Flavour Physics – Lecture 2

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1. Lecture 1: Introduction to Flavour Physics
2. Lecture 2: Lattice Computations in Flavour Physics
   1. Correlation Functions
   2. Inversions of the Dirac Operator
   3. The Scaling Trajectory
   4. Determination of Quark Masses
   5. Comment on the use of Perturbation Theory
   6. Towards Lattice Phenomenology - Leptonic and Semileptonic Decays
   7. (Partially) Twisted Boundary Conditions
3. Lecture 3: Light-quark physics
4. Lecture 4: Heavy-quark physics

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

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

  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:

$$Z = \int [dA_\mu]\,[d\psi]\,[d\bar\psi]\,e^{iS}\ .$$

- These formulae are written in Minkowski space, whereas Lattice calculations are performed in Euclidean space $(\exp(iS) \to \exp(-S)$ etc.).
- The physics which can be studied depends on the choice of the multilocal operator O.
- The functional integral is performed by discretising space-time and using Monte-Carlo Integration.

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Consider two-point correlation functions of the form:

$$C_2(t) = \int d^3x\, e^{i\vec{p}\cdot\vec{x}}\, \langle 0|\, J(\vec{x},t)\, J^\dagger(\vec{0},0)\, |0\rangle \;,$$

where J and $J^\dagger$ are any interpolating operators for the hadron H which we wish to study and the time t is taken to be positive.

- We assume that H is the lightest hadron which can be created by $J^\dagger$.
- We take $t > 0$, but it should be remembered that lattice simulations are frequently performed on periodic lattices, so that both time-orderings contribute.

Two-Point Correlation Functions (Cont.)

$$C_2(t) = \int d^3x\, e^{i\vec{p}\cdot\vec{x}}\, \langle 0|\, J(\vec{x},t)\, J^\dagger(\vec{0},0)\, |0\rangle\ ,$$

Inserting a complete set of states $\{|n\rangle\}$:

$$\begin{aligned} C_2(t) &= \sum_n \int d^3x\, e^{i\vec{p}\cdot\vec{x}}\, \langle 0|\, J(\vec{x},t)\, |n\rangle\, \langle n| J^\dagger(\vec{0},0)\, |0\rangle \\ &= \int d^3x\, e^{i\vec{p}\cdot\vec{x}}\, \langle 0|\, J(\vec{x},t)\, |H\rangle\, \langle H| J^\dagger(\vec{0},0)\, |0\rangle + \cdots \end{aligned}$$

where the $\cdots$ represent contributions from heavier states with the same quantum numbers as H.

Finally using translational invariance:

$$C_2(t) = \frac{1}{2E}\, e^{-iEt} \left| \langle 0| J(\vec{0},0) |H(p)\rangle \right|^2 + \cdots\ ,$$

where $E = \sqrt{m_H^2 + \vec{p}^{\,2}}$.

Two-Point Correlation Functions (Cont.)

$$C_2(t) = \frac{1}{2E}\, e^{-iEt} \left| \langle 0|J(\vec{0},0)|H(p)\rangle \right|^2 + \cdots \;.$$

- In Euclidean space $\exp(-iEt) \to \exp(-Et)$.
- 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 $J = \bar{u}\gamma^\mu\gamma^5 d$ then the decay constant of the π-meson can be evaluated,

  $$\left| \langle 0|\,\bar{u}\gamma^\mu\gamma^5 d\,|\pi^+(p)\rangle \right| = f_\pi\, p^\mu \;,$$

  (the physical value of $f_\pi \simeq$ is 132 MeV).

