High precision scale setting in lattice QCD

Lukas Varnhorst for the BMW collaboration

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BMW collaboration

Aix*Marseille université

SFB TR55

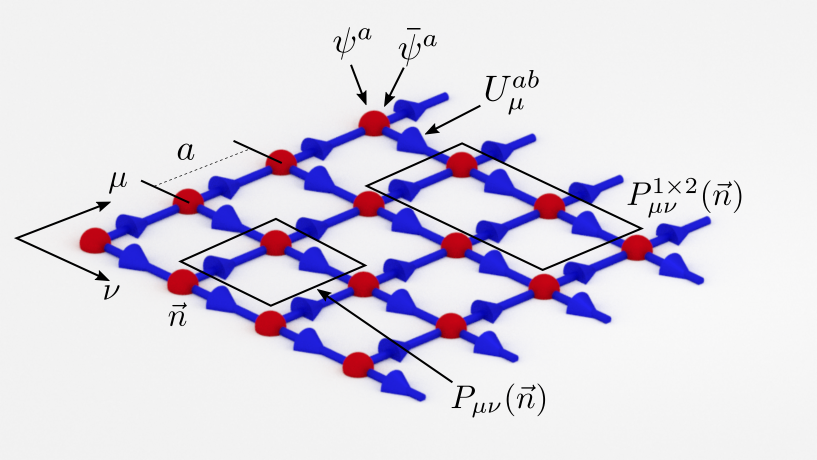
Talk based on:

S. Borsanyi, Z. Fodor, J. N. Guenther, C. Hoelbling,
S. D. Katz, L. Lellouch, T. Lippert, K. Miura, L. Parato and
K. K. Szabo, F. Stokes, B. C. Toth, Cs. Torok, L. Varnhorst,

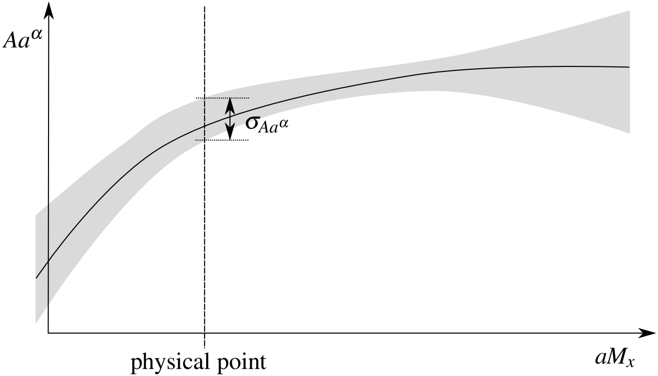
"Leading-order hadronic vacuum polarization contribution to the muon magnetic momentfrom lattice QCD,"

[arXiv:2002.12347 [hep-lat]].

Lattice QCD

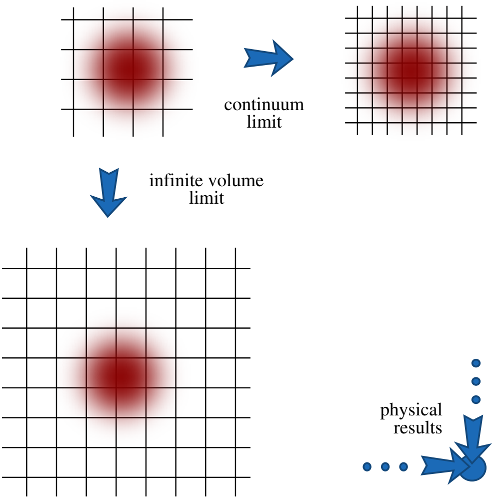

ψ^a
$\bar{\psi}^a$
U_μ^{ab}
a
μ
$P_{\mu\nu}^{1\times 2}(\vec{n})$
ν
$\vec{n}$
$P_{\mu\nu}(\vec{n})$

The need for a high precission scale setting



Important limits

Calculations can only be done with a finite number of lattice sites $\rightarrow$ Extrapolations to small lattice spacing and large volumina necessary.



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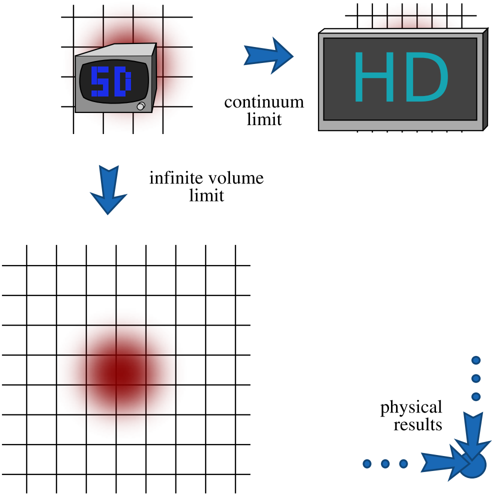

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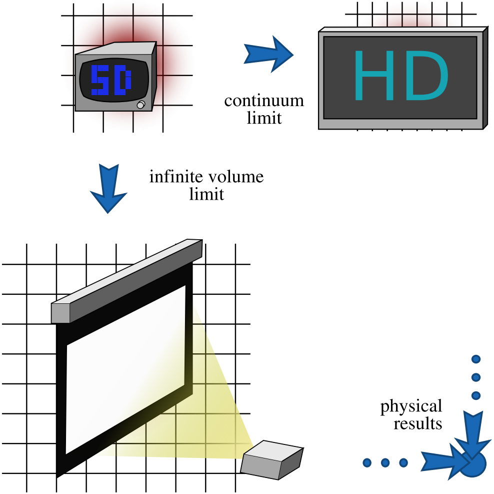
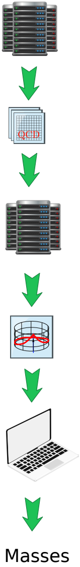


