Obtaining physical results from Lattice QCD simulations

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Outline of talk

- In this talk I will present some of the theoretical framework supporting the determination of physical quantities from lattice simulations.

1. Brief introduction to lattice QCD simulations
2. Brief introduction to the Operator Product Expansion
3. Renormalization
4. Finite-volume effects

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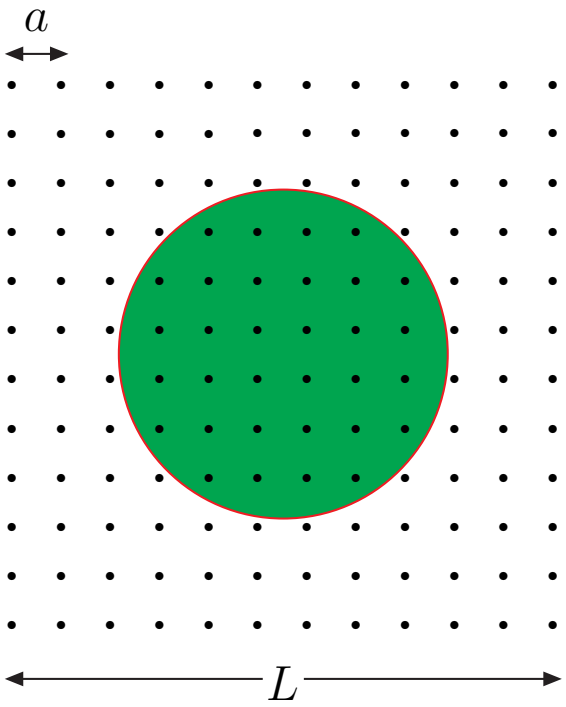
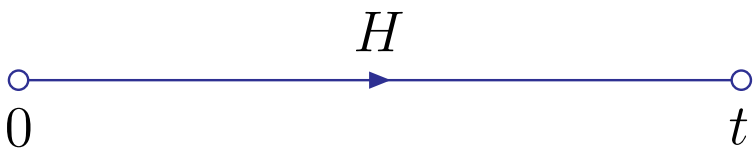


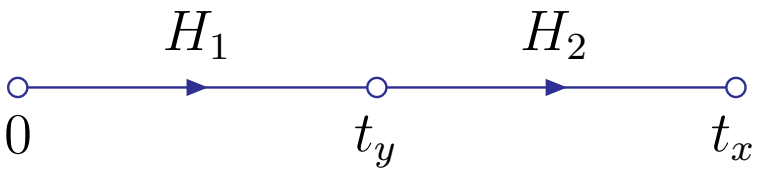
- Lattice phenomenology starts with the evaluation of correlation functions of the form:

$$\langle 0|\, O(x_1,x_2,\cdots,x_n)\,|0\rangle \quad = \quad \frac{1}{Z}\int [dA_\mu]\,[d\psi]\,[d\bar{\psi}]\,e^{-S}\,O(x_1,x_2,\cdots,x_n)\ ,$$

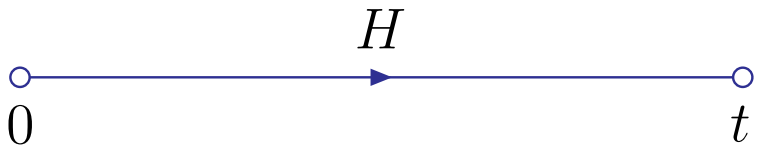
where $O(x_1,x_2,\cdots,x_n)$ is a multilocal operator composed of quark and gluon fields and Z is the partition function.

- The physics which can be studied depends on the choice of the multilocal operator O.





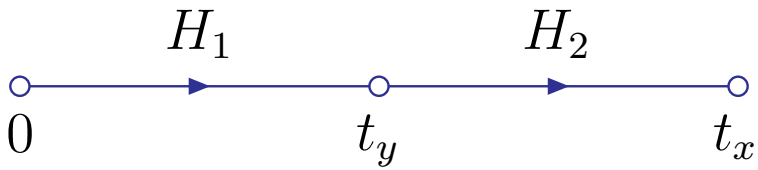
- The functional integral is performed by discretising Euclidean space-time and using Monte-Carlo Integration.



$$
\begin{aligned}
C_2(t) &= \int d^3x\, e^{i\vec{p}\cdot\vec{x}}\, \langle 0|\, \phi(\vec{x},t)\, \phi^\dagger(\vec{0},0)\, |0\rangle \\
&= \sum_n \int d^3x\, e^{i\vec{p}\cdot\vec{x}}\, \langle 0|\, \phi(\vec{x},t)\, |n\rangle\, \langle n|\phi^\dagger(\vec{0},0)\, |0\rangle \\
&= \int d^3x e^{i\vec{p}\cdot\vec{x}}\, \langle 0|\, \phi(\vec{x},t)\, |H\rangle\, \langle H|\phi^\dagger(\vec{0},0)\, |0\rangle + \cdots \\
= \frac{1}{2E}\, e^{-iEt} \left|\langle 0|\phi(\vec{0},0)|H(p)\rangle\right|^2 + \cdots &\Rightarrow \frac{1}{2E}\, e^{-Et} \left|\langle 0|\phi(\vec{0},0)|H(p)\rangle\right|^2 + \cdots \quad \text{(Euclidean)}
\end{aligned}
$$

where $E = \sqrt{m_H^2 + \vec{p}^{\,2}}$ and we have taken H to be the lightest state created by $\phi^\dagger$.
The $\cdots$ represent contributions from heavier states.

