Strong isospin breaking: comparing $N_f = 1{+}1{+}1$ simulations and the RM123 method

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in collaboration with

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Motivation

- HVP contribution to $g-2$ has reached subpercent precision
- Strong and electromagnetic isospin breaking effects contribute great part of the HVP computation
  - Developing strategies to compute isospin breaking effects becomes increasingly important
- Currently two ways to include IB effects:
  - Exact methods: explicit QCD+QED simulations
  - Perturbative methods: RM123 method
- RC⋆ collaboration showed that simulating QCD+QED leads to a signficant error reduction with respect to the RM123 method [RC⋆, JHEP 10 (2025) 158]

My work: compare $N_f = 1{+}1{+}1$ simulation with $N_f = 2{+}1$ plus RM123 method

- Which way to introduce **strong** isospin breaking effects is more efficient?

RM123 method

- Trick to compute derivatives with respect to action parameters [RM123 collaboration, JHEP 04 (2012) 124]

Original simulation: $N_f = 2{+}1$ (isoQCD)

$$\langle O\rangle_0 = \frac{\int \mathcal{D}U\mathcal{D}\psi\mathcal{D}\bar\psi\; O\; e^{-S_0}}{\int \mathcal{D}U\mathcal{D}\psi\mathcal{D}\bar\psi\; e^{-S_0}}.$$

$$S_0 = S_G + \sum_{f=u,d,s} \bar\psi_f D\psi_f + m_l \sum_x [\bar u u + \bar d d](x) + m_s \sum_x \bar s s(x)$$

$$m_l = \frac{1}{2}(m_u + m_d)$$

Target simulation: $N_f = 1{+}1{+}1$ (SIB)

$$\langle O\rangle_{\Delta m} = \frac{\int \mathcal{D}U\mathcal{D}\psi\mathcal{D}\bar\psi\; O\; e^{-S_0 - S_{\mathrm{IB}}(\Delta m)}}{\int \mathcal{D}U\mathcal{D}\psi\mathcal{D}\bar\psi\; e^{-S_0 - S_{\mathrm{IB}}(\Delta m)}}$$

$$S_{\mathrm{IB}}(\Delta m) = -\Delta m \sum_x [\bar u u - \bar d d](x)$$

$$\Delta m = \frac{1}{2}(m_d - m_u)$$

- Alternative: Taylor expand observable and approximate by truncating at first order

$$\langle O\rangle_{\Delta m} = \langle O\rangle_0 + \left.\frac{\partial\langle O\rangle_{\Delta m}}{\partial\Delta m}\right|_{\Delta m=0} \Delta m + \mathcal{O}(\Delta m^2)$$

- Obtain derivative by Taylor expanding path integral

$$\langle O\rangle_{\Delta m} = \frac{\int \mathcal{D}U\mathcal{D}\psi\mathcal{D}\bar\psi\; O(1+\Delta m S_{\mathrm{IB}})e^{-S_0}}{\int \mathcal{D}U\mathcal{D}\psi\mathcal{D}\bar\psi\; (1+\Delta m S_{\mathrm{IB}})e^{-S_0}} + \mathcal{O}(\Delta m^2) = \langle O\rangle_0 + \Delta m\langle O S_{\mathrm{IB}}\rangle_0 + \mathcal{O}(\Delta m^2)$$

- $\frac{\partial\langle O\rangle}{\partial\Delta m} = \langle O S_{\mathrm{IB}}\rangle_0$ can be obtained from $\Delta m = 0$ simulation, but normally has bigger variance
  - ↳ Are $N_f{=}1{+}1{+}1$ simulations more efficient or detect higher orders in Δm?

CLS ensembles

- Lattice QCD ensembles from the CLS initiative [M. Bruno et al. (2014)]
  - $N_f = 2{+}1$ flavors with $O(a)$ improved Wilson fermions and tree-level improved Lüscher-Weisz gauge action [Sheikholeslami and Wohlert (1985), Bulava and Schaefer (2013)] [Lüscher and Weisz (1985)]

- Comparison done with CLS ensemble N451

ID	β	V	a	M_π	$M_{K^\pm}$	M_{K^0}	$M_\pi L$	N_{cfg}
N451 ($N_f = 2+1$)	3.46	$48^3 \times 128$	0.07634 fm	286 MeV	468 MeV	468 MeV	4.0	1011
Y450 ($N_f = 1+1+1$)	3.46	$48^3 \times 128$	0.07634 fm	286 MeV	461 MeV	474 MeV	4.0	450

- We generated a new ensemble Y450 based in N451 but with up-down mass difference Δm

$$m_u = m_l - \Delta m \qquad \Delta m = \frac{1}{2}(m_d - m_u) \qquad \frac{\Delta m_R}{m_{l,R}} \approx 0.18$$
$$m_d = m_l + \Delta m$$

- All three quarks simulated with rational HMC

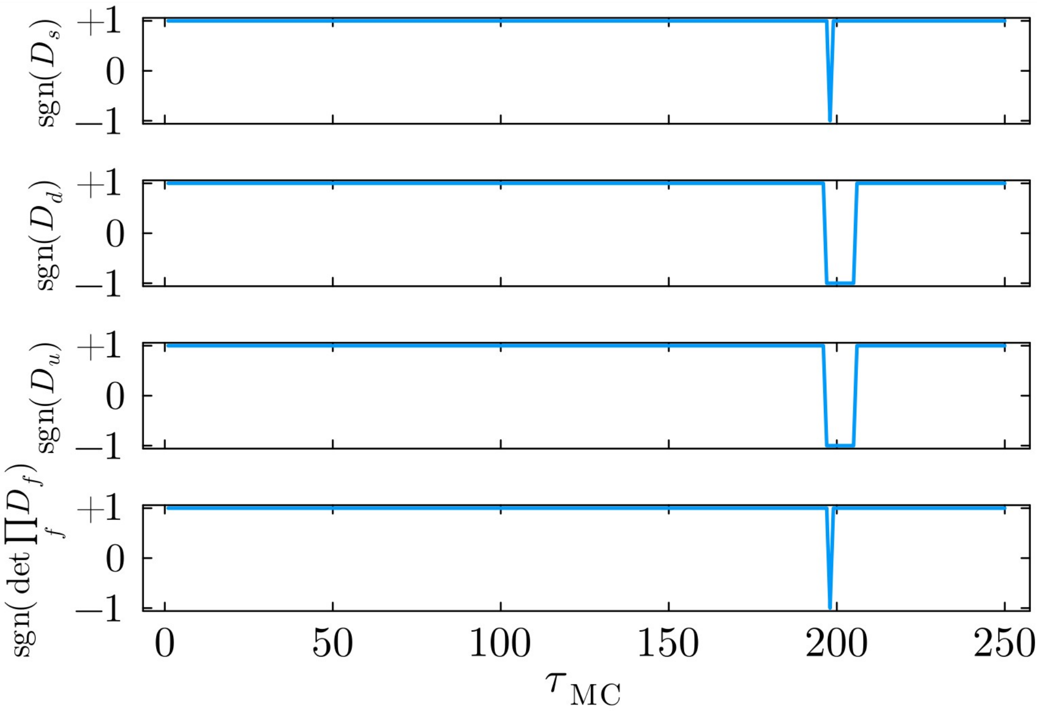
- Y450 takes ~3× more computing time than N451 to generate
  - 28 vs 11 pseudofermion actions

