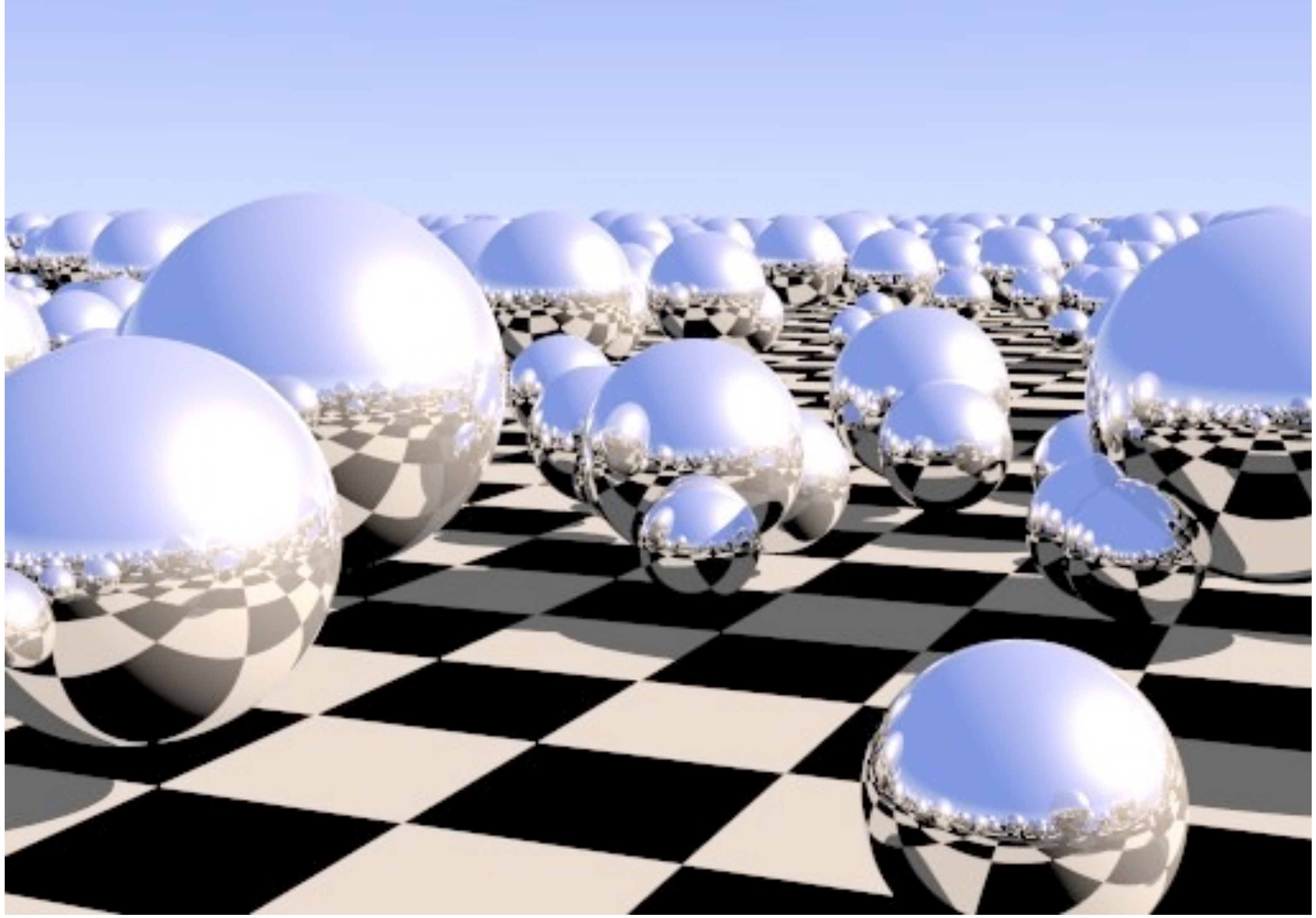


Many many mesons

William Detmold

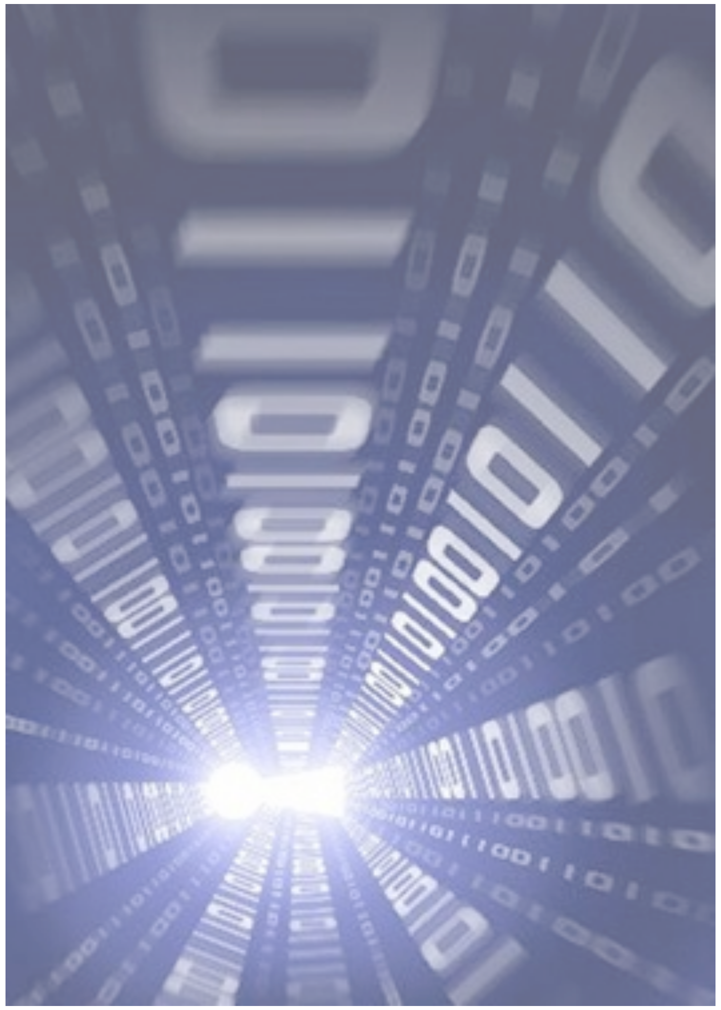
The College of William and Mary &
Thomas Jefferson National Accelerator Facility

Jefferson Lab

Extreme Computing and its Implications for the Nuclear Physics/Applied Mathematics/Computer Science Interface, INT, July 8th 2011

QCD @ the Exascale

- Goal: understanding nuclear physics from QCD
  - Multi hadron systems define nuclear physics
  - Complexity and precision frontier
- What do we want to know?
  - Spectra
  - Properties/matrix elements
  - Reactions



Nuclear physics from QCD

Nuclear physics from QCD

- Can we compute the mass of ^{208}Pb in QCD?

Nuclear physics from QCD

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$$\langle 0|T q_1(t) \ldots q_{624}(t) \overline{q}_1(0) \ldots \overline{q}_{624}(0)|0\rangle$$

Nuclear physics from QCD

- Can we compute the mass of ^{208}Pb in QCD?

$$\langle 0|T q_1(t) \ldots q_{624}(t) \overline{q}_1(0) \ldots \overline{q}_{624}(0)|0\rangle$$

- Long time behaviour gives ground state energy up to EW effects

$$\xrightarrow{t\to\infty} \# \exp(-M_{Pb} t)$$

Nuclear physics from QCD

- Can we compute the mass of ^{208}Pb in QCD?

$$\langle 0|T q_1(t)\ldots q_{624}(t)\overline{q}_1(0)\ldots\overline{q}_{624}(0)|0\rangle$$

- Long time behaviour gives ground state energy up to EW effects

$$\stackrel{t\to\infty}{\longrightarrow} \#\exp(-M_{Pb}t)$$

- But...

Nuclear physics from QCD

Nuclear physics from QCD

- Contractions: $(A+Z)!(2A-Z)!$

Nuclear physics from QCD

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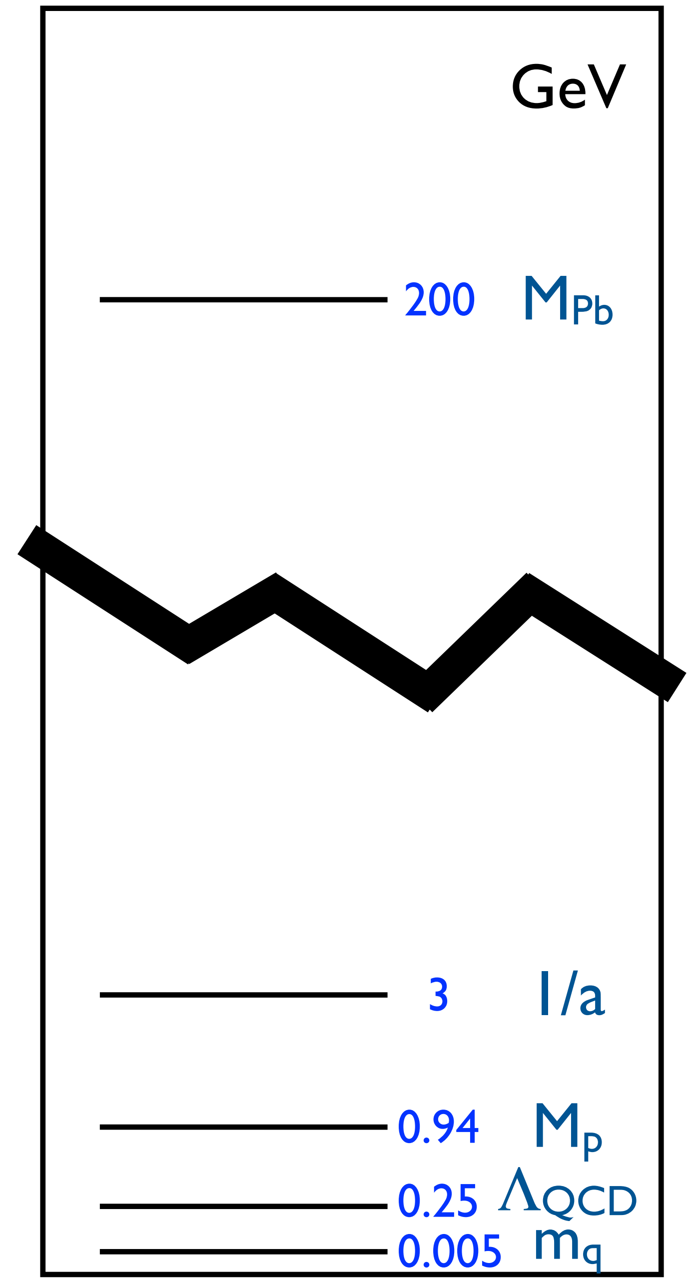
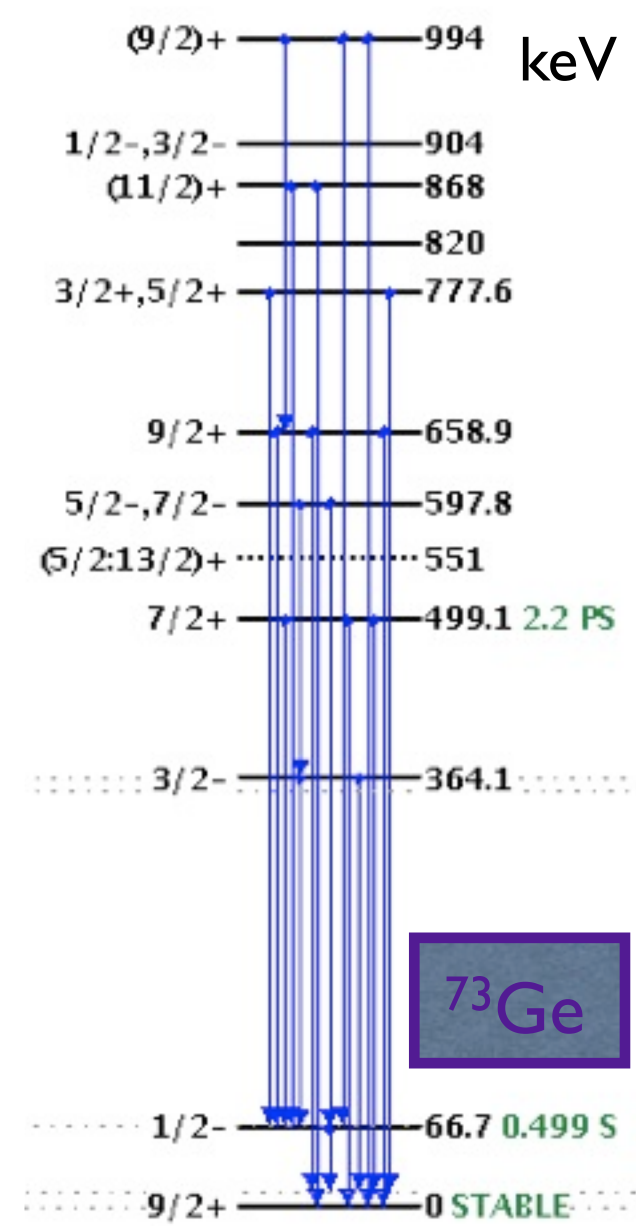
- Signals for very massive states (numerical precision)



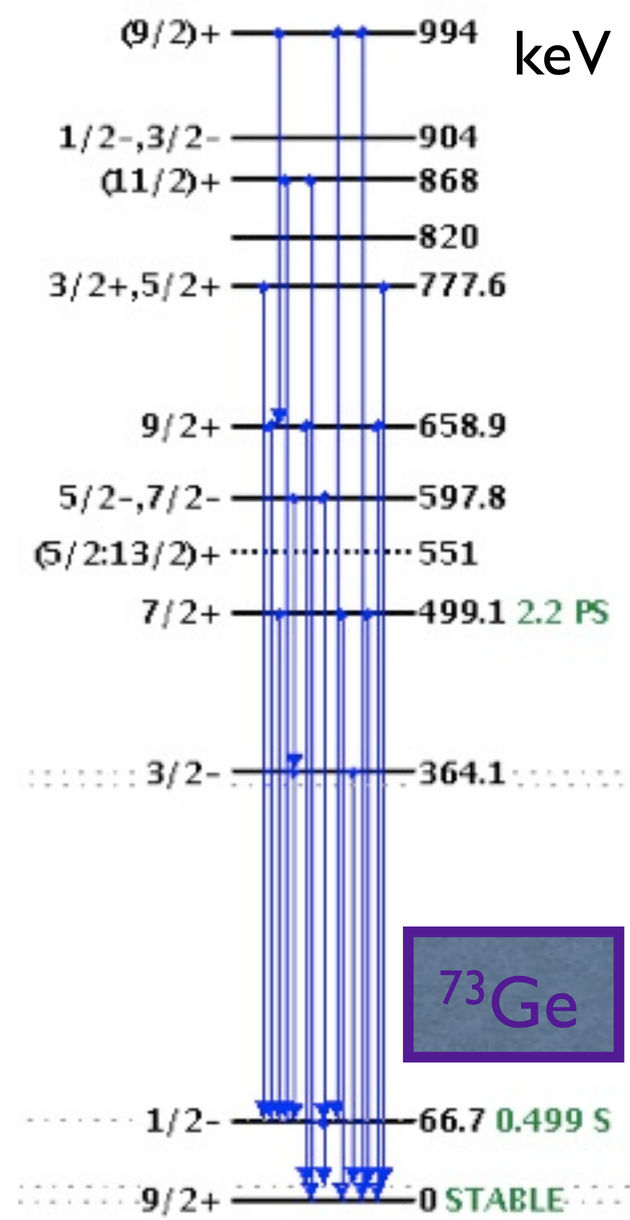
Nuclear physics from QCD

- Contractions: $(A+Z)!(2A-Z)!$
- Signals for very massive states (numerical precision)
- Small energy splittings



Nuclear physics from QCD

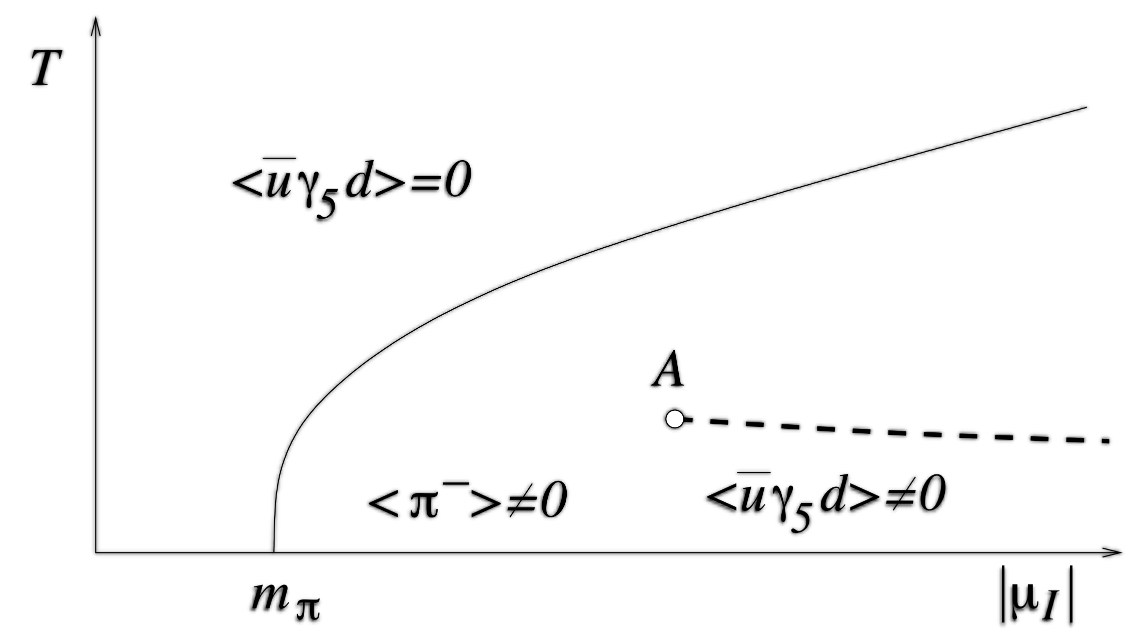
- Contractions: $(A+Z)!(2A-Z)!$
- Signals for very massive states (numerical precision)
- Small energy splittings
- Statistical noise: exponentially increases with A



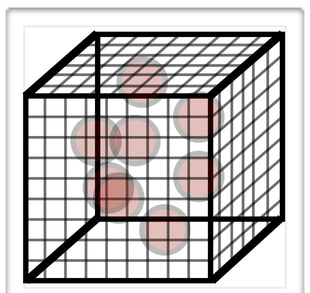
Many many mesons

- Many meson systems: a precursor to nuclei
- Meson condensates: interesting state of matter with a complex phase diagram
  - finite μ_I: BEC-BCS crossover
  - Vector condensation?