- By fitting $C(t)$ to the form above, both the energy (or, if $\vec{p} = 0$, the mass) and the modulus of the matrix element $\left|\langle 0|J(\vec{0},0)|H(p)\rangle\right|$ can be evaluated.
- Example: if $\phi = \bar{b}\,\gamma^\mu\gamma^5 u$ then the decay constant of the B-meson can be evaluated, $\left|\langle 0|\,\bar{b}\,\gamma^\mu\gamma^5 u\,|B^+(p)\rangle\right| = f_B\, p^\mu$.



$$C_3(t_x,t_y) = \int d^3x\, d^3y\, e^{i\vec{p}\cdot\vec{x}}\, e^{i\vec{q}\cdot\vec{y}}\, \langle 0|\, \phi_2(\vec{x},t_x)\, O(\vec{y},t_y)\, \phi_1^\dagger(\vec{0},0)\, |0\rangle\ ,$$

$$\simeq \frac{e^{-E_1 t_y}}{2E_1}\, \frac{e^{-E_2(t_x-t_y)}}{2E_2}\, \langle 0|\phi_2(0)|H_2(\vec{p})\rangle \langle H_2(\vec{p})|O(0)|H_1(\vec{p}+\vec{q})\rangle\, \langle H_1(\vec{p}+\vec{q})|\phi_1^\dagger(0)|0\rangle\ ,$$

for sufficiently large times t_y and $t_x - t_y$ and $E_1^2 = m_1^2 + (\vec{p}+\vec{q})^2$ and $E_2^2 = m_1^2 + \vec{p}^{\,2}$.

- Thus from 2- and 3-point functions we obtain transition matrix elements of the form $|\langle H_2|O|H_1\rangle|$.
- Important examples include $\langle \bar{K}^0|(\bar{s}\gamma_L^\mu d)\,(\bar{s}\gamma_{\mu L} d)|K^0\rangle$ and $\langle \pi^0|(\bar{s}\gamma^\mu u)|K^+\rangle$.

- In Lattice QCD, while it is natural to think in terms of the lattice spacing a, the input parameter is $\beta = 6/g^2(a)$.
- Imagine performing a simulation with $N_f = 2+1$ with $m_{ud} = m_u = m_d$ around their "physical" values.
- At each β, take two dimensionless quantities, e.g. m_π/m_Ω and m_K/m_Ω, and find the bare quark masses m_{ud} and m_s which give the corresponding physical values.These are then defined to be the physical (bare) quark masses at that β.
- Now consider a dimensionful quantity, e.g. m_Ω. The value of the lattice spacing is defined by

$$a^{-1} = \frac{1.672\,\mathrm{GeV}}{am_\Omega(\beta, m_{ud}, m_s)}$$

  where $am_\Omega(\beta, m_{ud}, m_s)$ is the computed value in lattice units.
- Other physical quantities computed at the physical bare-quark masses will now differ from their physical values by artefacts of $O(a^2)$.
- Repeating this procedure at different β defines a scaling trajectory. Other choices for the 3 physical quantities used to define the trajectory are clearly possible.
- If the simulations are performed with m_c and/or $m_u \neq m_d$ then the procedure has to be extended accordingly.

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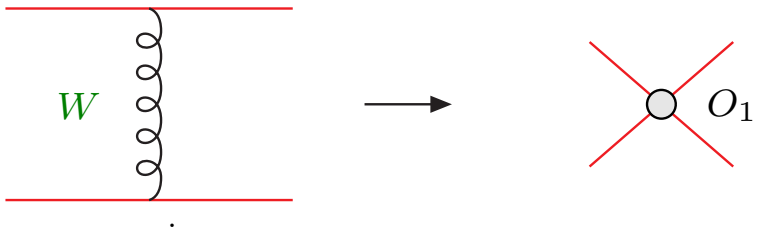
1. Brief introduction to lattice QCD simulations
2. Brief introduction to the Operator Product Expansion
3. Renormalization
4. Finite-volume effects

- Quarks interact strongly $\Rightarrow$ we have to consider QCD effects even in weak processes.
- Our inability to control (non-perturbative) QCD Effects is frequently the largest systematic error in attempts to obtain fundamental information from experimental studies of weak processes!
- Tree-Level:

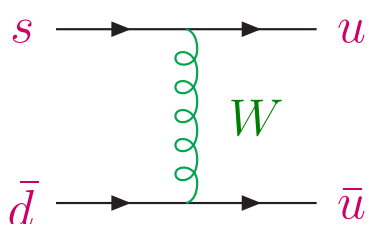


- Since $M_W \simeq 80\,\text{GeV}$, at low energies the momentum in the W-boson is much smaller than its mass $\Rightarrow$ the four quark interaction can be approximated by the local Fermi β-decay vertex with coupling

$$\frac{G_F}{\sqrt{2}} = \frac{g_2^2}{8M_W^2} \ .$$

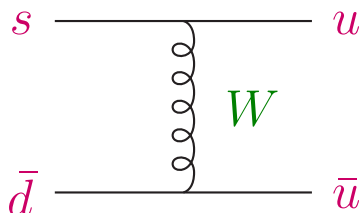
- *Asymptotic Freedom* $\Rightarrow$ we can treat QCD effects at short distances, $|x| \ll \Lambda_{QCD}^{-1}$ ($|x| < 0.1$ fm say) or corresponding momenta $|p| \gg \Lambda_{QCD}$ ($|p| > 2$ GeV say), using perturbation theory.
- The natural scale of strong interaction physics is of $O(1\ \mathrm{fm})$ however, and so in general, and for most of the processes discussed here, non-perturbative techniques must be used.
- For illustration consider $K \to \pi\pi$ decays, for which the tree-level amplitude is proportional to

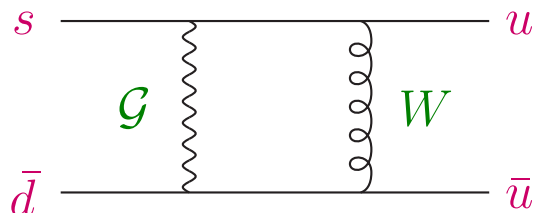
$$\frac{G_F}{\sqrt{2}} V_{ud}^* V_{us} \langle \pi\pi | (\bar{d}\gamma^\mu (1-\gamma^5) u)\, (\bar{u}\gamma_\mu (1-\gamma^5) s) | K \rangle \ .$$



- We therefore need to determine the matrix element of the operator

$$O_1 = (\bar{d}\gamma^\mu (1-\gamma^5) u)\, (\bar{u}\gamma_\mu (1-\gamma^5) s) \ .$$