<u>Number of pseudofermion actions</u>

	N451	Y450
	$l : 5$	$u : 11$ $d : 11$
	$s : 6$	$s : 6$
Total	11	28

$N_f = 1+1+1$ simulation: sign of det D

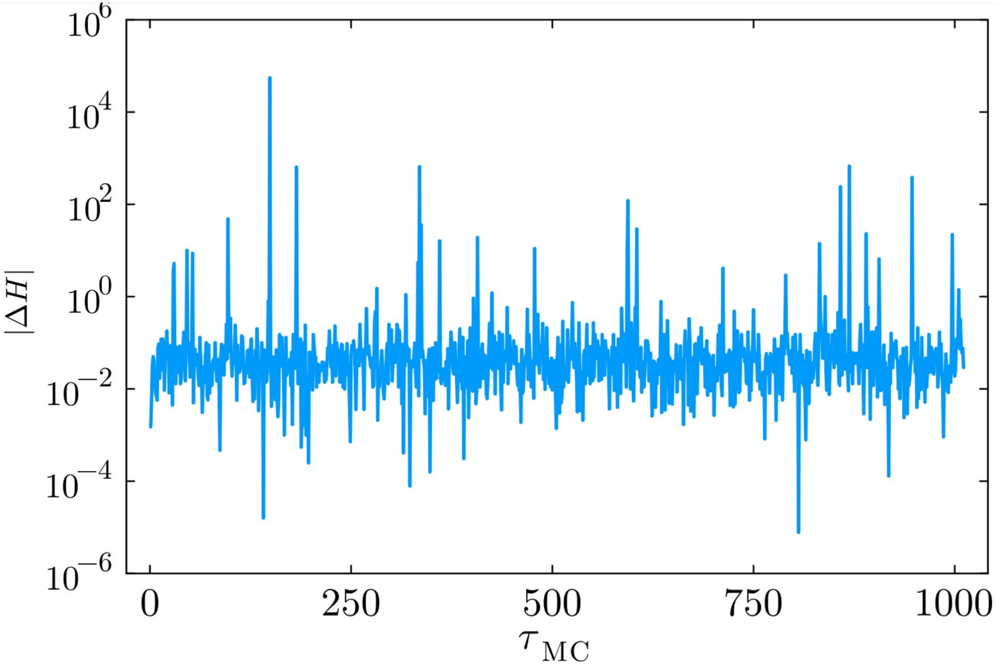
- Sign of the strange quark determinant is not necessarily positive in $N_f = 2+1$ with Wilson fermions
  - More of a potential problem for $N_f = 1+1+1$



- Only one configuration with $\mathrm{sign}(\det \prod_{f=u,d,s} D_f) = -1$
  - Additional reweighting factor -1

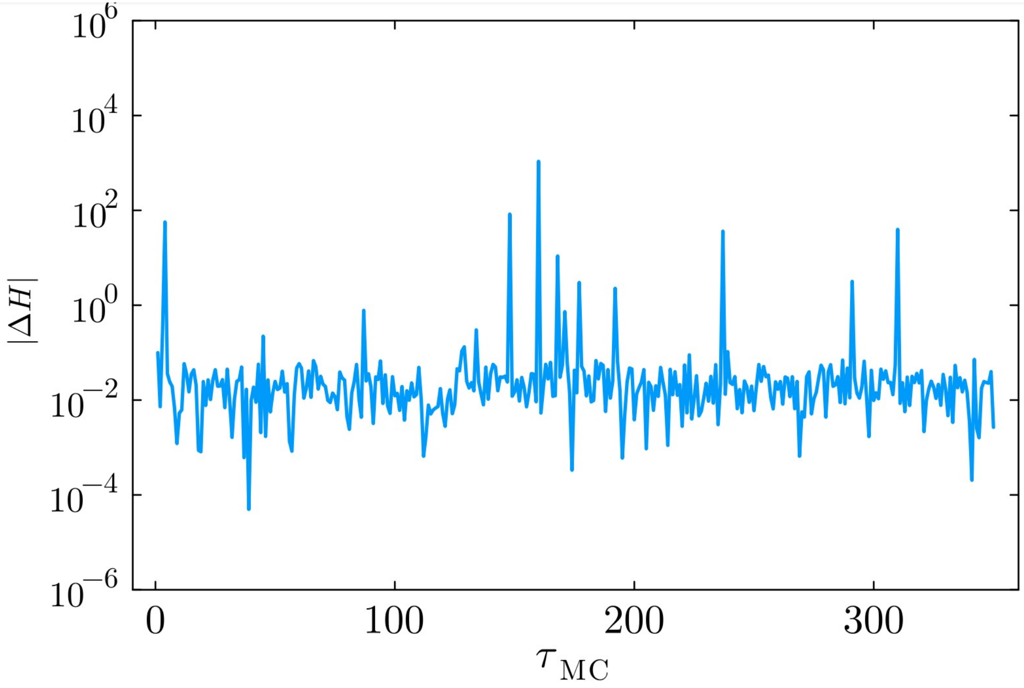
$N_f = 1{+}1{+}1$ simulation: stability

2+1



$p_{\mathrm{acc}} = 0.94$

1+1+1

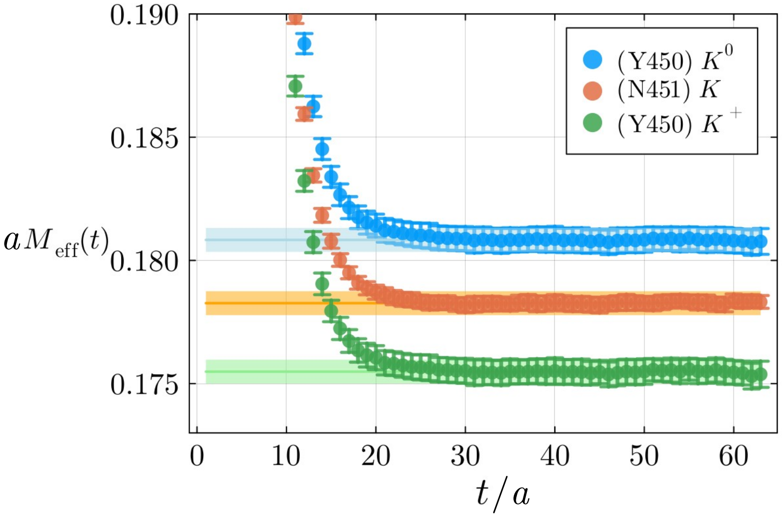


$p_{\mathrm{acc}} = 0.99$

- Tuned number of integration steps to obtain a stable MC chain without exploding forces