[Son & Stephanov]



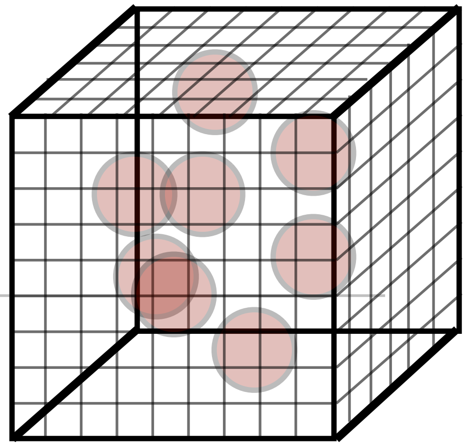
- Kaon condensation may be phenomenologically relevant in n-stars [Kaplan/Nelson]



Few meson (N<13) systems

Phys. Rev. Lett. 100:082004, 2008
Phys Rev D78:014507, 2008
Phys Rev D78:054514, 2008
Phys. Rev. Lett. 102:032004, 2009

Many boson systems



- Large volume expansion of ground state energy of n meson system to $1/L^7$
  - 2 & 3 body interactions (N body: $L^{-3(N-1)}$)
  - n=2: reproduces expansion of Lüscher

$$\Delta E_n = \frac{4\pi \overline{a}}{M\ L^3}\,{}^nC_2\left\{1 - \left(\frac{\overline{a}}{\pi\ L}\right)\mathcal{I} + \left(\frac{\overline{a}}{\pi\ L}\right)^2\left[\mathcal{I}^2 + (2n-5)\mathcal{J}\right] - \left(\frac{\overline{a}}{\pi\ L}\right)^3\left[\mathcal{I}^3 + (2n-7)\mathcal{I}\mathcal{J} + (5n^2-41n+63)\mathcal{K}\right]\right\} + {}^nC_3\frac{1}{L^6}\hat{\eta}_3^L + \mathcal{O}(L^{-7})$$

Scattering length

Geometric coefficients

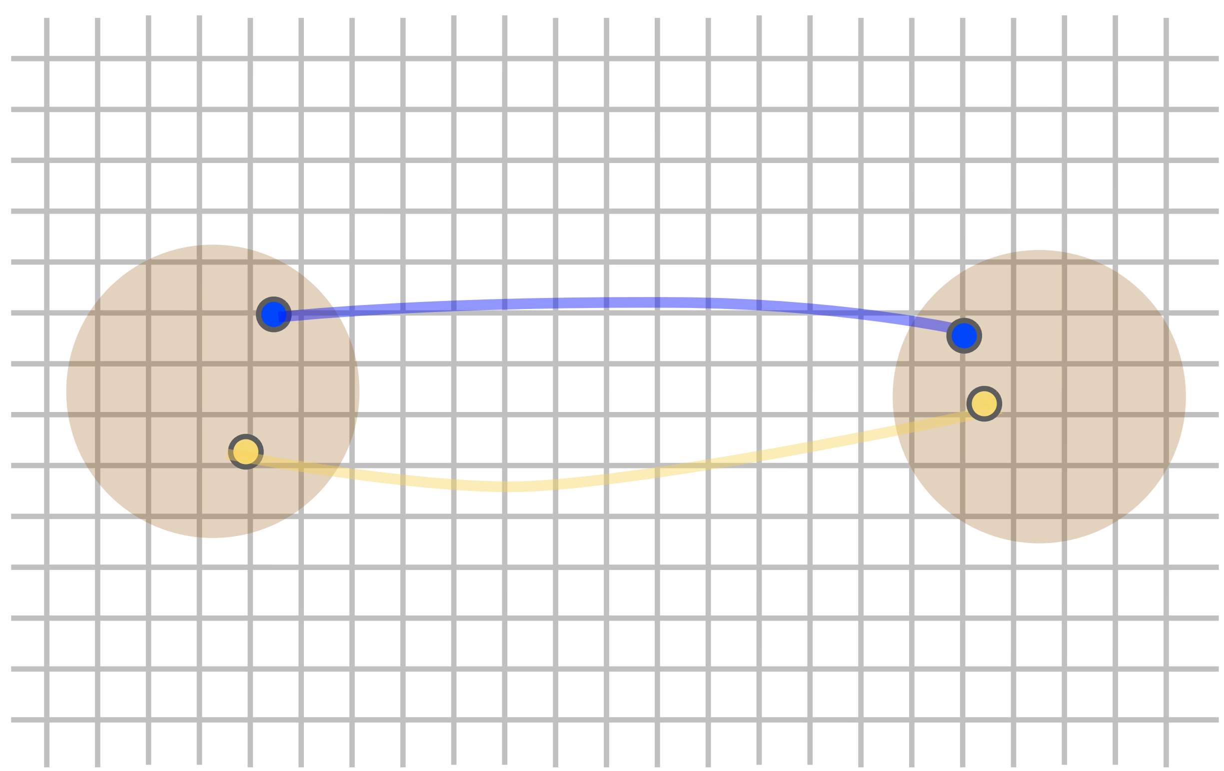
Three body Interaction

[Bogoliubov '47][Huang,Yang '57][Beane, WD, Savage PRD76;074507, 2007; WD+Savage PRD77:057502,2008]

Many mesons in LQCD

- Consider π^+ correlator ($m_u = m_d$)

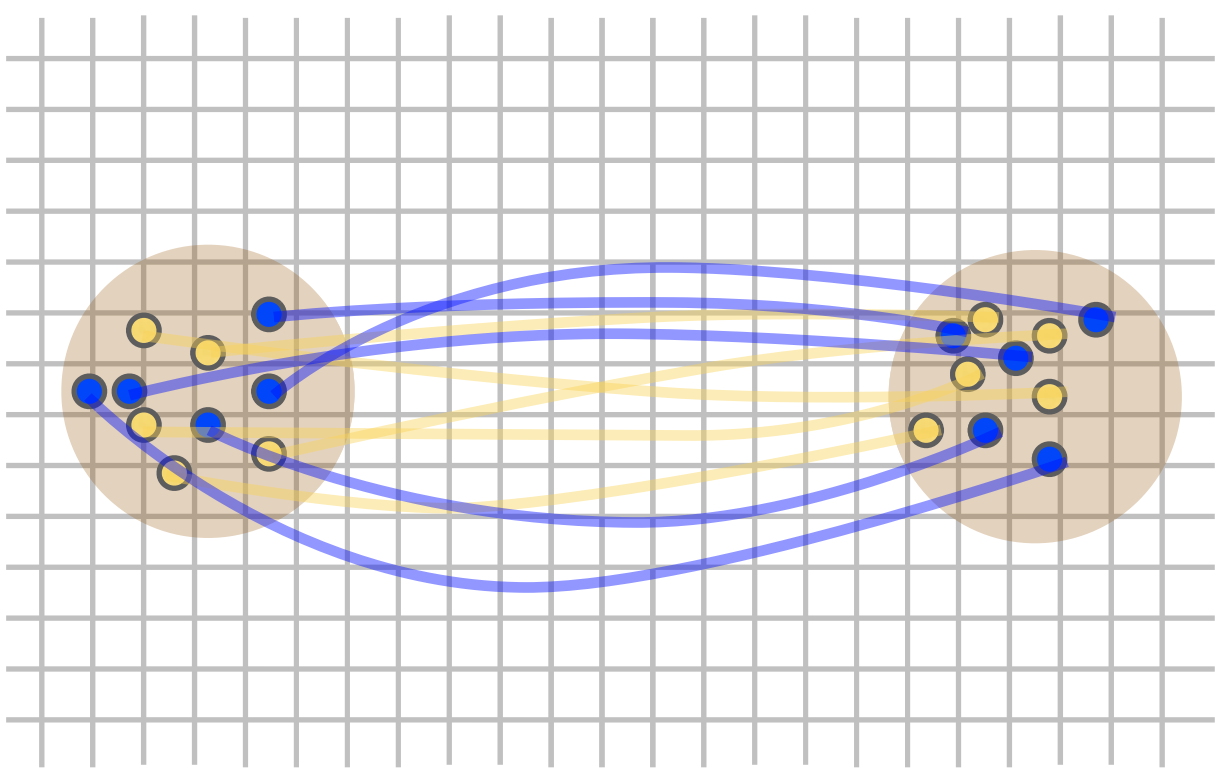
$$C\ \ (t) = \left\langle 0 \left| \left[\sum_{\mathbf{x}} \overline{d}\gamma_5 u(\mathbf{x},t)\overline{u}\gamma_5 d(\mathbf{0},0) \right] \ \right| 0 \right\rangle$$
$$\rightarrow A\ e^{-E\ \ t}$$



Many mesons in LQCD

- Consider n $\boldsymbol{\pi}^+$ correlator (m_u=m_d)

$$C_n(t) = \left\langle 0 \left| \left[\sum_{\mathbf{x}} \overline{d}\gamma_5 u(\mathbf{x},t)\overline{u}\gamma_5 d(\mathbf{0},0) \right]^n \right| 0 \right\rangle$$
$$\rightarrow A\ e^{-E_n t}$$



Many mesons in LQCD

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$$\to A\ e^{-E_n t}$$

- $n!^2$ Wick contractions: $(12!)^2 \sim 10^{17}$

$$C_3(t) = \mathrm{tr}\,[\Pi]^3 - 3\ \mathrm{tr}\,[\Pi]\,\mathrm{tr}\,[\Pi^2 + 2\ \mathrm{tr}\,[\Pi^3]$$

$$\Pi = \sum_{\mathbf{x}} \gamma_5 S(\mathbf{x}, t; 0) \gamma_5 S^\dagger(\mathbf{x}, t; 0)$$

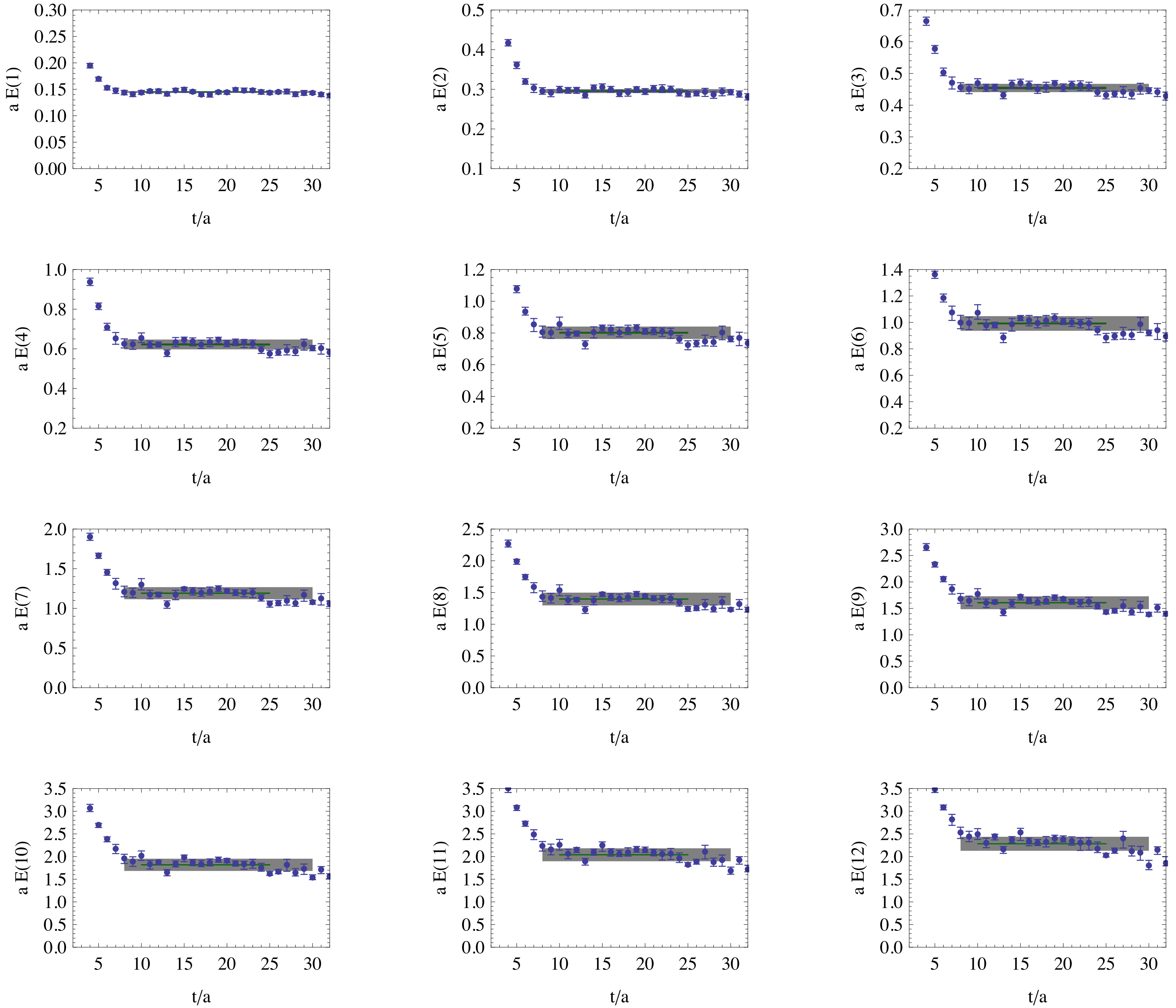
- Maximal isospin: only a single quark propagator

Lattice details

- Calculations use MILC gauge configurations
  - L=2.5 fm, a=0.12 fm, *rooted* staggered
  - also L=3.5 fm and a=0.09 fm
- NPLQCD: domain-wall quark propagators
  - $m_\pi \sim$ 291, 318, 352, 358, 491, 591 MeV
  - 24 propagators / lattice in best case
- $I_z=n=1,\ldots,12$ pion and (S=n) kaon systems