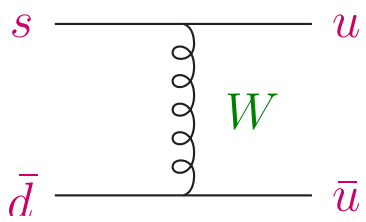
- Gluonic corrections generate a second operator $(\bar{d}T^a\gamma^\mu(1-\gamma^5)u)\,(\bar{u}T^a\gamma_\mu(1-\gamma^5)s)$, which by using Fierz Identities can be written as a linear combination of O_1 and O_2 where

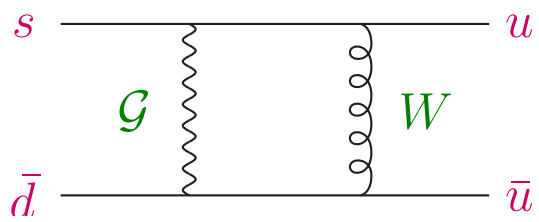
$$O_2 = (\bar{d}\gamma^\mu(1-\gamma^5)s)\,(\bar{u}\gamma_\mu(1-\gamma^5)u)\,.$$

- OPE $\Rightarrow$ the amplitude for a weak decay process can be written as

$$A_{if} = \frac{G_F}{\sqrt{2}}\,V_{CKM}\sum_i C_i(\mu)\langle f|\,O_i(\mu)\,|i\rangle\ .$$

- μ is the renormalization scale at which the operators O_i are defined.
- Non-perturbative QCD effects are contained in the matrix elements of the O_i, which are independent of the large momentum scale, in this case of M_W.
- The Wilson coefficient functions $C_i(\mu)$ are independent of the states i and f and are calculated in perturbation theory.
- Since physical amplitudes manifestly do not depend on μ, the μ-dependence in the operators $O_i(\mu)$ is cancelled by that in the coefficient functions $C_i(\mu)$.



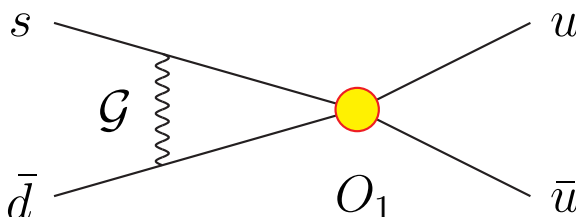


- For large loop-momenta k the right-hand graph is ultra-violet convergent:

$$\int_{k \text{ large}} \frac{1}{k}\,\frac{1}{k}\,\frac{1}{k^2}\,\frac{1}{k^2 - M_W^2}\,d^4k\ ,$$

  ($1/k$ for each quark propagator and $1/k^2$ for the gluon propagator.)
  We see that there is a term $\sim \log(M_W^2/p^2)$, where p is some infra-red scale.

- In the OPE we do not have the W-propagator.



Power Counting : $\int_{k \text{ large}} \frac{1}{k}\,\frac{1}{k}\,\frac{1}{k^2}\,d^4k \quad \Rightarrow \quad$ **divergence** $\quad \Rightarrow \quad \mu-$dependence.

- Infra-dependence is the same as in the full field-theory.

$$\log\left(\frac{M_W^2}{p^2}\right) = \log\left(\frac{M_W^2}{\mu^2}\right) + \log\left(\frac{\mu^2}{p^2}\right)$$

- The ir physics is contained in the matrix elements of the operators and the uv physics in the coefficient functions:

$$\log\left(\frac{M_W^2}{\mu^2}\right) \quad \to \quad C_i(\mu)$$

$$\log\left(\frac{\mu^2}{p^2}\right) \quad \to \quad \text{matrix element of } O_i$$

- In practice, the matrix elements are computed in lattice simulations with an ultraviolet cut-off of 2 – 4 GeV. Thus we have to resum *large logarithms* of the form $\alpha_s^n \log^n(M_W^2/\mu^2)$ in the coefficient functions $\Rightarrow$ factors of the type

$$\left[\frac{\alpha_s(M_W)}{\alpha_s(\mu)}\right]^{\gamma_0/2\beta_0} .$$

$$\left[\frac{\alpha_s(M_W)}{\alpha_s(\mu)}\right]^{\gamma_0/2\beta_0}$$

- γ_0 is the one-loop contribution to the *anomalous dimension* of the operator (proportional to the coefficient of $\log(\mu^2/p^2)$ in the evaluation of the one-loop graph above) and β_0 is the first term in the β-function, ($\beta \equiv \partial g/\partial \ln(\mu) = -\beta_0 g^3/16\pi^2$).
- In general when there is more than one operator contributing to the right hand side of the OPE, the mixing of the operators $\Rightarrow$ matrix equations.
- The factor above represents the sum of the *leading logarithms*, i.e. the sum of the terms $\alpha_s^n \log^n(M_W^2/\mu^2)$. For almost all the important processes, the first (or even higher) corrections have also been evaluated.
- These days, for most processes of interest, the perturbative calculations have been performed to several loops (2,3,4), $\mathrm{N}^n\mathrm{LO}$ calculations.

- The *effective Hamiltonian* for weak decays takes the form

$$\mathscr{H}_{\rm eff} \equiv \frac{G_F}{\sqrt{2}} V_{CKM} \sum_i C_i(\mu)\, O_i(\mu) \ .$$

- For some important physical quantities (e.g. ε'/ε), there may be as many as ten operators, whose matrix elements have to be estimated.
- Lattice simulations enable us to evaluate the matrix elements non-perturbatively. This is the subject of most of the remainder of these lectures.
- In weak decays the large scale, M_W, is of course fixed. For other processes, most notably for deep-inelastic lepton-hadron scattering, the OPE is useful in computing the behaviour of the amplitudes with the large scale (e.g. with the momentum transfer).