Strategy of Ω mass extraction



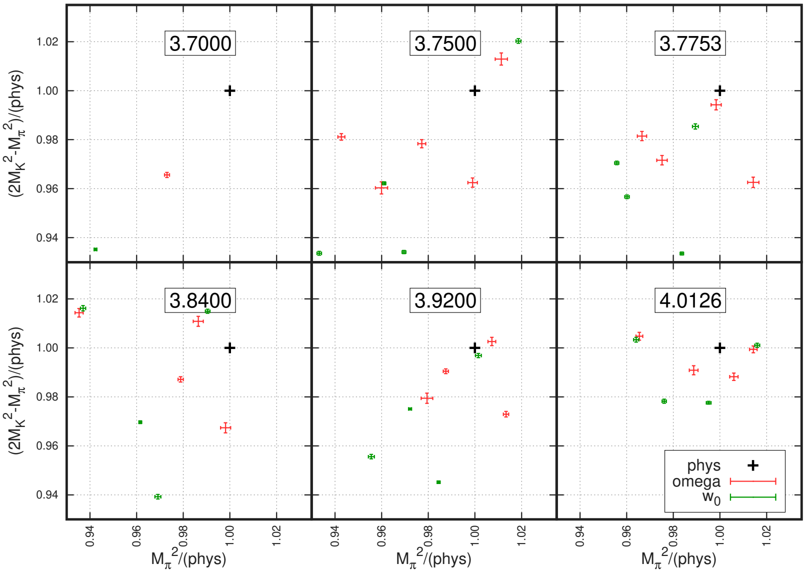
Determine the lattice scale with the Ω baryon mass

First discuss the isospin symmetric case

We used an action with the following properties:

- Symmanzik improved gauge action
- $N_f = 2 + 1 + 1$
- Four steps of stout smearing of the gauge fields in the Dirac operator
- Staggered fermions

Bracketing of the physical point



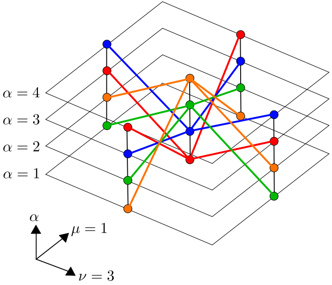
Staggered fermions

"Naïve" fermion action:

$$S_F = \sum_{x\in\Lambda} \bar{\psi}(x) \left(\sum_{\mu=1}^{4} \gamma_\mu \frac{U_\mu(x)\psi(x+\hat{\mu}) - U_\mu^\dagger(x-\hat{\mu})\psi(x-\hat{\mu})}{2a} + m\psi(x) \right)$$

12 component fermion fields $\psi_\alpha^a(x)$ and $\bar{\psi}_\alpha^a(x)$. It describes 16 Dirac fermions.

Staggered transformation $\psi(x) = \gamma_1^{x_1}\gamma_2^{x_2}\gamma_3^{x_3}\gamma_4^{x_4}\psi'(x)$ and $\bar{\psi}(x) = \bar{\psi}'(x)\gamma_4^{x_4}\gamma_3^{x_3}\gamma_2^{x_2}\gamma_1^{x_1}$ mixes spatial position with Dirac indizes:



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$$S_F = \sum_{x\in\Lambda} \bar{\chi}(x) \left(\sum_{\mu=1}^{4} \eta_\mu(x) \frac{U_\mu(x)\chi(x+\hat{\mu}) - U_\mu^\dagger(x-\hat{\mu})\chi(x-\hat{\mu})}{2a} + m\chi(x) \right)$$

with $\eta_\mu(x) = (-1)^{x_1+\cdots x_{\mu-1}}$. $\bar{\chi}(x)$ and $\chi(x)$ are 3 component fields and they describes 4 Dirac fermions.

Staggered fermions

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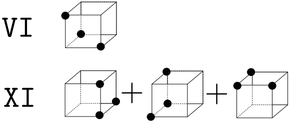
Baryon operators

Interpolating operator for baryons: Products of three quark fields. But: Dirac structure is encoded in spatial indices.