$K^+ - K^0$ mass splitting: explicit SIB

How broken is the 1+1+1 ensemble? ⇒ Edinburgh consensus



	QCD	isoQCD
M_{π^+}	135.0 MeV	135.0 MeV
M_{K^+}	491.6 MeV	494.6 MeV
M_{K^0}	497.6 MeV	494.6 MeV
$M_{D_s^+}$	1967 MeV	1967 MeV
$M_{B_s^0}$	5367 MeV	5367 MeV
f_{π^+}	130.5 MeV	130.5 MeV

[FLAG 2024 Tab. 6]

FLAG defines physical IB in QCD when kaon mass splitting is 6 MeV

$$M_{K^0} - M_{K^\pm} = 6 \text{ MeV} \qquad \text{(FLAG2024)}$$

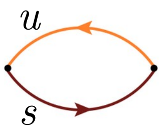
$$M_{K^0} - M_{K^\pm} = 14.026(52) \text{ MeV} \qquad \text{(Y450)}$$

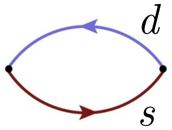
Our 1+1+1 ensemble is $\times 2.3$ more broken

↳ More sensitive to higher order effects in Δm

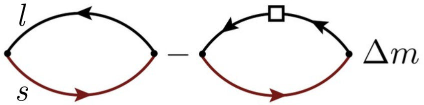
$K^+ - K^0$ mass splitting: explicit SIB

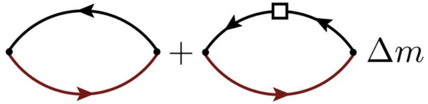
- In 1+1+1 one computes the regular two point function

$C_{K^+K^-} =$ 

$C_{K^0K^0} =$ 

- In 2+1 one needs an insertion of S_{IB}

$C_{K^+K^-} = +$ 

$C_{K^0K^0} = +$ 

Compute kaon mass derivative...

- with the RM123 method in 2+1: $\left.\frac{\partial \Delta M_K}{\partial(2\Delta m)}\right|_{\Delta m=0} = 3.9061(90)$ (1011 configs)
- by finite differences in 1+1+1: $\left.\frac{\partial \Delta M_K}{\partial(2\Delta m)}\right|_{\Delta m=0} \approx \frac{M_{K^0} - M_{K^\pm}}{2\Delta m} = 3.8960(140)$ (450 configs)

⇨ Good agreement at current level of statistics

⇨ No benefit in uncertainty by simulating 1+1+1

HVP contribution to $g-2$

- HVP in the time-momentum representation:

$$a_\mu^{\mathrm{hvp}} = \left(\frac{\alpha}{\pi}\right)^2 \int_0^\infty dt\, \tilde{K}(t;m_\mu)\, G(t) \qquad \delta_{kl} G^{(m,n)}(t) = -\int d^3x\, \langle J_k^m(t,\vec{x}) J_l^n(0)\rangle$$

$$J_\mu^\gamma = \frac{2}{3}\bar{u}\gamma_\mu u - \frac{1}{3}\bar{d}\gamma_\mu d - \frac{1}{3}\bar{s}\gamma_\mu s + \frac{2}{3}\bar{c}\gamma_\mu c + \dots$$

- Convenient to decompose into SU(3) flavor currents

$$J_\mu^m \equiv \bar{\psi} T^m \gamma_\mu \psi, \quad \bar{\psi} = (\bar{u}, \bar{d}, \bar{s}, \bar{c}, \bar{b}) \qquad T^m\text{: Gell–Mann matrices}$$

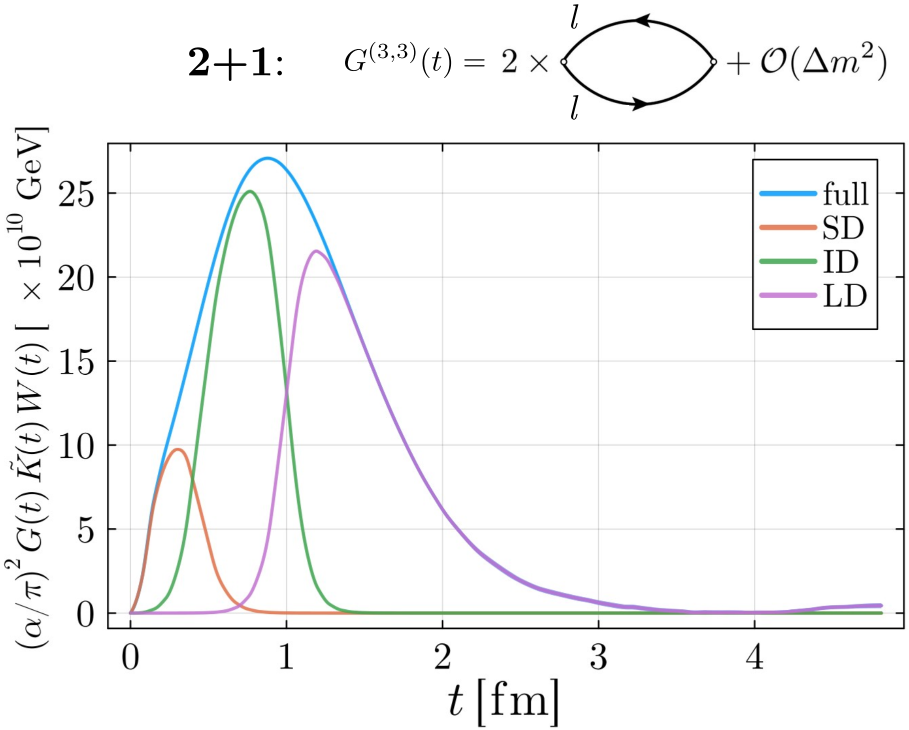
$$\text{isovector:} \quad J_\mu^3 = \frac{1}{2}(\bar{u}\gamma_\mu u - \bar{d}\gamma_\mu d) \qquad \text{isoscalar:} \quad J_\mu^8 = \frac{1}{2\sqrt{3}}(\bar{u}\gamma_\mu u + \bar{d}\gamma_\mu d - 2\bar{s}\gamma_\mu s)$$