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- The quark masses $m_q(a)$ and QCD coupling constant $g(a)$ obtained as above are bare parameters with a^{-1} as the ultraviolet cut-off and with discretised QCD as the bare theory.
- In perturbative calculations it is particularly convenient, and therefore conventional, to use the $\overline{\mathrm{MS}}$ renormalisation scheme.
  - Note that the $\overline{\mathrm{MS}}$ scheme is purely perturbative; we cannot perform simulations in $4+2\varepsilon$ dimensions.
  - Originally, providing both a^{-1} and μ are sufficiently large, renormalised quantities in the $\overline{\mathrm{MS}}$ scheme were obtained from the bare lattice ones using perturbation theory, e.g.

$$m^{\overline{\mathrm{MS}}}(\mu) = Z_m(a\mu)\, m^{\mathrm{latt}}(a)\,.$$

  - However, lattice perturbation theory frequently converges slowly (e.g. partly because of tadpole diagrams) and is technically complicated, e.g. for a scalar propagator,

$$\frac{1}{k^2+m^2} \to \frac{1}{\sum_\mu \{\frac{4}{a^2}\sin^2\frac{k_\mu a}{2}\}+m^2}\,.$$

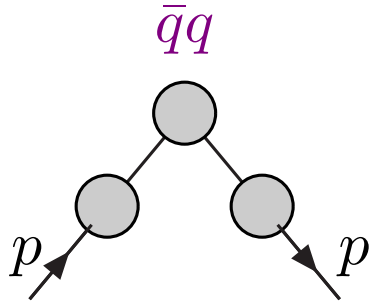
- $\Rightarrow$ *Non-perturbative renormalisation*

A General Method for Nonperturbative Renormalisation of Lattice Operators
G.Martinelli, C.Pittori, CTS, M.Testa and A.Vladikas Nuclear Physics B445 (1995) 81

- There are finite operators, such as V_μ and A_μ whose normalisation is fixed by Ward Identities (also Z_S/Z_P).
- Consider an operator O, which depends on the scale a, but which does not mix under renormalization with other operators:

$$O_R(\mu) = Z_O(\mu a)\, O_{\rm Latt}(a)\,.$$

  The task is to determine Z_O .
- In the Rome-Southampton RI-Mom scheme, we impose that the matrix element of the operator between parton states, in the Landau gauge say, is equal to the tree level value for some specified external momenta.
  - These external momenta correspond to the renormalisation scale.
- I will illustrate the idea by considering the scalar density $S = \bar{q}q$.
  - Since $m_q(\bar{q}q)$ does not need renormalization, $Z_m Z_S = 1$, so from the determination of Z_S we obtain Z_m.



(i) Fix the gauge (to the Landau gauge say).

(ii) Evaluate the unamputated Green function:

$$G(x,y) = \langle 0 \,|u(x)\,[\bar{u}(0)d(0)]\,\bar{d}(y)\,|\,0\rangle$$

and Fourier transform to momentum space, at momentum p as in the diagram,
$\Rightarrow\ G(p)$.

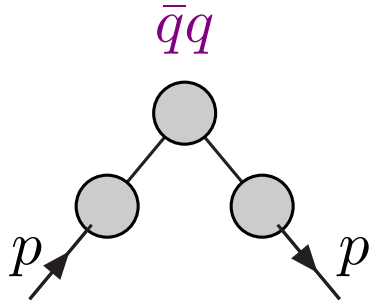
(iii) Amputate the Green function:

$$\Pi^{ij}_{S,\alpha\beta}(p) = S^{-1}(p)\,G(p)\,S^{-1}(p)\,,$$

where α,β (i,j) are spinor (colour) indices.
At tree level $\Pi^{ij}_{\alpha\beta}(p) = \delta_{\alpha\beta}\,\delta^{ij}$ and it is convenient to define

$$\Lambda_S(p) = \frac{1}{12}\,\mathrm{Tr}\,[\Pi_S(p)\,I]\,,$$

so that at tree-level $\Lambda_S = 1$.



- So far we have calculated the amputated Green function, in diagrammatic language, we have calculated the one-particle irreducible vertex diagrams.
- In order to determine the renormalization constant we need to multiply by $\sqrt{Z_q}$ for each external quark (i.e. there are two such factors).

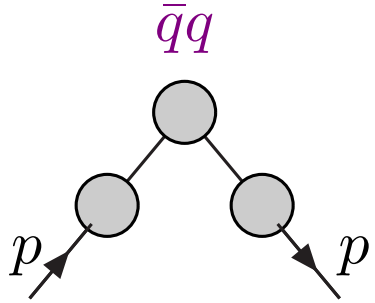
(iv) We now evaluate Z_q. There are a number of ways of doing this, perhaps the best is to use the non-renormalization of the conserved vector current:

$$Z_q \Lambda_{V_C} = 1 \quad \text{where} \quad \Lambda_{V_C} = \frac{1}{48} \mathrm{Tr} \left[\Pi_{V_C^\mu}(p) \gamma^\mu \right].$$

- This is equivalent to the definition

$$Z_q = -\frac{i}{48} \mathrm{tr} \left(\gamma_\rho \frac{\partial S^{-1}_{\mathrm{latt}}}{\partial p_\rho} \right)$$

at $p^2 = \mu^2$.



- We now have all the ingredients necessary to impose the renormalization condition. We define the renormalized scalar density S_R by $S_R(\mu) = Z_S(\mu a) S_{\rm Latt}(a)$ where

$$Z_S \frac{\Lambda_S(p)}{\Lambda_{V_C}(p)} = 1\,,$$

  for $p^2 = \mu^2$.
- The scalar density has a non-zero anomalous dimension and therefore Z_S depends on the scale μ.
- The renormalization scheme here is a MOM scheme. We called it the RI-MOM scheme, where the RI stands for *Regularization Independent* to underline the fact that the renormalized operators do not depend on the bare theory (i.e. the lattice theory).