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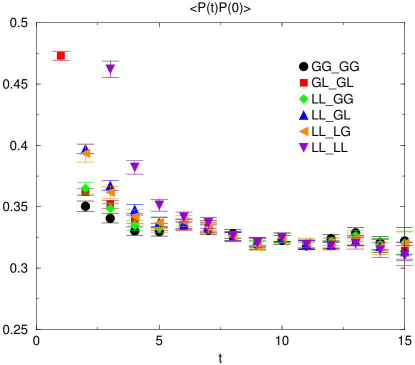
At zero momentum

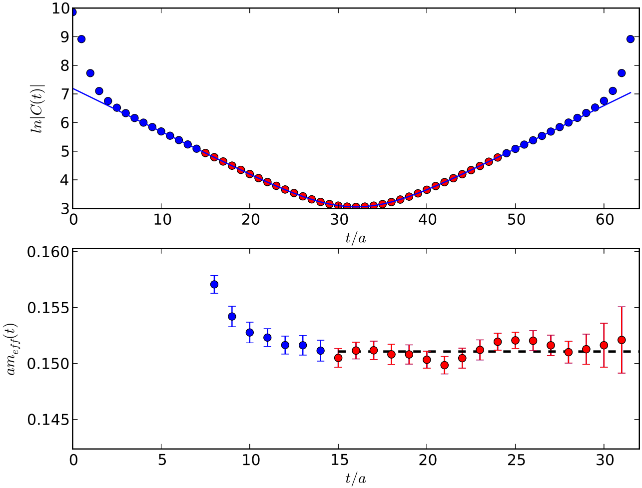
$$C_2(t) = \text{Constant} \times e^{-mt}$$

so that it is sensible to define the *effective mass*

$$m_{\text{eff}}(t) = \log\left(\frac{C(t)}{C(t+1)}\right).$$



Effective Mass Plot for a Pseudoscalar Meson. UKQCD Collaboration.

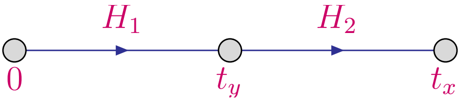


- Kaon correlation function and effective mass from RBC-UKQCD's simulation on a $32^3 \times 64$ DWF lattice with $a^{-1} = 2.28\,$GeV.

Consider now a three-point correlation function of the form:

$$C_3(t_x,t_y) = \int d^3x\, d^3y\; e^{i\vec{p}\cdot\vec{x}}\; e^{i\vec{q}\cdot\vec{y}}\; \langle 0|\, J_2(\vec{x},t_x)\, O(\vec{y},t_y)\, J_1^\dagger(\vec{0},0)\,|0\rangle\;,$$

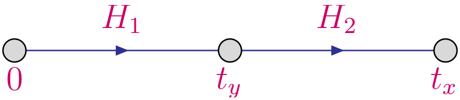
where $J_{1,2}$ may be interpolating operators for different particles and we assume that $t_x > t_y > 0$.



For sufficiently large times t_y and $t_x - t_y$

$$C_3(t_x,t_y) \simeq \frac{e^{-E_1 t_y}}{2E_1}\,\frac{e^{-E_2(t_x-t_y)}}{2E_2}\,\langle 0|J_2(0)|H_2(\vec{p})\rangle$$
$$\times\langle H_2(\vec{p})|O(0)|H_1(\vec{p}+\vec{q})\rangle\;\langle H_1(\vec{p}+\vec{q})|J_1^\dagger(0)|0\rangle\;,$$

where $E_1^2 = m_1^2 + (\vec{p}+\vec{q})^2$ and $E_2^2 = m_1^2 + \vec{p}^{\,2}$.



- From the evaluation of two-point functions we have the masses and the matrix elements of the form $|\langle 0|J|H(\vec{p})\rangle|$. Thus, from the evaluation of three-point functions we obtain matrix elements of the form $|\langle H_2|O|H_1\rangle|$.
- Important examples include:
  - $K^0-\bar{K}^0$ ($B^0-\bar{B}^0$) mixing. In this case

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

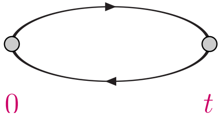
  - Semileptonic and rare radiative decays of hadrons of the form $B\to\pi,\rho+$leptons or $B\to K^*\gamma$. Now O is a quark bilinear operator such as $\bar{b}\gamma^\mu(1-\gamma^5)u$ or an *electroweak penguin* operator.