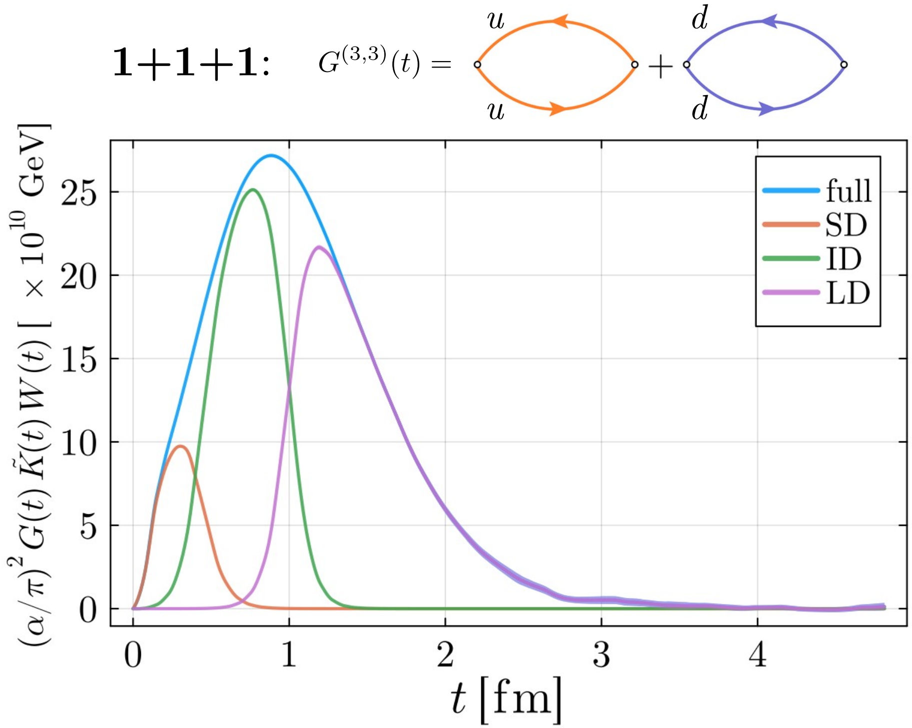
$$G^{(\gamma,\gamma)} = G^{(3,3)} + \frac{1}{3}G^{(8,8)} + \frac{2}{\sqrt{3}}G^{(3,8)} + \dots \qquad a_\mu^{\mathrm{hvp}} = a_\mu^{(3,3)} + \frac{1}{3}a_\mu^{(8,8)} + \frac{2}{\sqrt{3}}a_\mu^{(3,8)} + \cdots$$

- Only strong isospin breaking effects at first order come from $a_\mu^{(3,8)}$

HVP contribution to $g-2$: G^{33}

- Isovector-isovector contribution to HVP: possible test for higher order SIB effects





Ensemble	full	SD	ID	LD	configs
N451 (2+1)	485.8(3.6)	47.707(21)	185.16(21)	252.9(3.5)	1011
Y450 (1+1+1)	480.1(5.5)	47.704(23)	185.51(35)	246.9(5.5)	450

- Agreement between 2+1 and 1+1+1
- Both ensembles have similar error at equivalent statistics

SIB contribution to HVP: G^{38} and R_{38K}

- Strong isospin breaking contribution to HVP at first order comes from $a_\mu^{(3,8)}$ $\qquad a_\mu^{(3,8)}\Big|_{\text{isoQCD}} = 0$

$$a_\mu^{(3,8)} = \frac{\partial a_\mu^{(3,8)}}{\partial e^2} e^2 + \frac{\partial a_\mu^{(3,8)}}{\partial \Delta m} \Delta m + \mathcal{O}(\varepsilon^2) \qquad \varepsilon \equiv (\Delta m, e^2)$$

- Separation between QCD and QCD+QED is scheme-dependent, but one can define a scheme-independent, renormalized quantity R_{38K} [D. Erb et al, JHEP 10 (2025) 157]

See also:

- **D. Erb's talk Wed 11:10**
- **S. Lahrtz's talk Wed 11:30**

$$\Delta M_K^{\text{phys}} = \frac{\partial \Delta M_K}{\partial e^2} e^2 + \frac{\partial \Delta M_K}{\partial \Delta m} \Delta m + \mathcal{O}(\varepsilon^2)$$

$$a_\mu^{(3,8)} = \frac{\partial a_\mu^{(3,8)}}{\partial e^2} e^2 + R_{38K} \cdot \left(\Delta M_K^{\text{phys}} - \frac{\partial \Delta M_K}{\partial e^2} e^2 \right) \qquad R_{38K} \equiv \frac{1}{\frac{\partial \Delta M_K}{\partial \Delta m}} \cdot \frac{\partial a_\mu^{(3,8)}}{\partial \Delta m} = \frac{\partial a_\mu^{(3,8)}}{\partial \Delta M_K}$$

$\Rightarrow$ R_{38K} can be used for comparison across different collaborations

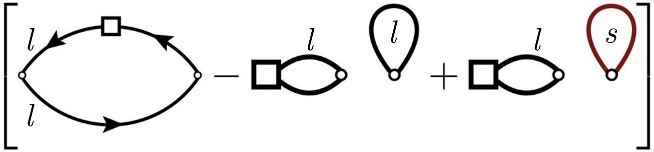
(even with different definitions of isoQCD and renormalization conventions)

SIB contribution to HVP: G^{38} and R_{38K}

- Strong isospin breaking contribution to HVP at first order comes from $a_\mu^{(3,8)}$ $\qquad a_\mu^{(3,8)}\Big|_{\text{isoQCD}} = 0$