- For any renormalisation method we require a delicate window for the momenta, ideally:

$$p \gg \Lambda_{\rm QCD} \qquad \text{and} \qquad p \ll a^{-1} \, .$$

- $p \gg \Lambda_{\rm QCD}$ is required in order for perturbation theory to be applicable, so that the results can be combined with the Wilson Coefficient functions, or to translate the results into the $\overline{\rm MS}$ scheme.
- $p \ll a^{-1}$ to keep the lattice artefacts small.
- *Step Scaling*, which we won't discuss today, allows us, in principle, to relax the first condition, $p \gg \Lambda_{\rm QCD}$.
  - The method has been used by a number of the large collaborations, including RBC/UKQCD.
- One, unattractive feature however, is that we need to fix the gauge. When considering operator mixing, we have to consider non-gauge invariant (but BRST invariant) operators.

- The RI-Mom Scheme was defined at an *exceptional* momentum, i.e. with a channel with a small (zero) momentum.
  Thus the matrix elements carry information about the physical mass spectrum which is unaccessible to perturbation theory.
- Although we showed in the RS paper that these non-perturbative effects are suppressed by powers of p^2, there is growing evidence that they present a numerical contamination which, as we strive for greater precision, should be evaluated.
- An extreme example is the pseudoscalar density where there are non-perturbative effects of the form

$$\frac{\langle 0|\bar{\psi}\psi|0\rangle}{mp^2}$$

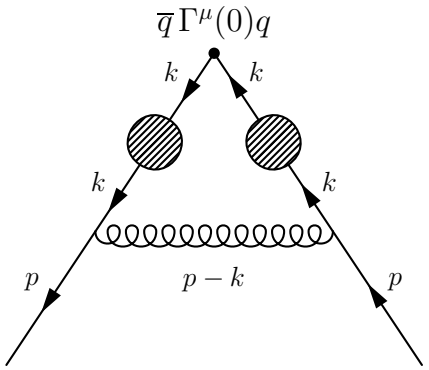
so that it is not possible to go to the chiral limit.

Giusti and Vladikas suggest taking combinations such as

$$\frac{m_1\Lambda_P(m_1) - m_2\Lambda_P(m_2)}{m_1 - m_2}\,.$$

Nonperturbative renormalization of quark bilinears and B_K using domain wall fermions

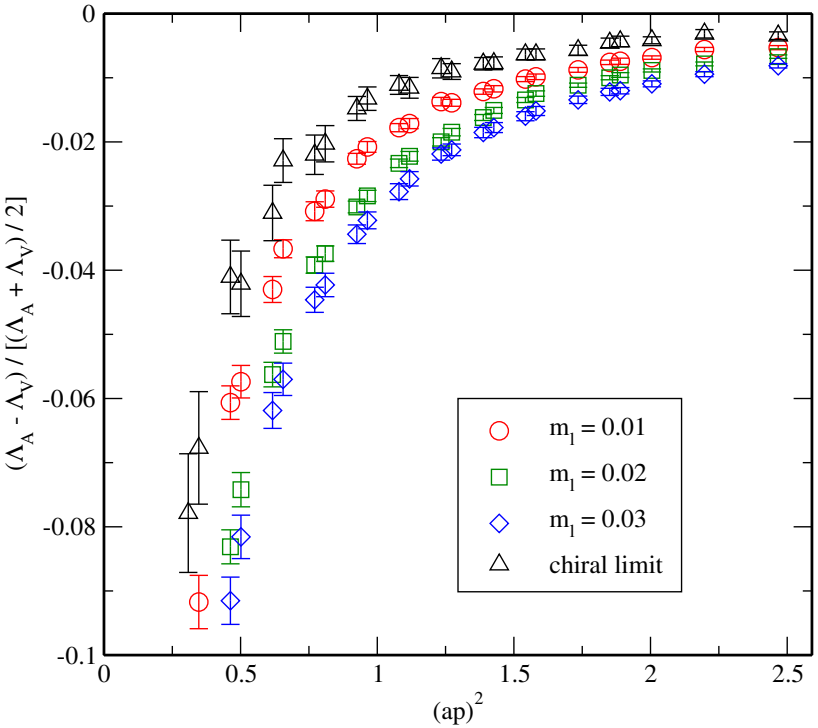
RBC-UKQCD, Y.Aoki, et al., arXiv:0712.1061

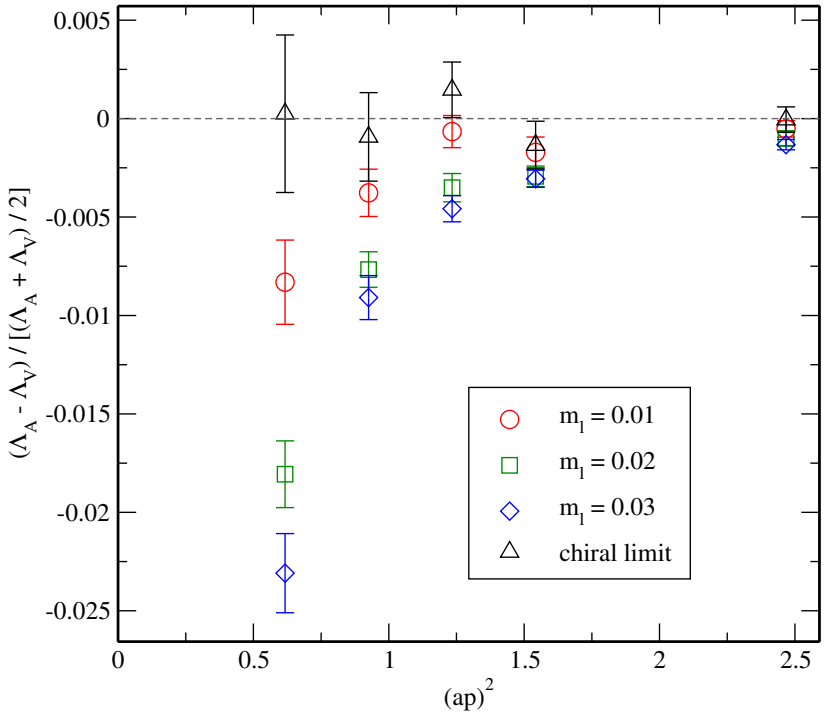


- One can imagine routing the large momentum p through the gluon to obtain

$$\frac{m^2}{p^2} \quad \text{or} \quad \frac{m\langle\bar{q}q\rangle}{p^4}$$

contributions.