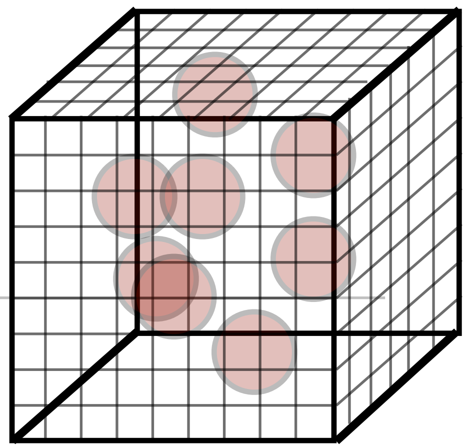
n-meson energies

- Effective energy plots: $\log[C_n(t)/C_n(t+1)]$



DWF on MILC
m_π = 319 MeV
a=0.09 fm, 28^3x96

Bosons in a box



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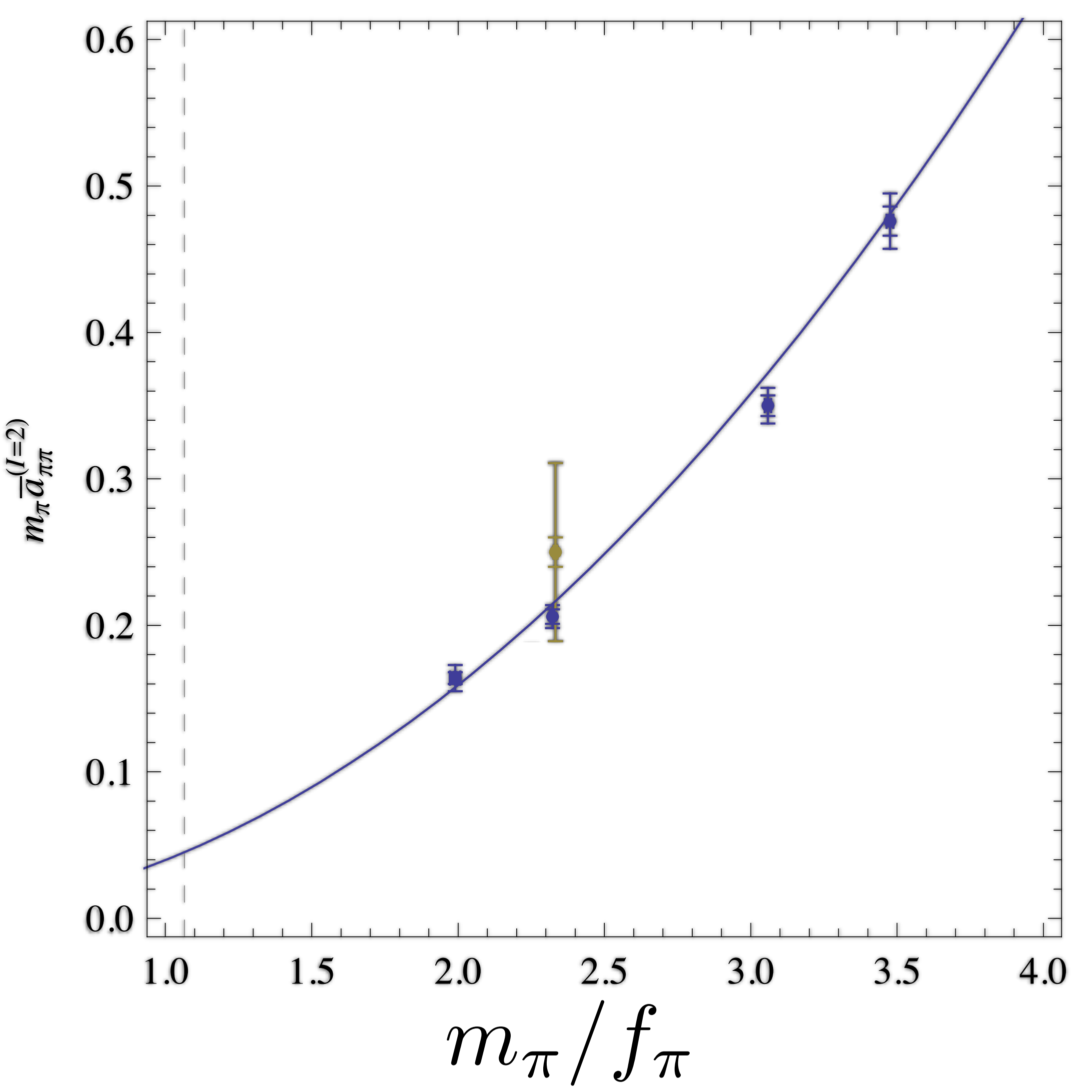
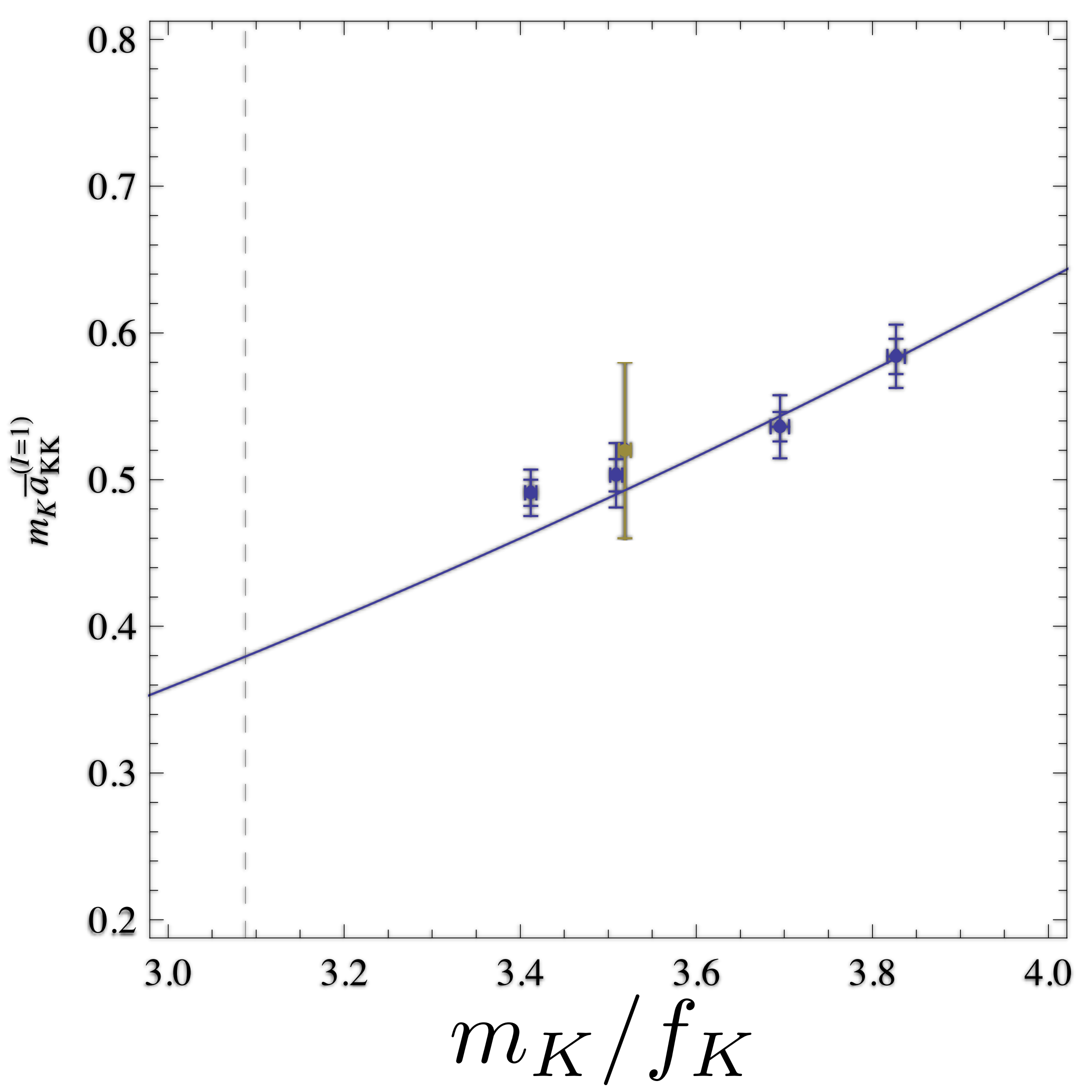
[Bogoliubov '47][Huang, Yang '57][Beane, WD, Savage PRD76;074507, 2007; WD+Savage PRD77:057502,2008]

$2\pi^+$ and $2K^-$ interaction

- Scattering lengths

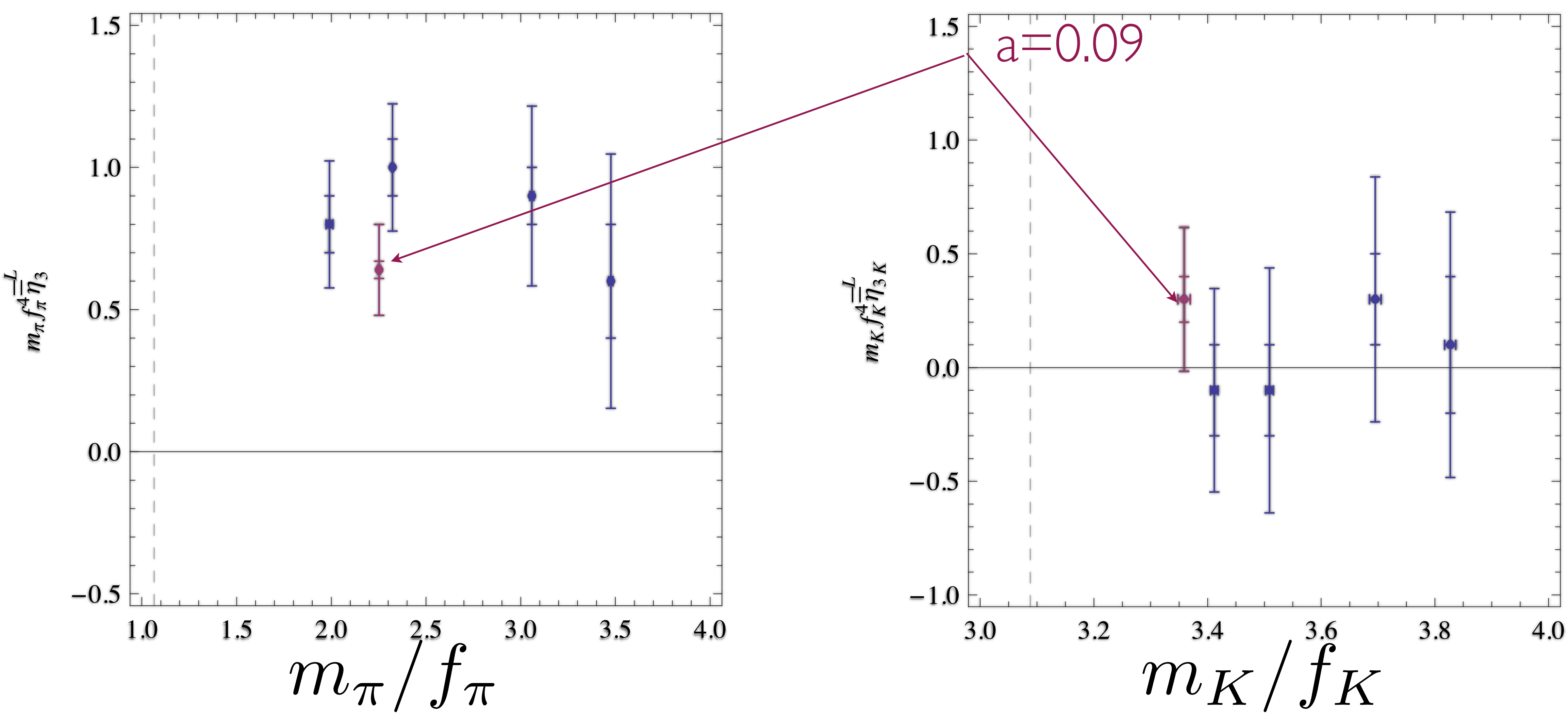




curves: Weinberg

$3\pi^+$ and $3K^-$ interaction

- First QCD three body interaction



Naïve dimension analysis: 1

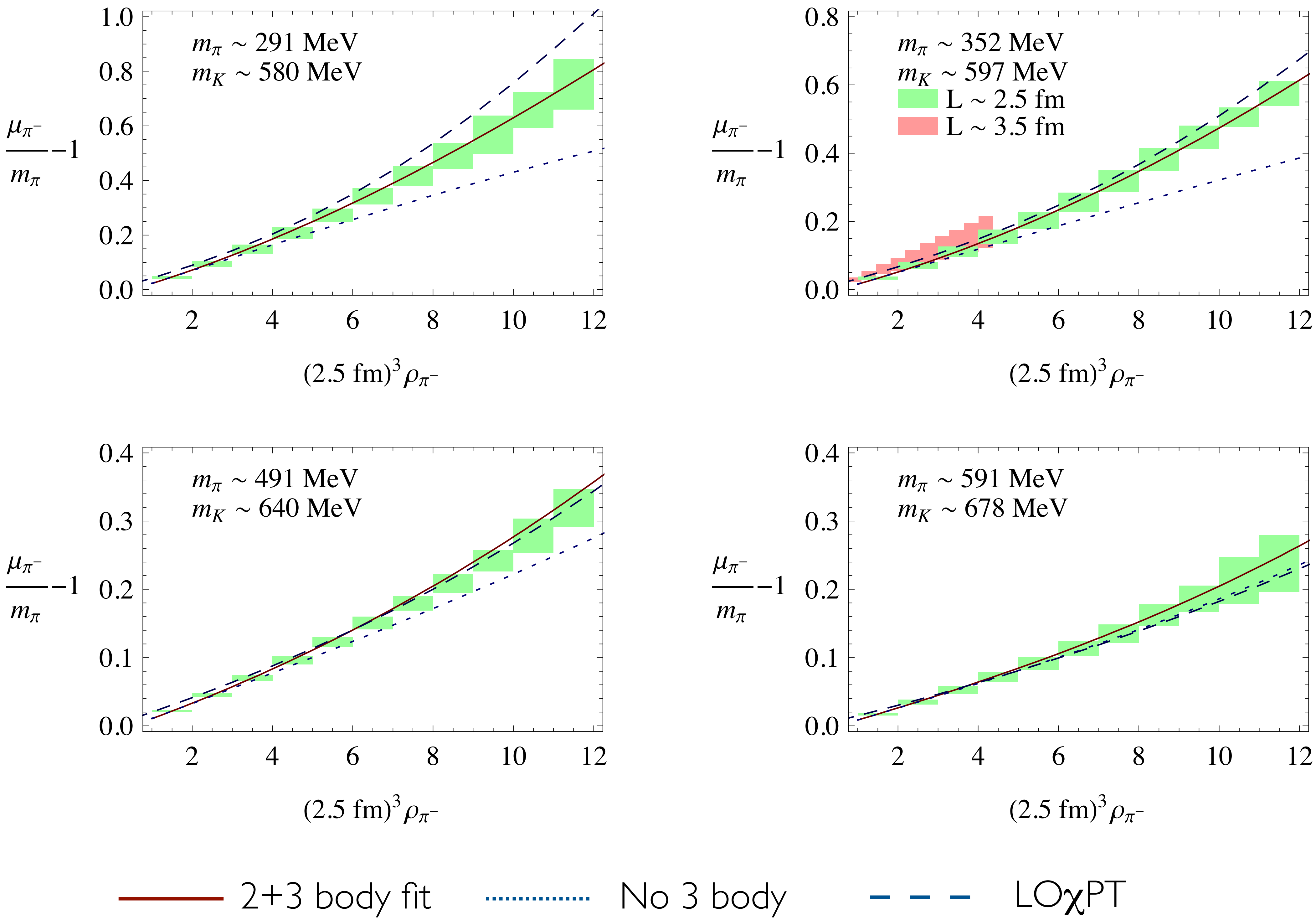
Equation of State

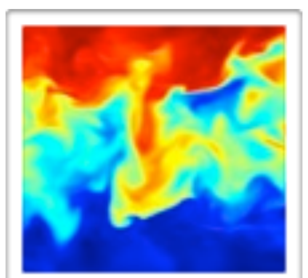
- For large n: Bose-Einstein condensate
- 1/L expansion: analytic form of EOS
- Chemical potential $\mu(\rho)$ (and pressure) numerically using finite difference

$$\mu = \left.\frac{d\ E}{d\ n}\right|_{V\ \mathrm{const}} \qquad p = -\left.\frac{dE}{dV}\right|_{n\ \mathrm{const}} = -\frac{1}{3L^2}\left.\frac{dE}{dL}\right|_{n\ \mathrm{const}}$$

- Compare with LOχPT [Son & Stephanov]

Isospin Chemical Potential





Mixed systems: pions & kaons

[W Detmold, B Smigielski arXiv:1103.4362 (to appear in PRD)]

n pions and *m* kaons

- Weakly interacting two species systems: pions and kaons - complexity
- $E_{n,m}$ of *n* pions and *m* kaons depends on three 2-body and four 3-body interaction parameters
  - Perturbative form is known for weakly interacting case *[Smigielski & Wasem '08]*
- Matching to lattice energies allows for extraction of interaction parameters

LQCD calculations

- One ensemble of anisotropic clover lattices
  - Dynamical N_f=2+1 lattices from JLab
  - m_π=390 MeV, a_s=0.123 fm, ξ=3.5, $20^3 \times 128$
  - ~30K measurements: ~75 sources on ~400 cfgs
- Anti-periodic BCs for quarks (periodic for mesons)
  - Correlators have complicated time dependence
- Correlators for all sets of $\{n,m\}$ with $n+m<13$

LQCD correlators

- Extend single species construction

$$C_{N,M}(t) = \left\langle \left(\sum_x \pi^-(x,t)\right)^N \left(\sum_x K^-(x,t)\right)^M \left(\pi^+(0,t)\right)^N \left(K^+(0,t)\right)^M \right\rangle$$

(projects p_{tot}=0 @ sink)

where

$$\pi^+ = \overline{u}\gamma_5 d, \qquad K^+ = \overline{u}\gamma_5 s$$

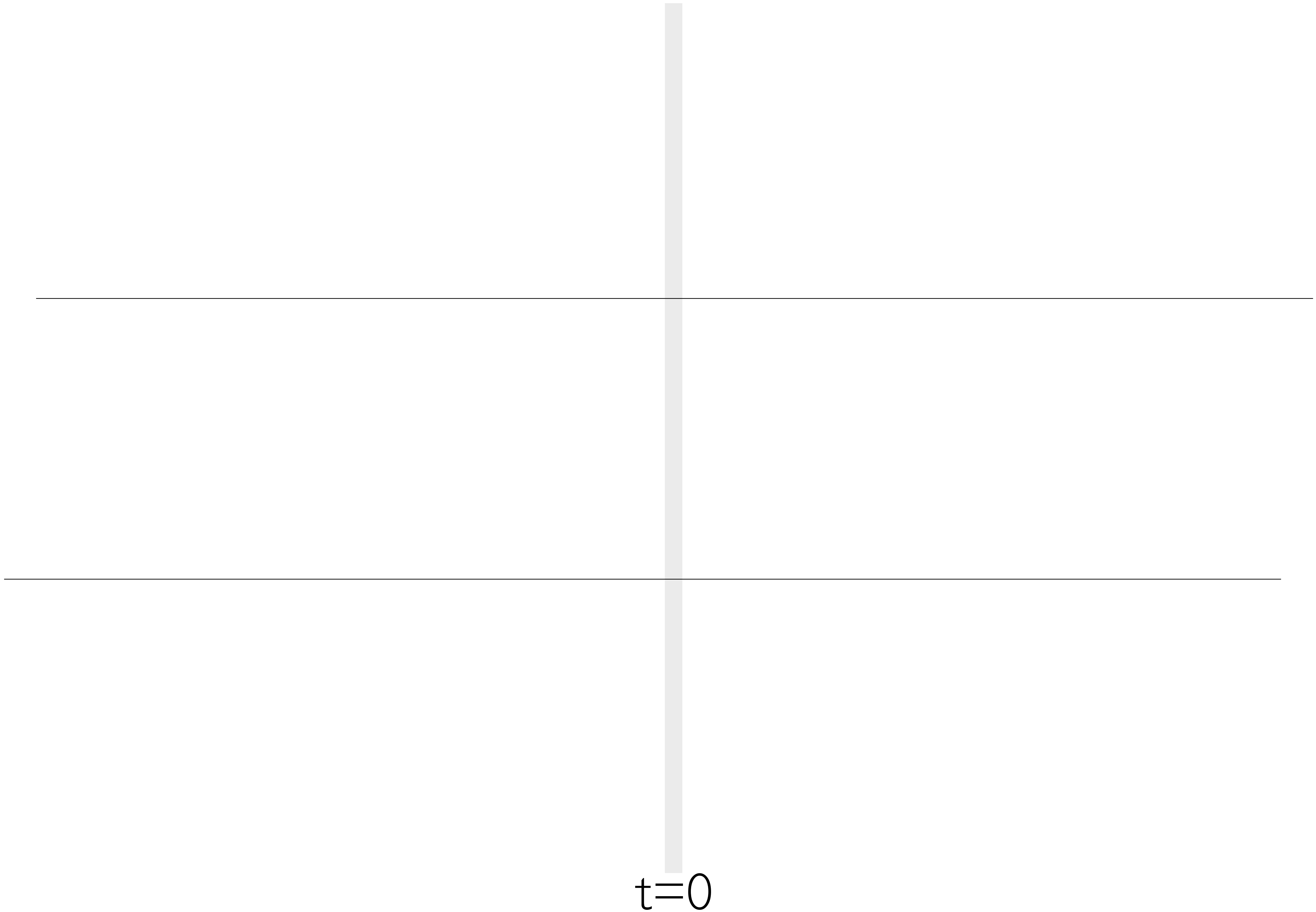
- Reduced symmetry: contractions significantly more complex – n=6 pions, m=6 kaons: 1500 terms!

