$ $m_s \simeq 100 \text{ MeV}$

A remarkable relation:

$$\left(\left(\frac{\mathbf{m}_{d}}{\mathbf{m}_{s}}\right)^{1/2} \simeq \left(\frac{\mathbf{m}_{u}}{\mathbf{m}_{c}}\right)^{1/4} \simeq \mathbf{V}_{us} \simeq 0.22$$

- The actual values of the mass difference $m_d - m_u$ and quark charges Q_d , Q_u implies $M_n > M_p$ and guarantees



the stability of matter

IB effects cannot be neglected at present in flavor physics phenomenology



 $f_{\rm K}/f_{\rm m} = 1.193(3)$



 $f_{+}(0) = 0.9704(33)$





EXPERIMENTS	K	net Kaon WG	ν _{us} κ π
	$\left \frac{V_{us} f_K}{V_{ud} f_\pi} \right = 0.2758$	8(5) 0.2% V	$f_{us} f_+(0) = 0.2163(5)$







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The (m_d-m_u) expansion

- Identify the isospin breaking term in the QCD action

- Expand the functional integral in powers of Δm

d

$$\left\langle O\right\rangle = \frac{\int D\phi \ O e^{-S_{0} + \Delta m \hat{S}}}{\int D\phi \ e^{-S_{0} + \Delta m \hat{S}}} \stackrel{\text{1st}}{\simeq} \frac{\int D\phi \ O e^{-S_{0}} \left(1 + \Delta m \hat{S}\right)}{\int D\phi \ e^{-S_{0}} \left(1 + \Delta m \hat{S}\right)} \approx \frac{\left\langle O\right\rangle_{0} + \Delta m \left\langle O \hat{S}\right\rangle_{0}}{1 + \Delta m \left\langle S\right\rangle_{0}}$$

Corrections to quark propagators at leading order in Δm :

 $= \longrightarrow + \Delta m \longrightarrow + \cdots$

 \longrightarrow $-\Delta m \longrightarrow + \cdots$

The expansion for the quark propagator



In the electro-quenched approximation:

$$\Delta \longrightarrow \pm = (e_f e)^2 \left[\underbrace{\swarrow}_{f} + \underbrace{\swarrow}_{f} \right] - [m_f - m_f^0] \longrightarrow \mp [m_f^{cr} - m_0^{cr}] \longrightarrow 11$$



The charged-neutral pion mass splitting

The charged and neutral pion masses



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The charged-neutral pion mass splitting

We obtain:

$$M_{\pi^+} - M_{\pi^0} = 4.21(23)_{stat}(13)_{syst}$$
 MeV
= 4.21(26) MeV

where the errors are statistical and systematic (estimated from chiral and continuum extrapolations and FSE).

The result is in good agreement with the experimental determination

$$\left[M_{\pi^{+}} - M_{\pi^{0}}\right]^{\exp} = 4.5936(5) \text{ MeV}$$

It suggests, a posteriori, that the effect of having neglected the disconnected contribution of $O(a_{em}m_{ud})$ is small





The charged-neutral kaon mass splitting and (m_d-m_u)

The charged and neutral kaon masses



Kaon mass splitting: results

$$\begin{bmatrix} M_{K^{+}} - M_{K^{0}} \end{bmatrix}^{QED} = 2.07(15) \text{ MeV}$$
$$\begin{bmatrix} M_{K^{+}} - M_{K^{0}} \end{bmatrix}^{exp} = -3.934(20) \text{ MeV}$$
$$\begin{bmatrix} M_{K^{+}} - M_{K^{0}} \end{bmatrix}^{QCD} = -6.00(15) \text{ MeV}$$





$$\hat{S} = \sum_{x} \left(\overline{u}u - \overline{d}d \right)$$



The up and down quark masses and related...