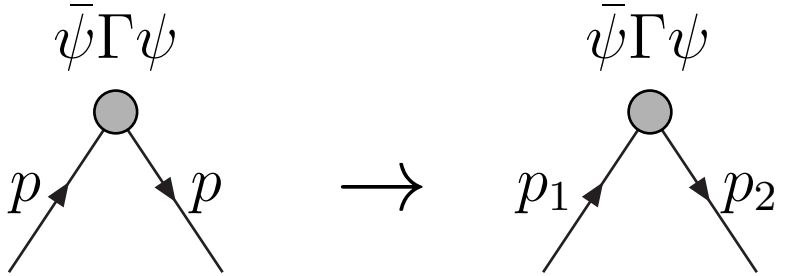




Both panels show $\dfrac{2(\Lambda_V - \Lambda_A)}{\Lambda_V + \Lambda_A}$ as a function of p^2.

- LH panel is for exceptional momenta whereas the RH panel is from an exploratory study with $p_1^2 = p_2^2 = p^2$ (RI-SMOM).

Renormalization of quark bilinear operators in a MOM-scheme with a non-exceptional subtraction point
C.Sturm, Y.Aoki, N.H.Christ, T.Izubuchi, CTS, and A.Soni; arXiv:0901.2599 [hep-ph]



$$p_1^2 = p_2^2 = (p_1 - p_2)^2$$

- In this paper we develop the scheme with the non-exceptional subtraction point

$$p_1^2 = p_2^2 = (p_1 - p_2)^2 .$$

- We calculate the one-loop conversion factors between this scheme and the $\overline{\rm MS}$ scheme. This is entirely a continuum exercise.

- An important requirement is that the chiral Ward Identities are satisfied by the renormalized quantities.
- The wave-function renormalization is fixed by imposing the RI′-MOM condition

$$\frac{1}{12p^2}\mathrm{tr}[S_R^{-1}(p)\ \not{p}] = -1\,.$$

The definition of S differs by factors of i w.r.t. the Rome-Southampton paper.

- The renormalization conditions on S and P are

$$\frac{1}{12}\mathrm{tr}[\Lambda_{P,R}(p_1,p_2)] = 1 \quad \text{and} \quad \frac{1}{12i}\mathrm{tr}[\Lambda_{P,R}(p_1,p_2)\gamma_5] = 1\,.$$

These conditions respect the chiral symmetry between S and P (e.g. the matching factors to $\bar{\mathrm{MS}}$ are the same.

- In order to preserve the WI, and in particular that $m\bar{\psi}\psi$ remains unrenormalized, we impose the mass renormalization condition

$$\frac{1}{12m_R}\mathrm{tr}[S_R^{-1}(p)] = 1 + \frac{1}{24m_R}\mathrm{tr}[q_\mu \Lambda^\mu_{A,R}(p_1,p_2)\gamma_5]\,.$$

- For the vector and axial currents the normalization conditions are:

$$\frac{1}{12q^2}\mathrm{tr}[q_\mu \Lambda^\mu_{V,R}(p_1,p_2)\ \not{q}] = 1 \quad \text{and} \quad \frac{1}{12q^2}\mathrm{tr}[q_\mu \Lambda^\mu_{A,R}(p_1,p_2)\gamma_5\ \not{q}] = 1\,.$$

  With these conditions the vector and axial currents satisfy the WI.
- The validity of the Ward Identities is demonstrated explicitly at one-loop order.
- For the tensor current there are no WI to satisfy and we simply impose

$$\frac{1}{144}Tr[\Lambda^{\mu\nu}_{T,R}\sigma_{\mu\nu}] = 1\,.$$

- Using the RI-MOM scheme we find that we are left with a large error in our value of the quark masses due to the uncertainty in the conversion from RI-MOM to $\overline{\text{MS}}$.

$$C_m(\text{RI/MOM} \to \overline{\text{MS}}) = 1 - 4\frac{\alpha_s}{4\pi}C_F + O(\alpha_s^2) = 1 + 12\% + 7\% + 6\% + \ldots$$

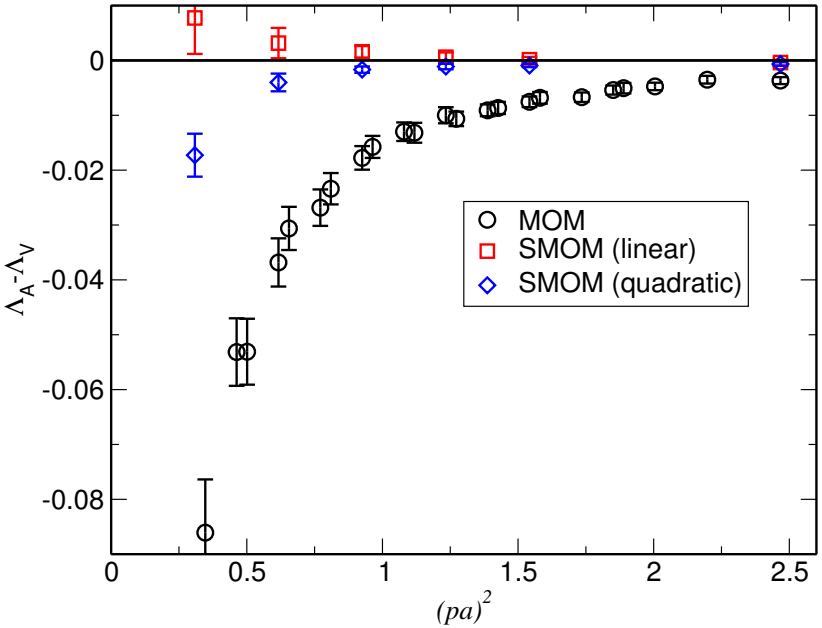
  Why?