  - can compute order Δm with the RM123 method on $N_f = 2{+}1$ ensemble

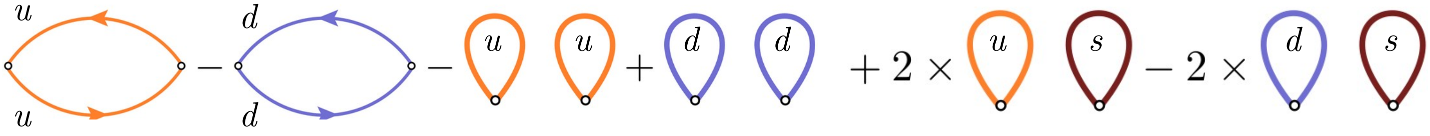
$G^{(3,8)}(t) = 4 \times$



$\Delta m + \mathcal{O}(\Delta m^2)$

  - and to all orders on $N_f = 1{+}1{+}1$ ensemble

$G^{(3,8)}(t) =$



- Disconnected contribution is noisy at long distance

  - Need to do spectral reconstruction

SIB contribution to HVP: G^{38} and R_{38K}

- Spectral decomposition of G^{38}

$$G^{38}(t;\Delta m) = \langle 0|\, J^3_\mu(t) J^8_\mu(0)\,|0\rangle = \sum_n \langle 0|\, J^3_\mu(0)\,|n\rangle \langle n|\, J^8_\mu(0)\,|0\rangle\, e^{-E_n t}$$

- Perfect isospin symmetry at $\Delta m = 0 \to \langle 0|\, J^8_\mu\,|\rho\rangle = 0 = \langle \omega|\, J^3_\mu\,|0\rangle \Rightarrow G^{38}(t;\Delta m = 0) = 0$

- At $\Delta m \neq 0$ there is $\rho - \omega$ mixing

$$G^{38}(t;\Delta m) = A_{3\rho}A_{8\rho}e^{-E_\rho t} + A_{3\omega}A_{8\omega}e^{-E_\omega t} + \ldots$$

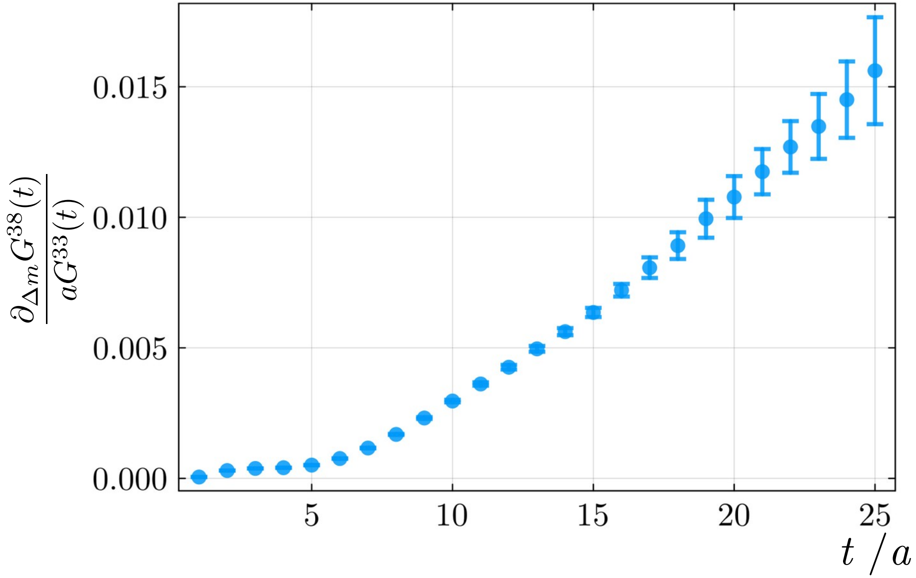
$$\partial_{\Delta m} G^{38}(t;\Delta m)\Big|_{\Delta m = 0} = A_{3\rho}A'_{8\rho}e^{-E_\rho t} + A'_{3\omega}A_{8\omega}e^{-E_\omega t}$$

- One can derive (see backup)

$$\frac{\partial_{\Delta m} G^{38}(t)}{G^{33}(t)} \sim A + Bt$$

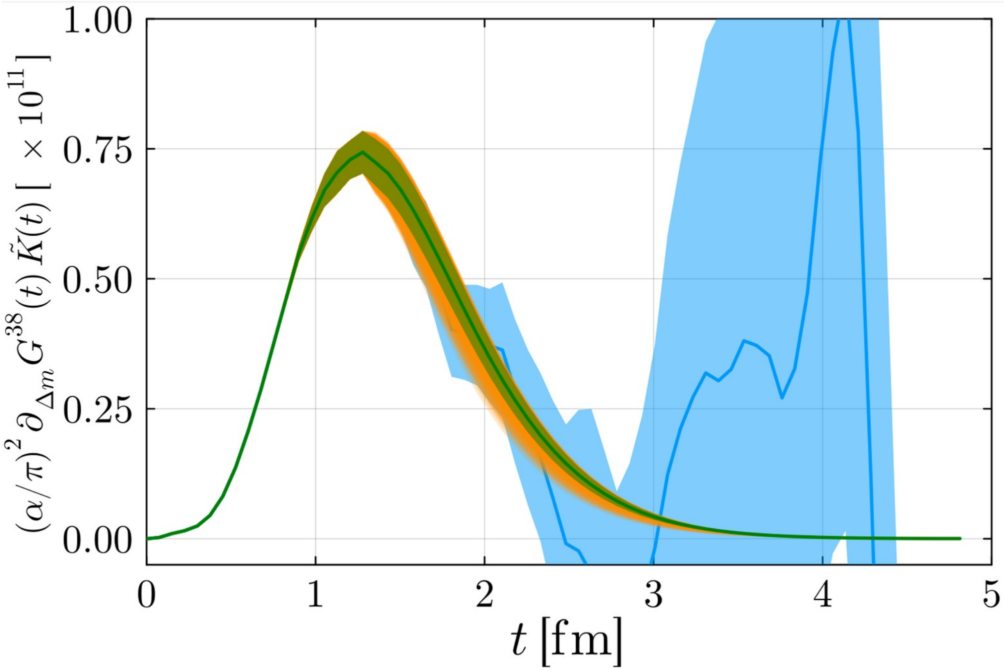
$\Rightarrow$ can fit A and B and reconstruct long distance:

$$\partial_{\Delta m} G^{38}(t) = (A_{\text{fit}} + B_{\text{fit}} t) G^{33}(t)$$