- Can show the expected behaviour is

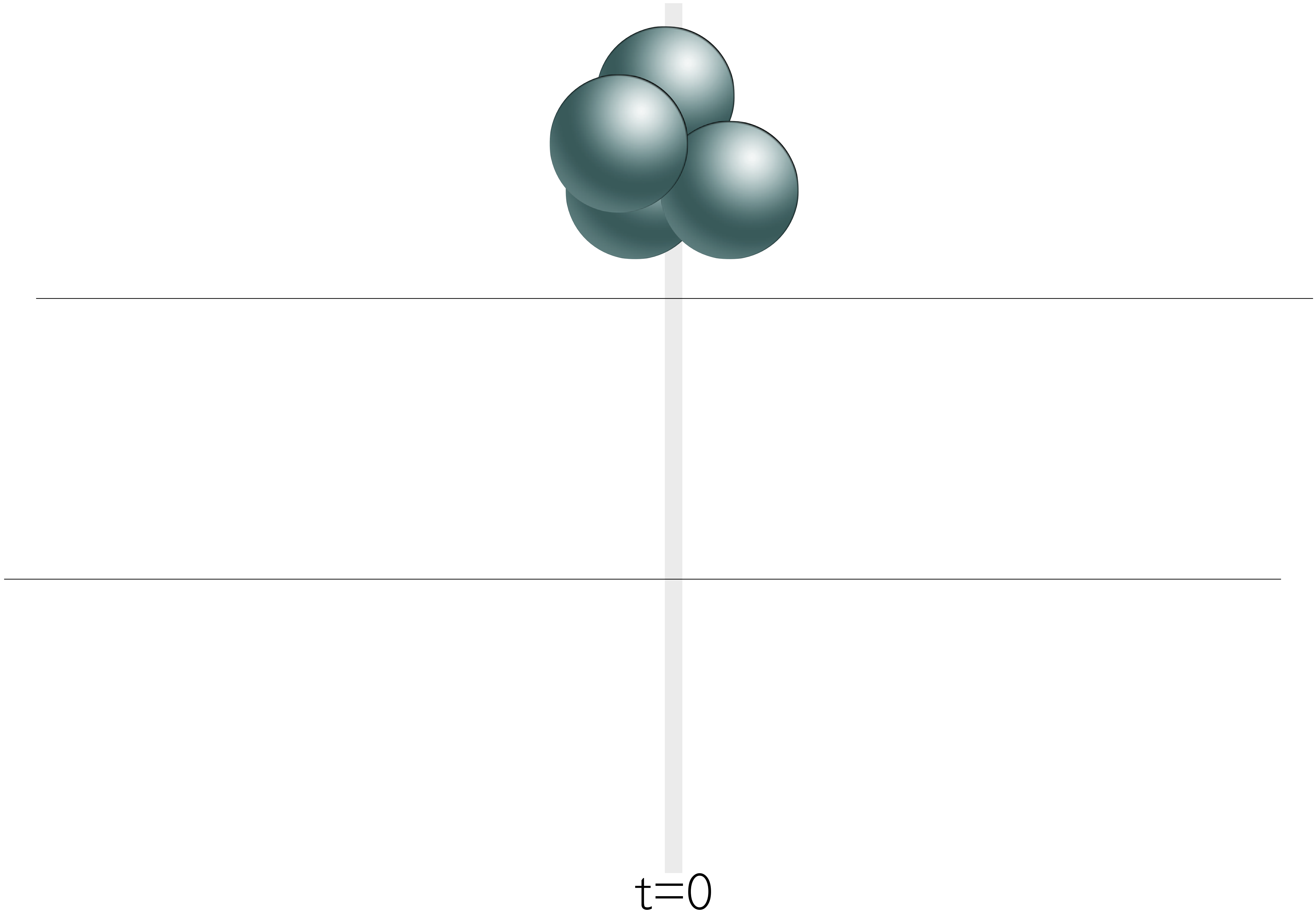
$$C_{N,M}(t) = \frac{1}{2}\sum_{m=0}^{M}\sum_{n=0}^{N} Z_{n,m}^{N-n,M-m} e^{-(E_{N-n,M-m}+E_{n,m})T/2} \cosh\left(\left(E_{N-n,M-m} - E_{n,m}\right)(t-T/2)\right)$$

$$+\frac{1}{2} Z_{\frac{N}{2},\frac{M}{2}}^{\frac{N}{2},\frac{M}{2}} \; e^{\left(E_{N/2,M/2}\right)T/2} \; \delta_{N,2l}\delta_{M,2k} + \ldots$$