Calculating Correlation Functions

- Imagine that we have generated a set of N gluon configurations $\{U_\mu(x)\}$ corresponding to some lattice action.
- In order to calculate the correlation functions we need to determine quark propagators $\{S^{ij}_{\alpha\beta}(x,y)\}$ corresponding to each configuration.
  - α, β are spinor labels (α, β=1,2,3,4).
  - i,j are colour labels (i,$j = 1,2,3$).
  - x, y are points on the lattice.
- As a simple example imagine that we want to evaluate the correlation function:

$$C(t) = \sum_{\vec{x}} \langle 0 \,|\, \phi(\vec{x},t)\, \phi^\dagger(\vec{0},0) \,|\, 0 \rangle \,,$$

where ϕ is a pseudoscalar density $\phi(x) = \bar{d(x)}\gamma^5 u(x)$.



$$C(t) = -\sum_{\vec{x}} \mathrm{Tr}\,\{S((\vec{x},t),(\vec{0},0))\,\gamma^5\, S((\vec{0},0),(\vec{x},t))\,\gamma^5\} \,.$$

- To evaluate the propagators we have to *invert* huge sparse matrices, solving

$$D^{ik}_{\alpha\gamma}(x,z)S^{kj}_{\gamma\beta}(z,y)=\delta_{xy}\delta^{ij}\delta_{\alpha\beta}\,,$$

  where D is the Dirac operator.

- This equation is of the form $M\cdot S=I$ where M and S are matrices. The standard algorithms (e.g. Conjugate Gradient) solve instead

$$M\cdot v=b\,,$$

  where the vector v is the solution and b is a given vector. In this was we obtain $S^{ij}_{\alpha\beta}(x,y)$ for single choices of j,β and y.

- To obtain the propagator for all values of j and β requires $3\times4=12$ such inversions (generally affordable).

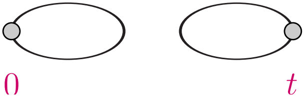
- To obtain the all-to-all propagators for all y requires $L^3\times T$ such inversions for each configuration. Not affordable without approximations.

- Thus we typically have the set of propagators $\{S(x,0)\}$, where I have put the *source* at the origin.

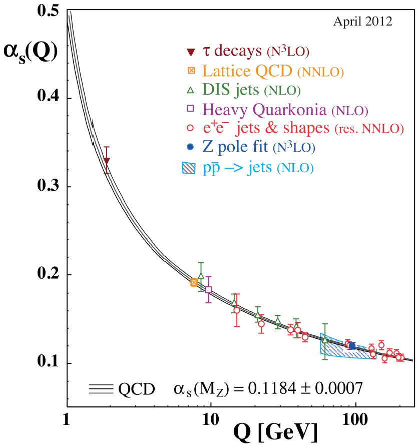
- γ^5*-Hermiticity:* $S(y,x)=\gamma^5\,S^\dagger(x,y)\,\gamma^5$.

Inversions (Side Remarks)

- For the purposes of this illustration I imagine solving $M \cdot S = I$, but for many applications it is necessary to solve $M \cdot S = B$, where B is a given matrix. Same techniques apply.
- It is advantageous to squeeze as much physics as possible from each configuration (volume averaging).
  - Having a point source is not in this spirit.
  - Other possible sources exist; e.g. gauge-fixed wall sources, Z_2 noise sources etc.
- Disconnected diagrams are a major difficulty. For example for the flavour-singlet meson we also have the diagram:



$$\mathscr{L}_{\rm QCD} = -\frac{1}{4} G_{\mu\nu} G^{\mu\nu} + \sum_{\text{flavours}, f} \bar{\psi}_f (i\not{D} - m_f) + \text{Gauge Fixing Term} + \text{Fadeev-Popov Ghost}$$



$$G^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + g f_{abc} A^b_\mu A^c_\nu$$
$$D_\mu = \partial_\mu - i g T_a A^a_\mu .$$

- QCD parameters, g and the quark masses, can only be fixed by using physical measurements.
- $\alpha_S(\mu)$ decreases logarithmically with the renormalization scale μ.
- Running of $\alpha_S(\mu) \Rightarrow$ given $g(\mu)$ we know μ; given μ we know $g(\mu)$.