The charged-neutral

D meson mass splitting







Quantum Chromodynamics (QCD)



LQCD

- non-perturbative approach based only on first principles
- free parameters of the fundamental theory [10 = 6 (quark masses) + 4 (CKM)]



Numerical simulations in LQCD

$$\langle O \rangle = \frac{1}{Z} \int D\varphi \ O(\varphi) \ e^{-S(\varphi)}$$
$$\downarrow$$
$$Monte Carlo methods$$
$$\downarrow$$
$$\downarrow$$
$$\langle O \rangle \simeq \frac{1}{N_c} \sum_{i=1}^{N_c} O(\varphi_i)$$

Path-Integral formalism in Euclidean space-time

Importance Sampling

 $P(\varphi) = \frac{e^{-S(\varphi)}}{Z}$

Metropolis and *Molecular Dynamics* algorithms



Hadron masses and matrix elements

$$G(t) = \sum_{\mathbf{x}} \langle A_0(\mathbf{x},t) A^{\dagger}_0(\mathbf{0},0) \rangle =$$

The operator $A_0 = \bar{u}\gamma_0\gamma_5 d$ can excite 1- π , 3- π etc. states

$$= \sum_{\mathbf{x}} \sum_{n} \frac{\langle 0 | e^{iPx} A_{0}(0) e^{-iPx} | n \rangle \langle n | A^{\dagger}_{0}(0) | 0 \rangle}{2E_{n}}$$

$$= \sum_{n} \frac{|\langle 0 | A_{0} | n \rangle|^{2}}{2m_{n}} \exp[-m_{n}t] \xrightarrow{A^{\dagger}_{0}(0)} A^{\dagger}_{0}(0) \xrightarrow{A_{0}(\mathbf{x},t)}$$

$$t \rightarrow \infty |\langle 0 | A_{0} | \pi \rangle|^{2} \qquad \text{for all } f_{\pi}^{2} m_{\pi} = f_{\pi} = f_{\pi}^{2} m_{\pi}$$

$$\xrightarrow{\rightarrow} \frac{|\langle \mathbf{v} | \mathbf{A}_0 | \mathbf{n} / |}{2 m_{\pi}} \exp[-m_{\pi} t] = \frac{\mathbf{I}_{\pi} \cdot \mathbf{I} \mathbf{I}_{\pi}}{2} \exp[-m_{\pi} t]$$

$$G(t) = \sum_{\mathbf{x}} \langle A_0(\mathbf{x}, t) A^{\dagger}_0(\mathbf{0}, 0) \rangle \rightarrow$$

$$\rightarrow \frac{|\langle 0 | A_0 | \pi \rangle|^2}{2 m_{\pi}} \exp[-m_{\pi} t] = \frac{f_{\pi}^2 m_{\pi}}{2} \exp[-m_{\pi} t]$$



3-point functions



 $\begin{aligned} \mathbf{K}^{\dagger}(\mathbf{t}_1) &= \sum_{\mathbf{x}} \mathbf{K}^{\dagger}(\mathbf{x}, \mathbf{t}_1) \exp[-\mathbf{i}\mathbf{p}_{\mathbf{K}}\mathbf{x}] \\ \Pi(\mathbf{t}_2) &= \sum_{\mathbf{x}} \Pi(\mathbf{x}, \mathbf{t}_2) \exp[+\mathbf{i}\mathbf{p}_{\pi}\mathbf{x}] \end{aligned}$

$$\langle \Pi(\mathbf{t_2}) \, \mathbf{J}_{\mu}^{\mathbf{weak}}(0) \, \mathbf{K}^{\dagger}(\mathbf{t_1}) \, \rangle \longrightarrow$$

 $\frac{\langle 0|\Pi|\pi\rangle\langle K| K^{\dagger}|0\rangle \exp[-E_{K}t_{1}-E_{\pi}t_{2}]}{(2E_{K})(2E_{\pi})} \times \langle \pi(\mathbf{p}_{\pi}) | J_{\mu}^{\text{weak}}(0) | K(\mathbf{p}_{K}) \rangle$

Also e.m. form factors, structure functions, etc



IB effects due to the m_d-m_u mass difference Very precise on the lattice because of the statistical correlation