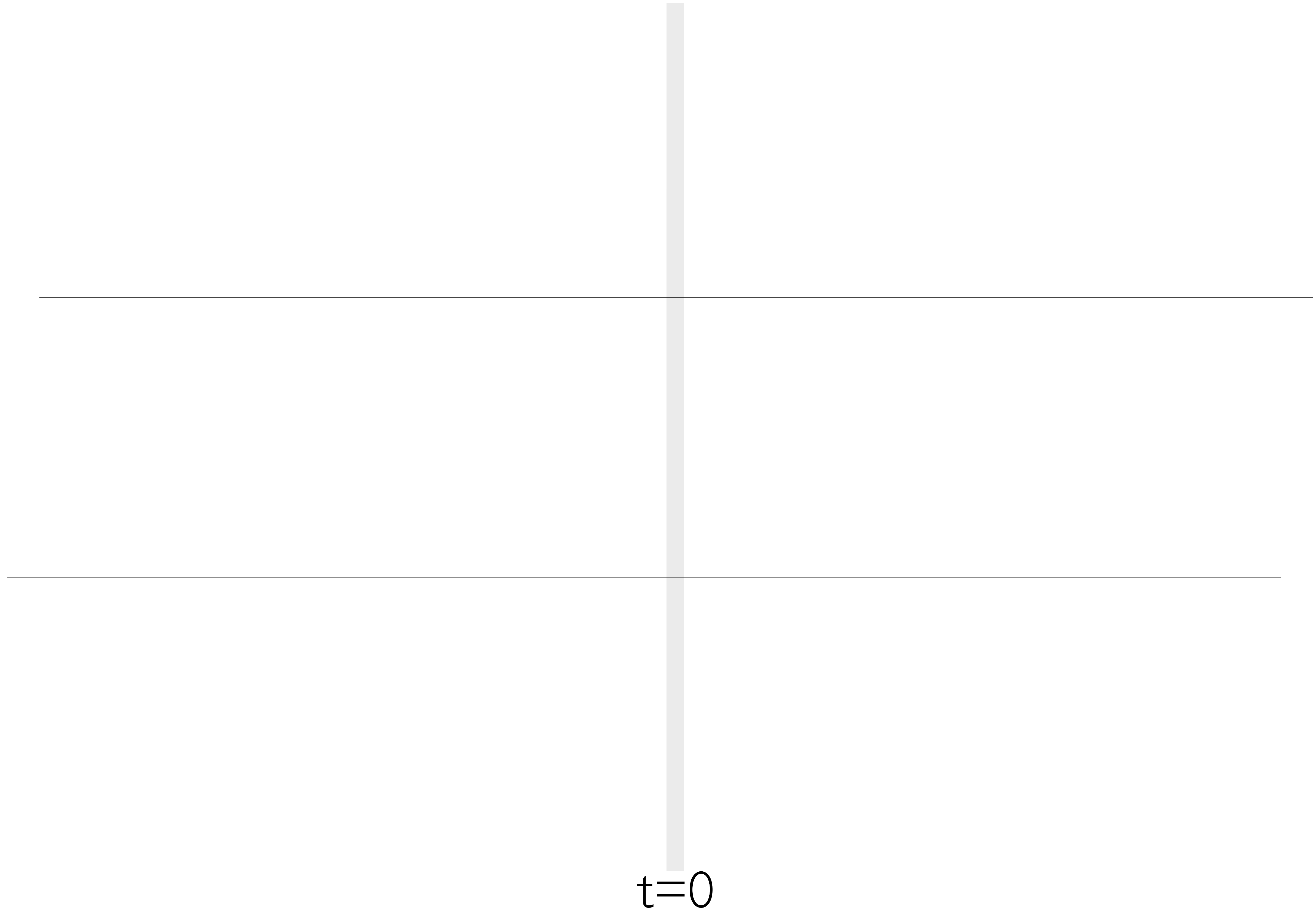
Four pion correlation



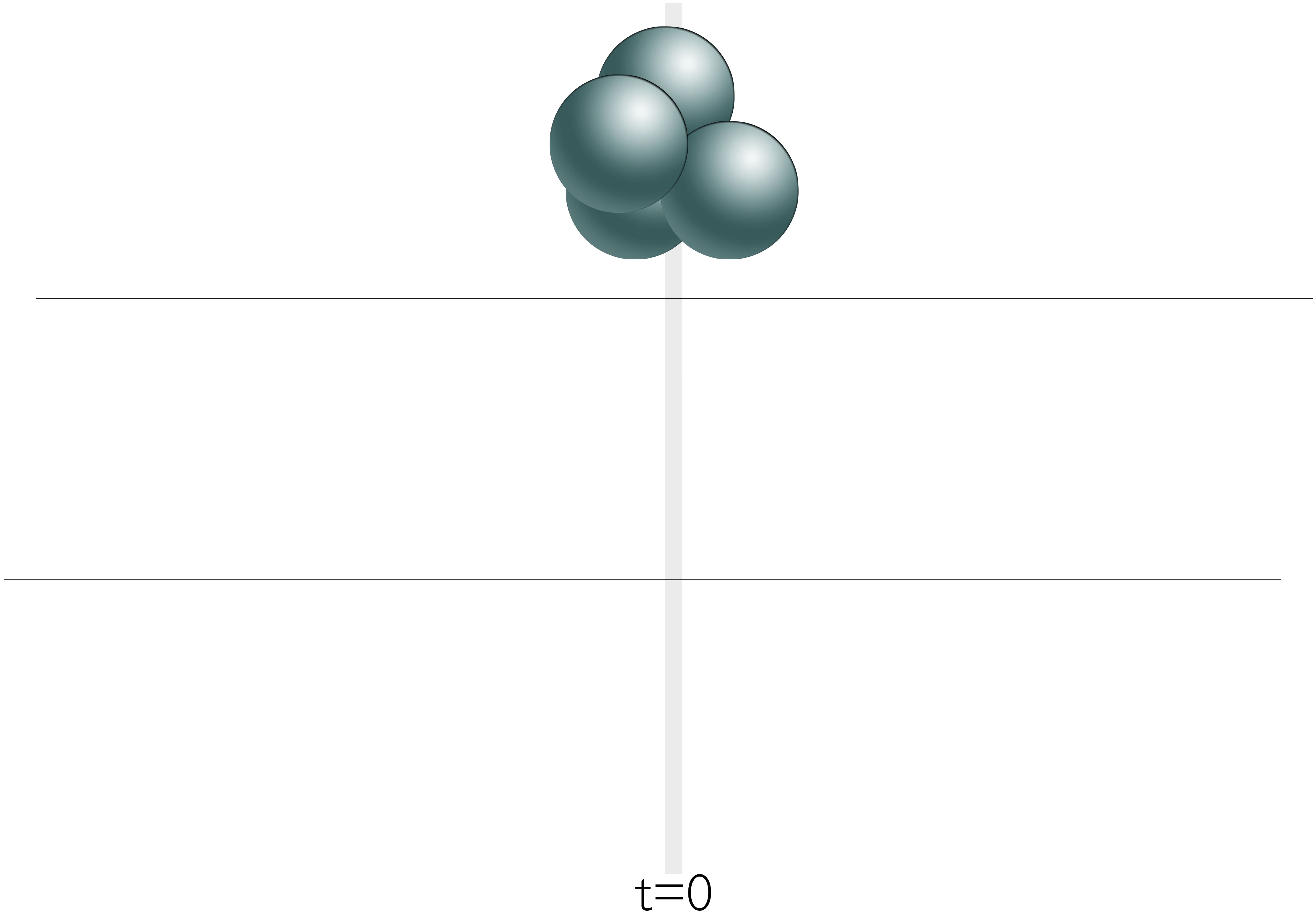
Four pion correlation



Four pion correlation

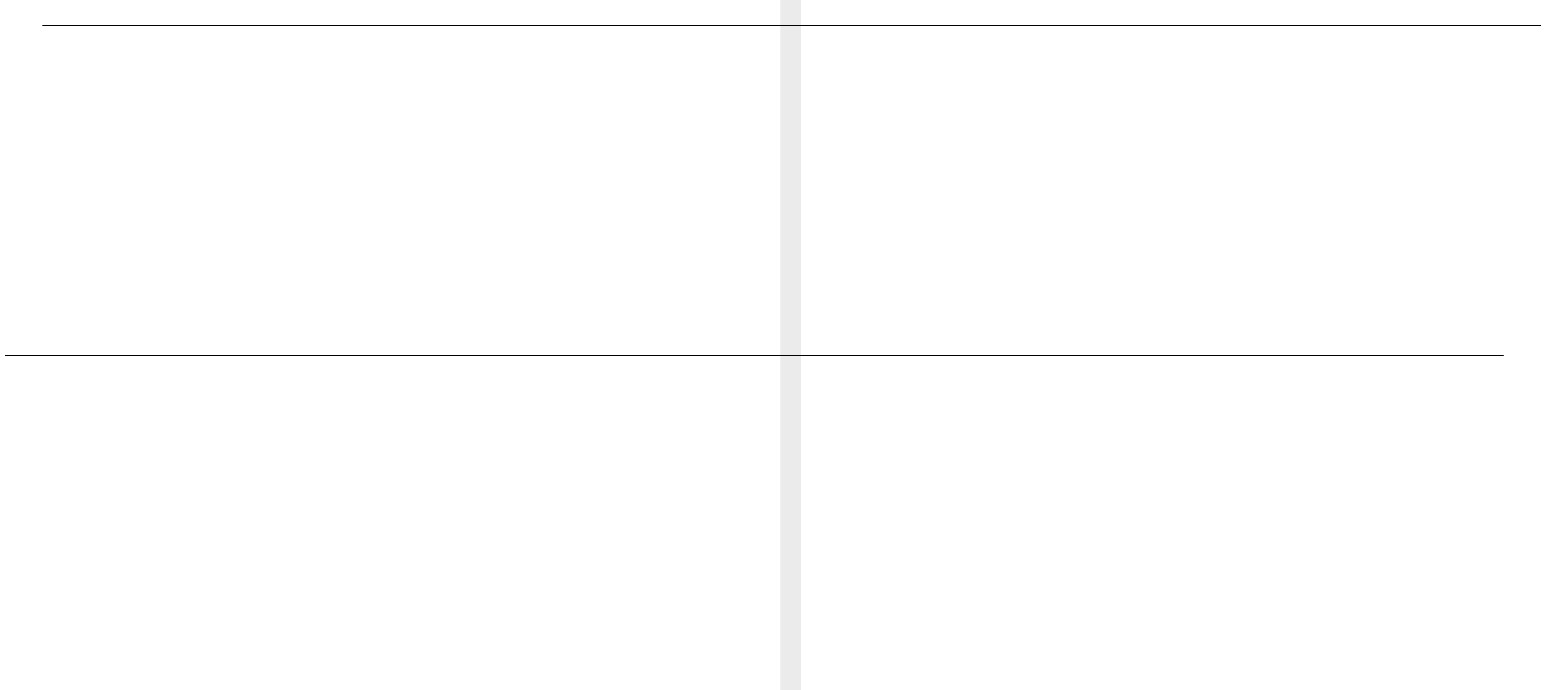


Four pion correlation



Four pion correlation

$$Z_{4\pi}\left(e^{-4E_{4\pi}t}+e^{-4E_{4\pi}(T-t)}\right)$$



t=0

Four pion correlation

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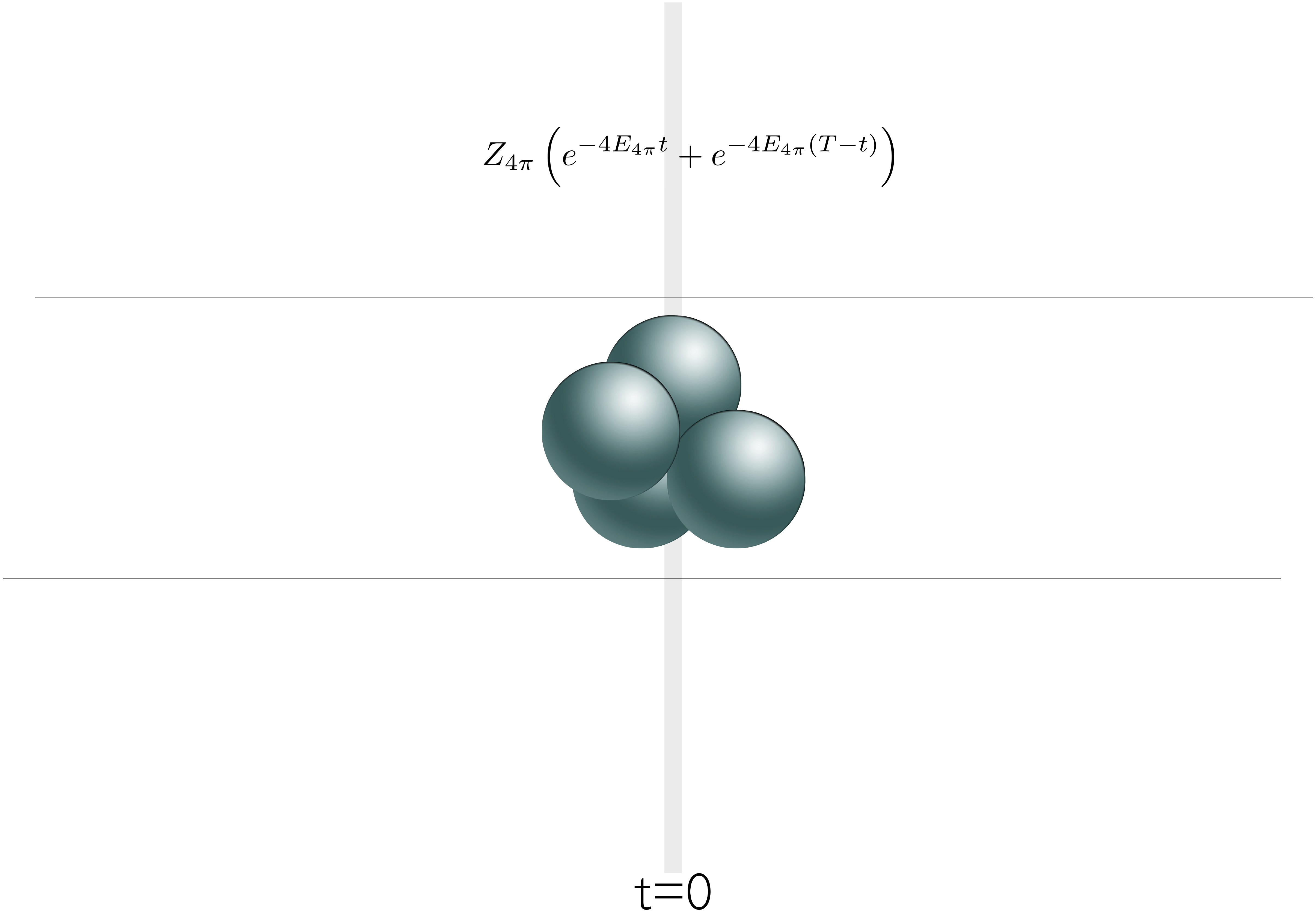

Four pion correlation

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t=0

Four pion correlation

$$Z_{4\pi}\left(e^{-4E_{4\pi}t}+e^{-4E_{4\pi}(T-t)}\right)$$

$$Z_{3/1\pi}\left(e^{-E_{3\pi}t}e^{-E_{1\pi}(T-t)}+e^{-E_{3\pi}(T-t)}e^{-E_{1\pi}t}\right)$$

t=0

Four pion correlation

$$Z_{4\pi}\left(e^{-4E_{4\pi}t}+e^{-4E_{4\pi}(T-t)}\right)$$

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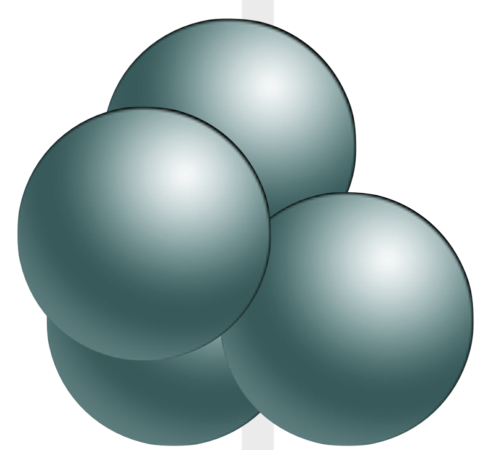

t=0

Four pion correlation

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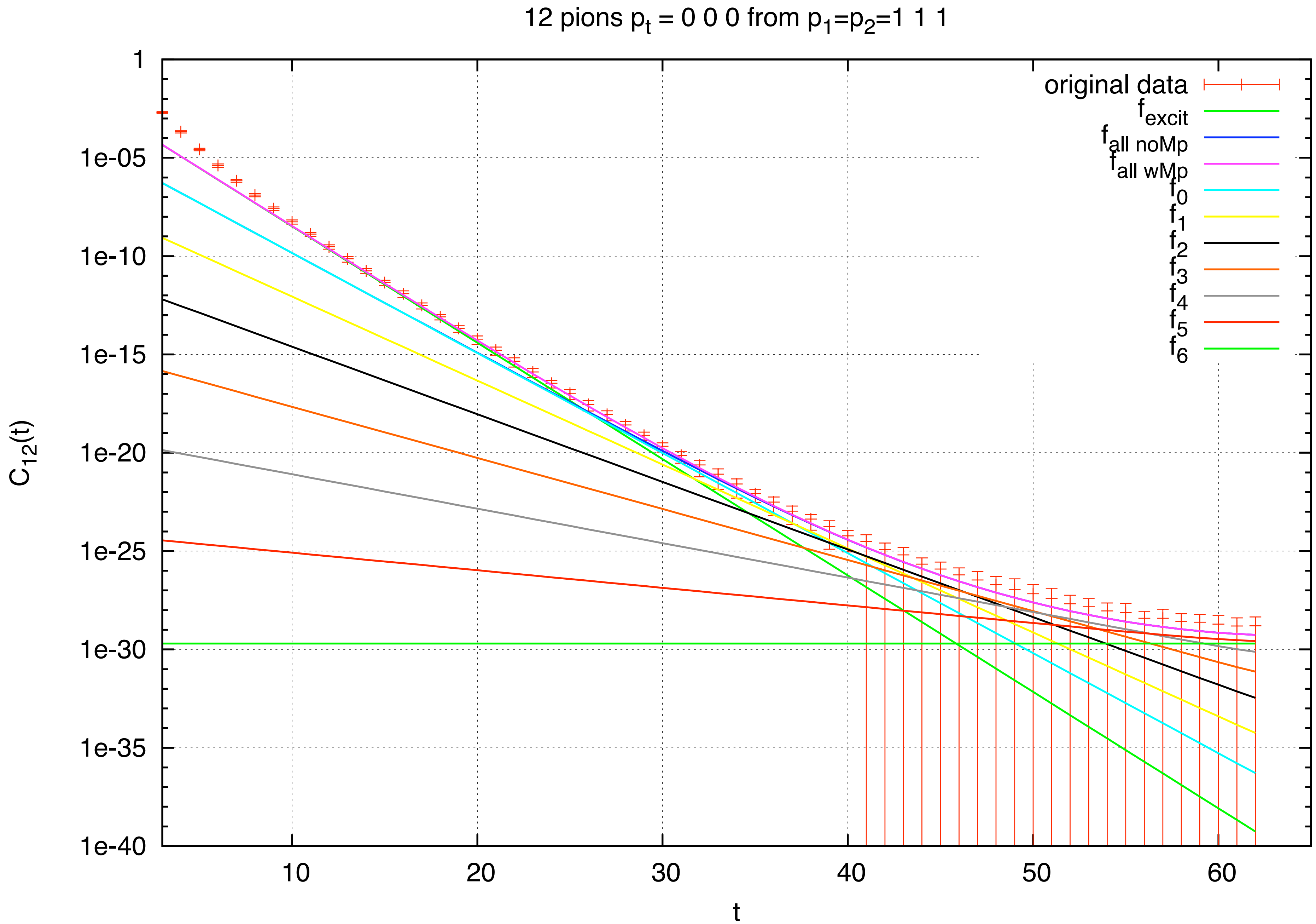
$$Z_{2/2\pi}e^{-E_{2\pi}t}e^{-E_{2\pi}(T-t)}=Z_{2/2\pi}e^{-E_{2\pi}T}$$

t=0

Analysis

- Extracting the eigen-energies (or interaction parameters) from these correlators is difficult
- Correlations between different {*n*,*m*}
- Huge parameter space, O(90) observables
  - $C_{4\pi,2K}$ involves 18 parameters
  - Cascading fit of more and more {*n*,*m*}
  - Augment χ^2 via Bayesian priors, VarPro

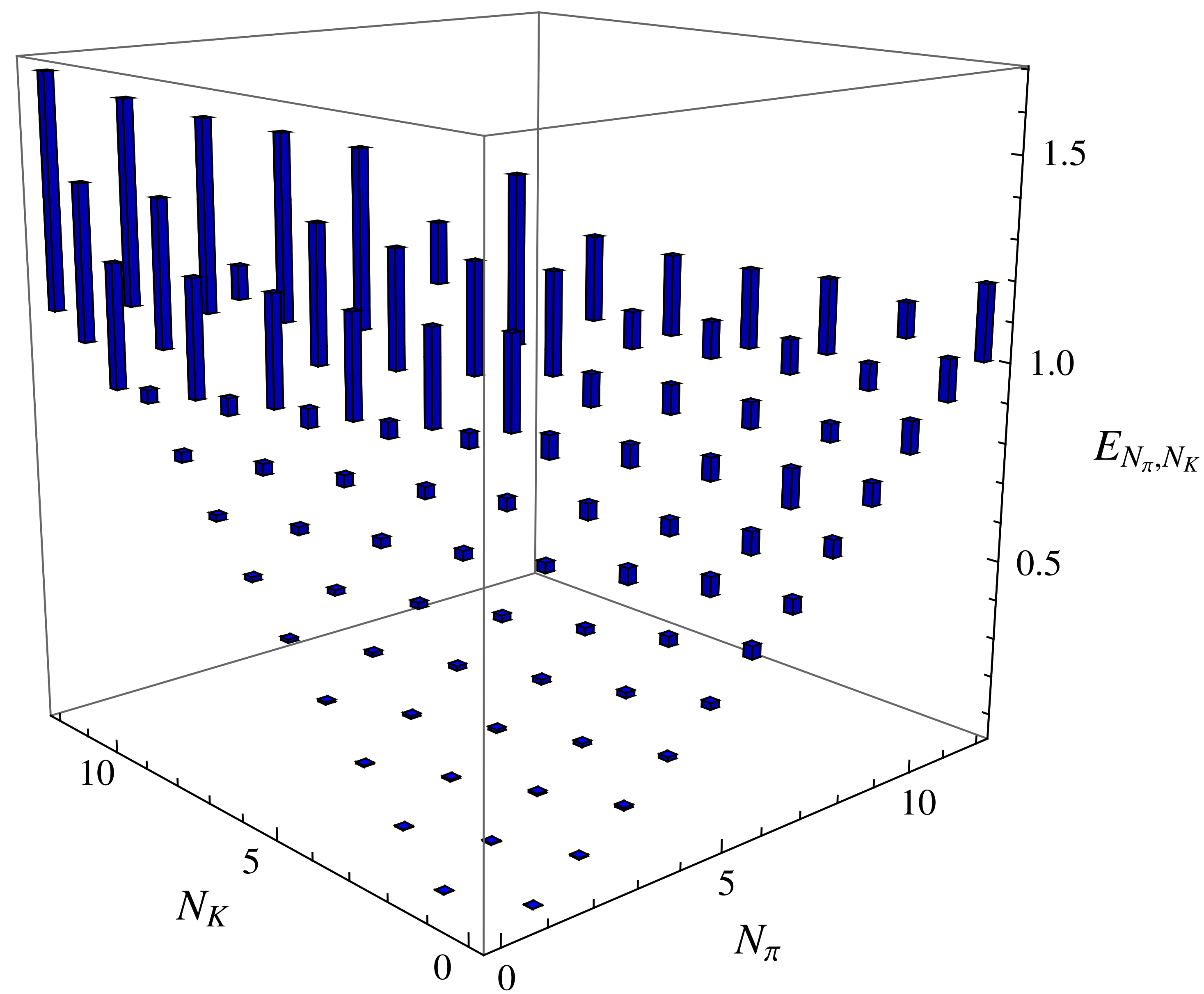
Thermal pollution



At no point does the ground state dominate the correlator!!!

Extracted energies

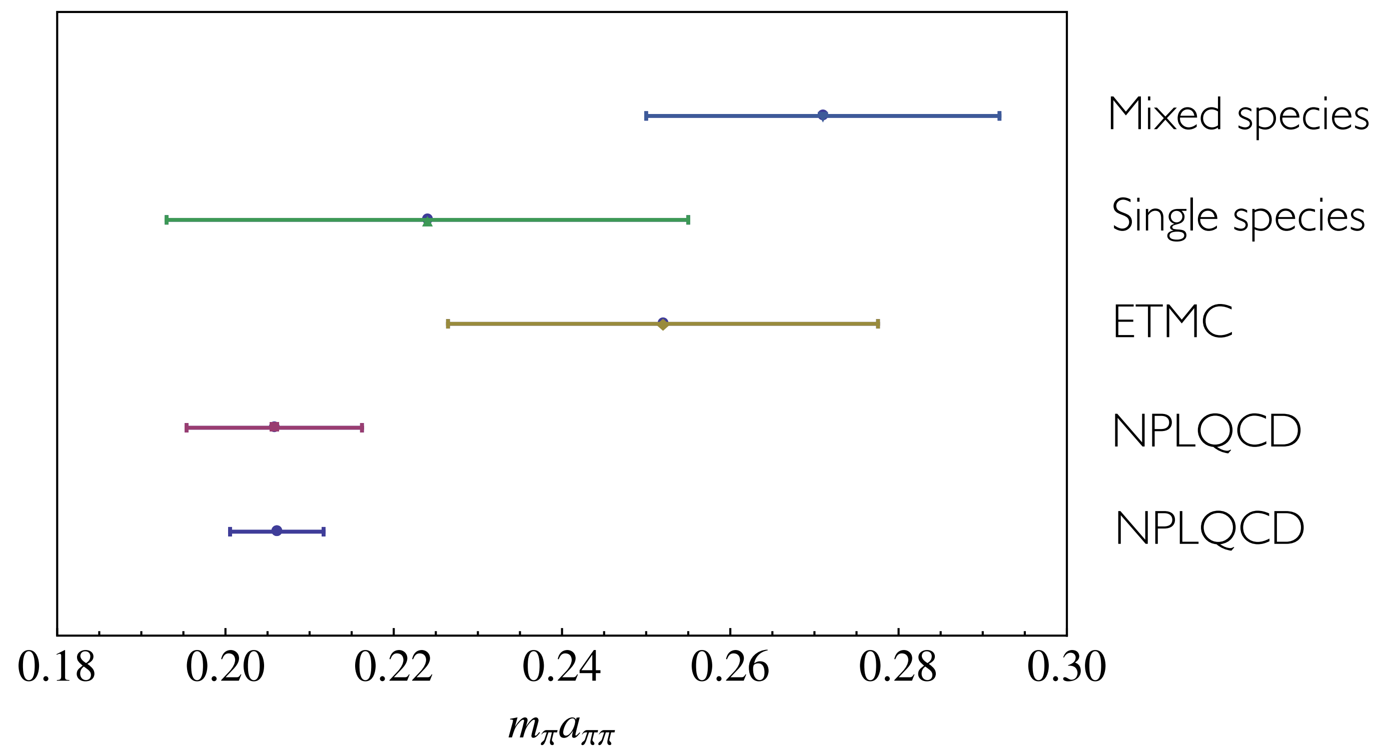
- Boxes correspond to extracted energies and their uncertainties