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- In Lattice QCD, while it is natural to think in terms of the lattice spacing a, the input parameter is $\beta = 6/g^2(a)$.
- $g(a)$ is the bare coupling constant in the bare theory defined by the particular discretization of QCD used in the simulation. a^{-1} is the ultraviolet cut-off in momentum space.
- Imagine now that we are performing a simulation with $N_f = 2+1$ and that we are in an ideal world in which we can perform simulations with $m_{ud} = m_u = m_d$ around their “physical" values. The procedure for defining a physical scaling trajectory is then relatively simple.

The scaling trajectory (Cont.)

- At each β, choose 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
  $$a^{-1} = \frac{1.672\,\mathrm{GeV}}{m_\Omega(\beta, m_{ud}, m_s)}$$
  where $m_\Omega(\beta, m_{ud}, m_s)$ is the measured 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 different scaling 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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- Quark Masses are fundamental parameters of the Standard Model of Particle Physics:

$$\mathscr{L} = \sum_{k=1}^{N_F} \overline{q}_k (i \not{D} - m_k) q_k - \frac{1}{4} G_{\mu\nu} G^{\mu\nu} + \mathrm{GF} + \mathrm{FP}\,.$$

- Unlike the leptons, quarks are confined inside hadrons and are therefore not observed as physical particles ⇒ quark masses cannot be measured directly.
- Quark masses therefore have to be obtained indirectly through their influence on hadronic quantities.
- Any quantitative statement about the value of a quark mass must make careful reference to the theoretical framework that is used to define it ⇒ *renormalization scheme* and *renormalization scale* μ.

  The most commonly used renormalization scheme for QCD perturbation theory is the $\overline{\mathrm{MS}}$ scheme.

- Physics is independent of renormalization schemes and scales and in practice we need $\mu \gg \Lambda_{\rm QCD}$ so that the μ dependence in $m_q(\mu)$ can be determined in perturbation theory.

$$\mu^2 \frac{dm_q(\mu)}{d\mu^2} = -\gamma(\alpha_s(\mu))\, m_q(\mu)$$

The *anomalous dimension* γ is known to four-loop order of perturbation. theory

Vermaseren, Larin & van Ritbergen

Chetyrkin, Kniehl & Steinhauser

$$\gamma(\alpha_s) = \sum_{r=1}^{\infty} \gamma_r \left(\frac{\alpha_s}{4\pi}\right)^r$$

The coefficients $\gamma_1 - \gamma_4$ are known.

- (Here I imagine doing $N_F = 2+1$ simulations for illustration.)
- By *calibrating* the lattice, i.e. fixing $m_{ud}(a)$, $m_s(a)$ and a such that 3 physical quantities, e.g. m_π, m_K and m_Ω take their physical values, we know the value of the physical bare quark masses for our discretization of QCD.

$$m^{\overline{\text{MS}}}(\mu) = Z_m(a\mu)m^{\text{latt}}(a)$$

- In principle, for large a, μ we can obtain $m^{\overline{\text{MS}}}(\mu)$ from $m^{\text{latt}}(a)$ using perturbation theory, but
  - lattice perturbation theory frequently converges slowly;
  - higher order calculations in lattice perturbation theory are difficult to perform;
  - the precision of lattice calculations is such that Non-Perturbative Renormalization (NPR) is necessary. R.Sommer's Lectures
- We cannot perform simulations in $4+2\varepsilon$ dimensions and hence we have to perform NPR into an intermediate scheme and then use continuum perturbation perturbation theory to match the result onto that in the $\overline{\text{MS}}$ scheme.
- Step-scaling enables us to obtain the result in the intermediate scheme at larger values of μ and hence to decrease the uncertainty in the matching factor.

G. Colangelo et al., arXiv:1011.4408

$$\begin{aligned} m_{ud}^{\overline{\rm MS}}(2\,{\rm GeV}) &= 3.43 \pm 0.11\,{\rm MeV} \\ m_{s}^{\overline{\rm MS}}(2\,{\rm GeV}) &= 94 \pm 3\,{\rm MeV} \\ \frac{m_s}{m_{ud}} &= 27.4 \pm 0.4\,. \end{aligned}$$

- FLAG2 to appear soon.