Disconnected Wick contractions generated by the insertion of $\hat{S} = \Sigma_x(\bar{u}u-\bar{d}d)$ vanish due to isospin

 $\langle O \rangle \simeq \langle O \rangle_0 + \Delta m \langle O \hat{S} \rangle_0$

 $(\mathbf{x})_{u} - (\mathbf{x})_{d} = 0$

 $\frac{\langle O \rangle - \langle O \rangle_0}{\langle O \rangle} = \Delta m$

symmetry:

An example: the charged and neutral pions

Because of the u \leftrightarrow d symmetry, the corrections cancel at 1st order





This is certainly not the case at 2nd order:

$$C_{\pi^0\pi^0}(t) - C_{\pi^+\pi^-}(t) = -2\left[\textcircled{\otimes} - \textcircled{\otimes} \textcircled{\otimes}\right] + \mathcal{O}(\Delta m_{ud})^3$$

The charged and neutral kaons





Electromagnetic

corrections

LATTICE QED

- Non-compact QED: the dynamical variable is the gauge potential $A_{\mu}(x)$ in a fixed (covariant) gauge
- The covariant derivatives are defined by introducing the QED links:

$$A_{\mu}(\mathbf{X}) \rightarrow E_{\mu}(\mathbf{X}) = e^{-i\boldsymbol{a}\boldsymbol{e}\boldsymbol{A}_{\mu}(\mathbf{X})}$$

$$aD_{\mu}^{+}q_{f}(\mathbf{x}) = \left[E_{\mu}(\mathbf{x})\right]^{e_{f}}q_{f}(\mathbf{x}+a\hat{\mu}) - q_{f}(\mathbf{x})$$

- Gauge transformations for the quarks and photon fields are:

$$q_{f}(\mathbf{x}) \rightarrow e^{i \boldsymbol{\varepsilon}_{f} \lambda(\mathbf{x})} q_{f}(\mathbf{x})$$
$$\overline{q}_{f}(\mathbf{x}) \rightarrow e^{-i \boldsymbol{\varepsilon}_{f} \lambda(\mathbf{x})} \overline{q}_{f}(\mathbf{x})$$

$$A_{\mu}(\mathbf{x}) \rightarrow A_{\mu}(\mathbf{x}) + \nabla_{\mu}^{+}\lambda(\mathbf{x}) =$$
$$= A_{\mu}(\mathbf{x}) + (\lambda(\mathbf{x} + a\hat{\mu}) - \lambda(\mathbf{x}))/a$$

- The QED link then transforms as: $E_{\mu}(x) \rightarrow e^{-iae[A_{\mu}(x)+\nabla_{\mu}\lambda(x)]} = e^{i\theta\lambda(x)}E_{\mu}(x)e^{-i\theta\lambda(x+a\hat{\mu})}$ and $D_{\mu}^{+}q_{f}(x) = (\partial_{\mu} - iee_{f}A_{\mu}(x))q_{f}(x) + O(a)$ is manifestly covariant.

LATTICE QED

- For non-compact QED the pure gauge action is:

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

$$= -\frac{1}{4} \sum_{\mathbf{x};\mu\nu} \left[A_{\nu}(\mathbf{x}) \nabla_{\mu}^{-} \left(\nabla_{\mu}^{+} A_{\nu}(\mathbf{x}) - \nabla_{\nu}^{+} A_{\mu}(\mathbf{x}) \right) - A_{\mu}(\mathbf{x}) \nabla_{\nu}^{-} \left(\nabla_{\mu}^{+} A_{\nu}(\mathbf{x}) - \nabla_{\nu}^{+} A_{\mu}(\mathbf{x}) \right) \right]$$

- By using a covariant gauge fixing one gets:

- Imposing periodic b.c. and looking at the action in momentum space reveals a problem with the zero momentum mode:

$$S_{QED} = \frac{1}{2} \sum_{k;\mu\nu} \tilde{A}_{\nu}^{*}(k) \left(2\sin(k_{\mu}/2)\right)^{2} \tilde{A}_{\nu}(k)$$