Interaction parameters

- Energies allow us to interaction parameters

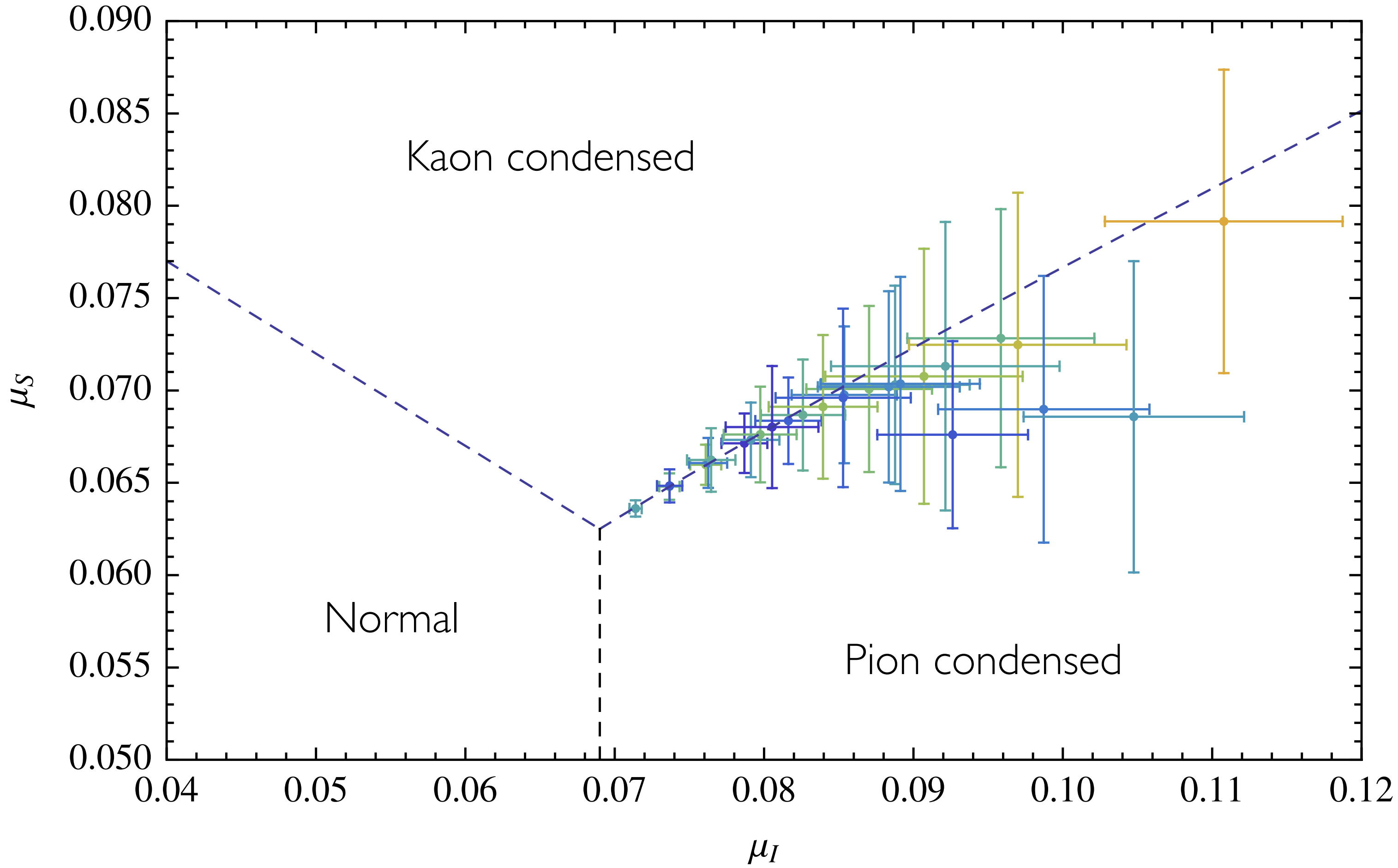
$$
\begin{aligned}
m_K \bar{a}_{KK} &= 0.461 \pm 0.010, \\
m_\pi \bar{a}_{\pi\pi} &= 0.271 \pm 0.021, \\
m_{\pi K} \bar{a}_{\pi K} &= 0.166 \pm 0.016, \\
m_K \bar{\eta}_{3,KKK} f_K^4 &= -0.08 \pm 0.12, \\
m_\pi \bar{\eta}_{3,\pi\pi\pi} f_\pi^4 &= 0.68 \pm 0.33, \\
\frac{m_\pi m_K}{m_\pi + 2m_K} \bar{\eta}_{3,\pi KK} f_{\pi KK}^4 &= 0.22 \pm 0.17, \\
\frac{m_\pi m_K}{2m_\pi + m_K} \bar{\eta}_{3,\pi\pi K} f_{\pi\pi K}^4 &= 0.45 \pm 0.26.
\end{aligned}
$$



- Single species parameters consistent with literature
- Predictions for mixed interactions

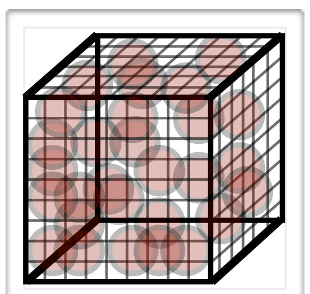
Chemical potentials

- LOχPT phase diagram for μ_I, μ_S [Kogut & Toublan, PRD 64, 034007 (2001)]



blue=small n+m
orange=large n+m

- QCD calculations probe interesting region



Many meson systems

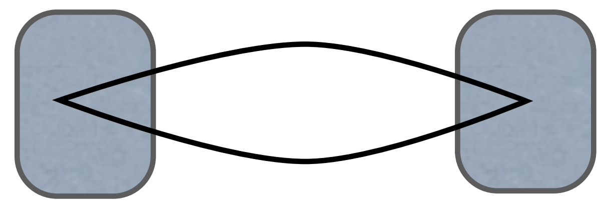
[WD, Savage, Phys. Rev. D82, 014501, 2010]

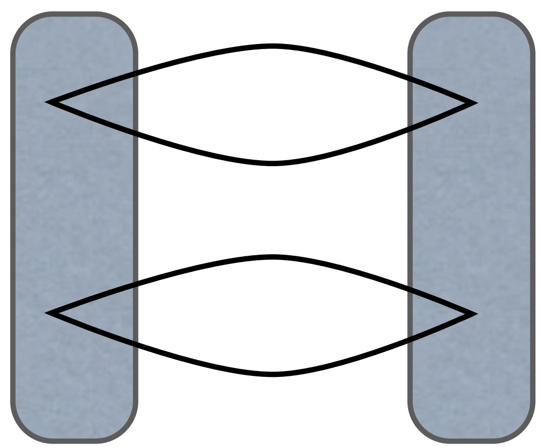
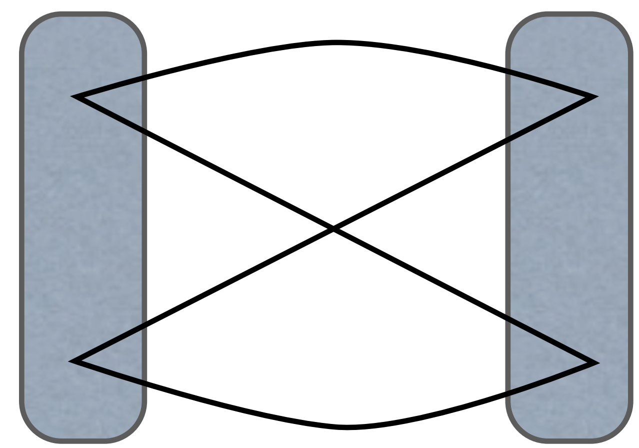
[WD + Zhifeng Shi, in progress]

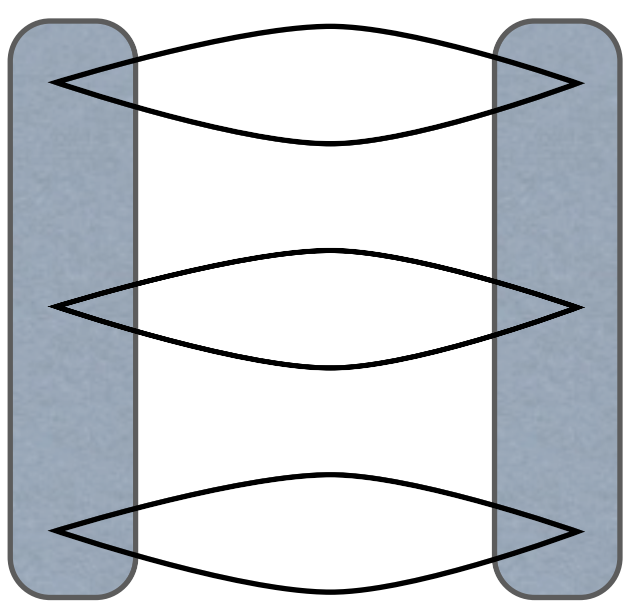
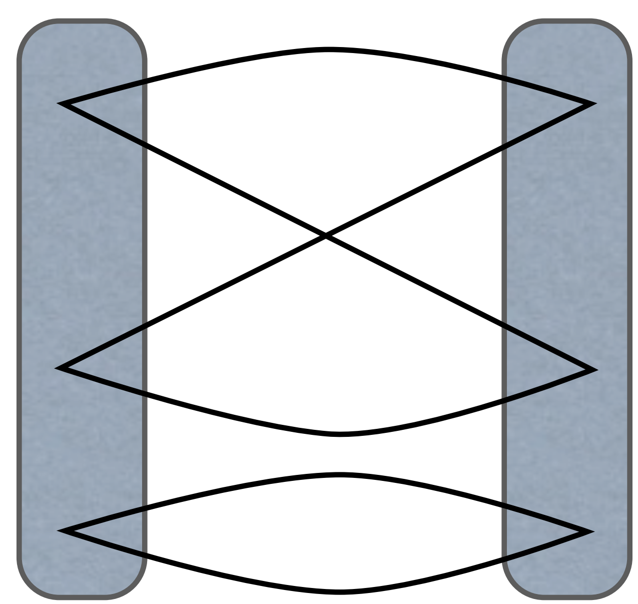
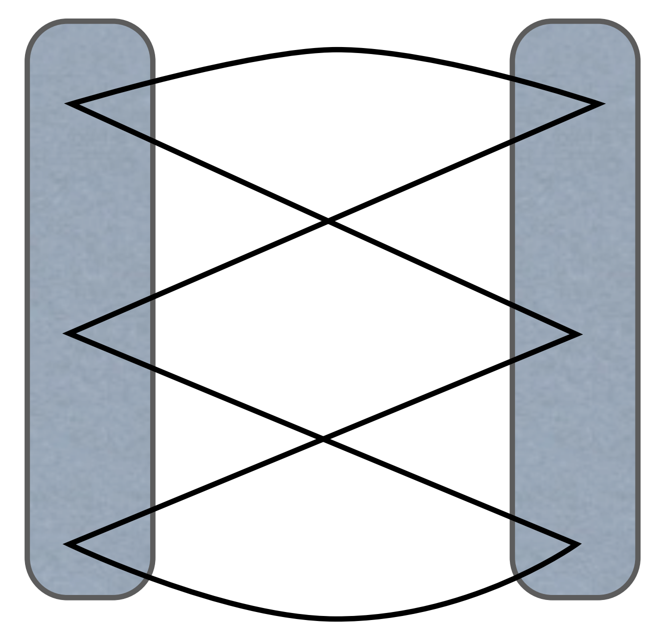
Large systems

- How do we deal with complexity of contractions?
  - One species: $N_{\text{terms}} \sim e^{\pi\sqrt{2n/3}}/\sqrt{n}$
  - Two-species is harder, more is unfeasible
- How do we go beyond n=12?
  - Previous method fails because of Pauli principle
  - Avoid by using multiple propagator sources but this leads to contraction complexity

Few pion contractions

$C_{1\pi}(t) =$ 

$C_{2\pi}(t) =$  $-$ 

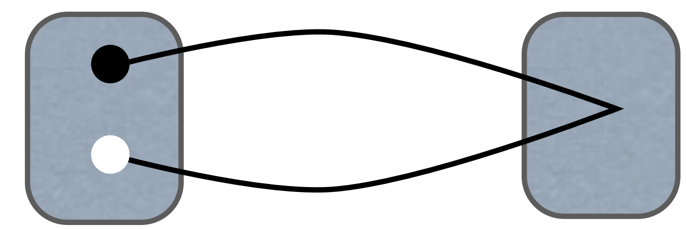
$C_{3\pi}(t) =$  -3  -2 

Blocks

- Define a partly contracted pion correlator

$$\Pi \equiv R_1 = \sum_{\mathbf{x}} S_u(\mathbf{x},t;x_0)\gamma_5 S_d(x_0;\mathbf{x},t)\gamma_5 = \sum_{\mathbf{x}} S_u(\mathbf{x},t;x_0) S_d^\dagger(\mathbf{x},t;x_0)$$

  - Time-dependent 12x12 matrix (spin-colour indices)



- Correlators

$$C_1(t) = \langle \Pi \rangle, \quad C_2(t) = \langle \Pi \rangle^2 - \langle \Pi^2 \rangle, \ldots$$

- Functional definition

$$\Pi_{ij} = \bar{u}_i(x) u_k(x_0) \frac{\delta}{\delta \bar{u}_j(x) \delta u_k(x_0)} C_1(t)$$

- Generalises to

$$(R_n)_{ij} \equiv \bar{u}_i(x) u_k(x_0) \frac{\delta}{\delta \bar{u}_j(x) \delta u_k(x_0)} C_n(t)$$

Recursion relation

[WD, Savage, Phys. Rev. D82, 014501, 2010]

- The block objects <u>*are*</u> simply related
- Recursion relation

$$R_{n+1} = \langle R_n \rangle \ R_1 - n \ R_n \ R_1$$

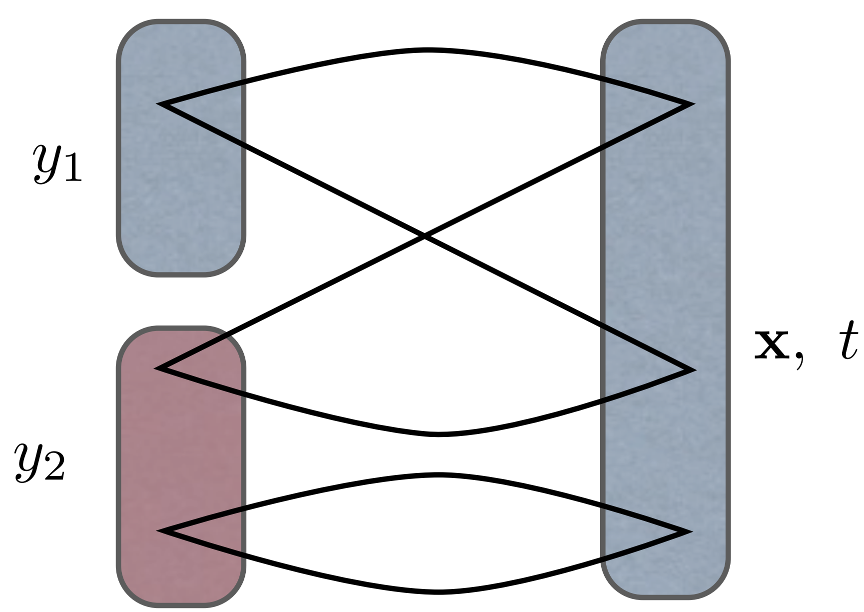
- Initial condition is that $R_1 = \Pi, \qquad R_j = 0, \, \forall j < 1$
- Can also construct a descending recursion as we know that R_{13}=0

Multi-source systems

- To get beyond n=12, need to consider multi-source systems
- Consider two sources first

$$C_{(n_1\pi_1^+\ ,\ n_2\pi_2^+)}(t) = \left\langle \left(\sum_{\mathbf{x}} \pi^+(\mathbf{x},t) \right)^{n_1+n_2} \left(\pi^-(\mathbf{y_1},0) \right)^{n_1} \left(\pi^-(\mathbf{y_2},0) \right)^{n_2} \right\rangle$$

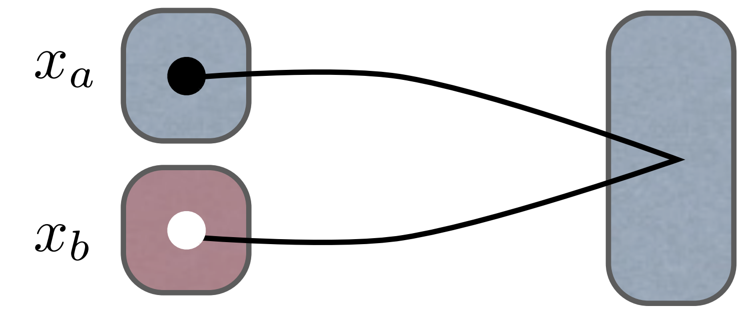
- $C_{(1,2)}(t)$ contains contractions like



Multi-source systems

- Multiple types of blocks needed

$$A_{ab} = \sum_{\mathbf{x}} S_u(\mathbf{x}, t; x_a) S_d^\dagger(\mathbf{x}, t; x_b)$$