Classification of staggered baryon operators in [1]. For the Ω baryon, there are two candidates:



E.g. for the XI operator

$$O_{\mathrm{VI}} = \frac{1}{6}\epsilon^{abc}(D_1\chi^a(x))(D_2\chi^b(x))(D_3\chi^c(x))$$

$$D_i = \frac{1}{2}(\chi(x-\hat{i}) + \chi(x+\hat{i}))$$

In [2] an additional flavor DOF is used to construct a operator Ba

$$O_{\mathrm{Ba}} = [2\delta_{\alpha1}\delta_{\beta2}\delta_{\gamma3} - \delta_{\alpha3}\delta_{\beta1}\delta_{\gamma2} - \delta_{\alpha2}\delta_{\beta3}\delta_{\gamma1} + (\cdots\beta\leftrightarrow\gamma\cdots)] \times$$
$$\epsilon^{abc}\left((D_1\chi^a_\alpha(x))(D_{12}\chi^b_\beta(x))(D_{13}\chi^c_\gamma(x)) - (D_2\chi^a_\alpha(x))(D_{21}\chi^b_\beta(x))(D_{23}\chi^c_\gamma(x)) + (D_3\chi^a_\alpha(x))(D_{31}\chi^b_\beta(x))(D_{23}\chi^c_\gamma(x))\right)$$

[1] M. F. L. Golterman and J. Smit, "Lattice Baryons With Staggered Fermions," Nucl. Phys. B **255** (1985), 328-340
[2] J. A. Bailey, "Staggered baryon operators with flavor SU(3) quantum numbers," Phys. Rev. D **75** (2007), 114505 [arXiv:hep-lat/0611023 [hep-lat]]

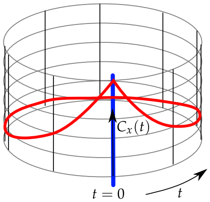
The Ω correlation function

The correlation function of a staggeered baryon has the form

$$H(t; A, M) = A_1 h_+(t; M_0) + A_2 h_-(t; M_2) + A_3 h_+(t; M_3) + A_4 h_-(t; M_4) + \cdots$$

with

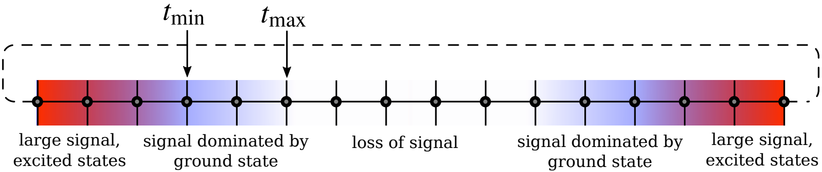
$$h_+(t, M) = e^{-Mt} + (-1)^{t-1} e^{-M(t-T)}$$
$$h_-(t, M) = -h_+(T-t, M)$$



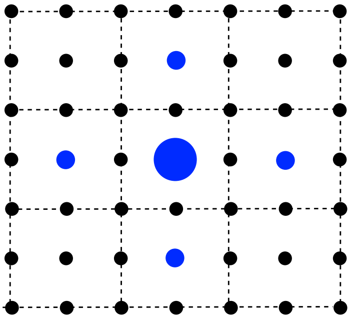
Mass can be estimated by effective mass

$$M_{\text{eff}}(t) = -\frac{1}{0.5} \log\left(\frac{H(t-1)}{H(t+1)}\right)$$

→ Asymptotic exponential decay



Quark smearing



Excited state contributions can be reduced by applying quark field smearing

Searing connects only next-to-neighbours to keep the taste structure intact.

Gauge fields are 3d stout smearied fields.

$$Wv(x) = (1-\sigma)v(x) + \frac{\sigma}{6}\sum_{\mu=1,2,3}\Big(U_\mu^{3\mathrm{d}}(x)U_\mu^{3\mathrm{d}}(x+\hat{\mu})v(x+2\hat{\mu}) + U_\mu^{3\mathrm{d}\dagger}(x-\hat{\mu})U_\mu^{3\mathrm{d}\dagger}(x-2\hat{\mu})v(x-2\hat{\mu})\Big)$$

But: Supression of excited states not enough

Extraction of the Ω mass:

4 state fit extraction

Fit propagator to

$$H(t;A,M) = A_1 h_+(t;M_0) + A_1 h_-(t;M_1) + A_2 h_+(t;M_2) + A_3 h_-(t;M_3)$$

with $h_+(t,M) = e^{-Mt} + (-1)^{t-1} e^{-M(t-T)}$ and $h_-(t,M) = -h_+(T-t,M)$.

Use priors for the excited state masses:

prior mean	rel. prior width
2012 MeV	0.10
2250 MeV	0.10
2400 MeV	0.15

GEVP based extraction

Construct matrix [1] from folded propagator H_t:

$$\mathcal{H}(t) = \begin{pmatrix} H_{t+0} & H_{t+1} & H_{t+2} & H_{t+3} \\ H_{t+1} & H_{t+2} & H_{t+3} & H_{t+4} \\ H_{t+2} & H_{t+3} & H_{t+4} & H_{t+5} \\ H_{t+3} & H_{t+4} & H_{t+5} & H_{t+6} \end{pmatrix}$$

and solve $\mathcal{H}(t_a)v(t_a,t_b) = \lambda(t_a,t_b)\mathcal{H}(t_b)v(t_a,t_b)$.

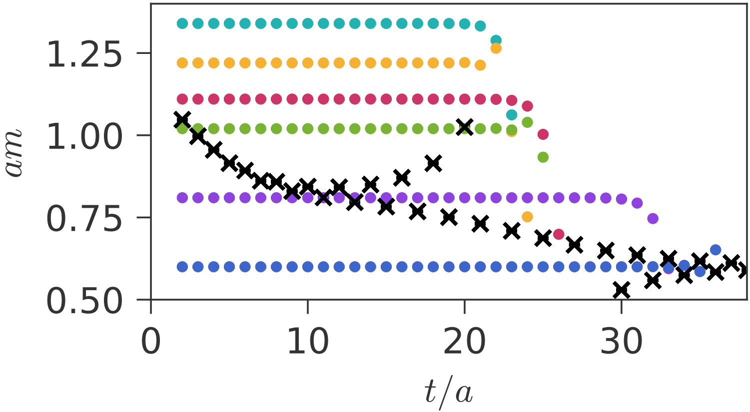
Then, extract mass from $C(t) = v^\dagger(t_a,t_b)\mathcal{H}(t)v(t_a,t_b)$ between t_0 and t_1.