The photon propagator is infrared divergent

LATTICE QED

 The infrared problem is not specific of the lattice regularization but it is general for QED in a finite volume with periodic b.c. Already at the classical level, the Gauss' law for a charged particle is inconsistent for the zero mode:

$$\nabla_{\mu}^{-} F_{\mu\nu}(\mathbf{X}) = j_{\nu}(\mathbf{X}) \longrightarrow \nabla_{i}^{-} E_{i}(\mathbf{X}) = \rho(\mathbf{X}) \longrightarrow$$

•
$$\mathbf{0} = \sum_{\mathbf{x}} \nabla_i^- E_i(\mathbf{x}) = \mathbf{e} \sum_{\mathbf{x}} \delta^3(t, \mathbf{x}) = \mathbf{e}$$

- A solution to the infrared problem consists in removing the zero mode:

$$D_{\mu\nu}^{\perp}(\mathbf{x}-\mathbf{y}) = \sum_{k\neq 0} \frac{\delta_{\mu\nu}}{\left[2\sin(k_{\rho}/2)\right]^{2}}$$

- We subtracted the zero mode in x-space and applied a stochastic technique

$$\boldsymbol{P}^{\perp}\phi(\boldsymbol{x}) \equiv \phi(\boldsymbol{x}) - \frac{1}{V} \sum_{\boldsymbol{y}} \phi(\boldsymbol{y})$$

$$\begin{bmatrix} -\nabla_{\rho}^{-}\nabla_{\rho}^{+} \end{bmatrix} \phi_{\mu}(\mathbf{X}) = \mathbf{P}^{\perp} \eta_{\mu}(\mathbf{X}) \checkmark \mathbf{P}^{\perp}$$
noise
$$\phi_{\mu}(\mathbf{X}) = \begin{bmatrix} \frac{\delta_{\mu\nu}}{-\nabla_{\rho}^{-}\nabla_{\rho}^{+}} \mathbf{P}^{\perp} \end{bmatrix} \eta_{\nu}(\mathbf{X}) = \sum_{\mathbf{y}} \mathbf{D}_{\mu\nu}^{\perp}(\mathbf{X} - \mathbf{y}) \eta_{\nu}(\mathbf{y})$$

The leading isospin breaking expansion

 The QCD + QED action is written in terms of the full covariant derivative:

$$D_{\mu}^{+}q_{f}(x) = \left[E_{\mu}(x)\right]^{e_{f}}U_{\mu}(x)q_{f}(x+\hat{\mu}) - q_{f}(x)$$
QED \checkmark QCD

- Since $E_{\mu}(x) = e^{-ieA_{\mu}(x)} = 1 - ieA_{\mu}(x) - 1/2 e^2 A_{\mu}^2(x) + ...$ the expansion of the lattice action up to $O(e^2)$ contains 2 contributions:

$$S_{f} = \sum_{x} \overline{q}_{f}(x) D_{f}[U, A] q_{f}(x) =$$

$$= S_{f}(e=0) + \sum_{x,\mu} \left[e_{f}eA_{\mu}(x) V_{\mu}^{f}(x) + \frac{(e_{f}e)^{2}}{2} A_{\mu}(x) A_{\mu}(x) T_{\mu}^{f}(x) + \dots \right]$$
Both contributions are required for gauge invariance
$$(e_{f}e)^{2} \xrightarrow{\swarrow} (e_{f}e)^{2} \xrightarrow{\swarrow} (e_{f}e)^{2} \xrightarrow{\swarrow} (e_{f}e)^{2} \xrightarrow{\checkmark} (e_{f}e$$

The leading isospin breaking expansion

- Switching on the e.m. interactions requires the introduction of new counterterms which renormalize the couplings of the theory:

$$\vec{g}^0 = \left(0, g^0_s, m^0_u, m^0_d, m^0_s, \ldots\right) \rightarrow \vec{g} = \left(\vec{e}^2, g_s, m_u, m_d, m_s, \ldots\right)$$