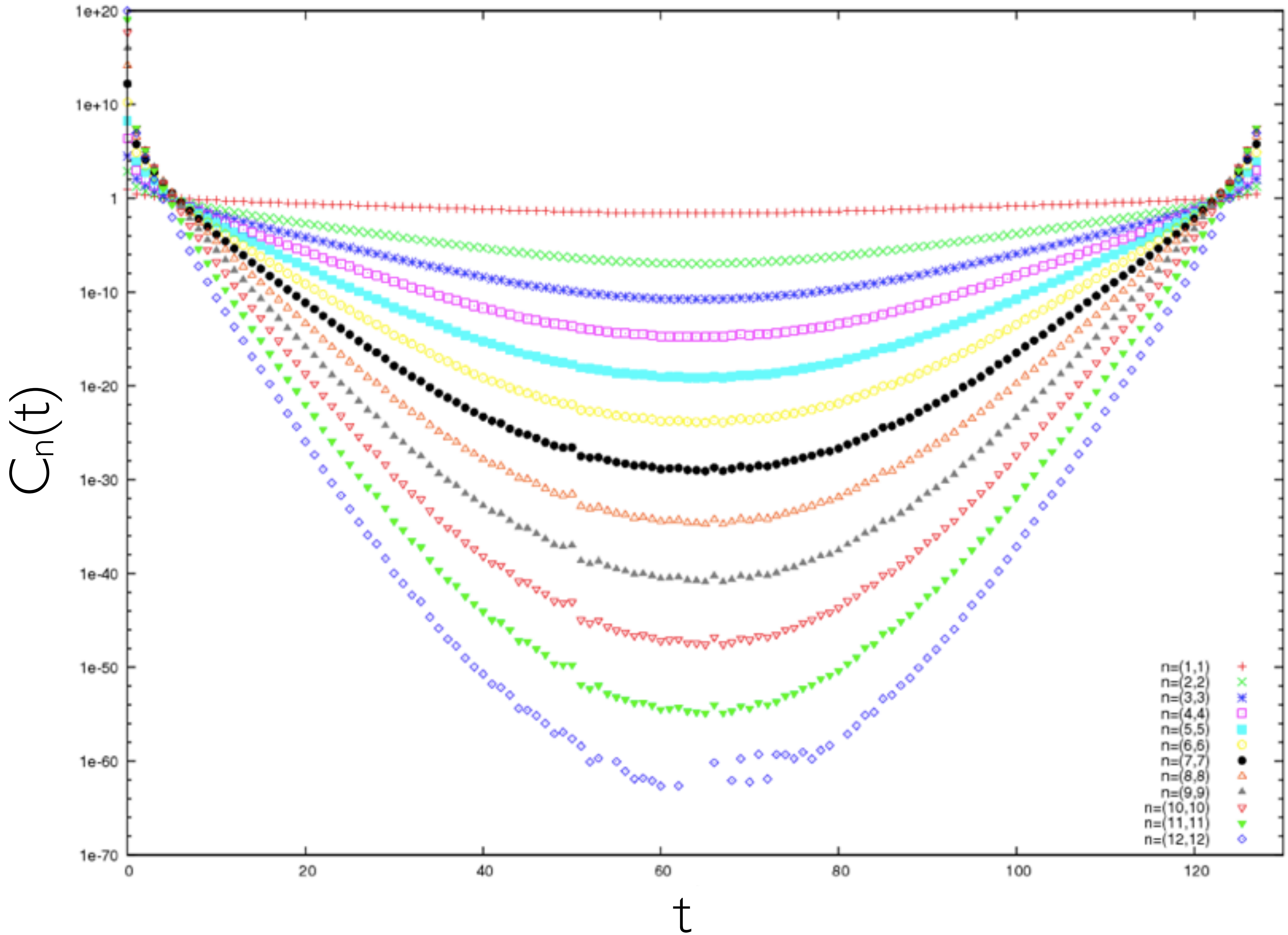
- Two species case has a simple recursion relation:
  First define

$$P_1 = \left(\begin{array}{c|c} A_{11}(t) & A_{12}(t) \\ \hline 0 & 0 \end{array} \right) \quad , \quad P_2 = \left(\begin{array}{c|c} 0 & 0 \\ \hline A_{21}(t) & A_{22}(t) \end{array} \right)$$

Then the generalisations of the R_n satisfy a recursion

$$\begin{aligned} Q_{(n_1+1,n_2)} = & \langle\, Q_{(n_1,n_2)} \,\rangle\, P_1 \;-\; (n_1+n_2)\, Q_{(n_1,n_2)}\;\; P_1 \\ & +\langle\, Q_{(n_1+1,n_2-1)} \,\rangle\, P_2 \;-\; (n_1+n_2)\, Q_{(n_1+1,n_2-1)}\;\; P_2 \end{aligned}$$

N=24 pions

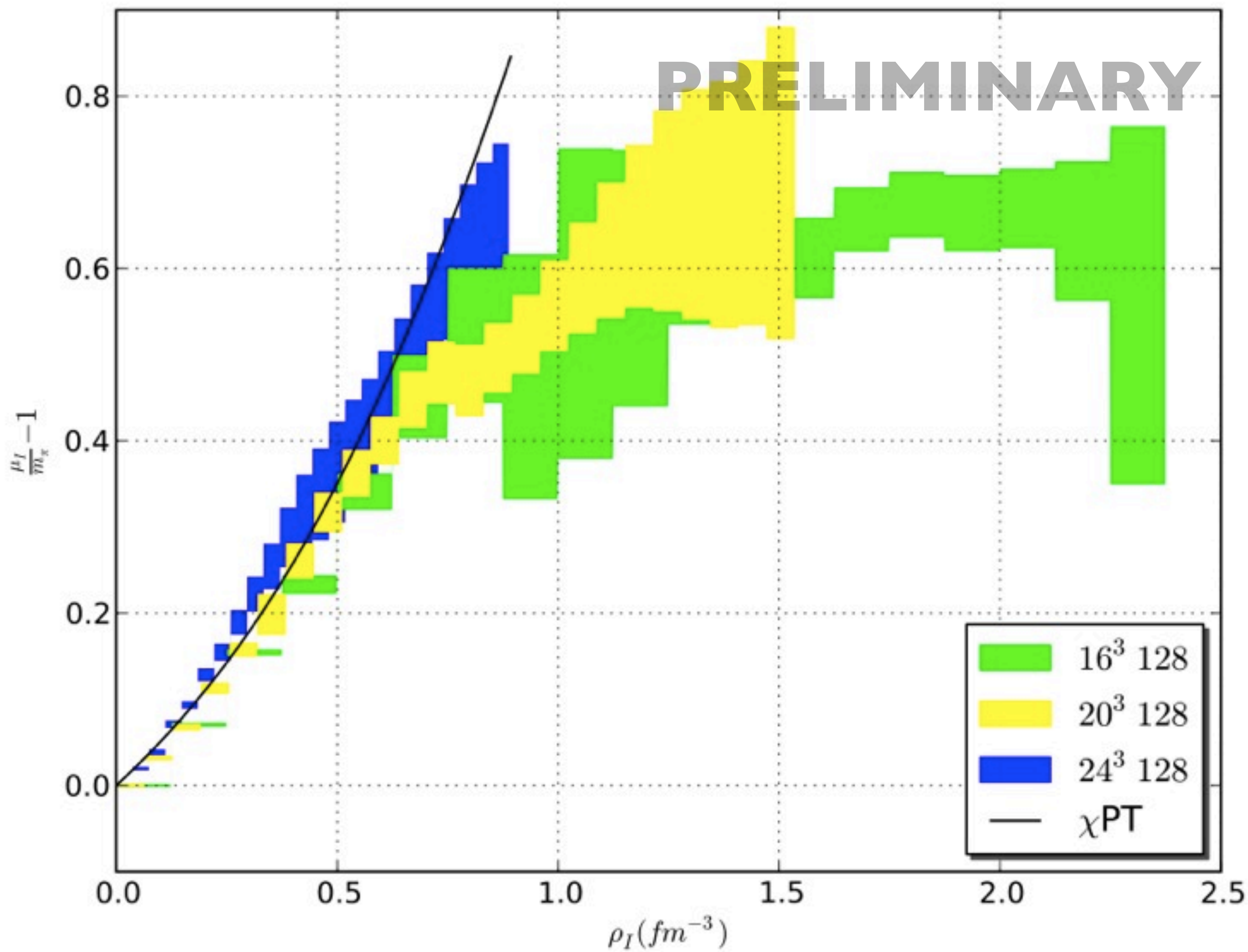


1e+20
1e+10
1
1e-10
1e-20
1e-30
1e-40
1e-50
1e-60
1e-70
0
20
40
60
80
100
120
$C_n(t)$
t
n=(1,1)
n=(2,2)
n=(3,3)
n=(4,4)
n=(5,5)
n=(6,6)
n=(7,7)
n=(8,8)
n=(9,9)
n=(10,10)
n=(11,11)
n=(12,12)

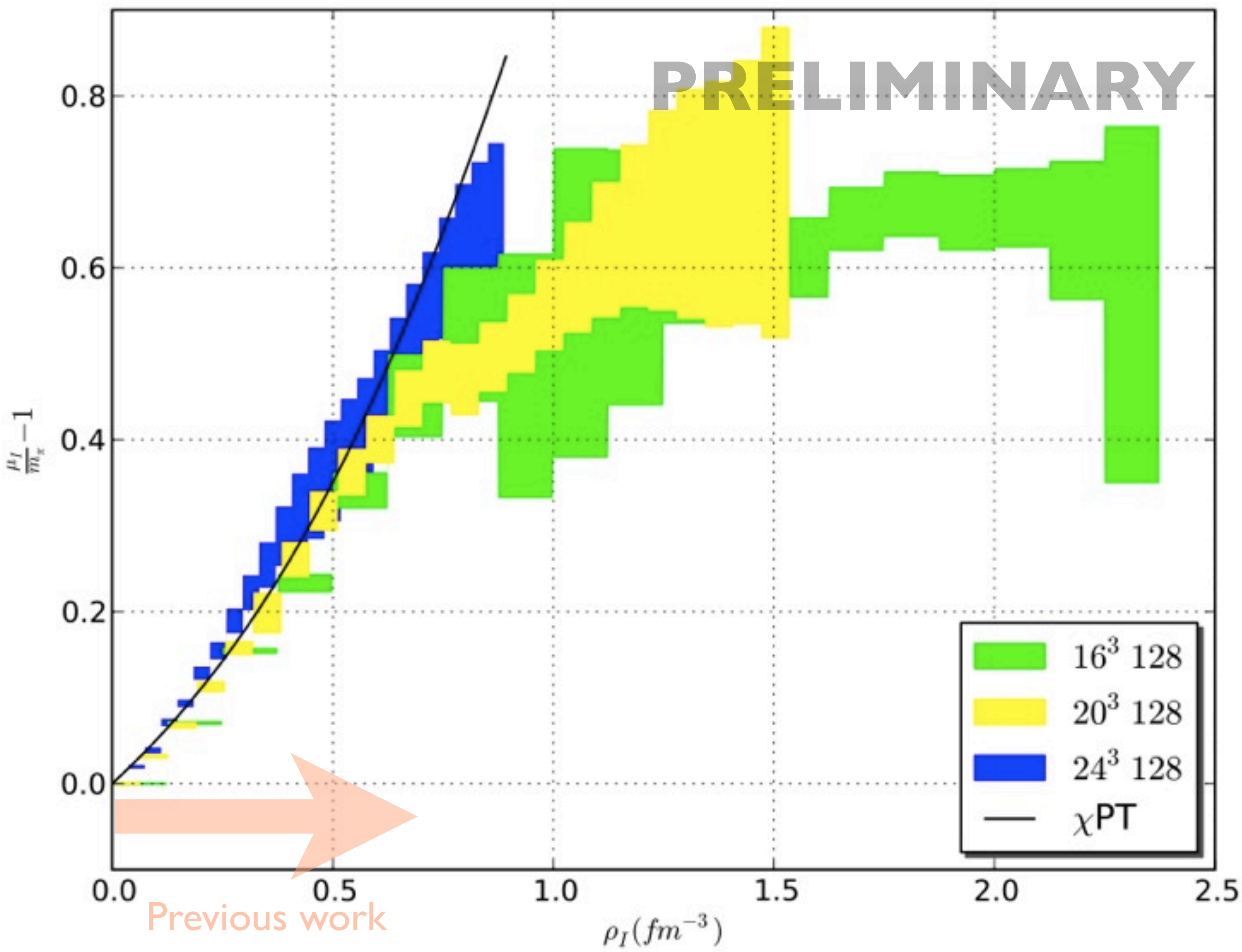
Higher density

- Recurrence relations become costly
  - Number of applications of recurrence grows fast
  - Make use of closed shells/descending recurrence
  - Beyond N ~ 36 is problematic ☹
- New method: scales as N log(N)
  - Limited only by computer representation of floats: $^{238}\pi^+$ requires ~250 decimal digit precision

Higher density: μ_I



Higher density: μ_I

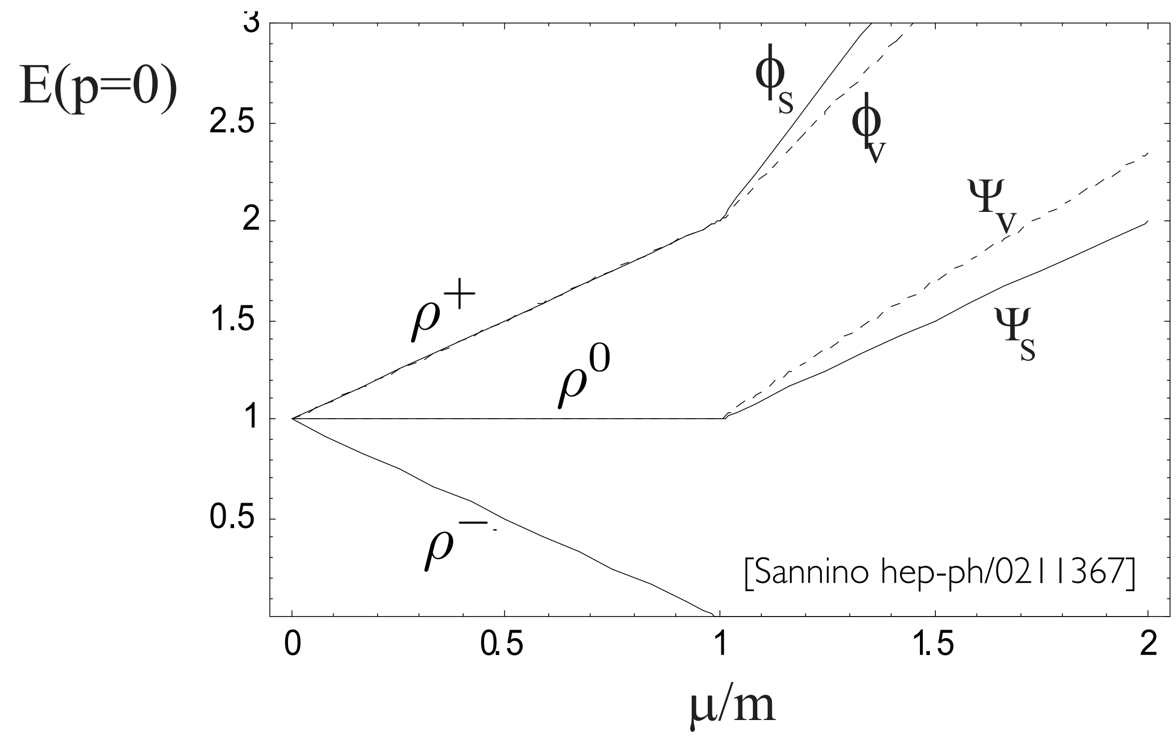


Vector condensation

- Possible explanation: condensation of ρ mesons
  - Ground state contains J=0 pairs of ρ's replacing π's
- Expected from general arguments [Voskresensky; Sannino,...]

$$\mathcal{L} = -\frac{1}{4}F^a_{\mu\nu}F^{a\mu\nu} + \frac{m^2}{2}A^a_\mu A^{a\mu} + \delta\,\epsilon^{abc}\partial_\mu A_{a\nu}A^\mu_b A^\nu_c - \frac{\lambda}{4}\left(A^a_\mu A^{a\mu}\right)^2 + \frac{\lambda'}{4}\left(A^a_\mu A^{a\nu}\right)^2$$