No assumption on the masses of the excited states.

[1] C. Aubin and K. Orginos, "A new approach for Delta form factors," AIP Conf. Proc. **1374** (2011) no.1, 621-624 doi:10.1063/1.3647217 [arXiv:1010.0202 [hep-lat]].

GEVP based extraction

Can improve overlap with groundstate significantly → Mock analysis:



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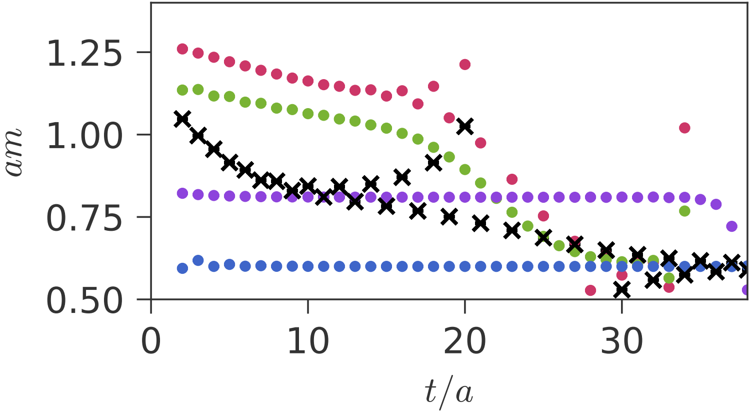
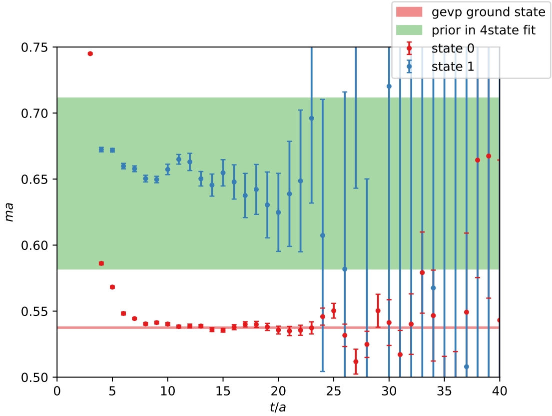


GEVP based extraction

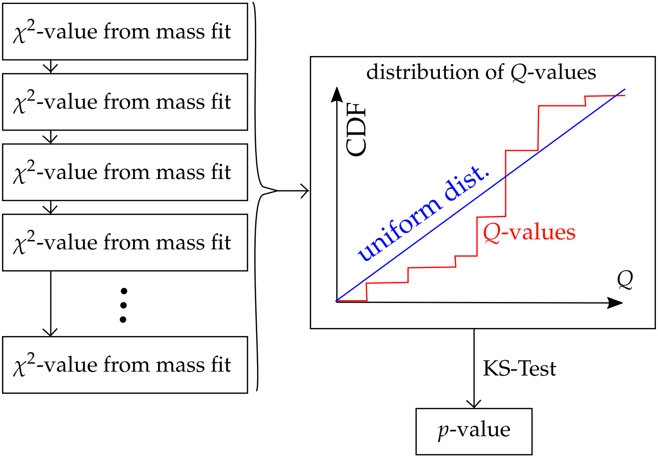
On real data ground state overlap can be significantly improved:



GEVP excited state agrees very well with prior in the 4 state fit.

GEVP based extraction

Method requires to tune the parameters for the GEP (t_a and t_b) and for the exponential fit (t_1 and t_2). We use a Kolmogorov-Smirnov test to determine the ranges.



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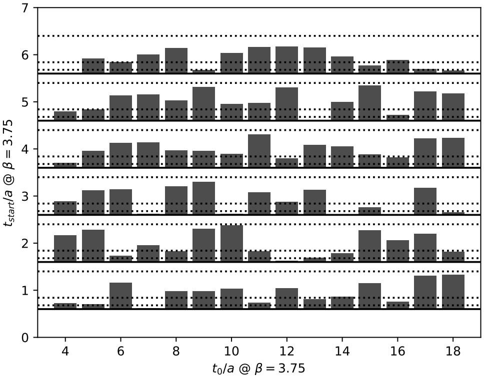