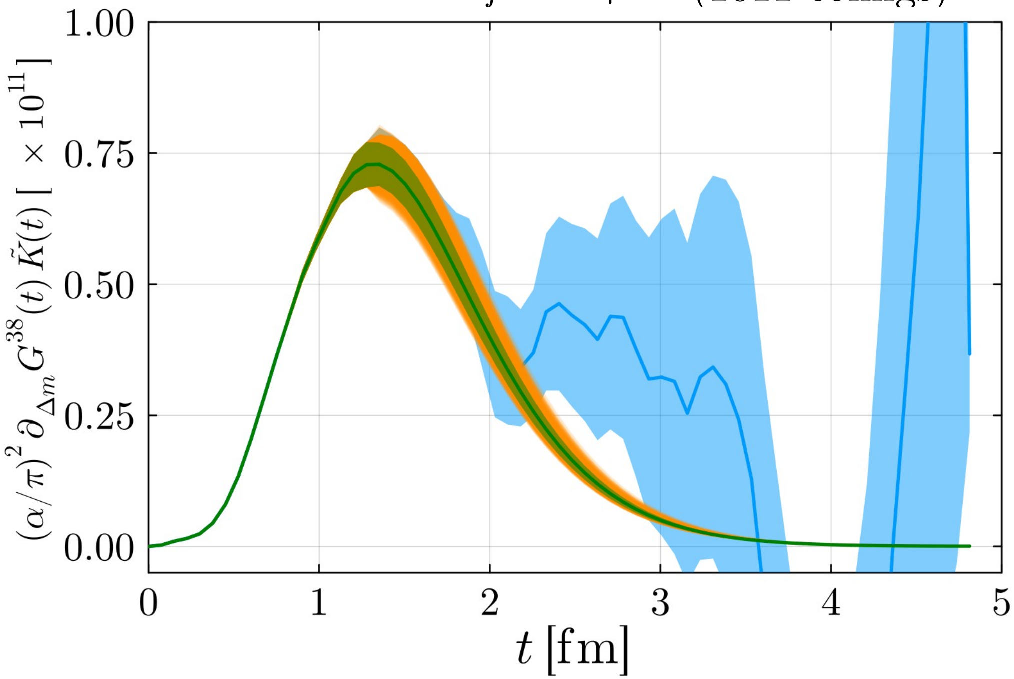
SIB contribution to HVP: G^{38} and R_{38K}

N_f = 1+1+1 (450 configs)



$R_{38K} = -2.45(15)(8)[17] \times 10^{-11}\ \mathrm{MeV}^{-1}$

N_f = 2+1 (1011 configs)



$R_{38K} = -2.51(13)(11)[17] \times 10^{-11}\ \mathrm{MeV}^{-1}$

- Good agreement between RM123 and $N_f = 1+1+1$ at current statistics

Conclusions and outlook

- Compared RM123 method in $N_f = 2{+}1$ with a simulation with $N_f{=}1{+}1{+}1$
- $N_f = 1{+}1{+}1$ takes around 3 times more computing time per configuration
  - ↳ more pseudofermion actions in the non-degenerate light sector
- We studied the kaon mass splitting, and the isovector and isospin-violating contributions to HVP
  - ↳ No sign of higher order SIB effects (even with $\sim\times 2$ more breaking than nature)
  - ↳ No benefit in uncertainty by simulating $N_f{=}1{+}1{+}1$
  - ↳ Standard RM123 method is robust
- Maybe combining strong isospin broken ensembles in a global fit together with other CLS ensembles could yield better derivatives

Thank you!

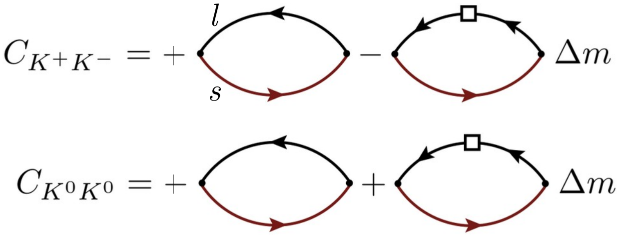
- Related talks by the Mainz group:
  - H. B. Meyer, Tue. 16:50
  - A. Conigli, Wed. 9:00
  - A. Beltran, Wed. 9:20
  - D. Erb, Wed. 11:10
  - S. Lahrtz, Wed. 11:30
  - A. De Santis, Wed. 9:00

Backup

$K^+ - K^0$ mass splitting: explicit SIB

- In 1+1+1 one computes the regular two point function

- In 2+1 one needs an insertion of S_{IB}



Compute kaon mass derivative...

- with the RM123 method in 2+1:

$$\frac{\partial \Delta M_K}{\partial(2\Delta m)}\Big|_{\Delta m=0} = 3.9061(90)$$

- by correlated finite differences in 1+1+1:

$$\frac{\partial \Delta M_K}{\partial(2\Delta m)}\Big|_{\Delta m=0} \approx \frac{M_{K^0} - M_{K^\pm}}{2\Delta m} = 3.8960(140)$$

⇒ Good agreement at current level of statistics

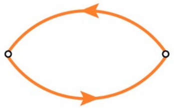
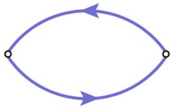
⇒ No benefit in uncertainty by simulating 1+1+1

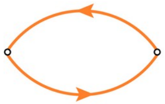
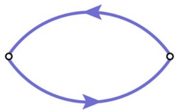
- by (independent) finite differences between 2+1 and 1+1+1:

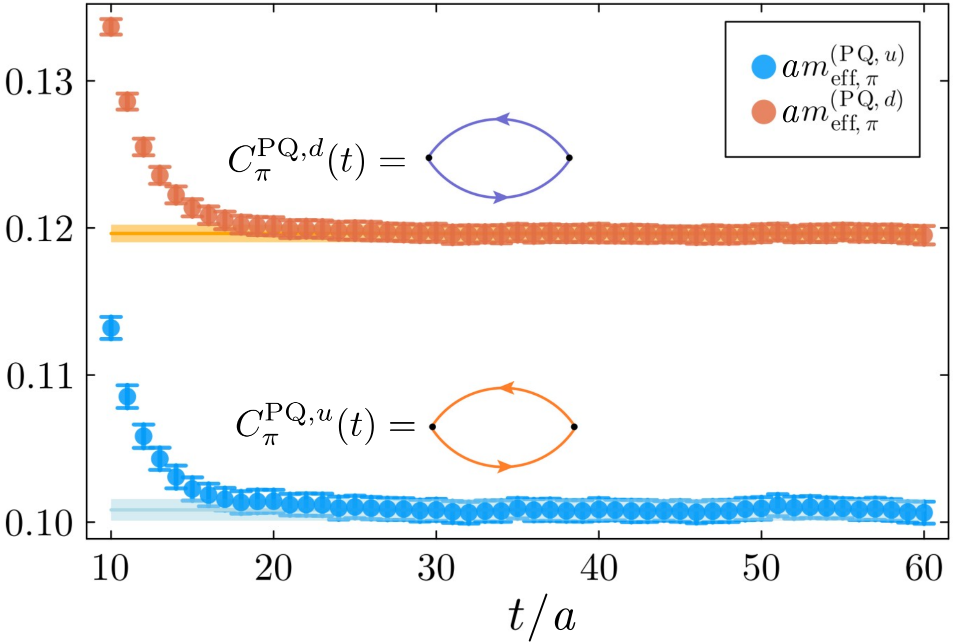
$$\frac{\partial \Delta M_K}{\partial(2\Delta m)}\Big|_{\Delta m=0} \approx \frac{M_{K^0}|_{\Delta m} - M_K|_{\Delta m=0}}{\Delta m} = 3.74(83)$$