Perturbation Theory - (slide shown at non-lattice conference)

- The precision of lattice calculations is now reaching the point where we need better interactions with the N^nLO QCD perturbation theory community.
- The traditional way of dividing responsibilities is:

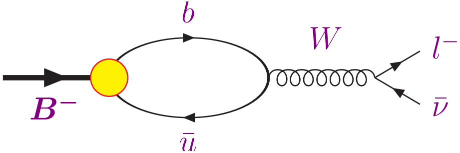
$$\text{Physics} \;=\; \underset{\substack{\uparrow \\ \text{Perturbative} \\ \text{QCD}}}{C} \;\times\; \underset{\substack{\uparrow \\ \text{Lattice} \\ \text{QCD}}}{\langle f\,|\,O\,|\,i\rangle}$$

- The two factors have to be calculated in the same scheme.
- Can we meet half way?

$$\begin{array}{c}\text{bare}\\ \text{lattice}\\ \text{operators}\end{array} \longrightarrow \;\textbf{?}\; \longleftarrow \begin{array}{c}\text{operators}\\ \text{renormalized}\\ \text{in } \overline{\text{MS}} \text{ scheme}\end{array}$$

- What is the best scheme for **?** (RI-SMOM, Schrödinger Functional, $\cdots$)?
- Recent examples of such collaborations following J.Gracey ...:
  - two-loop matching factor for m_q between the RI-SMOM schemes and $\overline{\text{MS}}$.
    M.Gorbahn and S.Jager, arXiv:1004:3997, L.Almeida and C.Sturm, arXiv:1004:4613
  - HPQCD + Karlsruhe Group in determination of quark masses.

- The difficulty in making predictions for weak decays of hadrons is in controlling the non-perturbative strong interaction effects.
- As a particularly simple example consider the leptonic decays of pseudoscalar mesons in general and of the B-meson in particular.



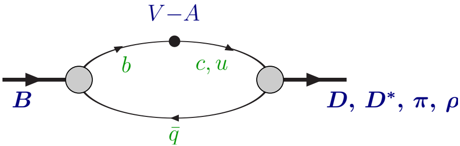
- Non-perturbative QCD effects are contained in the matrix element

$$\langle 0|\,\bar b\gamma^\mu(1-\gamma^5)u\,|B(p)\rangle\ .$$

- Lorentz Inv. + Parity $\Rightarrow\ \langle 0|\,\bar b\gamma^\mu u\,|B(p)\rangle = 0.$
- Similarly $\quad \langle 0|\,\bar b\gamma^\mu\gamma^5 u\,|B(p)\rangle = i f_B p^\mu\ .$

All QCD effects are contained in a single constant, f_B, the B-meson's *(leptonic) decay constant.* $(f_\pi \simeq 132\,\text{MeV})$

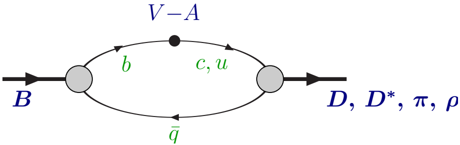
• These can be determined from either inclusive or exclusive decays. I start with a discussion of exclusive decays.



• Space-Time symmetries allow us to parametrise the non-perturbative strong interaction effects in terms of invariant form-factors. For example, for decays into a pseudoscalar meson P $(=\pi, D$ for example)

$$\langle P(k)|V^\mu|B(p)\rangle \;=\; f^+(q^2)\left[(p+k)^\mu - \frac{m_B^2-m_P^2}{q^2}\,q^\mu\right] + f^0(q^2)\,\frac{m_B^2-m_P^2}{q^2}\,q^\mu\,,$$

where $q = p - k$.



- For decays into a vector V $(=\rho, D^*$ for example), a conventional decomposition is

$$\langle V(k,\varepsilon)|V^\mu|B(p)\rangle = \frac{2V(q^2)}{m_B+m_V}\varepsilon^{\mu\gamma\delta\beta}\varepsilon^*_\beta p_\gamma k_\delta$$

$$\langle V(k,\varepsilon)|A^\mu|B(p)\rangle = i(m_B+m_V)A_1(q^2)\varepsilon^{*\mu} - i\frac{A_2(q^2)}{m_B+m_V}\varepsilon^*\cdot p\,(p+k)^\mu + i\frac{A(q^2)}{q^2}2m_V\varepsilon^*\cdot p\,q^\mu\ ,$$

where ε is the polarization vector of the final-state meson, and $q=p-k$.

$$\{A_3 = \frac{m_B+m_V}{2m_V}A_1 - \frac{m_B-m_V}{2m_V}A_2\ .\}$$

- It is usual to define the lattice theory with periodic boundary conditions for the fields

$$\phi(x_i+L)=\phi(x_i)\,.$$

This implies that components of momenta are quantized in units of $2\pi/L$.