- With the RI-SMOM scheme we only know the one-loop result

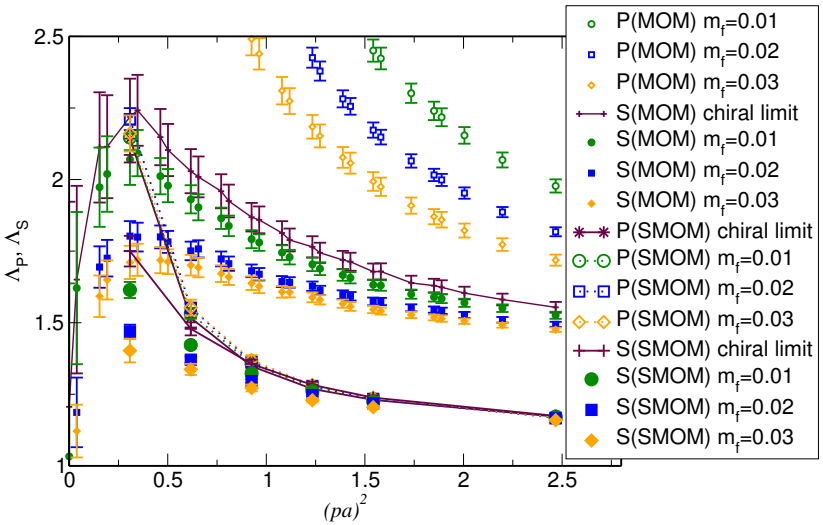
$$C_m(\text{RI/SMOM} \to \overline{\text{MS}}) = 1 - 0.484\frac{\alpha_s}{4\pi}C_F + O(\alpha_s^2) = 1 + 1.5\% + \ldots$$

  Is this an accident or evidence that the convergence is better.

Evidence for small chiral symmetry breaking



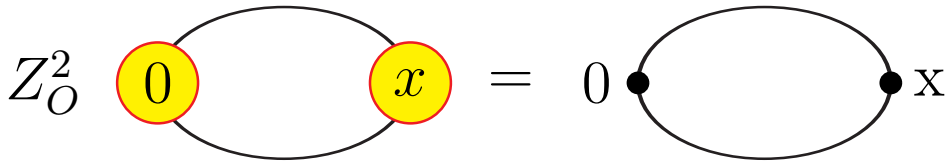
- $\Lambda_A - \Lambda_V$.



- Λ_S and Λ_P.

Y.Aoki arXiv:0901.2595 [hep-lat]

- In my view, we should investigate the best way to perform NPR in a gauge invariant way.
- One possibility is to compute correlation functions at short distances in configuration space and require that the renormalised operators give the lowest order perturbative contribution.



where the yellow circles represent the insertion of the lattice operator $O_{\rm Latt}$ and the right-hand diagram represents the lowest-order diagram in perturbation theory.

- The renormalization scale is now $1/|x|$, and the same constraints on the values of $1/x^2$ hold here as for the momenta in the RI-Mom scheme.
- The Alpha collaboration (and others) has been implementing a gauge invariant NPR, based on the use of the Schrödinger Functional.

One last point!

- Since we cannot perform simulations with lattice spacings $< 1/M_W$ or $1/m_t$ we exploit the standard technique of the Operator Product Expansion and write schematically:

$$\text{Physics} = \sum_i C_i(\mu) \times \langle f|O_i(\mu)|i\rangle \,.$$

- Until recently, the (perturbative) Wilson coefficients $C_i(\mu)$ were typically calculated with much greater precision than our knowledge of the matrix elements.
  - The C_i are typically calculated in schemes based on dimensional regularisation (such as $\overline{\text{MS}}$) which are intrinsically perturbative.
  - We can compute the matrix elements non-perturbatively, with the operators renormalised in schemes which have a non-perturbative definition (such as RI-MOM schemes) but not in purely perturbative schemes based on dim.reg.

  G.Martinelli, C.Pittori, CTS, M.Testa and A.Vladikas, hep-lat/9411010

- Thus the determination of the C_i in $\overline{\text{MS}}$-like schemes is not the complete perturbative calculation. Matching between $\overline{\text{MS}}$ and non-perturbatively defined schemes must also be performed.
  - This is beginning to be done.
  - We are now careful to present tables of matrix elements of operators renormalized in RI-MOM schemes, which can be used to gain better precision once improved perturbative calculations are performed.

Quantity	■	N_f=2+1+1	■	$N_f = 2+1$	■	$N_f = 2$
m_s(MeV)	2	93.9(1.1)	5	92.0(2.1)	2	101(3)
m_{ud}(MeV)	1	3.70(17)	5	3.373(80)	1	3.6(2)
m_s/m_{ud}	2	27.30(34)	4	27.43(31)	1	27.3(9)
m_d(MeV)	1	5.03(26)	Flag(4)	4.68(14)(7)	1	4.8(23)
m_u(MeV)	1	2.36(24)	Flag(4)	2.16(9)(7)	1	2.40(23)
m_u/m_d	1	0.470(56)	Flag(4)	0.46(2)(2)	1	0.50(4)
m_c/m_s	3	11.70(6)	2	11.82	1	11.74
$f_+^{K\pi}(0)$	1	0.9704(24)(22)	2	0.9667(27)	1	0.9560(57)(62)
f_{K^+}/f_{π^+}	3	1.193(3)	4	1.192(5)	1	1.205(6)(17)
f_K(MeV)	3	155.6(4)	3	155.9(9)	1	157.5(2.4)
f_π(MeV)			3	130.2(1.4)		
$\Sigma^{\frac{1}{3}}$(MeV)	1	280(8)(15)	4	274(3)	4	266(10)
F_π/F	1	1.076(2)(2)	5	1.064(7)	4	1.073(15)
$\bar{\ell}_3$	1	3.70(7)(26)	5	2.81(64)	3	3.41(82)
$\bar{\ell}_4$	1	4.67(3)(10)	5	4.10(45)	2	4.51(26)
$\hat{B}_K$	1	0.717(18)(16)	4	0.7625(97)	1	0.727(22)(12)

Outline of talk

1. Brief introduction to lattice QCD simulations
2. Brief introduction to the Operator Product Expansion
3. Renormalization
4. Finite-volume effects

- Let $f(p^2)$ be a smooth function. For a sufficiently large L:

$$\frac{1}{L}\sum_n f(p_n^2) = \int \frac{dp}{2\pi} f(p^2)\,,$$

  where $p_n = (2\pi/L)\,n$ and the relation holds "locally".