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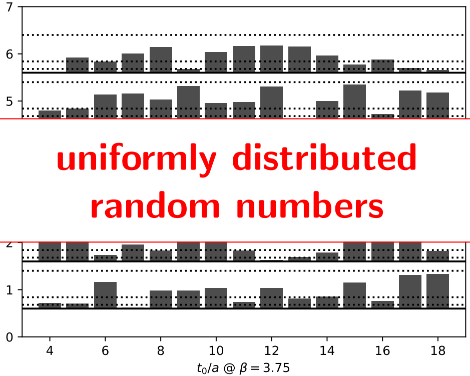

uniformly distributed random numbers

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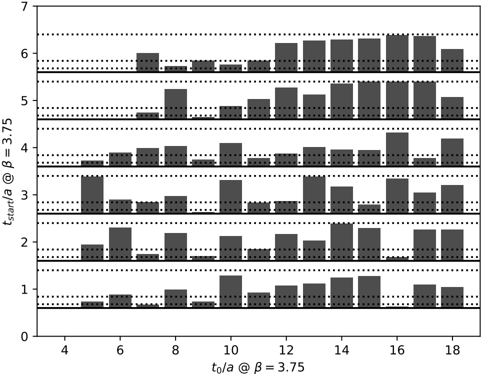
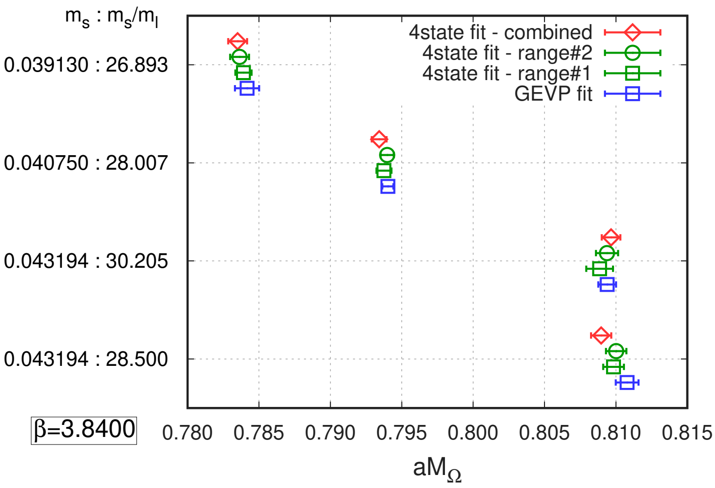


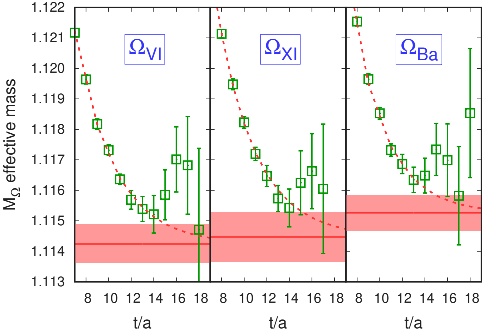
Comparison between methods

Good agreement between mass extraction with both methods:



Comparison of operators

We have investigate the 3 operators `VI`, `XI` and `Ba` on one ensemble with increased statistics:

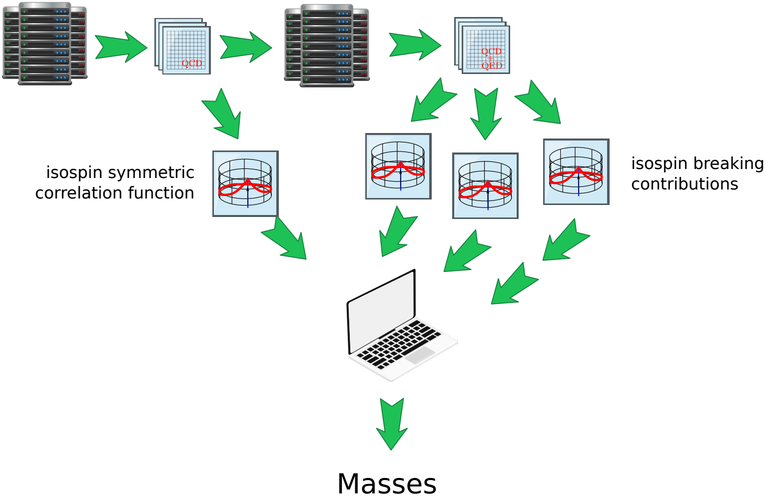


`VI` and `XI` couple to two tatstes, whereas `Ba` is constructed to couple only to one taste.

Difference safely within the 0.1% error on usual configurations. → Use `VI` for the main analysis.

checkpoint

The calcultation of the isospin corrected Ω masses



The path integral

The path integral in the full theory is

$$Z = \int \mathcal{D}U \, e^{-S_g[U]} \int DA \, e^{-S_\gamma[A]} \, \text{dets}$$

where

$$\text{dets} = \prod_f \det M_f^{1/4}$$

- Non-Compact formlation (photon field A_μ)
- Configurations generated with $m_u = m_d$ and without electromagnetism
- $S_\gamma[A]$ is the $\mathrm{QED_L}$, i.e. with the spatial zero modes removed
- Isospin correction added as derivatives

Full QCD+QED

- QCD + QED

$$\langle \mathcal{C} \rangle_{\mathrm{QCD+QED}} = \frac{\int \mathrm{d}U \int \mathrm{d}A \ \mathcal{C}(U,A) \ e^{-S_{\mathrm{g}}[U]} \, e^{-S_\gamma[A]} \ \det M(U,A)}{\int \mathrm{d}U \int \mathrm{d}A \ e^{-S_{\mathrm{g}}[U]} \, e^{-S_\gamma[A]} \ \det M(U,A)}$$