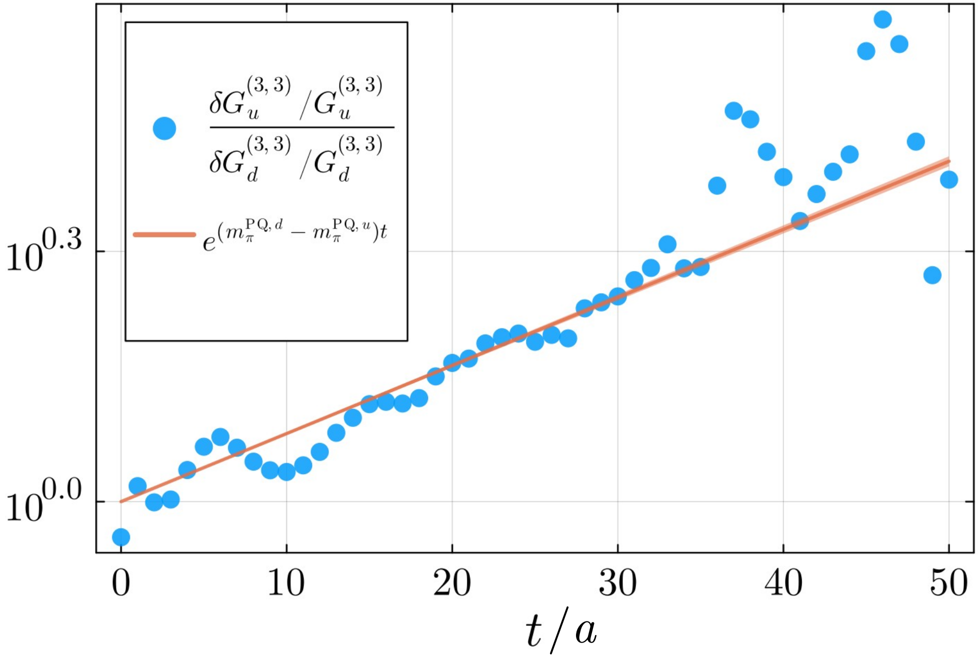
⇒ Exploiting correlations is important

HVP contribution to $g-2$: G^{33}

$G^{(3,3)}(t) =$  $+$ 

StN $\Big[$  $\Big]$ / StN $\Big[$  $\Big]$ $\underset{\sim}{\propto} \dfrac{e^{-(m_\rho - m_\pi^{\mathrm{PQ},u})t}}{e^{-(m_\rho - m_\pi^{\mathrm{PQ},d})t}} = e^{-\Delta m_\pi^{\mathrm{PQ},ud}\, t}$





Window	$a_\mu^{(3,3),u}$	$a_\mu^{(3,3),d}$
Full	491.1(7.7)	469.1(4.1)
SD	47.810(23)	47.590(22)
ID	187.70(39)	183.30(34)
LD	255.6(7.7)	238.2(3.9)

- Error of u contribution is larger than d (LD)
  - can be explained with Parisi-Lepage argument for StN
- A small light quark mass shift can change the error by a factor $\times 2$

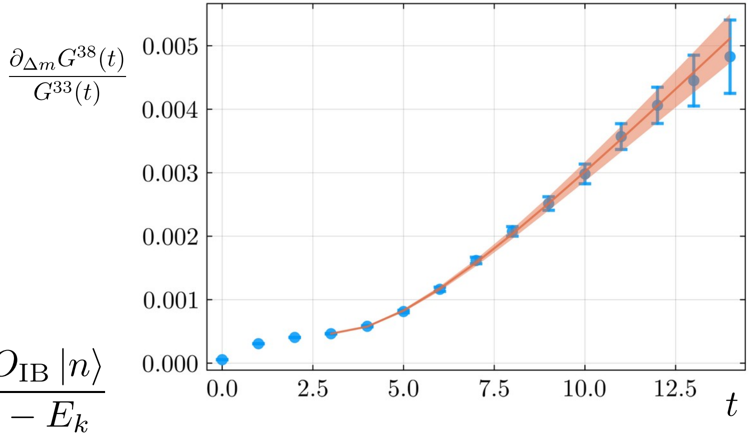
IB contribution to HVP: G^{38} and R_{38K}

$$G^{38}(t;\Delta m) = \langle 0| J^3_\mu(t) J^8_\mu(0) |0\rangle = \sum_n \langle 0| J^3_\mu(0) |n\rangle \langle n| J^8_\mu(0) |0\rangle e^{-E_n t}$$

- Perfect isospin symmetry at $\Delta m = 0 \to \langle 0| J^8_\mu |\rho\rangle = 0 = \langle \omega | J^3_\mu |0\rangle$ $\Rightarrow$ $G^{38}(t;\Delta m = 0) = 0$
- At $\Delta m \neq 0$ there is $\rho - \omega$ mixing

$$G^{38}(t;\Delta m) = A_{3\rho} A_{8\rho} e^{-E_\rho t} + A_{3\omega} A_{8\omega} e^{-E_\omega t} + \dots$$

$$\partial_{\Delta m} G^{38}(t;\Delta m)\Big|_{\Delta m=0} = A_{3\rho} A'_{8\rho} e^{-E_\rho t} + A'_{3\omega} A_{8\omega} e^{-E_\omega t}$$