- Example (one of our current simulations):

$$L=48a \quad \text{with} \quad a^{-1}=1.73\,\text{GeV} \quad \Rightarrow \quad \frac{2\pi}{L}=.225\,\text{GeV}$$

so that the available momenta for phenomenological studies (e.g. in the evaluation of form-factors) are limited.
(In addition we require pa to be small to avoid discretization errors.)

- Bedaque has advocated the use of twisted boundary conditions e.g.

$$q(x_i+L)=e^{i\theta_i}q(x_i)$$

so that the momentum spectrum is

$$p_i=n_i\frac{2\pi}{L}+\frac{\theta_i}{L}\,.$$

(Twist can be a matrix in flavour space, but action has to be single-valued.)

(Partially) Twisted Boundary Conditions (Cont.)

CTS and G.Villadoro, hep-lat/0411033

- Conclusion 1: For quantities which do not involve Final State Interactions (e.g. masses, decay constants, form-factors) the Finite-Volume corrections are exponentially small also with Twisted BC's.
- Conclusion 2: Moreover they are also exponentially small for *partially twisted boundary conditions* in which the sea quarks satisfy periodic BC's but the valence quarks satisfy twisted BC's $\Rightarrow$

We do not need to perform new simulations for every choice of $\{\theta_i\}$.

For example:

$$\frac{\Delta f_{K^\pm}}{f_{K^\pm}} \to \begin{cases} -\frac{9}{4}\frac{m_\pi^2}{f_\pi^2}\frac{e^{-m_\pi L}}{(2\pi m_\pi L)^{3/2}} & \text{(a)} \\ -\frac{m_\pi^2}{f_\pi^2}\frac{e^{-m_\pi L}}{(2\pi m_\pi L)^{3/2}}\left(\frac{1}{2}\sum_{i=1}^3 \cos\theta_i + \frac{3}{4}\right) & \text{(b)} \\ -\frac{m_\pi^2}{f_\pi^2}\frac{e^{-m_\pi L}}{(2\pi m_\pi L)^{3/2}}\left(\sum_{i=1}^3 \cos\theta_i - \frac{3}{4}\right) & \text{(c)} \end{cases}$$

d and s quarks satisfy periodic boundary conditions,
u quark is (a) untwisted, (b) fully twisted (c) partially twisted.

- The use of partially twisted boundary conditions opens up many interesting phenomenological applications.

It also works numerically!

  - Tests of the dispersion relation for pseudoscalars in the quenched approximation - de Divittis, Tantalo and Petronzio (2004)
  - Flynn, Juettner & CTS, using UKQCD $16^3 \times 32,\ N_F$=2 configurations:

$$L \simeq 1.7\,\mathrm{fm}, \quad a \simeq 0.1\,\mathrm{fm}, \quad \frac{m_\pi}{m_\rho} = 0.7,\ 0.57\ .$$

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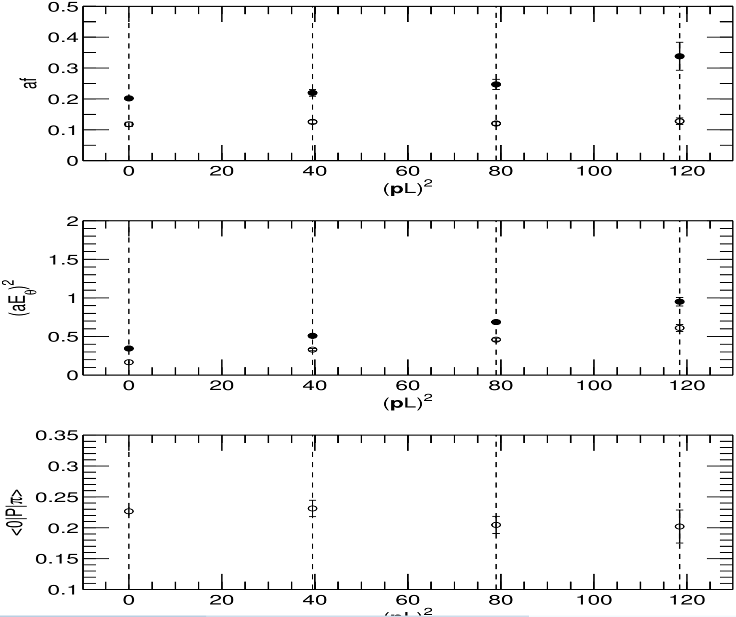