- Keep leading order in $\delta m = m_d - m_u$ and $e^2 = 4\pi\alpha$

$$\langle \mathcal{C} \rangle_{\mathrm{QCD+QED}}(\delta m, e) = \langle \mathcal{C} \rangle_{\mathrm{QCD+QED}} \Big|_{\substack{\delta m=0 \\ e=0}} + \delta m \cdot \frac{\partial}{\partial \delta m} \langle \mathcal{C} \rangle_{\mathrm{QCD+QED}} \Big|_{\substack{\delta m=0 \\ e=0}} + \\ + \frac{e^2}{2} \cdot \frac{\partial^2}{\partial e^2} \langle \mathcal{C} \rangle_{\mathrm{QCD+QED}} \Big|_{\substack{\delta m=0 \\ e=0}} + \mathcal{O}(e^4, e^2 \delta m, \delta m^2)$$

Dynamical QED as quenched QED expectation values

$$\langle \mathcal{C} \rangle_{\text{QCD+QED}} = \frac{\int \mathrm{d}U \int \mathrm{d}A \;\mathcal{C}(U,A)\; e^{-S_\mathrm{g}[U]}\, e^{-S_\gamma[A]}\, \det M(U,A)}{\int \mathrm{d}U \int \mathrm{d}A \; e^{-S_\mathrm{g}[U]}\, e^{-S_\gamma[A]}\, \det M(U,A)} =$$

$$= \frac{\int \mathrm{d}U \int \mathrm{d}A \;\mathcal{C}(U,A)\, \frac{\det M(U,A)}{\det M(U,0)}\; e^{-S_\gamma[A]}\; e^{-S_\mathrm{g}[U]}\, \det M(U,0)}{\int \mathrm{d}U \int \mathrm{d}A \; \frac{\det M(U,A)}{\det M(U,0)}\; e^{-S_\gamma[A]}\; e^{-S_\mathrm{g}[U]}\, \det M(U,0)} =$$

$$= \frac{\int \mathrm{d}U \;\left\langle \mathcal{C}(U,A)\, \frac{\det M(U,A)}{\det M(U,0)} \right\rangle_{A,\mathrm{q.}} \; e^{-S_\mathrm{g}[U]}\, \det M(U,0)}{\int \mathrm{d}U \;\left\langle \frac{\det M(U,A)}{\det M(U,0)} \right\rangle_{A,\mathrm{q.}} \; e^{-S_\mathrm{g}[U]}\, \det M(U,0)} =$$

$$= \frac{\left\langle \left\langle \mathcal{C}(U,A)\, \frac{\det M(U,A)}{\det M(U,0)} \right\rangle_{A,\mathrm{q.}} \right\rangle_U}{\left\langle \left\langle \frac{\det M(U,A)}{\det M(U,0)} \right\rangle_{A,\mathrm{q.}} \right\rangle_U}$$

Expansion up to $\mathcal{O}(e^2, \delta m)$

e_v: QED coupling in valence sector

e_s: QED coupling in sea sector

$$\mathcal{C}(U,A) \approx \mathcal{C}_0(U) + \frac{\delta m}{m_l} \cdot \mathcal{C}'_m(U) + e_v \cdot \mathcal{C}'_1(U,A) + \frac{e_v^2}{2} \cdot \mathcal{C}''_2(U,A)$$

$$\left(\prod_{f=u,d,s,c} \frac{\det M^{(f)}[U,A]}{\det M^{(f)}[U,0]} \right)^{1/4} \approx 1 + e_s \cdot \frac{d_1(U,A)}{d_0(U)} + \frac{e_s^2}{2} \cdot \frac{d_2(U,A)}{d_0(U)}$$

- $m_u = m_l - \frac{\delta m}{2}, \quad m_d = m_l + \frac{\delta m}{2} \quad \longrightarrow \quad \mathcal{O}(\delta m)$ sea effect vanishes

$$\langle \mathcal{C} \rangle_{\text{QCD+QED}} = \langle \mathcal{C}_0(U) \rangle_U + \frac{\delta m}{m_l} \cdot \langle \mathcal{C}'_m(U) \rangle_U + \frac{e_v^2}{2} \cdot \left\langle \langle \mathcal{C}''_2(U,A) \rangle_{A,\text{q.}} \right\rangle_U + $$
$$+ e_v e_s \cdot \left\langle \left\langle \mathcal{C}'_1(U,A) \cdot \frac{d_1(U,A)}{d_0(U)} \right\rangle_{A,\text{q.}} \right\rangle_U +$$
$$+ \frac{e_s^2}{2} \cdot \left\langle \left(\mathcal{C}_0(U) - \langle \mathcal{C}_0(U) \rangle_U \right) \cdot \left\langle \frac{d_2(U,A)}{d_0(U)} \right\rangle_{A,\text{q.}} \right\rangle_U$$