- For any observable, the leading isospin breaking expansion reads,

$$O(\vec{g}) = O(\vec{g}^0) + \left[e^2 \frac{\partial}{\partial e^2} + \left(g_s^2 - (g_s^0)^2 \right) \frac{\partial}{\partial g_s^2} + \left(m_f - m_f^0 \right) \frac{\partial}{\partial m_f} + \dots \right] O(\vec{g}) \Big|_{\vec{g} = \vec{g}^0}$$

or, in terms of renormalized couplings,

$$O(\vec{\hat{g}}) = O(\vec{\hat{g}}^0) + \left[\hat{e}^2 \frac{\partial}{\partial \hat{e}^2} + \left(\hat{g}_s^2 - \left(\frac{Z_{g_s}}{Z_{g_s}^0} g_s^0\right)^2\right) \frac{\partial}{\partial \hat{g}_s^2} + \left(m_f - \frac{Z_{m_f}}{Z_{m_f}^0} m_f^0\right) \frac{\partial}{\partial \hat{m}_f} + \dots \right] O(\vec{g})\Big|_{\vec{g} = \vec{g}^0}$$

ETMC gauge ensembles Nf=2+1+1



ensemble	β	V/a^4	$M_{\pi}(\text{MeV})$	$M_K({ m MeV})$	$M_D({ m MeV})$
A30.32	1.90	$32^3 \times 64$	275 (10)	568 (22)	2012 (77)
A40.32			316 (12)	578 (22)	2008 (77)
A50.32			350 (13)	586(22)	2014 (77)
A40.24		$24^3 \times 48$	322 (13)	582 (23)	2017 (77)
A60.24			386 (15)	599(23)	2018 (77)
A80.24			442 (17)	618 (24)	2032 (78)
A100.24			495 (19)	639 (24)	2044 (78)
A40.20		$20^3 \times 48$	330 (13)	586 (23)	2029 (79)
B25.32	1.95	$32^3 \times 64$	259 (9)	546 (19)	1942 (67)
B35.32			302 (10)	555 (19)	1945 (67)
B55.32			375 (13)	578 (20)	1957 (68)
B75.32			436 (15)	599 (21)	1970 (68)
B85.24		$24^3 \times 48$	468 (16)	613 (21)	1972 (68)
D15.48	2.10	$48^3 \times 96$	223 (6)	529 (14)	1929 (49)
D20.48			255 (7)	535 (14)	1933 (50)
D30.48			318 (8)	550 (14)	1937 (49)

Finite size effects (FSE)

In pure QCD, the existence of a mass gap renders FSE exponentially small ~ $e^{-M_{\pi}\cdot L}$ (in most of the cases)

The QED photon is massless, the e.m. interactions are long ranged and FSE are only power suppressed.

With our regularization of the zero mode, FSE are expressed by:

$$M_{PS}^2(T,L) \sim_{T,L\to+\infty} M_{PS}^2 \left\{ 1 - q^2 \alpha_{em} \left[\frac{\kappa}{M_{PS}L} \left(1 + \frac{2}{M_{PS}L} \right) \right] \right\}$$

$$\kappa = 2.837297(1)$$

QED_L (i.e.
$$A_{\mu}(k_0, \vec{k} = \vec{0}) \equiv 0$$
 for all k_0)

Sz. Borsanyi *et al.* arXiv:1406.4088 [hep-ph]

The charged and neutral pion masses





Comparison with other approaches/results

- Other lattice studies of QCD + QED have been /are being performed.
- They are based on the "standard" approach: QED is introduced directly in the Monte Carlo simulation, like QCD.
- <u>Advantages</u> of our approach:
- \bullet The small parameters Δm and e are factorized in the expansion
- No need to generate new gauge configurations
- IB is introduced only where needed (no large overall FSE due to e.m.)
- Specific diagrammatic contributions can be easily isolated.
- E.g. separation between strong and e.m. IB effects
- <u>Disadvantages</u>:
- More vertices and correlations functions to be computed