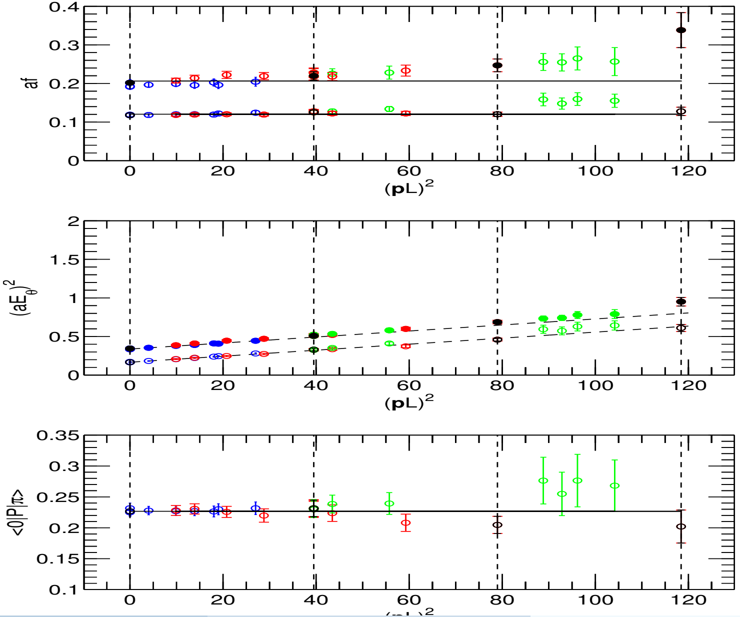

0.4
0.3
0.2
0.1
0
af
0
20
40
60
80
100
120
$(pL)^2$
2
1.5
1
0.5
0
$(aE_\theta)^2$
0
20
40
60
80
100
120
$(pL)^2$
0.35
0.3
0.25
0.2
0.15
0.1
<0|P|π>
0
20
40
60
80
100
120

(Partially) Twisted Boundary Conditions (cont.)

- Conclusion 3: For some amplitudes which involve final state interactions, it is not possible in general to extract the physical matrix elements using twisted boundary conditions (at least without new ideas).
- An important example: $K\to\pi\pi$ decays in the $I=0$ channel. The boundary conditions break isospin symmetry $\Rightarrow$ energy eigenstates are no longer states with definite I.
  - Consider the $\pi\pi$-state to be in the center of mass frame and let the u (d) quark satisfy twisted (periodic) boundary conditions.
  - In the free theory $\vec{p}_{\pi^0}=\vec{0}$ and $\vec{p}_{\pi^\pm}=\pm\vec{\theta}/L$. $\Rightarrow E_{\pi^0\pi^0}=2m_\pi$ and $E_{\pi^+\pi^-}=2\sqrt{m_\pi^2+\theta^2/L^2}$.
  - In the interacting theory $\pi^+\pi^-\leftrightarrow\pi^0\pi^0$ transitions complicate the analysis very significantly
    $\Rightarrow$ it is not possible to determine physical $K\to\pi\pi$ amplitudes using twisted boundary conditions with FV corrections under control.

Exercise - Finite Volume Effects in 1 Dimension

- 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 the approach developed with Steve and Changhoan Kim, this is the starting point for all calculations of FV effects.
- Calculate the leading finite-volume effects for

$$f(p^2) = \frac{1}{p^2 + m^2}\,.$$