- In actual lattice calculations the spacing between momenta are $O(\text{few}\,100\,\text{MeV})$ so we would not expect such a local relation to be sufficiently accurate.
- However using the Poisson summation formula:

$$\sum_{n=-\infty}^{\infty} \delta(x-n) = \sum_{n=-\infty}^{\infty} \exp(2\pi i n x)$$

  we obtain the powerful exact relation

$$\frac{1}{L}\sum_{n=-\infty}^{\infty} f(p_n^2) = \int_{-\infty}^{\infty} \frac{dp}{2\pi} f(p^2) + \sum_{n\neq 0} \int_{-\infty}^{\infty} \frac{dp}{2\pi} f(p^2) e^{inpL}\,,$$

  which implies that

$$\boxed{\frac{1}{L}\sum_n f(p_n^2) = \int_{-\infty}^{\infty} \frac{dp}{2\pi} f(p^2)\,,}$$

  up to exponentially small corrections in L.
  - In our approach, this is the starting point for all calculations of FV effects.

$$\frac{1}{L}\sum_{n=-\infty}^{\infty} f(p_n^2) = \int_{-\infty}^{\infty}\frac{dp}{2\pi}\, f(p^2) + \sum_{n\neq 0}\int_{-\infty}^{\infty}\frac{dp}{2\pi}\, f(p^2)e^{inpL},$$

Consider a term with $n > 0$:

$$\begin{aligned}\int \frac{dp}{2\pi}\,\frac{e^{inpL}}{p^2+m^2} &= \int \frac{dp}{2\pi}\,\frac{e^{inpL}}{(p+im)(p-im)} \\ &= \frac{1}{2m}e^{-nmL}\end{aligned}$$

- Note that the finite-volume corrections are much smaller than would be expected from density of states arguments.
- The exponentially small FV corrections can also frequently be estimated using Chiral Perturbation Theory.

If the function $f(p^2)$ has no singularities on the real axis, then the Poisson-Summation formula implies that

$$\frac{1}{L}\sum_n f(p_n^2) = \int_{-\infty}^{\infty} \frac{dp}{2\pi} f(p^2)\,,$$

up to terms which are exponentially small in L.

Numerical Examples:

$f(p^2)$	Sum ($L=32$)	Integral	Difference
e^{-p^2}	0.282095	0.282095	$O(10^{-10})$
$e^{-p^2/16}$	1.12838	1.12838	$O(10^{-12})$
$e^{-(p/(2\pi/L))^2}$	0.0553949	0.0553892	$O(5\times 10^{-6})$
$\frac{1}{p^2+1}$	0.5	0.5	0
$\frac{1}{p^2+(2\pi/L)^2}$	2.55601	2.54648	$O(10^{-2})$

- Note that the contribution to the sum from the term with $p_n = 0$ is 1/32=0.031 for all the Gaussians and yet the sum approximates the integral very well.
- In the last row the contribution from the term with $p_n = 0$ is 0.81.

When there is a singularity the summation formula has a correction term. For example:

$$\frac{1}{L}\sum_n \frac{f(p_n^2)}{k^2-p_n^2} = \mathscr{P}\int_{-\infty}^{\infty}\frac{dp}{2\pi}\,\frac{f(p^2)}{k^2-p^2} + \frac{f(k^2)\cot(kL/2)}{2k}\,.$$

(This is the one-dimensional version of the key ingredient in the Lüscher quantisation formula.)

Numerical Examples:

$f(p^2)$	$k/(2\pi/L)$	Sum ($L=32$)	Integral	cot term	Difference
e^{-p^2}	0.5	0.560578	0.560578	0	$O(10^{-12})$
e^{-p^2}	0.4	2.61766	0.561875	2.05578	$O(10^{-12})$
$e^{-(p/(2\pi/L))^2}$	0.5	2.43916	2.43915	0	$O(10^{-5})$
$e^{-(p/(2\pi/L))^2}$	0.4	4.34832	2.58565	1.76266	$O(10^{-5})$

- The contribution from the single term at $p_n = 0$ for $k = 0.4\,(2\pi/L)$ is about 5.
- The optimal choice of volume appears to be $L = \pi/k$!

- These are based on the Poisson summation formula:

$$\frac{1}{L}\sum_{n=-\infty}^{\infty} f(p_n^2) = \int_{-\infty}^{\infty}\frac{dp}{2\pi}\,f(p^2) + \sum_{n\neq 0}\int_{-\infty}^{\infty}\frac{dp}{2\pi}\,f(p^2)e^{inpL},$$

- For single-hadron states the finite-volume corrections decrease exponentially with the volume $\propto e^{-m_\pi L}$. For multi-hadron states, the finite-volume corrections generally fall as powers of the volume.
- For two-hadron states, there is a huge literature following the seminal work by Lüscher and the effects are generally understood.
  - The spectrum of two-pion states in a finite volume is given by the scattering phase-shifts. M. Luscher, Commun. Math. Phys. 105 (1986) 153, Nucl. Phys. B354 (1991) 531.
  - The $K \to \pi\pi$ amplitudes are obtained from the finite-volume matrix elements by the Lellouch-Lüscher factor which contains the derivative of the phase-shift. L.Lellouch & M.Lüscher, hep-lat/:0003023, C.h.Kim, CTS & S.R.Sharpe, hep-lat/0507006 $\cdots$
  - Recently we have also determined the finite-volume corrections for $\Delta m_K = m_{K_L} - m_{K_S}$. N.H.Christ, X.Feng, G.Martinelli & CTS, arXiv:1504.01170
- For three-hadron states, there has been a major effort by Hansen and Sharpe leading to much theoretical clarification.

M.Hansen & S.Sharpe, arXiv:1408.4933, 1409.7012, 1504.04248

- In this talk I have sketched some of the theoretical framework which enables us to extract physical quantities in flavour physics or hadronic structure from simulations of lattice QCD.