QCD+QED

$$\langle\mathcal{C}\rangle_{\text{QCD+QED}} \approx \langle\mathcal{C}\rangle\big|_0 + \frac{\delta m}{m_l}\cdot\langle\mathcal{C}\rangle'_m + \frac{e_v^2}{2}\cdot\langle\mathcal{C}\rangle''_{20} + e_v e_s\cdot\langle\mathcal{C}\rangle''_{11} + \frac{e_s^2}{2}\cdot\langle\mathcal{C}\rangle''_{02}$$

$$\langle\mathcal{C}\rangle\big|_0 = \langle\mathcal{C}_0(U)\rangle_U$$

$$\langle\mathcal{C}\rangle'_m = \left\langle\mathcal{C}'_m(U)\right\rangle_U$$

$$\langle\mathcal{C}\rangle''_{20} = \left\langle\left\langle\mathcal{C}''_2(U,A)\right\rangle_{A,\text{q.}}\right\rangle_U$$

$$\langle\mathcal{C}\rangle''_{11} = \left\langle\left\langle\mathcal{C}'_1(U,A)\cdot\frac{d_1(U,A)}{d_0(U)}\right\rangle_{A,\text{q.}}\right\rangle_U$$

$$\langle\mathcal{C}\rangle''_{02} = \left\langle\left(\mathcal{C}_0(U) - \langle\mathcal{C}_0(U)\rangle_U\right)\cdot\left\langle\frac{d_2(U,A)}{d_0(U)}\right\rangle_{A,\text{q.}}\right\rangle_U$$

Strategy:

- Take isospin symmetric $SU(3)$ configurations: U
- Measure $\mathcal{C}_0(U)$ and $\mathcal{C}'_m(U)$
- For each U, generate quenched $U(1)$ fields: A
- Measure $\mathcal{C}'_1(U,A)$, $\mathcal{C}''_2(U,A)$, $\frac{d_1(U,A)}{d_0(U)}$ and $\frac{d_2(U,A)}{d_0(U)}$

Isospin breaking for hadron masses

Consider effective mass $\mathcal{M}[H]$ (H: correlation function) as observable:

$$M_0 = \mathcal{M}[\langle H_0 \rangle_0]$$

$$M''_{02} = \left.\frac{\delta \mathcal{M}[H]}{\delta H}\right|_{\langle H_0 \rangle_0} \langle H \rangle''_{02} = \left.\frac{\delta \mathcal{M}[H]}{\delta H}\right|_{\langle H_0 \rangle_0} \left\langle (H_0 - \langle H_0 \rangle_0) \frac{\mathrm{dets}''_2}{\mathrm{dets}_0} \right\rangle$$

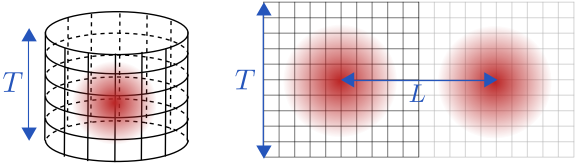
$$M''_{20} \approx \frac{1}{e_v^2} (\mathcal{M}[\frac{1}{2} \langle H_+ + H_- \rangle_0] - \mathcal{M}[\langle H_0 \rangle_0])$$

$$M''_{11} \approx \left.\frac{\delta \mathcal{M}[H]}{\delta H}\right|_{\langle H_+ + H_- \rangle_0} \left\langle \frac{H_+ - H_-}{2 e_v} \frac{\mathrm{dets}'_1}{\mathrm{dets}_0} \right\rangle_0$$

$$M'_m \approx \frac{m_l}{\delta m} (\mathcal{M}[\langle H_{\delta m} \rangle_0] - \mathcal{M}[\langle H_0 \rangle_0])$$

Note that derivatives of $\mathcal{M}[H]$ can be calculated analytical.

Finite-Volume-Corrections



QED in a box with periodic boundary condition → mirror particle. Full calculation for e.g. charged scalar particles yields ($\kappa = 2.837\ldots$) [1,2]

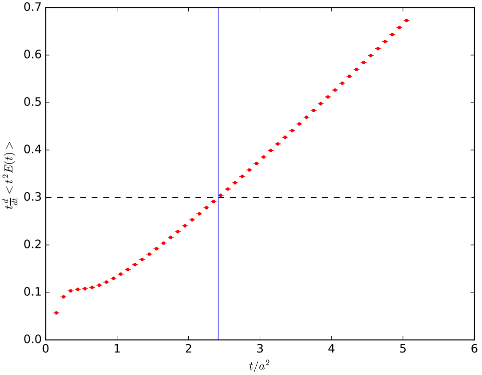
$$M(L) - M(\infty) = -\frac{(Qe)^2 c}{8\pi}\left[\frac{1}{L} + \frac{2}{ML^2} + \mathcal{O}(L^{-3})\right]$$

QCD has a mass gap → Finite volume corrections to masses scale exponential with the decay length determined by the lightest propagating degree of freedom.

[1] Z. Davoudi and M. J. Savage, "Finite-Volume Electromagnetic Corrections to the Masses of Mesons, Baryons and Nuclei," Phys. Rev. D **90** (2014) no.5, 054503 doi:10.1103/PhysRevD.90.054503 [arXiv:1402.6741 [hep-lat]].
[2] S. Borsanyi *et al.*, "Ab initio calculation of the neutron-proton mass difference," Science **347** (2015) 1452 doi:10.1126/science.1257050 [arXiv:1406.4088 [hep-lat]].

The scale w_0

Very promising for high precision scale setting: w_0.



- Apply Wilson flow to "smooth out" the gauge fields and bring them closer to the classical solution. [1]
- Monitor the action density.
- Define w_0 to be the value of $\sqrt{t}$ where $\tau \frac{\mathrm{d}}{\mathrm{d}\tau} \langle \tau^2 E(t) \rangle = 0.3$. [2]
- Closely related to t_0. [1]

[1] M. Lüscher, "Properties and uses of the Wilson flow in lattice QCD," JHEP **1008** (2010) 071 Erratum: [JHEP **1403** (2014) 092] [arXiv:1006.4518 [hep-lat]].
[2] S. Borsanyi *et al.*, "High-precision scale setting in lattice QCD," JHEP **1209** (2012) 010 [arXiv:1203.4469 [hep-lat]].