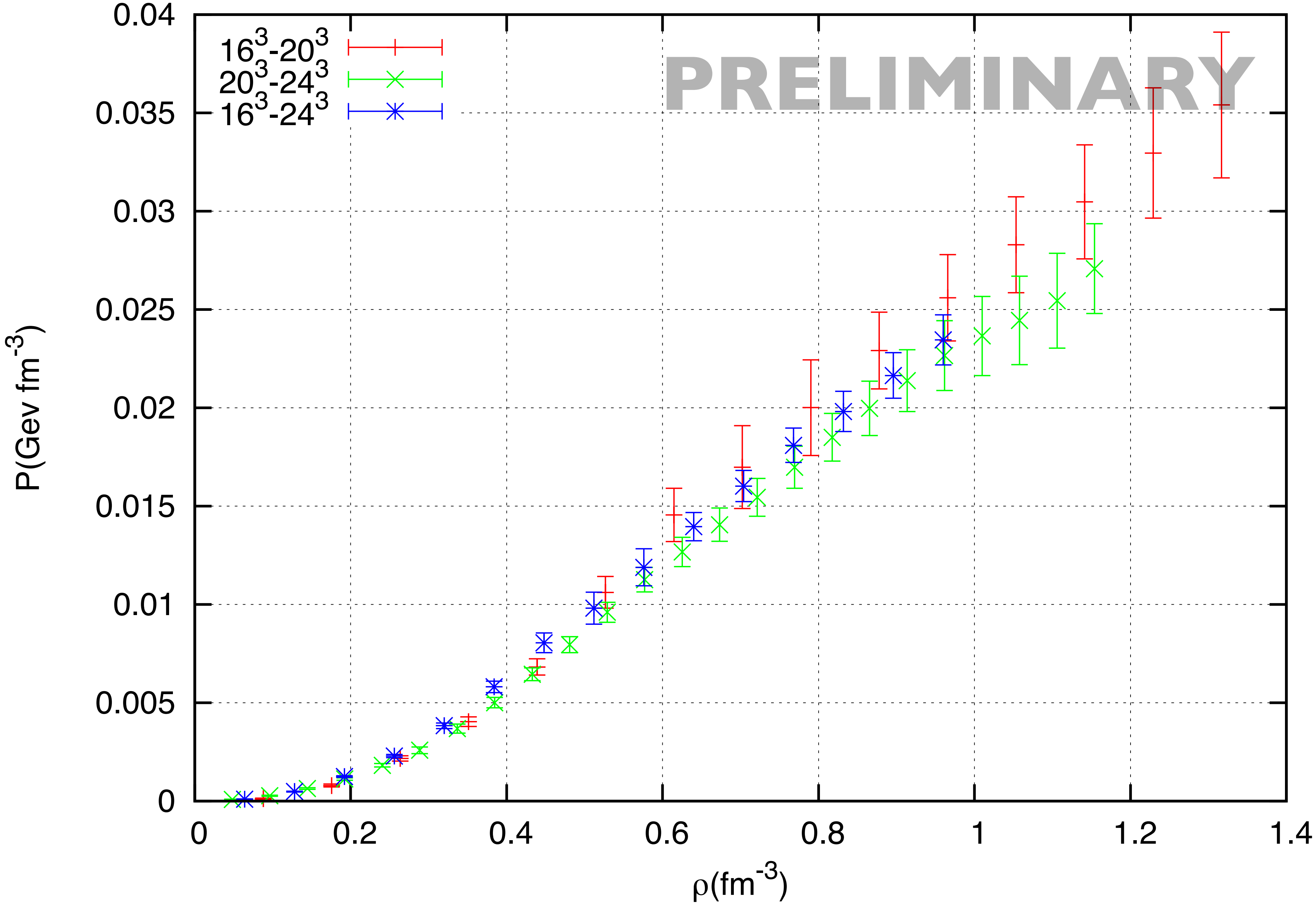
$$\partial_\nu A_\rho \to \partial_\nu A_\rho - i\,[B_\nu\ , A_\rho] \qquad B_\nu = \mu\,\delta_{\nu 0}T^3$$



- Similar expectation from ChPT+vector mesons
- Also seen in AdS models of QCD [Aharony et al.]

Pressure

- Measurements of E_n(L=16,20,24) access pressure



Matrix elements in
multi-hadron systems

[WD + Huey-Wen Lin, in progress]

Properties of multi-hadron systems

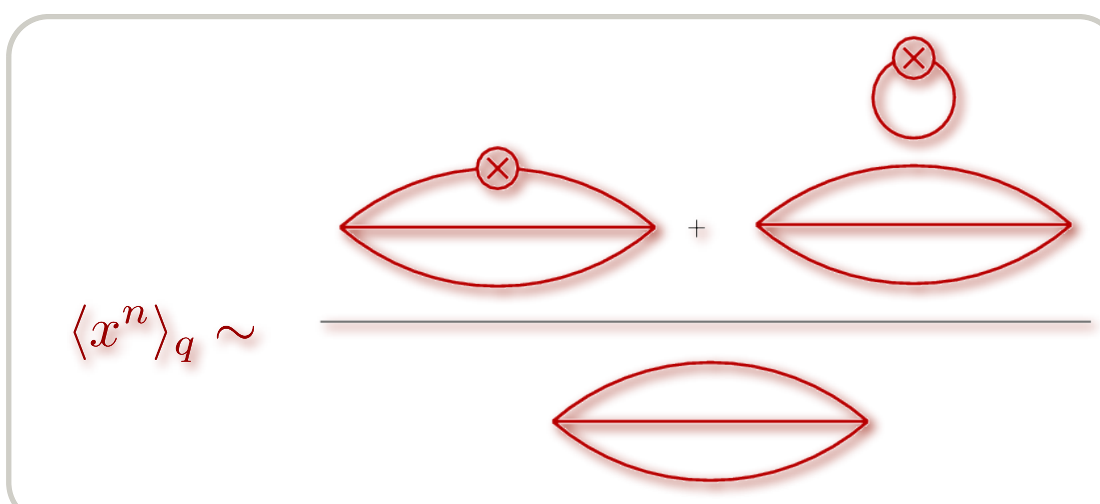
- Many important EW interactions with nuclei
  - μ_d, $np \rightarrow d\gamma$, V_{ud}, $0\nu\beta\beta$
- How can we probe multi-hadron systems?
  - External fields
  - Three-point functions
- Generically difficult

Example: momentum fraction

- Mellin moments of parton distributions defined by forward matrix elements of local operators

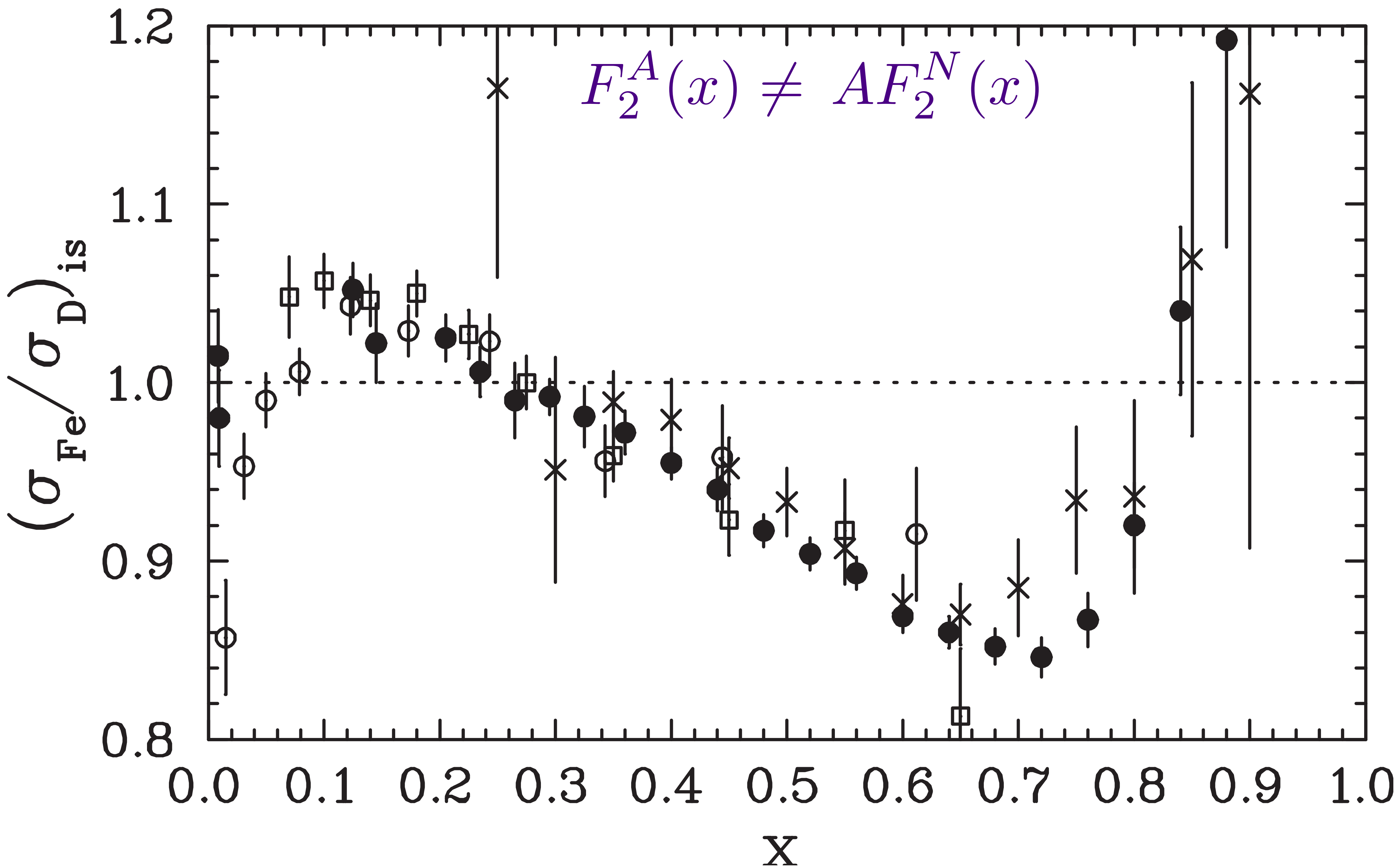
$$\langle x^n \rangle_H = \int_{-1}^{1} dx\, x^n q_H(x) \qquad \langle H|\overline{\psi}\gamma^{\{\mu_0} D^{\mu_1} \ldots D^{\mu_n\}}|H\rangle = p^{\{\mu_0} \ldots p^{\mu_n\}} \langle x^n \rangle_H$$

- n=1 corresponds to LC momentum fraction carried by quarks inside H (renormalisation scale dependent)
- Intensively studied in QCD using 3-pt functions (also possible using background fields



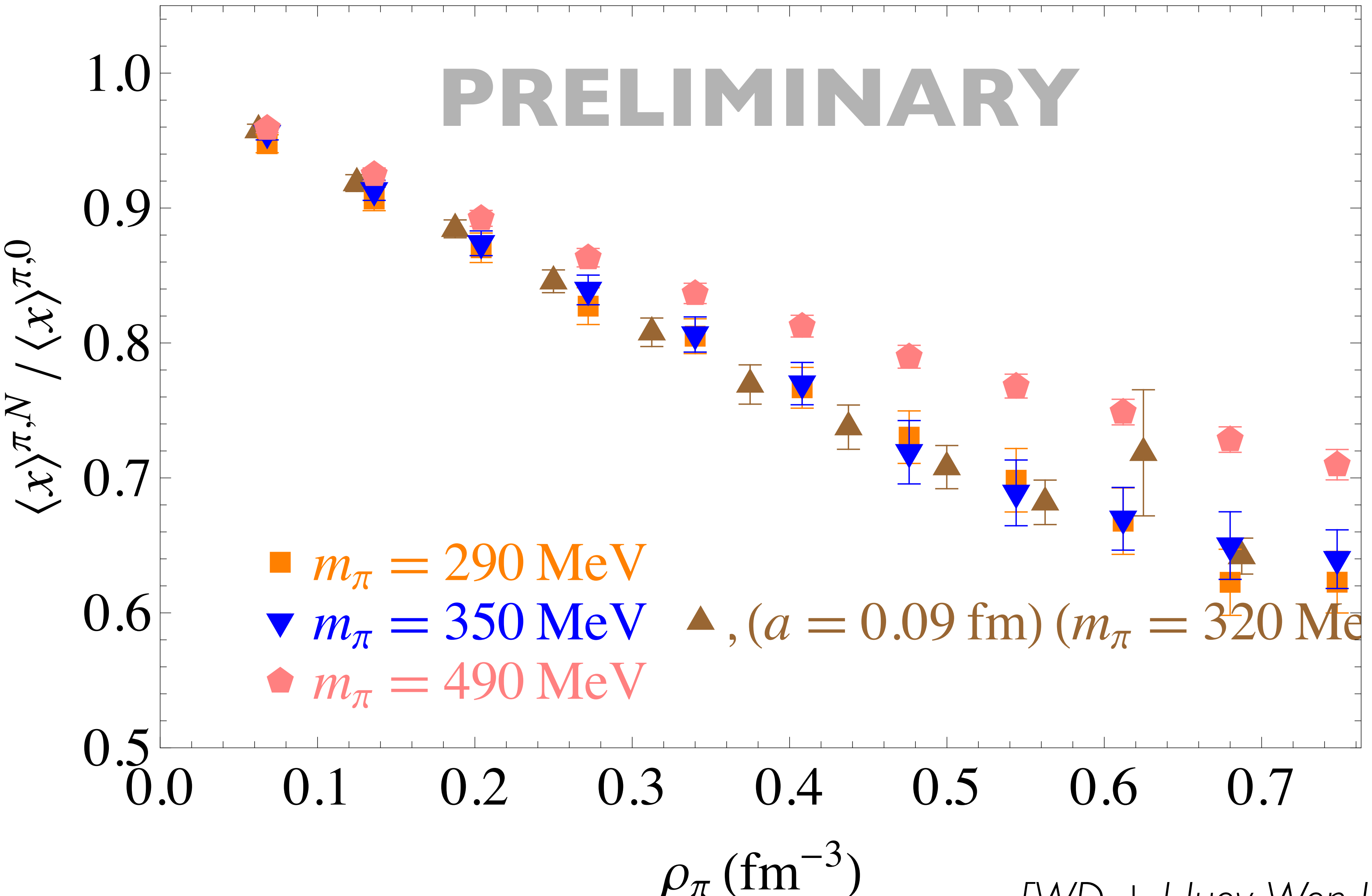
EMC effect

- Medium modification of parton distributions



Pionic EMC effect

- LC momentum fraction carried by quarks in a pion in a dense medium c.f. in free space

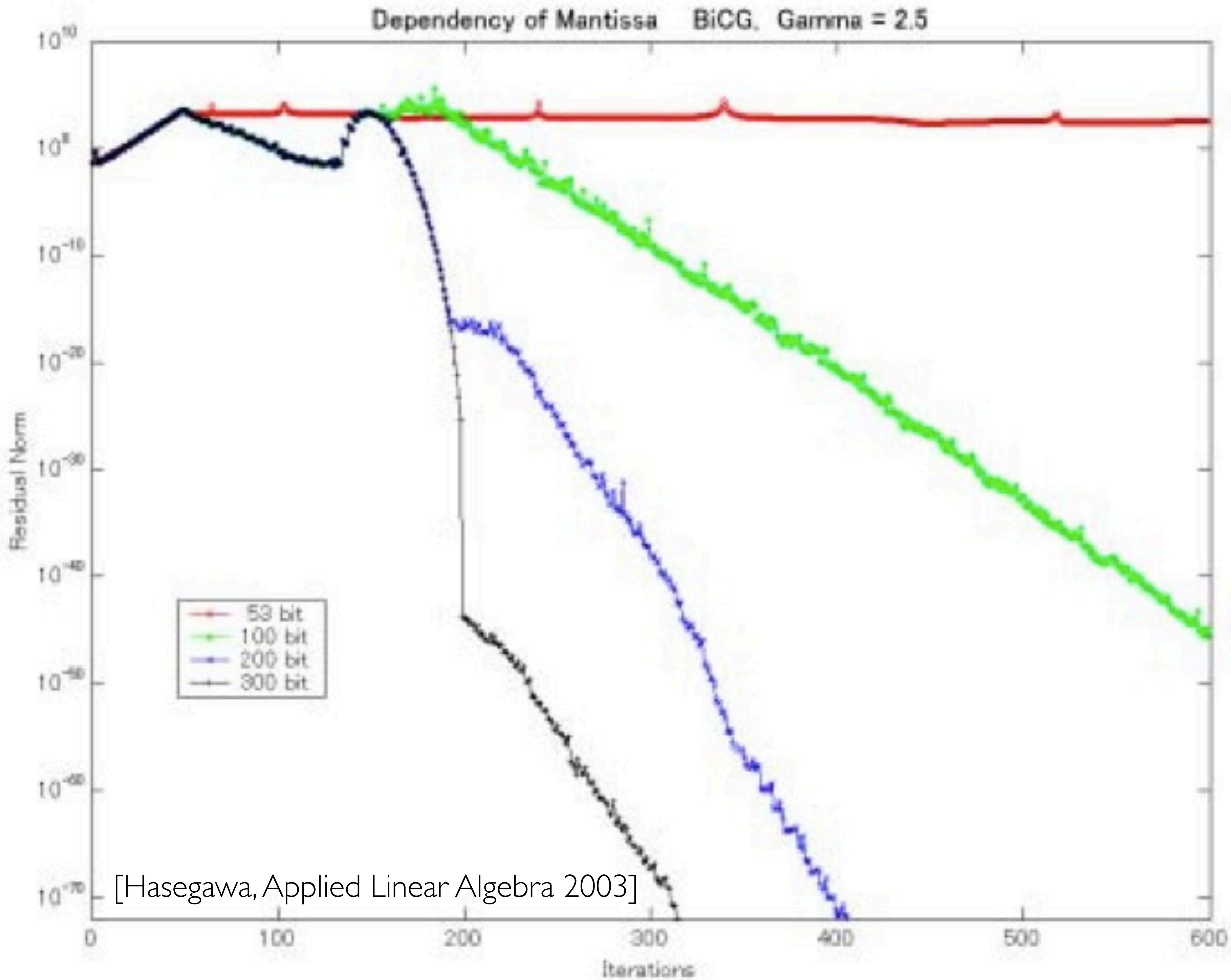


[WD + Huey-Wen Lin, in progress]

Outlook

- What lessons have pions taught us?
- Contractions require tricks
- Thermal effects ~ exp(-$m_\pi L_4$)
    - Particularly bad in multi-hadron states
    - Always present (pions from the sea)
- Precision
    - Contraction of propagators
    - Ultimately: HMC, propagator calculations

BiCG vs precision



N=200 Toeplitz matrix, $|ev_{min}|=0.8$ $|ev_{max}|\sim 5$