Consider perturbation of states: $|n\rangle_{\Delta m} = |n\rangle + \Delta m \sum_{k\neq n} |k\rangle \frac{\langle k| O_{\mathrm{IB}} |n\rangle}{E_n - E_k}$

$$\partial_{\Delta m} G^{38}(t;\Delta m)\Big|_{\Delta m=0} = A_{3\rho} A_{8\omega} s_{\omega\rho} \frac{e^{-E_\rho t} - e^{-E_\omega t}}{E_\rho - E_\omega} + a_\rho e^{-E_\rho t} + a_\omega e^{-E_\omega t}$$

$$e^{-E_\omega t} \approx e^{-E_\rho t}(1 - \Delta E t)$$

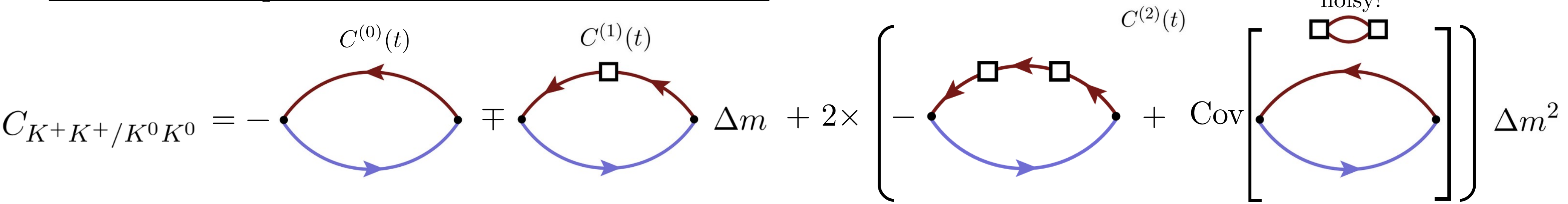
$$\partial_{\Delta m} G^{38}(t;\Delta m)\Big|_{\Delta m=0} = \left[a_\rho + a_\omega + \left(A_{3\rho} A_{8\omega} s_{\rho\omega} - a_\omega \Delta E\right) t\right] e^{-E_\rho t} \equiv (A + Bt)\, e^{-E_\rho t}$$

$$\frac{\partial_{\Delta m} G^{38}(t)}{G^{33}(t)} \sim A + Bt$$

$K^+ - K^0$ mass splitting: RM123 (N451)

Diagrams obtained with github.com/djukanovic/qct

Power series expansion of kaon correlation function

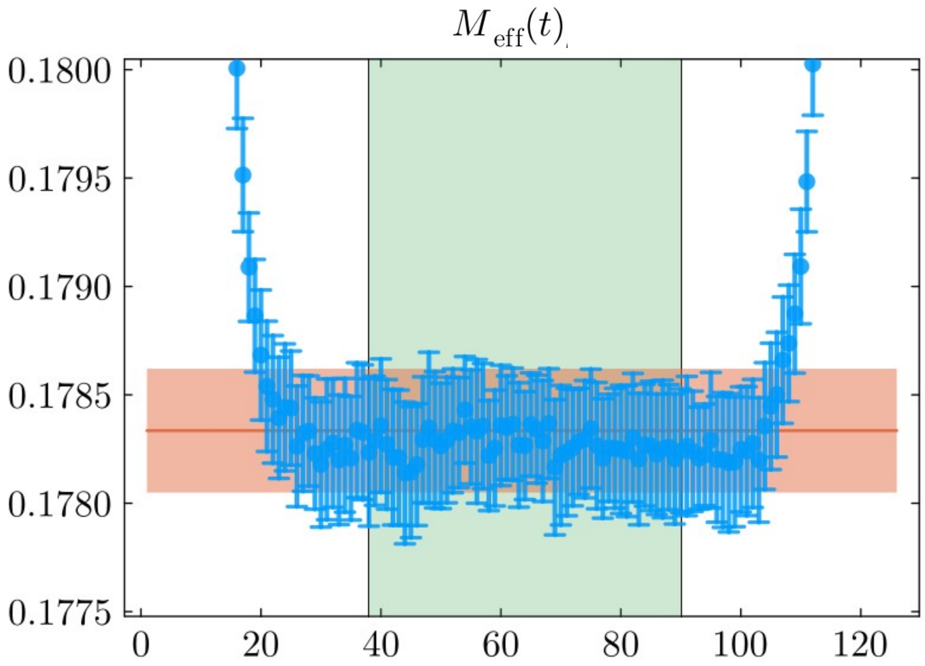


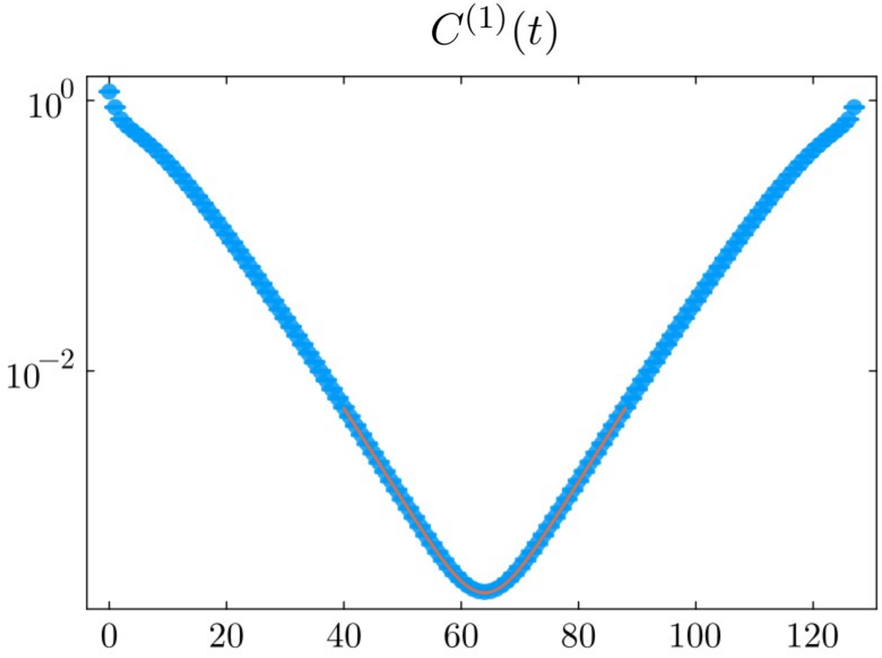
- $M_{K^0} - M_{K^\pm}$ does not have correction of order Δm^2 (neither connected nor disc.)
  - no deviation expected with respect to explicit simulation
- $M_{K^0} + M_{K^\pm}$ has no correction of order Δm but does have for order Δm^2
  - can test whether second order (valence-valence and sea-sea) is important
- Can obtain kaon mass derivative by fitting to:

$$C^{(0)} = A^{(0)} \cosh\left(M_K^{(0)}(t - T/2)\right)$$

$$C^{(1)} = A^{(1)} \cosh\left(M_K^{(0)}(t - T/2)\right) + A^{(0)} M_K^{(1)}(t - T/2) \sinh\left(M_K^{(0)}(t - T/2)\right)$$

$K^+ - K^0$ mass splitting: RM123 (N451)





Errors obtained with Γ method (ADerrors.jl)

$$M_K^{(0)} = 0.17834(29), \qquad A^{(0)} = -0.000000872(14)$$

$$M_K^{(1)} = 3.9061(90), \qquad A^{(1)} = 0.0002282(41)$$