Isospin splitting of w_0

In general we have

$$\langle W_{\tau=w_0^2(e)} \rangle = 0.3 \quad \text{with} \quad W_\tau = \frac{\mathrm{d}(\tau^2 E)}{\mathrm{d}\log\tau}$$

We then expanded

$$\langle W_\tau \rangle = \langle W_\tau \rangle_0 + e_s^2 \left\langle (W_\tau - \langle W_\tau \rangle_0) \frac{\text{dets}_2''}{\text{dets}_0} \right\rangle_0$$

$$w_0(e_s) = w_0 + e_s^2 \delta w_0$$

$$W_{\tau=w_0^2(e_s)} = W_{\tau=w_0^2} + e_s^2 \cdot 2 w_0 \delta w_0 \cdot \left. \frac{\mathrm{d}W}{\mathrm{d}\tau} \right|_{\tau=w_0^2}$$

So that

$$\delta w_0 = -\left[\frac{1}{2\sqrt{\tau}} \left\langle \frac{\mathrm{d}W}{\mathrm{d}\tau} \right\rangle_0^{-1} \left\langle (W_\tau - \langle W_\tau \rangle_0 \frac{\text{dets}_2''}{\text{dets}_0} \right\rangle_0 \right]_{\tau=w_0^2}$$

Global fits

Using `Type I` fit:

$$Y = A + BX_l + CX_s + DX_{\delta m} + Ee_v^2 + Fe_v e_s + Ge_s^2$$

with

$$X_l = M_{\pi^0}^2/M_\Omega^2 - \left[M_{\pi^0}^2/M_\Omega^2\right]_*$$
$$X_s = M_{K_\chi}^2/M_\Omega^2 - \left[M_{K_\chi}^2/M_\Omega^2\right]_*$$
$$X_{\delta m} = \frac{(M_{K^0} - M_{K^+})^2}{M_\Omega^2}$$
$$M_{K_\chi}^2 = \frac{1}{2}(M_{K^0}^2 + M_{K^+}^2 - M_{\pi^+}^2)$$

The coefficients $A, \ldots, G$ themselfs depend on the lattice spacing and X_l and X_s.

Global fits

Using `Type I` fit:

$$Y = A + BX_l + CX_s + DX_{\delta m} + Ee_v^2 + Fe_v e_s + Ge_s^2$$

The coefficients $A, \dots, G$ themselfs depend on the lattice spacing and X_l and X_s.

$$\begin{aligned}
A &= A_0 + A_2 a^2 + A_4 a^4 \\
B &= B_0 + B_2 a^2 \\
C &= C_0 + C_2 a^2 \\
D &= D_0 + D_2 a^2 + D_4 a^4 + D_l X_l + D_s X_s \\
E &= E_0 + E_2 a^2 + E_4 a^4 + E_l X_l + E_s X_s \\
F &= F_0 + F_2 a^2 \\
G &= G_0 + G_2 a^2
\end{aligned}$$

Global fits

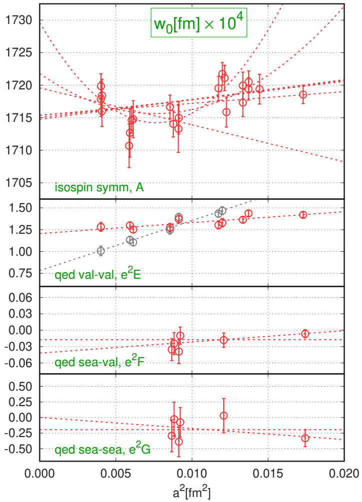
Using `Type I` fit:

$$Y = A + BX_l + CX_s + DX_{\delta m} + Ee_v^2 + Fe_v e_s + Ge_s^2$$

Write as coupled system of equations

$$\begin{aligned}
[Y]_0 &= [A + BX_l + CX_s]_0 \\
[Y]'_m &= [DX_{\delta m}]'_m \\
[Y]''_{20} &= [A + BX_l + CX_s + DX_{\delta m}]''_{20} + [E]_0 \\
[Y]''_{11} &= [A + BX_l + CX_s + DX_{\delta m}]''_{11} + [F]_0 \\
[Y]''_{02} &= [A + BX_l + CX_s + DX_{\delta m}]''_{02} + [G]_0
\end{aligned}$$

w_0 from Ω mass:



$$w_0 = 0.17236(29)(63)[70]\,\mathrm{fm}$$

Using Type I fit:

$$w_0 M_\Omega = A + BX_l + CX_s + Ee_v^2 + FXe_v e_s + Ge_s^2$$

with

$$X_l = M_{\pi^0}^2 / M_\Omega^2 - \left[M_{\pi^0}^2 / M_\Omega^2\right]_*$$

$$X_s = M_{K_\chi}^2 / M_\Omega^2 - \left[M_{K_\chi}^2 / M_\Omega^2\right]_*$$

$$M_{K_\chi}^2 = \frac{1}{2}(M_{K^0}^2 + M_{K^+}^2 - M_{\pi^+}^2)$$

Error by AIC weighted histogram method: