lattice QCD and the hadron spectrum

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finite lattice spacing

acts as a UV cutoff $\Lambda \sim \frac{1}{a}$ required, regularization of a renormalizable theory

appears as a scale $\hat{m} = am$

discretization errors $X(a) = X(0) + a\,\delta X_1 + \ldots$

extrapolate $a \to 0$

finite lattice volume

need $L \gg \frac{1}{m_\pi}$

impacts multi-hadron systems in an interesting way

carefully understand QFT in a finite volume

discretization choice

all should agree in the *a*→0 limit

impact at finite *a* depends on observable

choose a discretization appropriate to your quantities

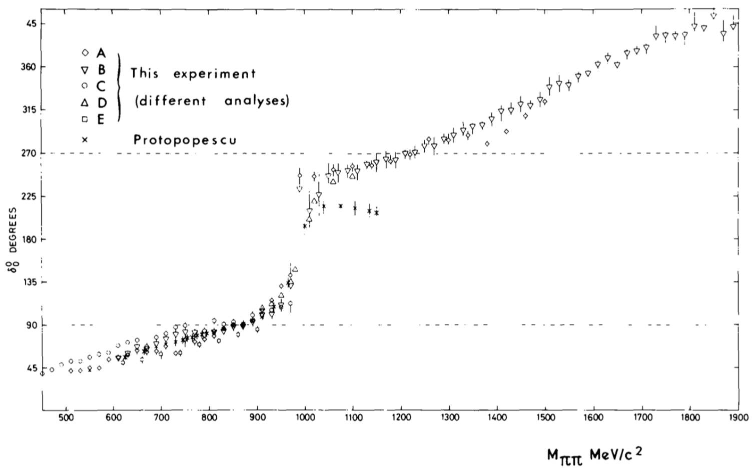
quark mass choice

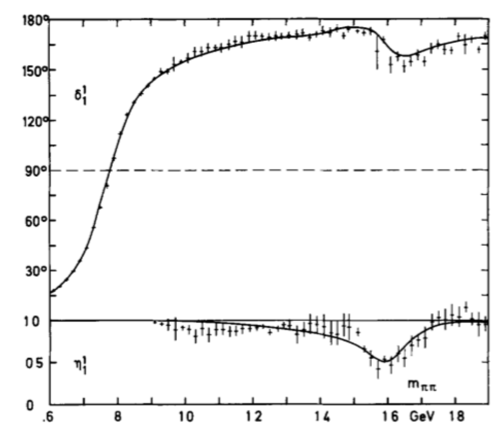
many calculations done with $m_{u,d} > m_{u,d}^{\text{phys}}$

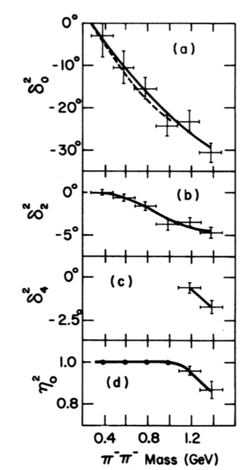
use quark mass as a tool to understand QCD

what quantities do we want to compute ?

scattering amplitudes !







not obvious how, try something simpler: **energy spectrum**

two-point correlation functions and the spectrum

consider $\langle 0 | \, O_{\mathrm{f}}(t) \; O_{\mathrm{i}}^{\dagger}(0) \, | 0 \rangle$

e.g. in our case:
operators with definite J^P quantum numbers
as color-singlet combinations of quark and gluon fields

e.g. as last time, $\bar{\psi}\gamma_5\psi$

two-point correlation functions and the spectrum

consider $\langle 0 | \, O_\mathrm{f}(t) \, O_\mathrm{i}^\dagger(0) \, | 0 \rangle$

Euclidean time-evolution $O(t) = e^{Ht} \, O(0) \, e^{-Ht}$

$$= \langle 0 | \, O_\mathrm{f}(0) \, e^{-Ht} \, O_\mathrm{i}^\dagger(0) \, | 0 \rangle$$

QCD Hamiltonian has a complete set of eigenstates $H | \mathfrak{n} \rangle = E_\mathfrak{n} | \mathfrak{n} \rangle$

$$1 = \sum_\mathfrak{n} | \mathfrak{n} \rangle \langle \mathfrak{n} |$$

(only discrete eigenstates ?)

presumably (color singlet) hadrons or systems of hadrons ?

the spectrum

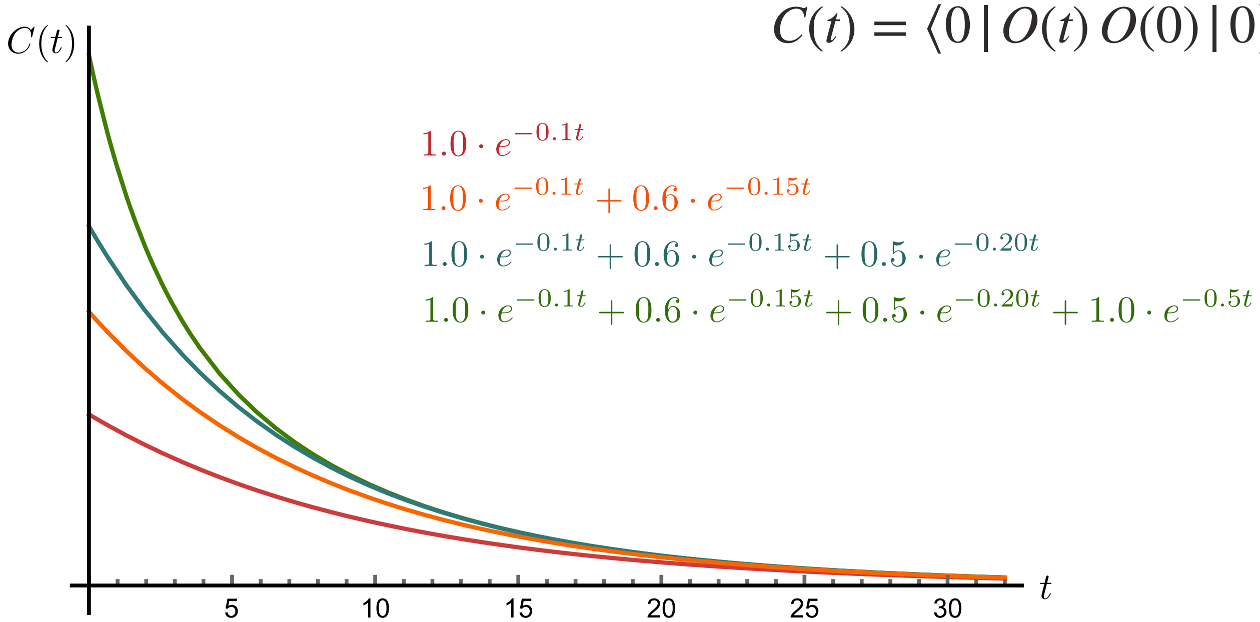
$$= \sum_\mathfrak{n} e^{-E_\mathfrak{n} t} \, \langle 0 | O_\mathrm{f}(0) | \mathfrak{n} \rangle \langle \mathfrak{n} | O_\mathrm{i}^\dagger(0) | 0 \rangle$$

amplitude for $O_\mathrm{i}^\dagger$
to 'interpolate' state $| \mathfrak{n} \rangle$
from the vacuum

time dependence of two point correlation functions

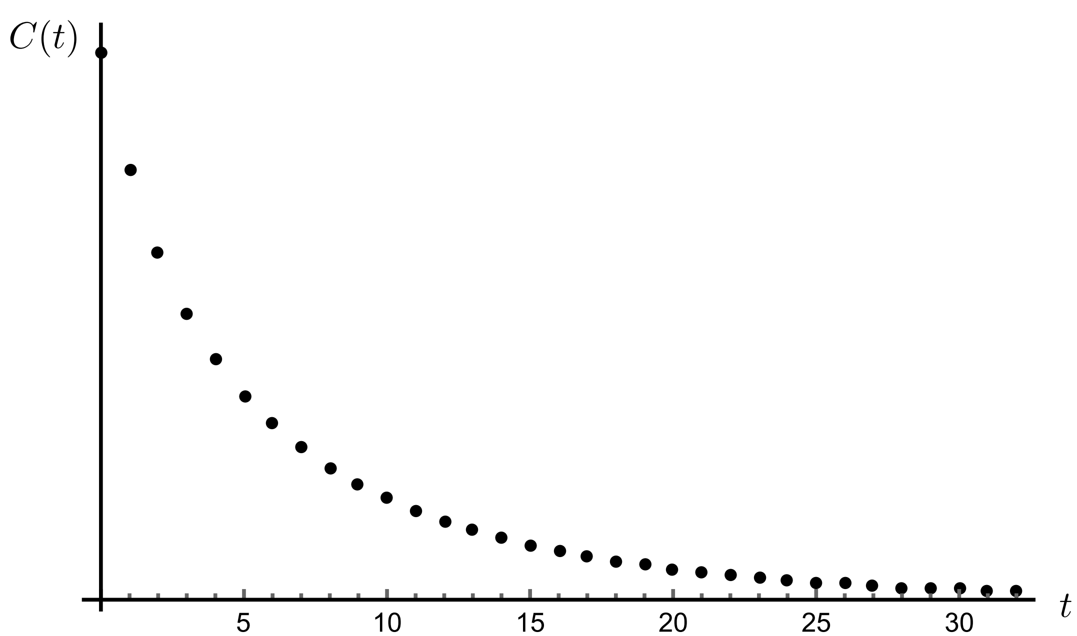
diagonal correlation function

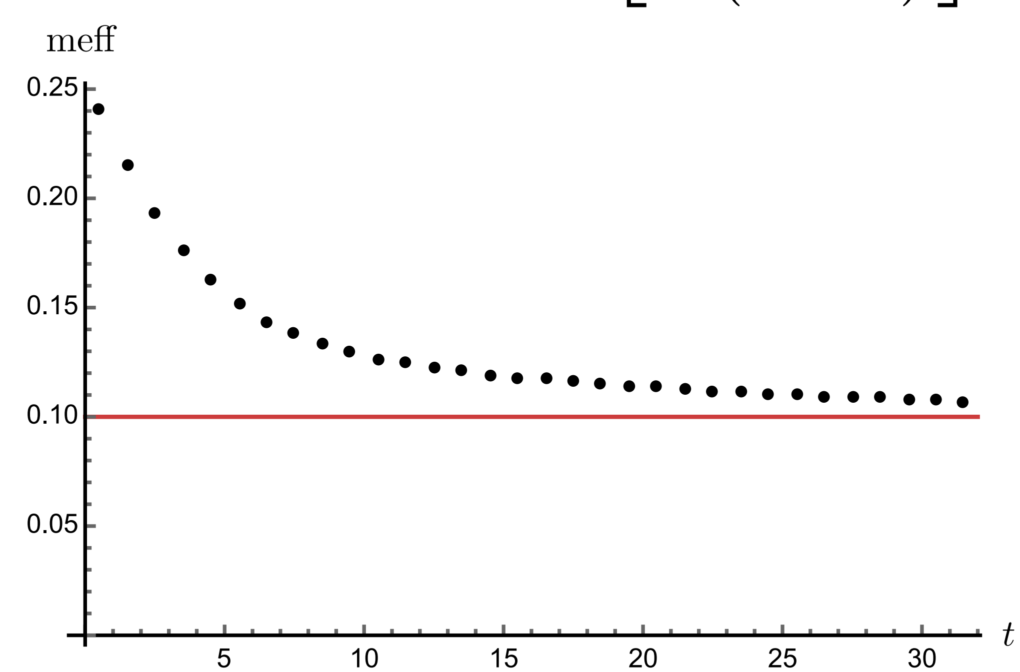
$$C(t) = \langle 0 | \mathcal{O}(t)\, \mathcal{O}(0) | 0 \rangle$$



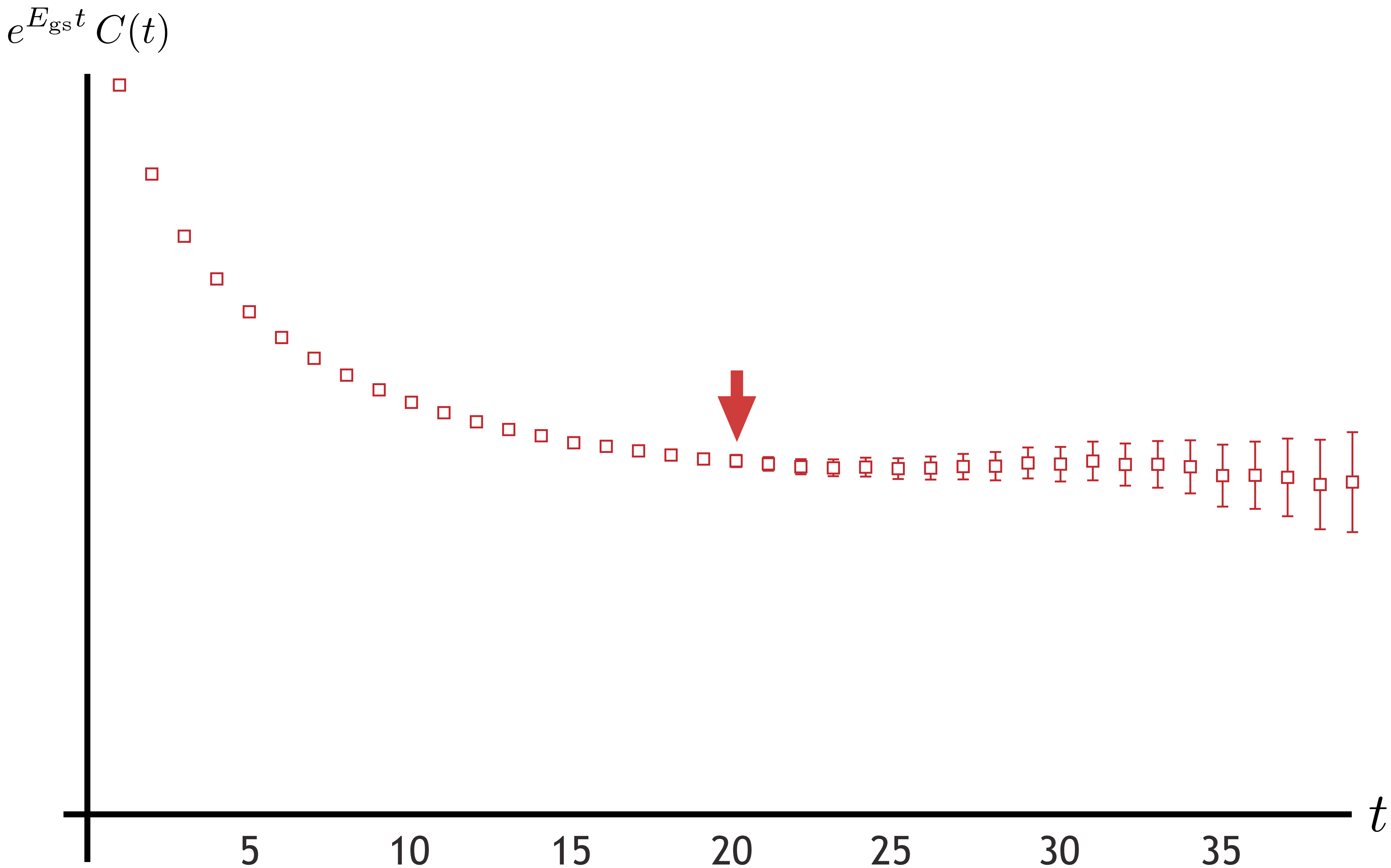
notice that as $t \to \infty$ $\quad C(t) \to c \cdot e^{-E_{\mathrm{gs}} t}$

useful to define the 'effective mass' $\quad \log\left[\frac{C(t)}{C(t+1)}\right]$



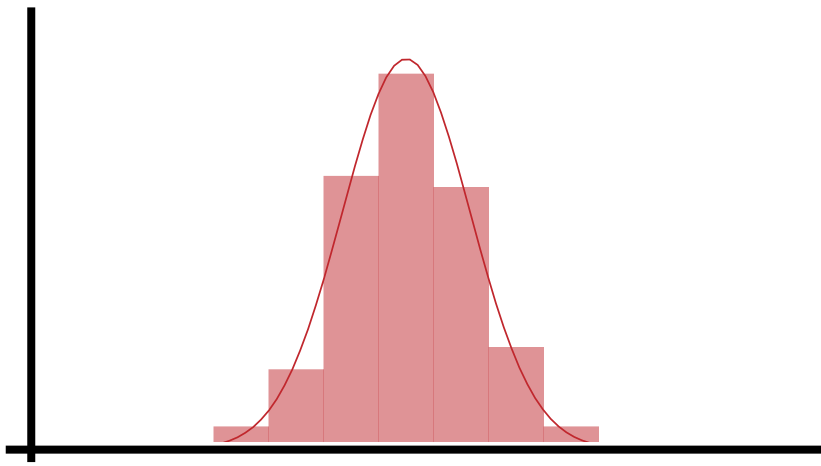


an actual lattice QCD two point correlation function



generally statistical noise increases with increasing t

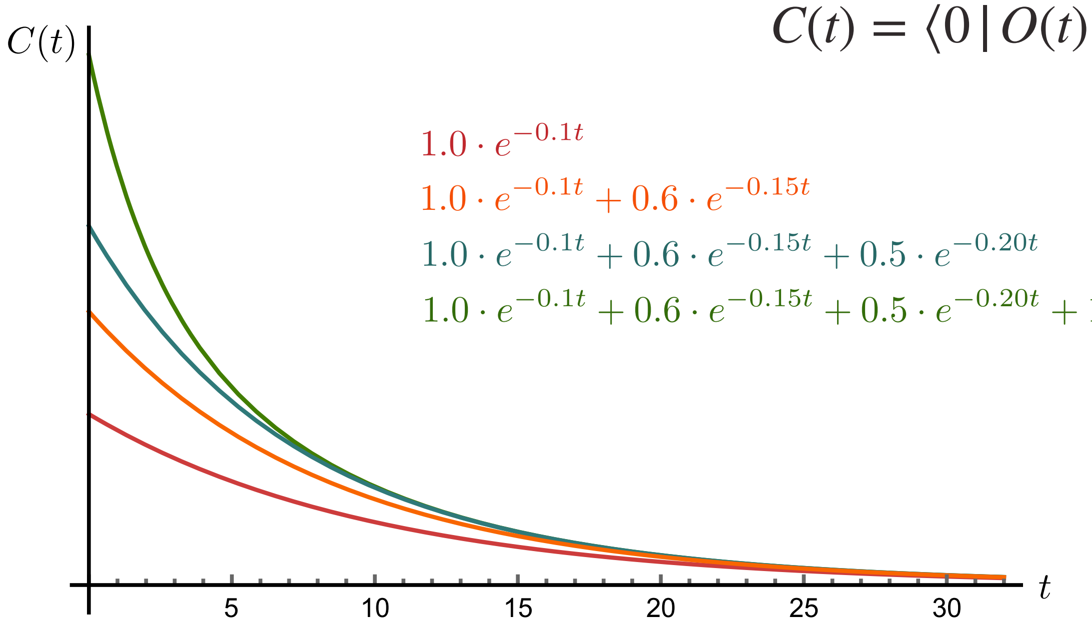
ensemble dist<u>n</u>



time dependence of two point correlation functions

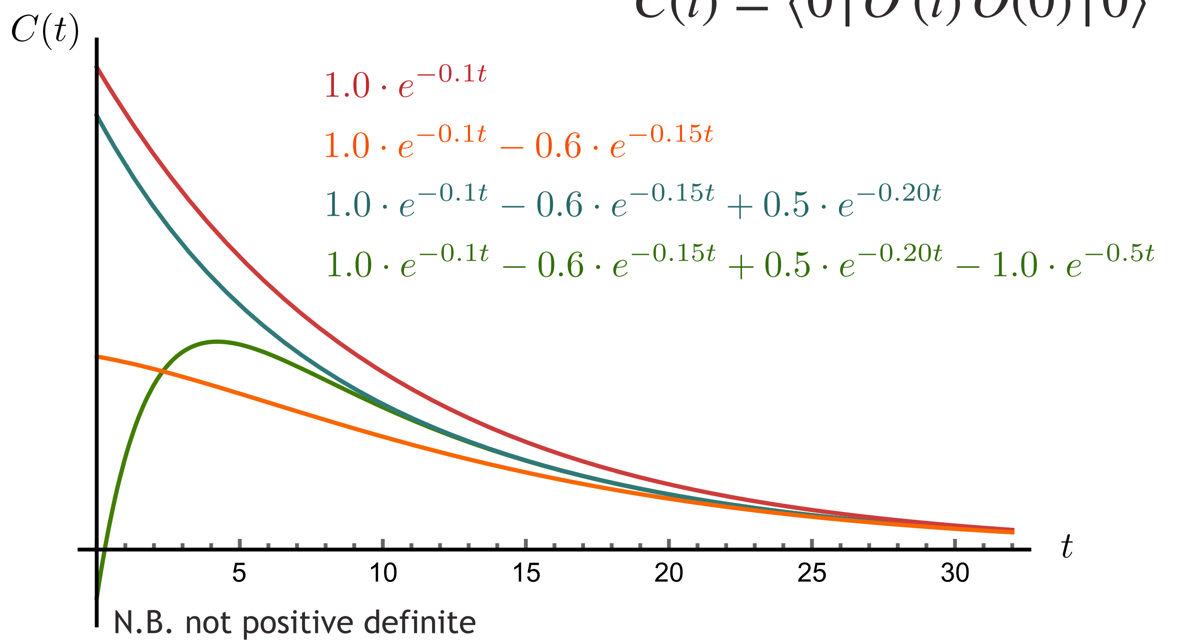
diagonal correlation function

$C(t) = \langle 0 | O(t)\, O(0) | 0 \rangle$



off-diagonal correlation function

$C(t) = \langle 0 | O'(t)\, O(0) | 0 \rangle$



suggests non-linear fitting to a sum of exponentials ...

? how many exponentials ?

? what if there are (near) degenerate states ?

... actually getting reliable results this way
for anything more than the ground state proves impractical ...

extracting the excited spectrum

a more powerful approach makes use of a **basis of operators** $\{O_1, O_2, O_3, \ldots\}$

there should be a **linear combination** which **optimally produces the ground-state**
and **another** which **optimally produces the first-excited-state**
etc ...

$$\Omega_{\mathfrak{n}}^\dagger = \sum_i v_i^{(\mathfrak{n})} O_i^\dagger$$

how do we find these optimizing weights ?

$$\Omega_\mathfrak{n}^\dagger = \sum_i v_i^{(\mathfrak{n})}\, O_i^\dagger \qquad \Omega_\mathfrak{n}^\dagger\big|0\big\rangle = \big|\mathfrak{n}\big\rangle + \sum_{\mathfrak{m}\neq\mathfrak{n}} \epsilon_\mathfrak{m}\big|\mathfrak{m}\big\rangle$$

with the $\epsilon_\mathfrak{m}$ as small as possible

‘optimal’ correlation function

$$\big\langle 0\big|\Omega_\mathfrak{n}(t)\,\Omega_\mathfrak{n}^\dagger(0)\big|0\big\rangle = e^{-E_\mathfrak{n} t} + \sum_{\mathfrak{m}\neq\mathfrak{n}} \big|\epsilon_\mathfrak{m}\big|^2 e^{-E_\mathfrak{m} t}$$

minimize this

$$= \sum_{ij} v_i^*\, \big\langle 0\big|O_i(t)\, O_j^\dagger(0)\big|0\big\rangle\, v_j = \sum_{ij} v_i^*\, C_{ij}(t)\, v_j$$

by varying the v_i

can avoid the trivial minimum ($v_i=0$) by fixing normalization $\sum_{ij} v_i^*\, C_{ij}(t_0)\, v_j = 1$

this choice will become clearer later

implement constraint via a Lagrange multiplier

minimize $\Lambda = \sum_{ij} v_i^*\, C_{ij}(t) v_j - \lambda\Big[\sum_{ij} v_i^*\, C_{ij}(t_0) v_j - 1\Big]$

⇒ generalized eigenvalue problem $\mathbf{C}(t)\mathbf{v} = \lambda(t)\mathbf{C}(t_0)\mathbf{v}$

generalized eigenvalue problem *a.k.a* "GEVP"

$$\mathbf{C}(t)\mathbf{v} = \lambda(t)\mathbf{C}(t_0)\mathbf{v}$$

eigenvalues, *a.k.a* **principal correlators** $\lambda_{\mathfrak{n}}(t) \sim e^{-E_{\mathfrak{n}}(t-t_0)}$

eigenvectors, *a.k.a* **optimized operator weights** $\Omega_{\mathfrak{n}}^\dagger = \sum_i v_i^{(\mathfrak{n})} O_i^\dagger$

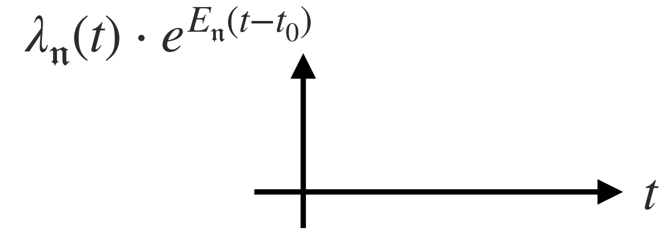
eigenvector orthogonality $\mathbf{v}^{(\mathfrak{n})} \cdot \mathbf{C}(t_0) \cdot \mathbf{v}^{(\mathfrak{m})} = \delta_{\mathfrak{n},\mathfrak{m}}$

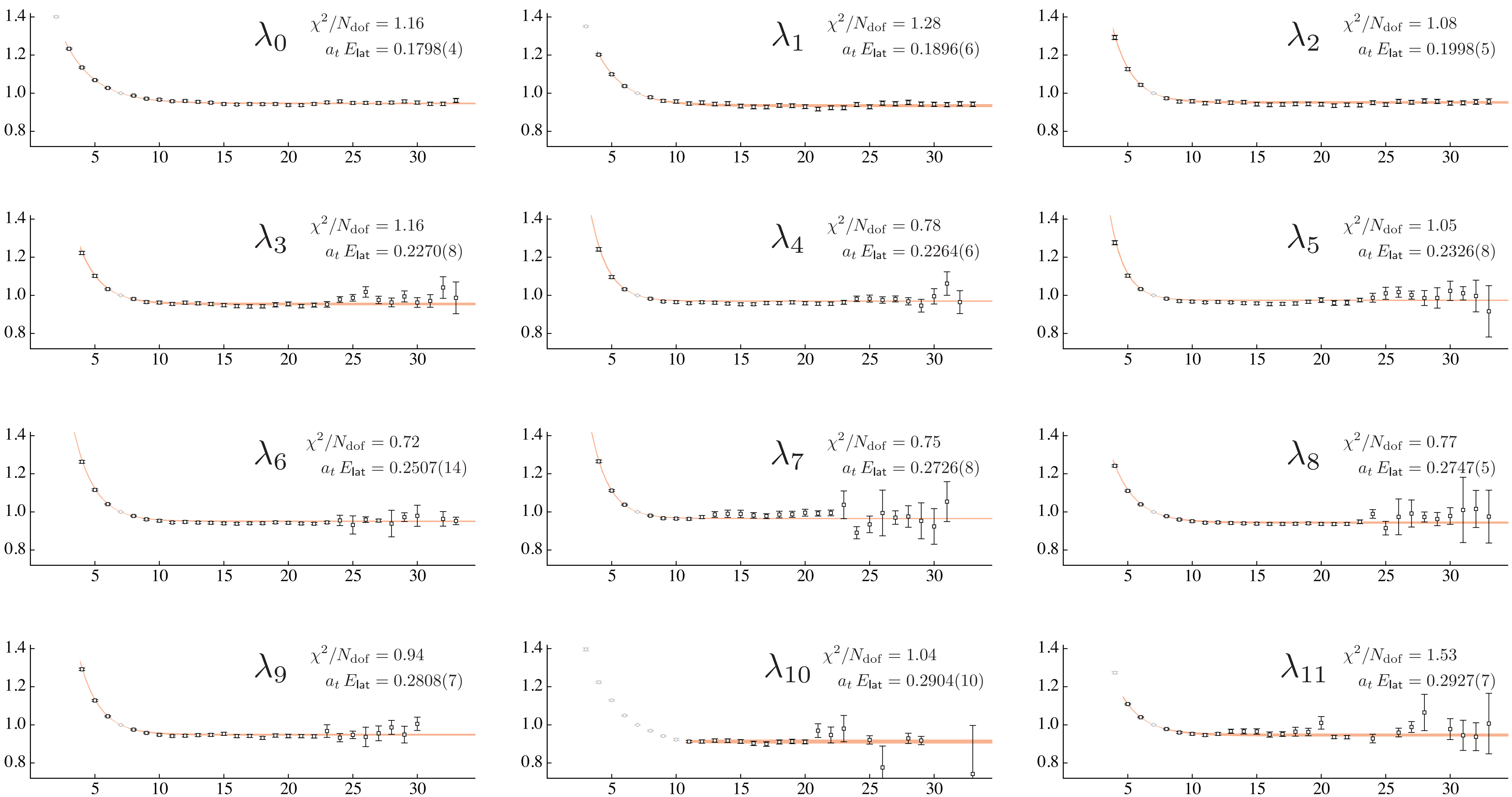
things to think about:

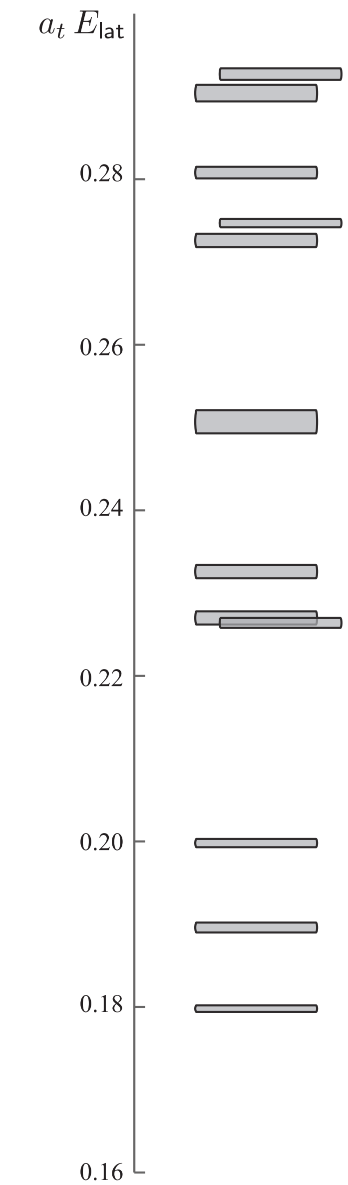
? how do you select the value of t_0 ?

? is there some limit in which this gives the exact answer ?

principal correlators







fitted with

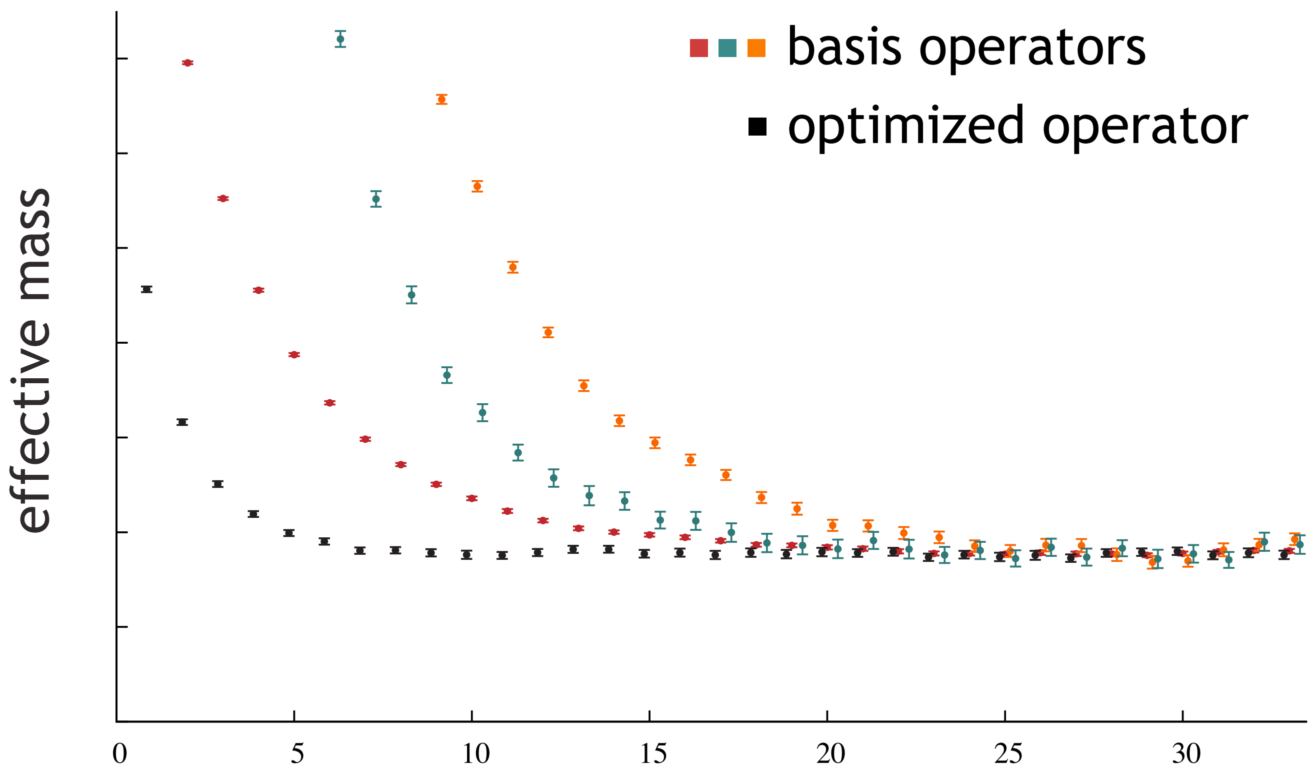
$$\lambda_n(t) = (1 - A_n)\, e^{-E_n(t-t_0)} + A_n\, e^{-E'_n(t-t_0)}$$

with $A_n \ll 1$ and $E'_n \gg E_n$

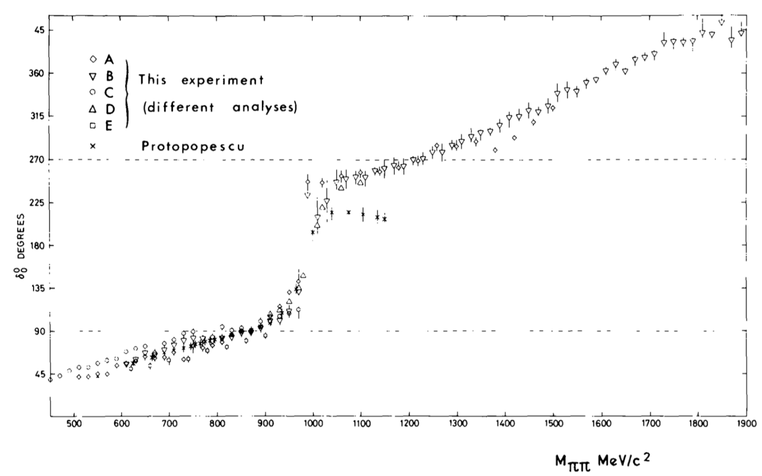
optimized operator construction

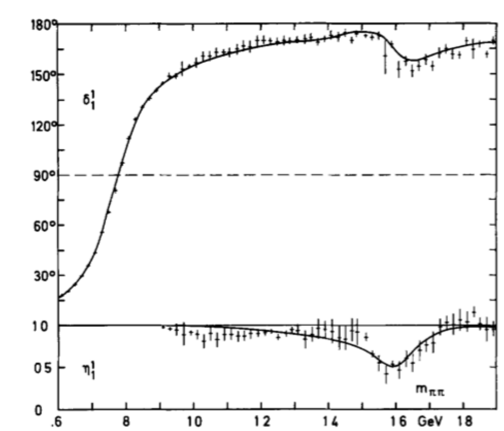
$$\Omega_{\mathfrak{n}}^{\dagger} = \sum_i v_i^{(\mathfrak{n})} O_i^{\dagger}$$

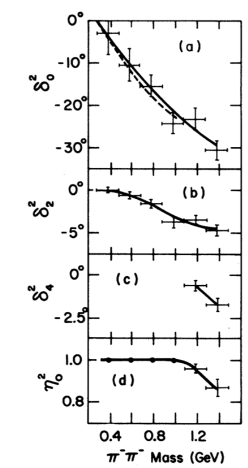
diagonal correlators



optimized operator saturated by the pion by timeslice 7 ok, so it looks like we should be able to compute spectra, but we wanted **scattering amplitudes !**







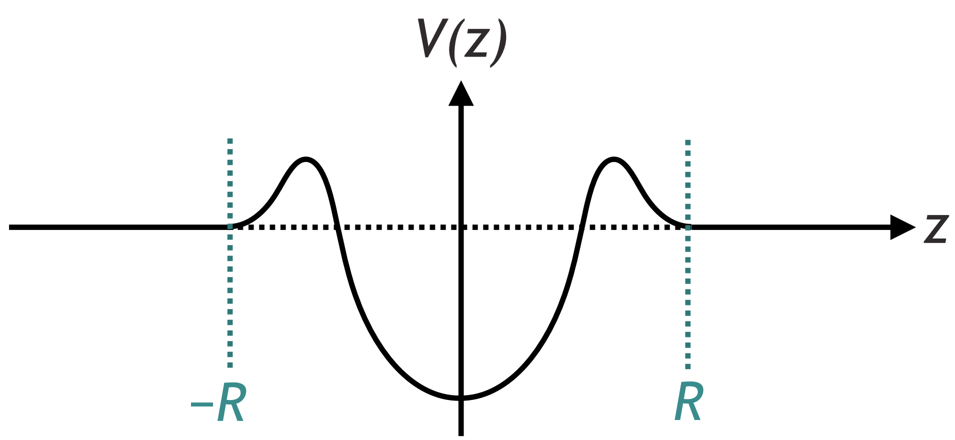
scattering in a finite volume ?

lattice defines a **(periodic) spatial volume** — usually a cube, side length a few fermi

spectra are discrete in a finite volume — no scattering continuum ?

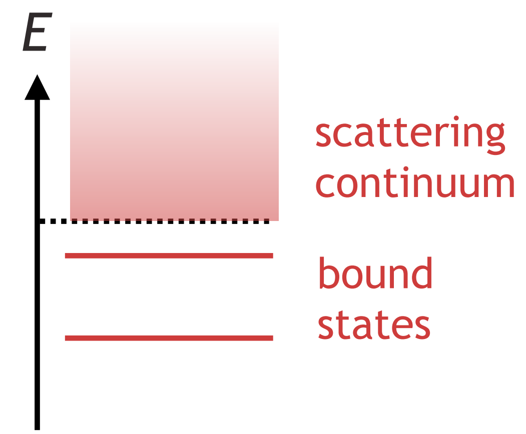
let’s get a conceptual picture by returning to our one-dim quantum mechanics problem

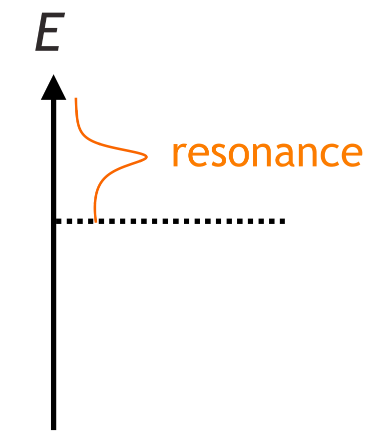
scattering



solve the Schrödinger equation

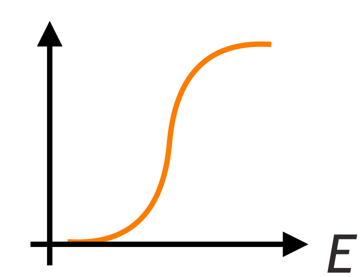
$$-\frac{1}{m}\frac{d^2\psi}{dz^2} + V(z)\psi(z) = E\psi(z)$$





$$\psi(|z| > R) \sim \cos\big(p\,|z| + \delta(p)\big)$$

phase-shift



‘scattering’ in a finite-volume

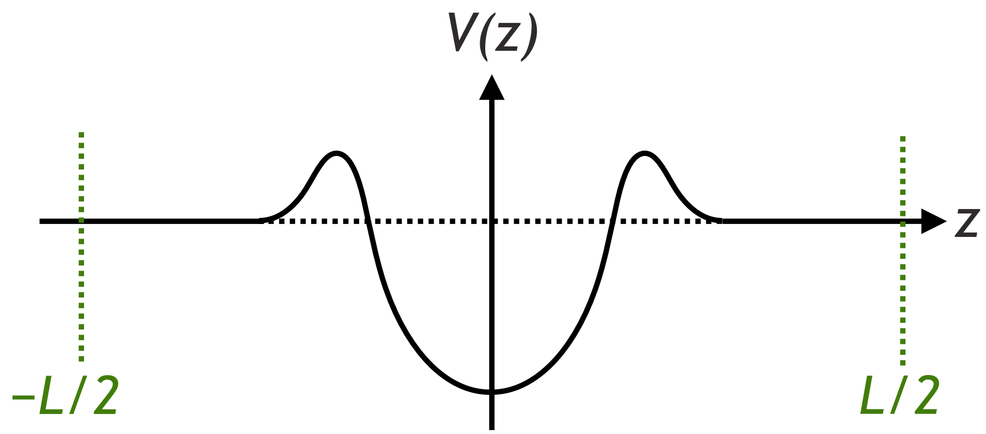
now put the system in a ‘box’ — periodic boundary condition at $z = \pm L/2$

$$\psi(|z| > R) \sim \cos\big(\, p\,|z| + \delta(p)\,\big)$$

$$\psi(L/2) = \psi(-L/2)$$
$$\frac{d\psi}{dz}(L/2) = \frac{d\psi}{dz}(-L/2)$$

momentum quantization condition

$$p = \frac{2\pi}{L} n - \frac{2}{L}\delta(p)$$



3+1 dim quantum field theory result

for elastic scattering in a cube the corresponding relationship is $\cot\delta_\ell(E) = \mathcal{M}_\ell\big(E(L), L\big)$

in the simplest case of a single partial wave being non-zero

Lüscher 1986

⋮

many subsequent works
see the RMP for a complete list

will present some complications later …

$k = \frac{1}{2}\sqrt{E^2 - 4m^2}$

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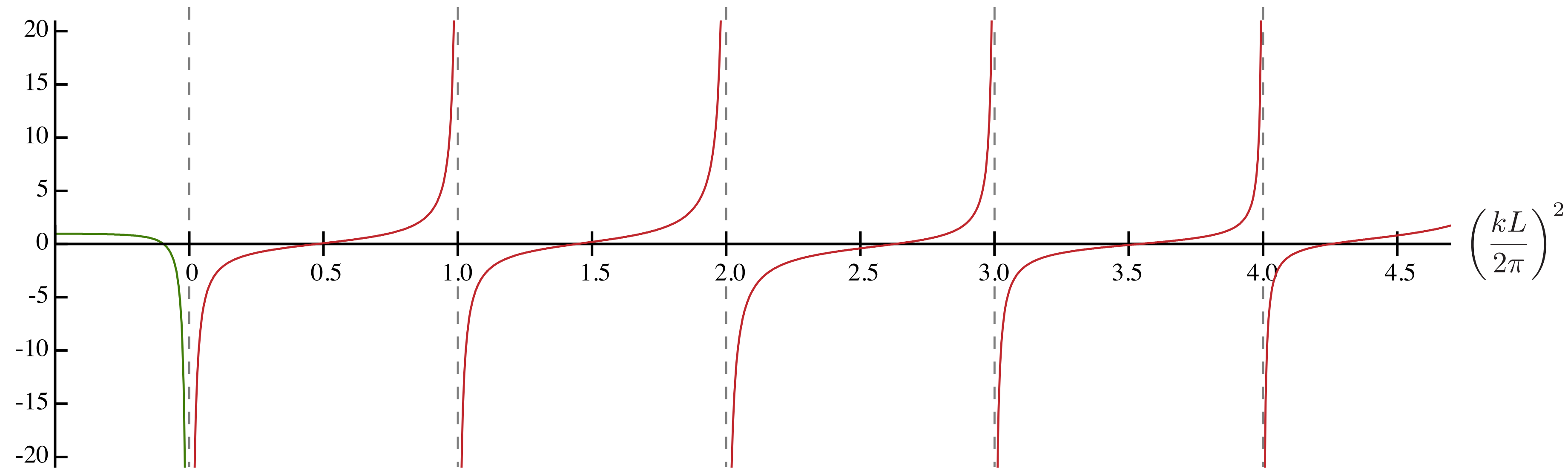
$$\cot\delta_\ell(E) = \mathcal{M}_\ell\big(E(L), L\big)$$

known function expressing the 'kinematics' of the finite-volume

e.g. $\mathcal{M}_0$



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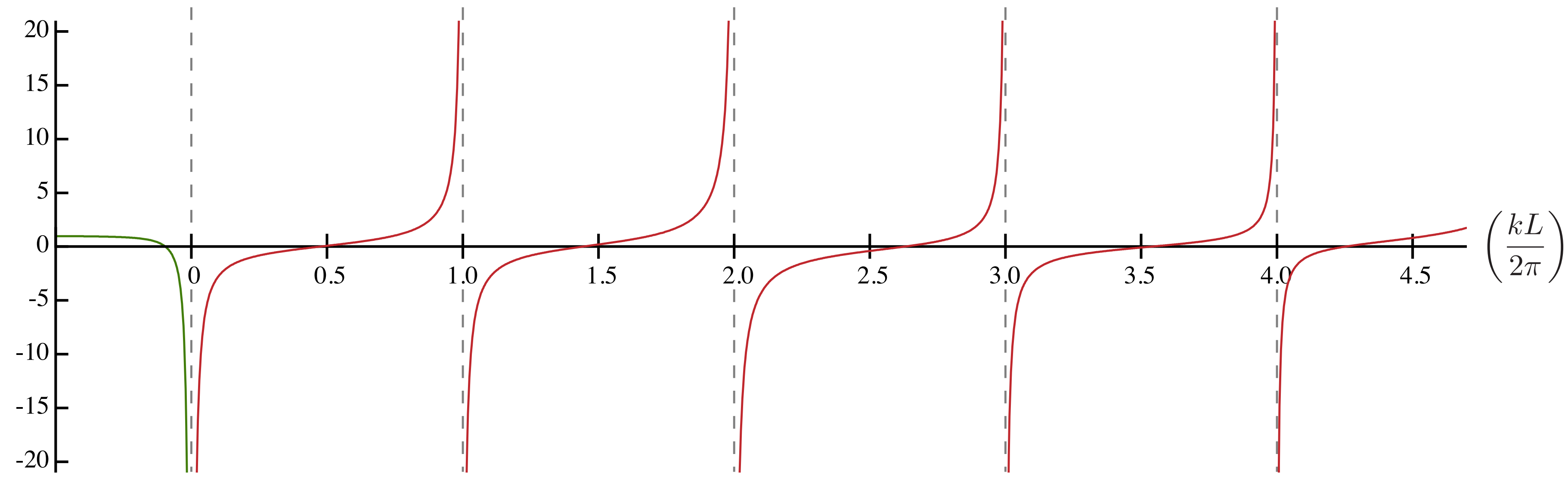
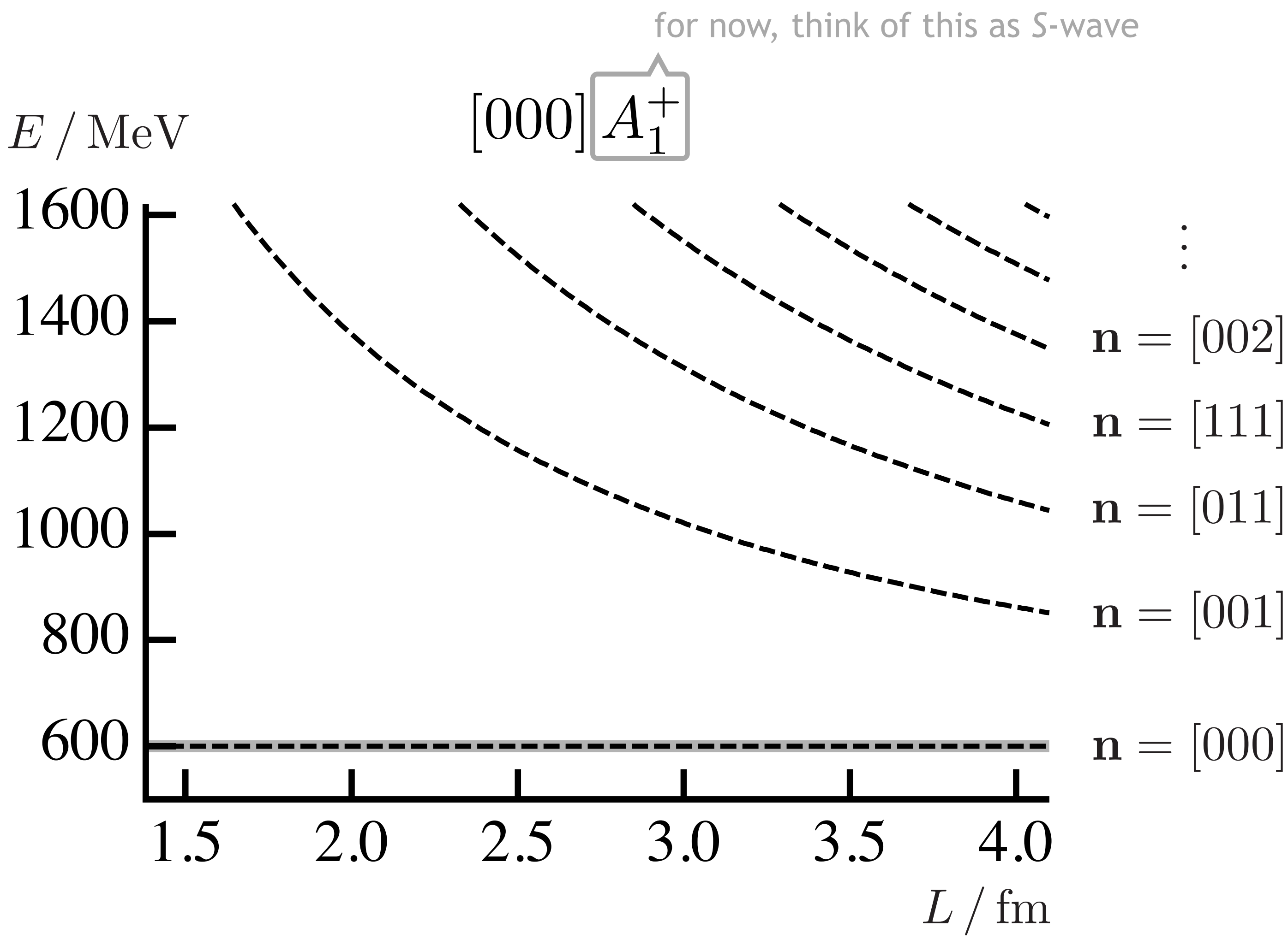


$k = \frac{1}{2}\sqrt{E^2 - 4m^2}$

so find the intersections of this curve with $\cot\delta(E)$

no interaction

scattering particles *m* = 300 MeV



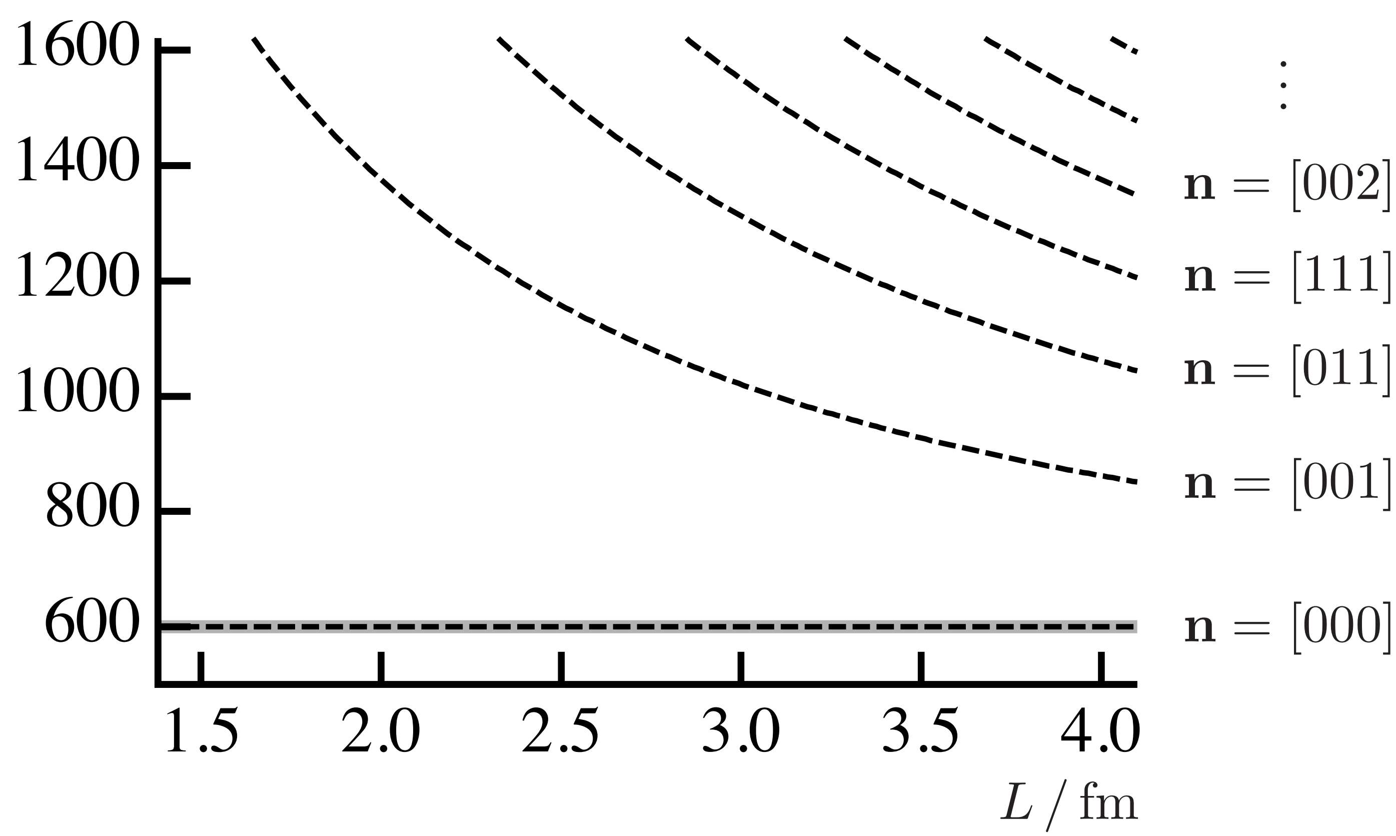
$$E_{\mathrm{ni}} = 2\sqrt{m^2 + \mathbf{p}^2} \qquad \mathbf{p} = \frac{2\pi}{L}\mathbf{n}$$

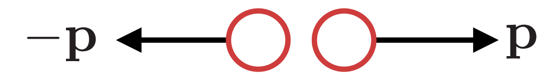
no interaction

scattering particles m = 300 MeV

for now, think of this as S-wave

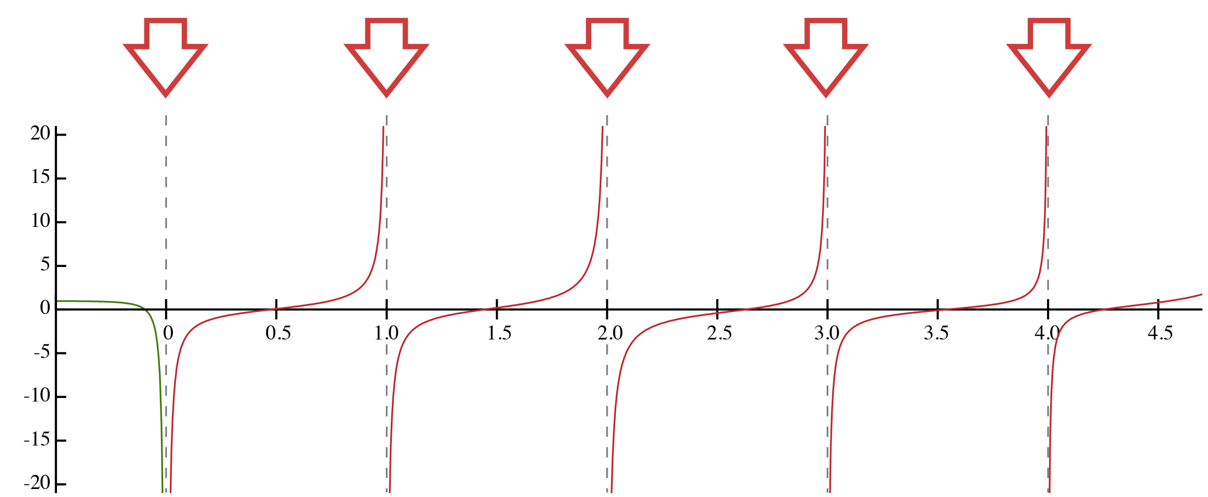
$[000]\ A_1^+$





$$E_{\mathrm{ni}} = 2\sqrt{m^2 + \mathbf{p}^2} \qquad \mathbf{p} = \frac{2\pi}{L}\mathbf{n}$$

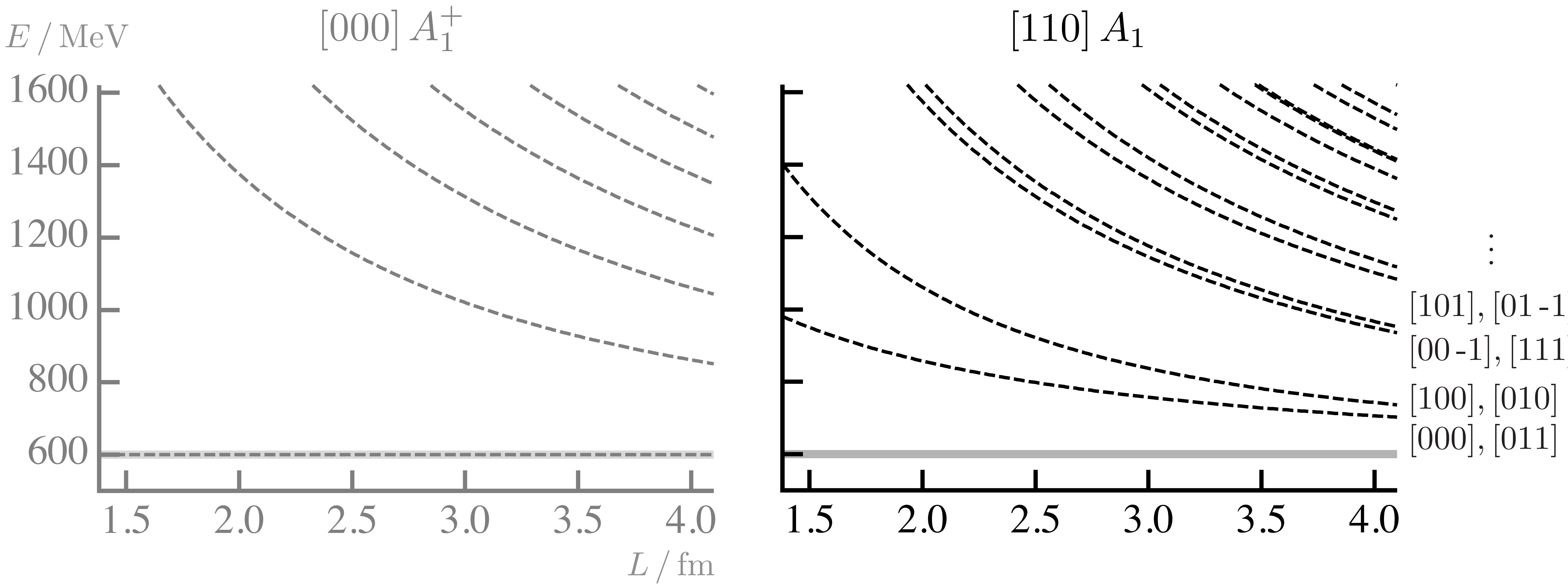
$$\cot\delta(E) = \mathcal{M}\big(E(L), L\big) \qquad \delta \to 0,\ \cot\delta \to \infty$$

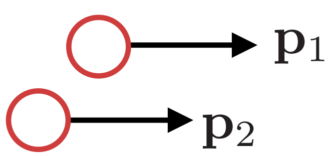


divergences correspond to non-interacting energies

no interaction — in a moving frame

$\cot \delta_\ell(E) = \mathcal{M}_\ell^{\mathbf{P}}\big(E(L), L\big)$





$$\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$$

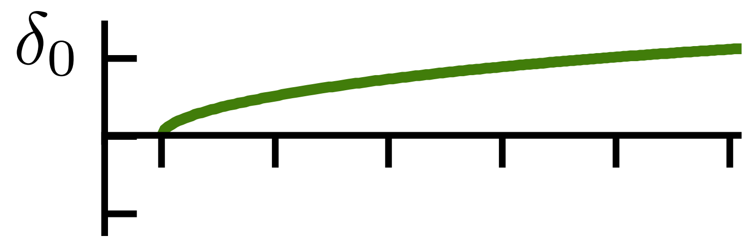
$$E_{\mathrm{ni}} = \sqrt{m^2 + \mathbf{p}_1^2} + \sqrt{m^2 + \mathbf{p}_2^2}$$

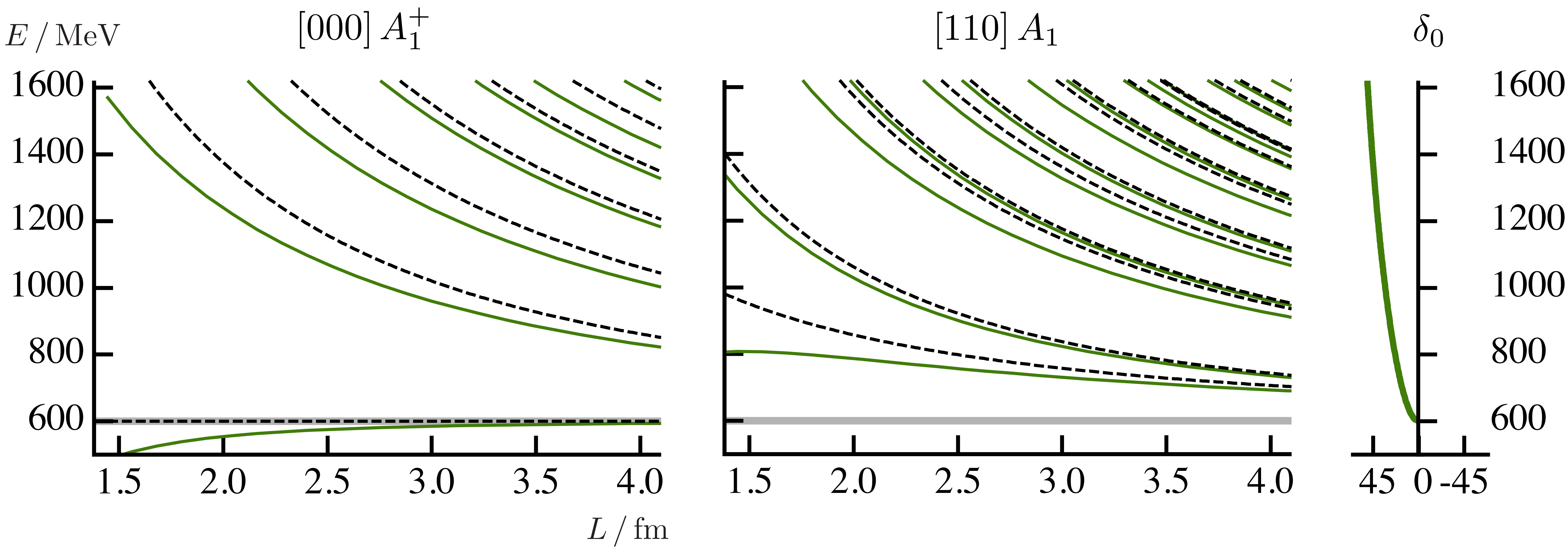
$$\mathbf{P} = \frac{2\pi}{L}\mathbf{n}$$

$$\mathbf{p}_{1,2} = \frac{2\pi}{L}\mathbf{n}_{1,2}$$

in the cm frame $E_{\mathrm{cm}} = \sqrt{E^2 - \mathbf{P}^2}$

find the finite-volume spectrum for a **fixed phase-shift**





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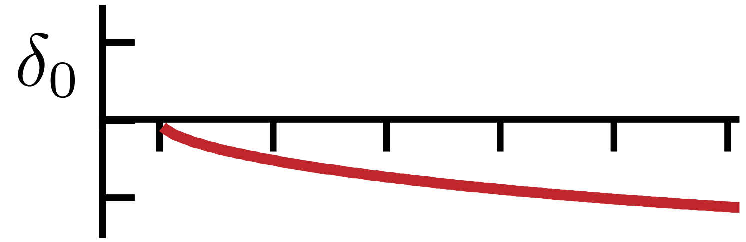
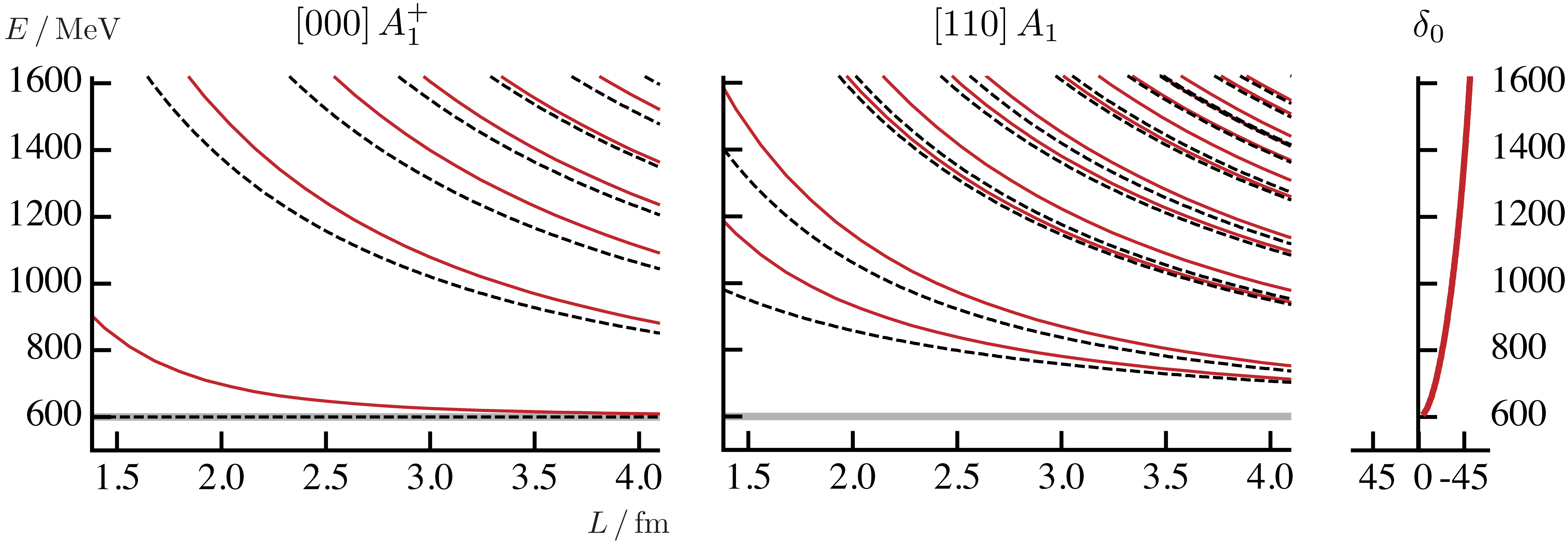
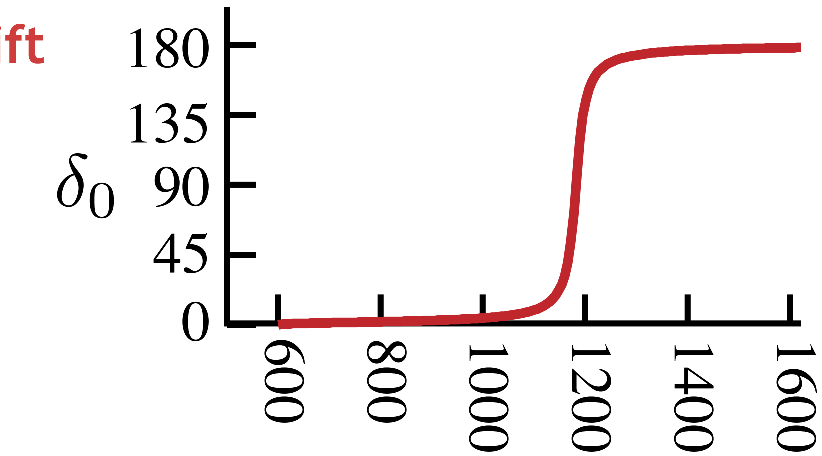




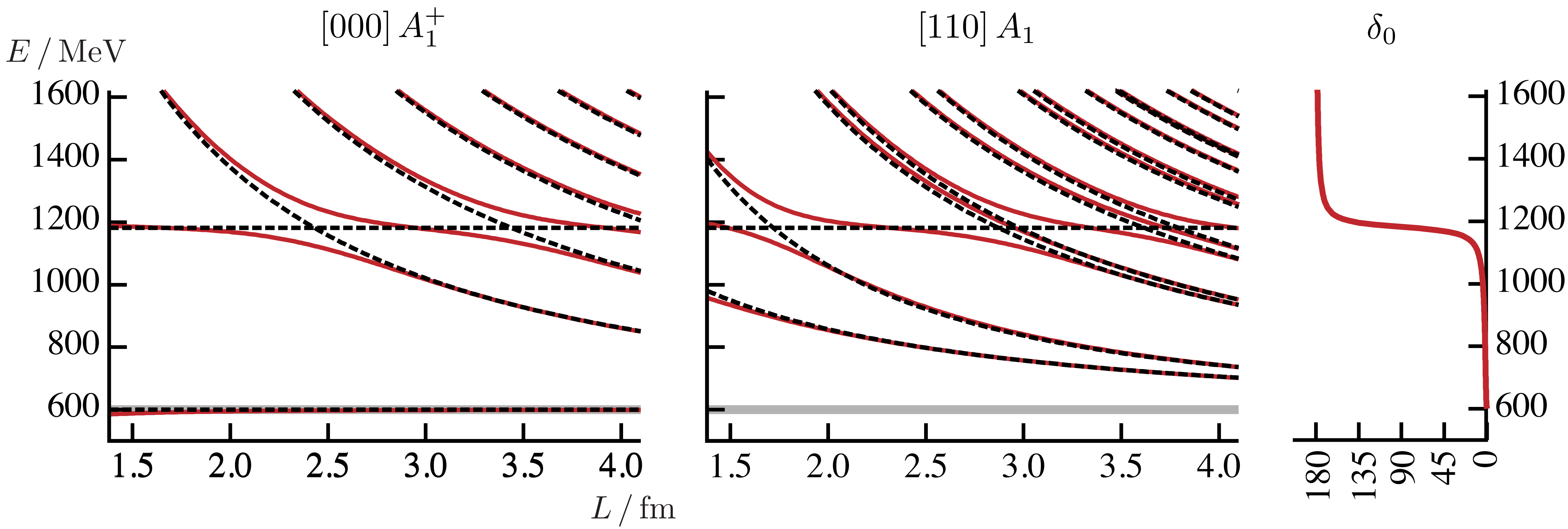
an elastic resonance

find the finite-volume spectrum for a **fixed phase-shift**



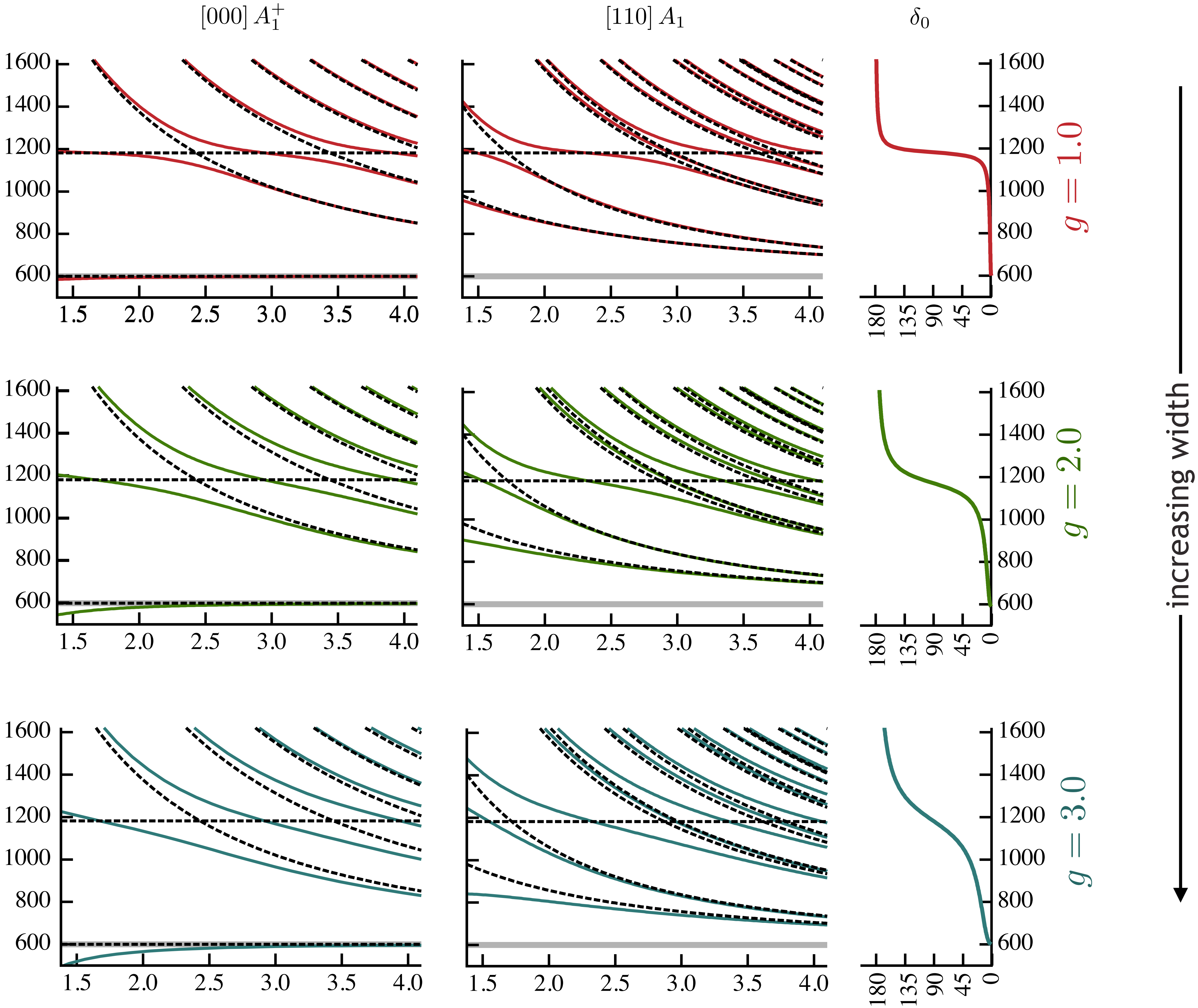
$$\tan\delta = \frac{E\,\Gamma(E)}{m_R^2 - E^2}$$

$$\Gamma(E) = \frac{g^2}{6\pi}\frac{m_R^2}{E^2}k(E)$$



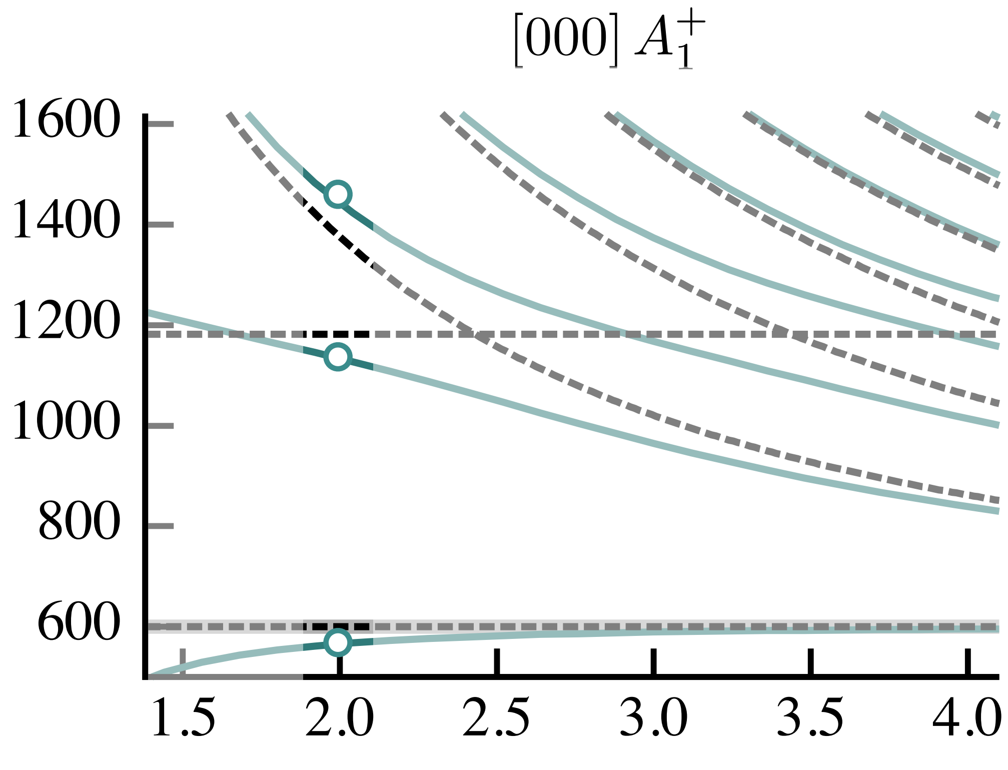
note the avoided level crossings

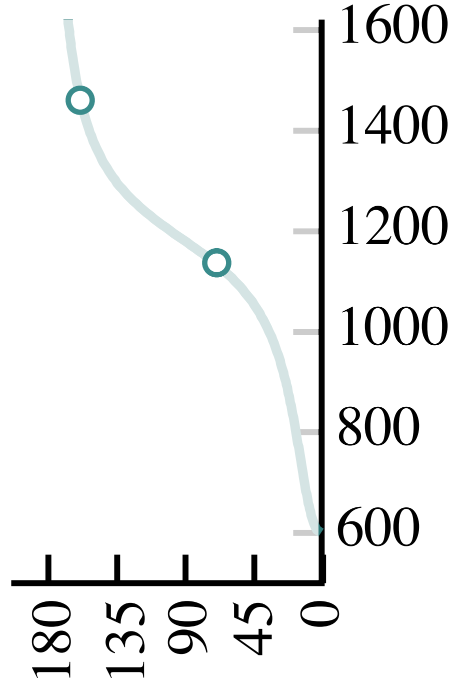
elastic resonance



$$\Gamma(E) = \frac{g^2}{6\pi}\frac{m_R^2}{E^2}k(E)$$

what about the reverse process — obtain the phase-shift from the finite-volume spectrum ?





an elastic resonance — finite-volume mapping

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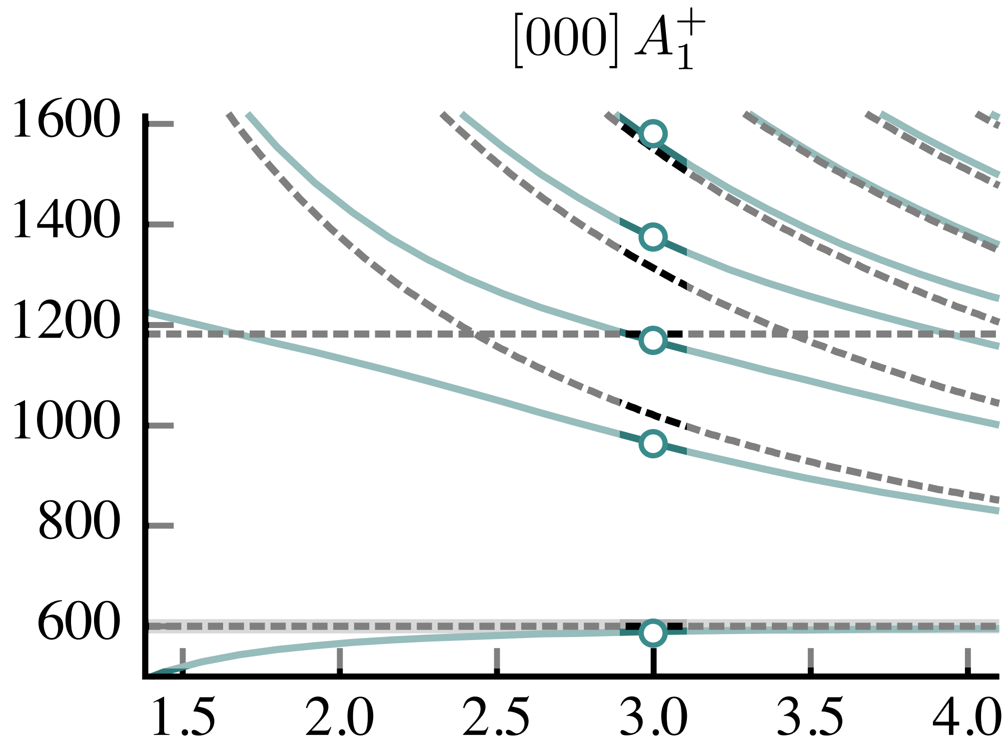

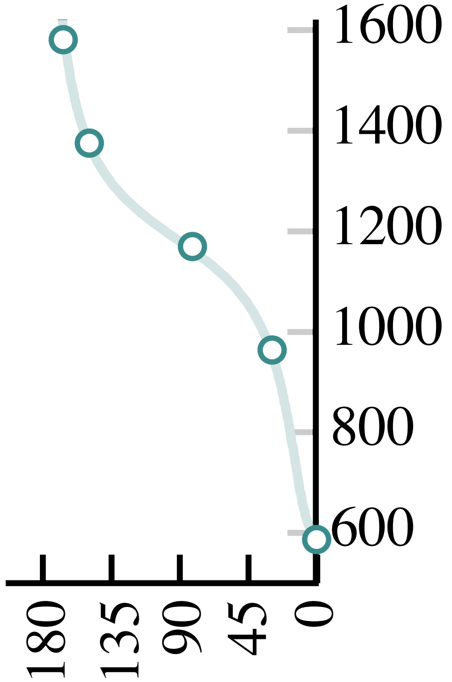

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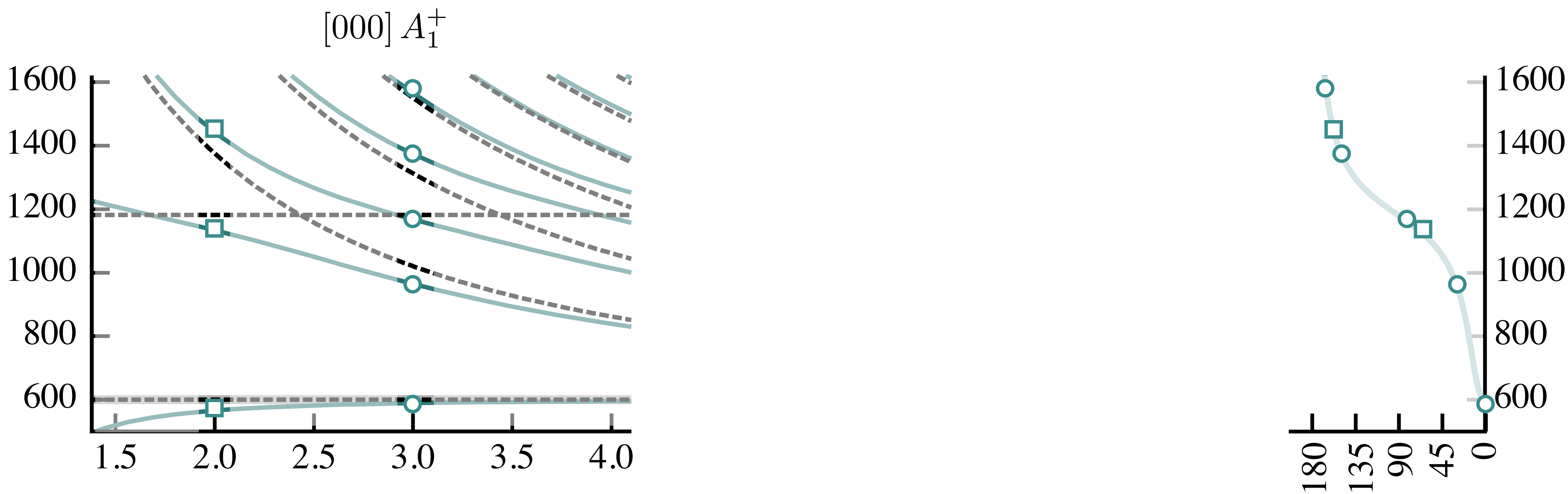
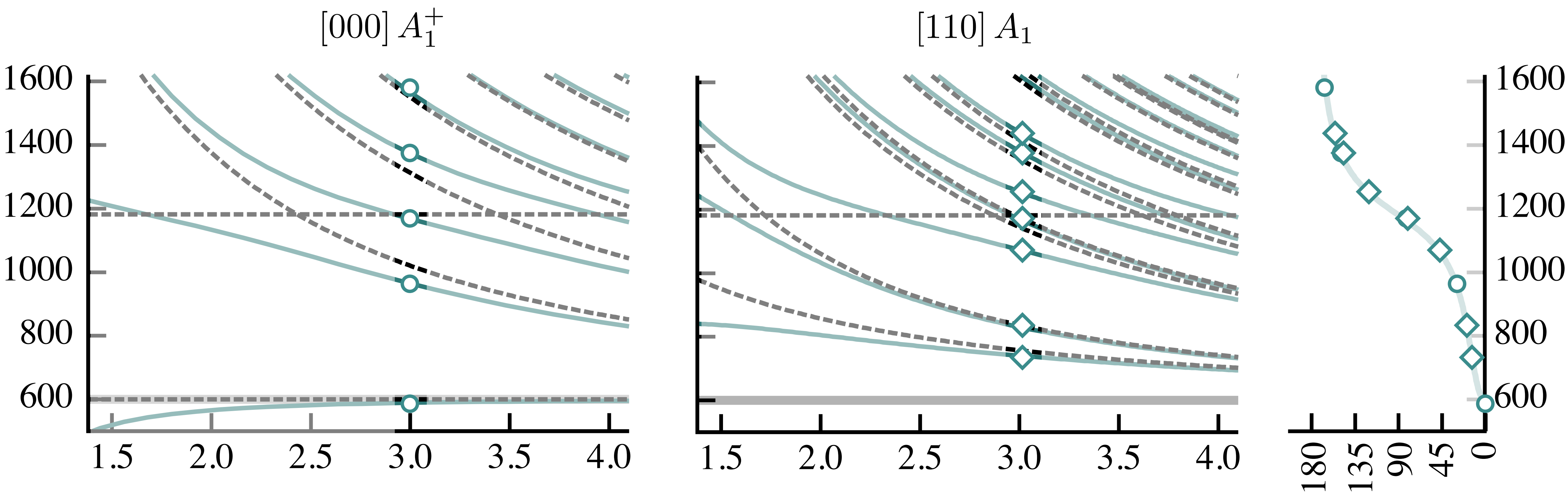


more volumes give more information,

but each new volume is a completely new lattice calculation and hence very computationally costly



determining the **moving-frame spectrum** provides much more information

it looks like given enough finite volume energies,
we can reconstruct the elastic scattering phase-shift …

some annoying technical stuff — breaking of rotational symmetry

a **finite cubic lattice** has a **smaller rotational symmetry group** than an infinite continuum

simpler example of the problem: a rotationally symmetric two-dim system $\psi(r,\theta) = R_m(r)\, e^{im\theta}$

now considered on a square grid — minimum rotation is by $\pi/2$

m and $m+4n$ transform the same !

back in 3D — **irreducible representations** of the reduced symmetry group contain multiple spins

cubic symmetry

$\Lambda(\mathrm{dim})$	$A_1(1)$	$T_1(3)$	$T_2(3)$	$E(2)$	$A_2(1)$
J	$\mathbf{0}, 4\ldots$	$\mathbf{1}, 3, 4\ldots$	$\mathbf{2}, 3, 4\ldots$	$\mathbf{2}, 4\ldots$	$\mathbf{3}\ldots$

subduction $\big|\Lambda, \rho\big\rangle = \sum_m S^{\Lambda,\rho}_{J,m} \big|J, m\big\rangle$

for non-zero momentum it's even worse
— in continuum have **little group**, those rotations which don't change ***p***

⇒ label by **helicity**

can subduce helicity states into irreps of the reduced cubic symmetry

PRD85 014507 (2012)

reduction of rotational symmetry is an important feature of the quantization condition too

for elastic scattering, what we previously presented as $\cot\delta_\ell(E) = \mathcal{M}_\ell\big(E(L), L\big)$

should actually be $0 = \det\Big[\cot\delta_\ell\,\delta_{\ell,\ell'}\,\delta_{m,m'} - \mathcal{M}_{\ell m;\ell' m'}\Big]$

which when subduced becomes $0 = \det\Big[\cot\delta_\ell\,\delta_{\ell,\ell'}\,\delta_{n,n'} - \mathcal{M}^{\Lambda}_{\ell n;\ell' n}\Big]$

features **all ℓ** subduced into irrep Λ

n = embedding of ℓ into Λ

e.g. [000] A_1

$$0 = \det\left[\begin{pmatrix} \cot\delta_0(E) & 0 & \cdots \\ 0 & \cot\delta_4(E) & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} - \begin{pmatrix} \mathcal{M}^{A_1}_{01;01}(E,L) & \mathcal{M}^{A_1}_{01;41}(E,L) & \cdots \\ \mathcal{M}^{A_1}_{41;01}(E,L) & \mathcal{M}^{A_1}_{41;41}(E,L) & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}\right]$$

what allows us to make progress is that $\delta_\ell(E) \sim k^{2\ell+1}$ at energies not too far from threshold

so higher angular momenta are naturally suppressed

in practice, truncate at some $\ell_{\max}$ ...

where are we … ?

matrix of correlation functions → finite volume spectra → elastic scattering amplitudes

$$\langle 0 | O_i(t)\, O_j^\dagger(0) | 0 \rangle$$

but what operator basis $\{O_i\}_{i=1\dots N}$ should we use ?

must be constructed
out of quark/gluon fields

easiest constructions with meson quantum numbers – **fermion bilinears** $\bar{\psi}\boldsymbol{\Gamma}\psi$

well motivated by
success of quark model

'looks' like a $q\bar{q}$ system

Γ = Dirac gamma
+ gauge-covariant derivatives

$D_\mu = \partial_\mu + igA_\mu$

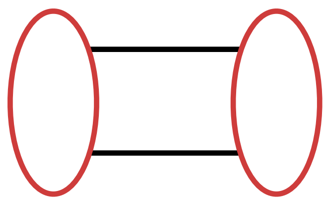
meson operators

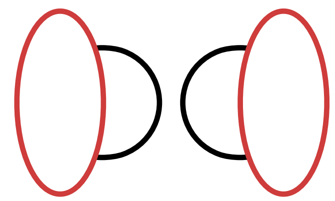
easiest constructions with meson quantum numbers — **fermion bilinears** $\bar{\psi}\boldsymbol{\Gamma}\psi$

well motivated by success of quark model

‘looks’ like a $q\bar{q}$ system

Wick contractions





‘annihilation’
required for isospin=0

quark propagation from t to t
⇒ matrix inversions on many t

meson operators

easiest constructions with meson quantum numbers – **fermion bilinears** $\bar{\psi}\Gamma\psi$

well motivated by success of quark model

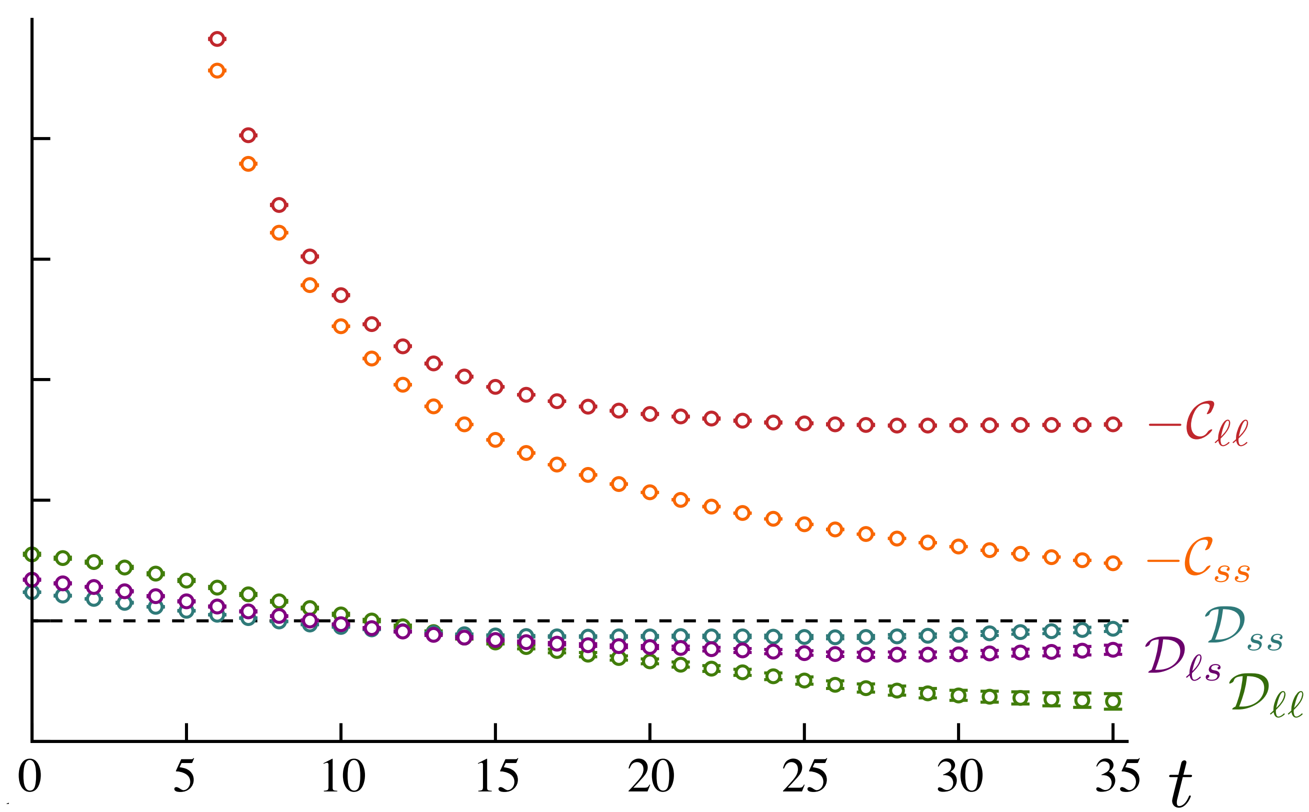
'looks' like a $q\bar{q}$ system

Wick contractions

'annihilation' required for isospin=0

quark propagation from *t* to *t*
⇒ matrix inversions on many *t*

an isospin=0 correlation function



turns out this is not enough …

meson operators

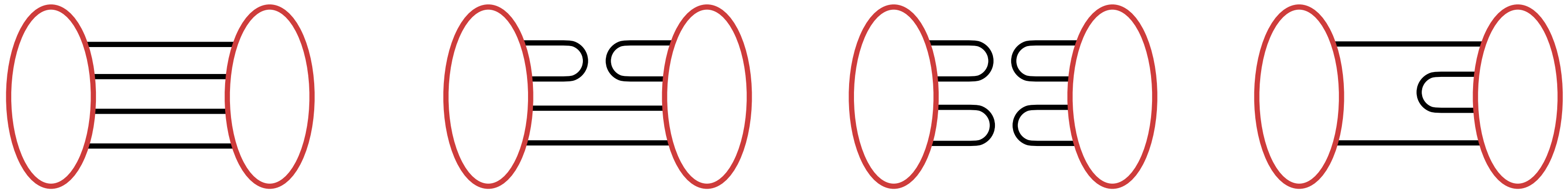
easiest constructions with meson quantum numbers – **fermion bilinears** $\bar{\psi}\boldsymbol{\Gamma}\psi$

but can also construct operators with **more quark fields**

e.g. 'local' tetraquark operators $\bar{\psi}_{\mathbf{x}}\bar{\psi}_{\mathbf{x}}\psi_{\mathbf{x}}\psi_{\mathbf{x}}$

e.g. 'meson-meson'-like operators $\sum_{\mathbf{x}} e^{i\mathbf{p}\cdot\mathbf{x}}\, \bar{\psi}_{\mathbf{x}}\boldsymbol{\Gamma}\psi_{\mathbf{x}} \sum_{\mathbf{y}} e^{i\mathbf{q}\cdot\mathbf{y}}\, \bar{\psi}_{\mathbf{y}}\boldsymbol{\Gamma}'\psi_{\mathbf{y}}$

schematic Wick contractions



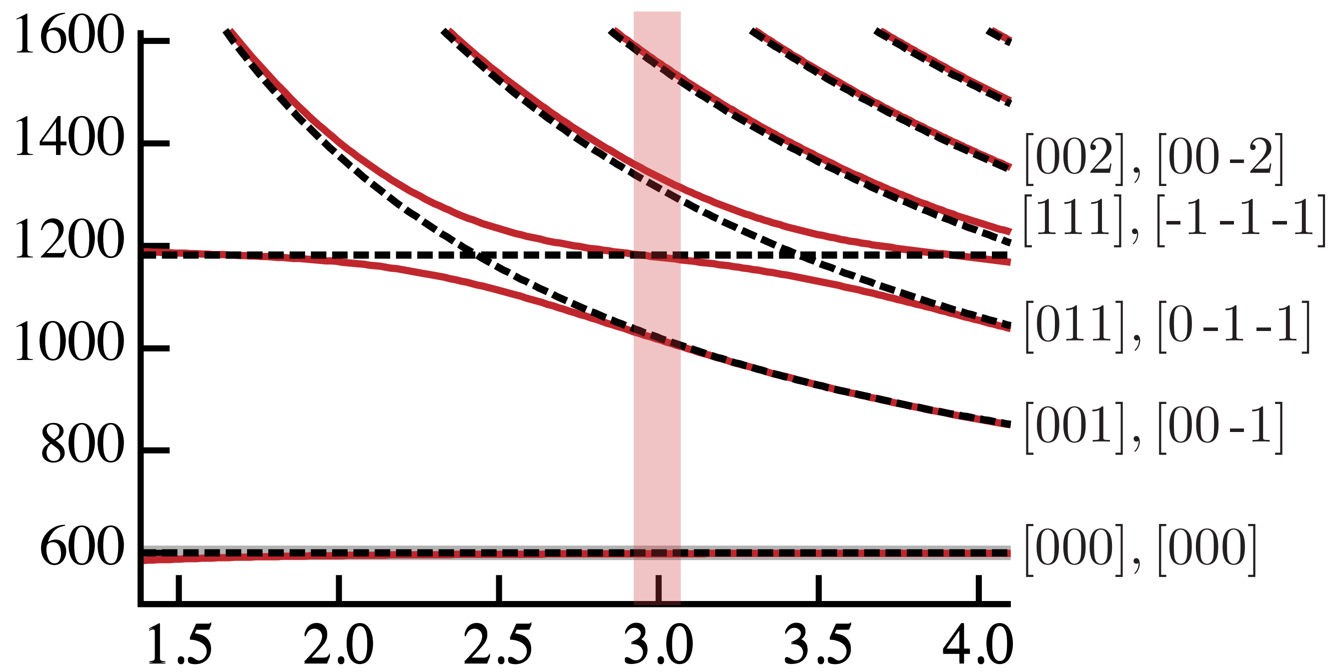
'annihilation' generally required

and can clearly include still more quark fields ad infinitum ...

... is there some organizing principle which suggests what operator basis we should use ?

the non-interacting spectrum as an operator basis guide

e.g. narrow resonance (in rest frame)



suppose we want to determine all states up to 1500 MeV on a 3 fm lattice

we might try an operator basis featuring ‘meson-meson’-like operators with back-to-back momentum up to [111]

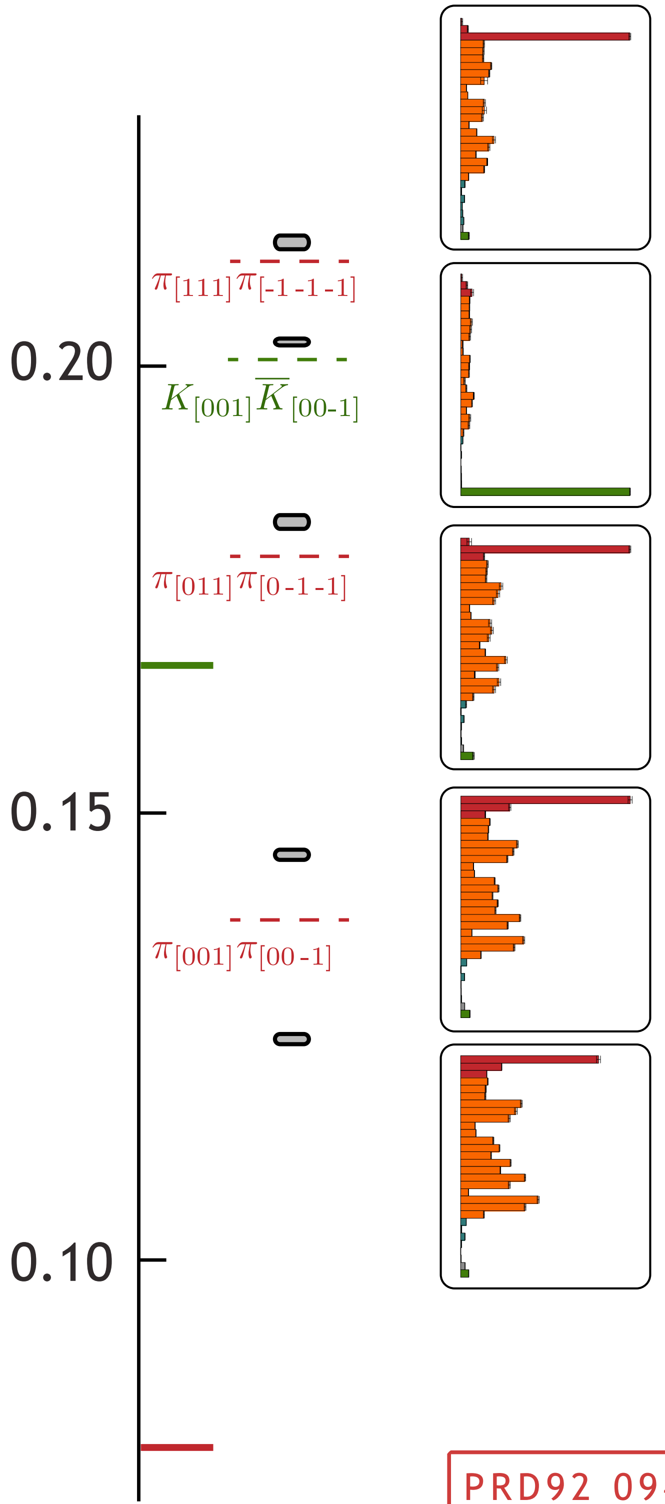
‘look like’ the expected meson-meson basis states

plus a set of $\bar{\psi}\Gamma\psi$ operators

‘look like’ a bound $q\bar{q}$-like basis state

isospin=1 T_1^- irrep spectrum

variational analysis of 30×30 correlation matrix: $3\times\pi\pi$, $26\times\bar{\psi}\Gamma\psi$, $1\times K\bar{K}$

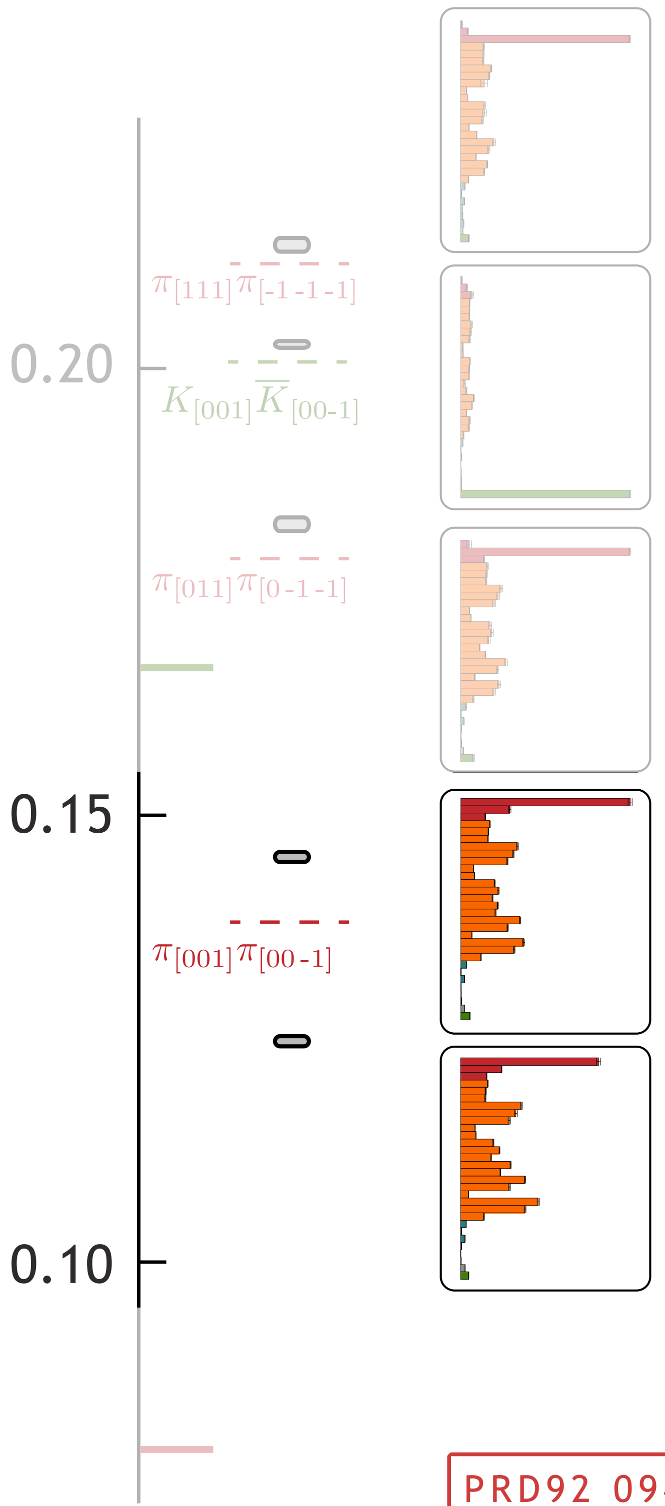


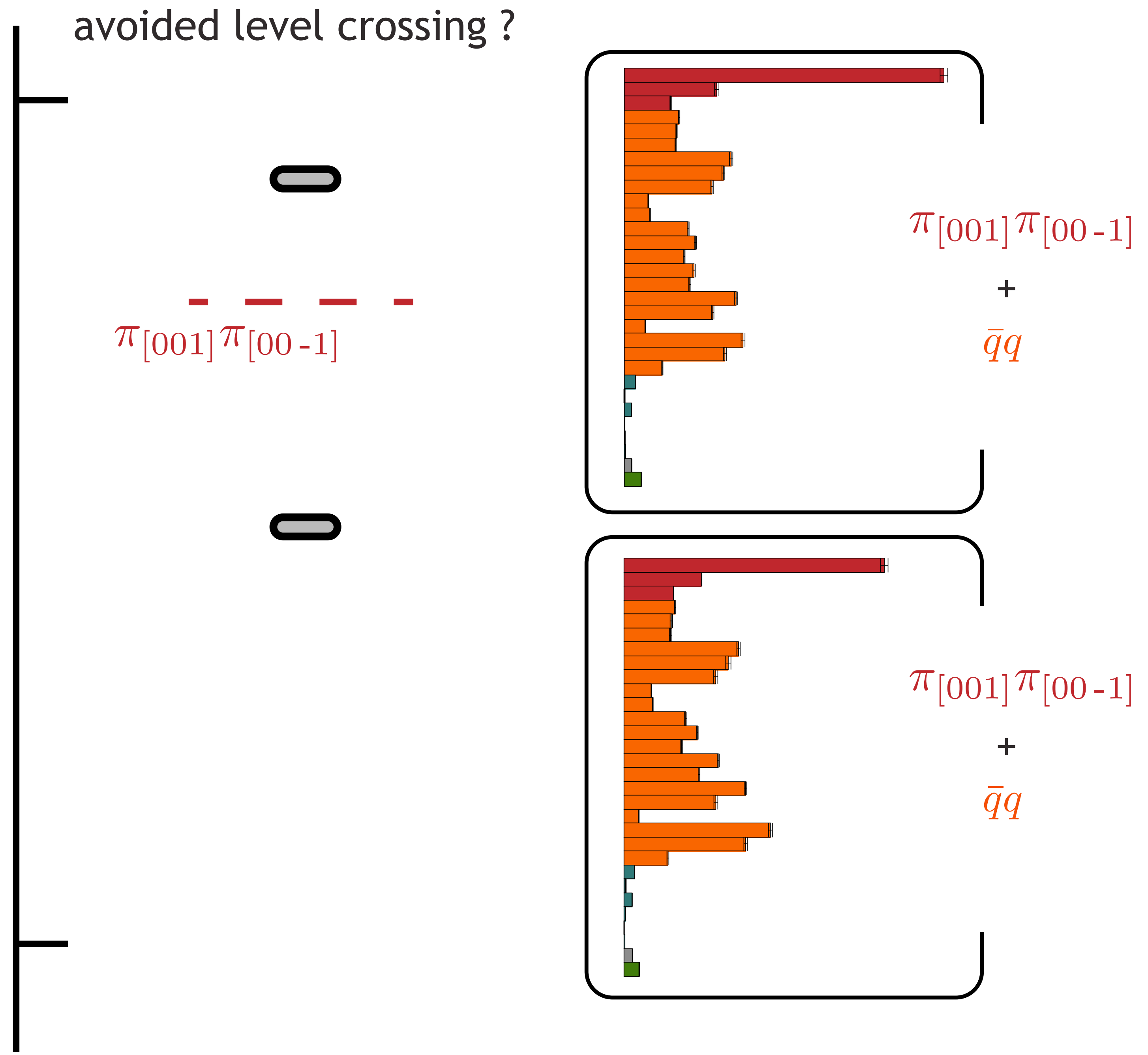
PRD92 094502 (2015)

$m_\pi = 0.039$
$m_K = 0.083$
$L \sim 3.8$ fm

isospin=1 T_1^- irrep spectrum

variational analysis of 30×30 correlation matrix: $3\times\pi\pi$, $26\times\bar{\psi}\Gamma\psi$, $1\times K\bar{K}$





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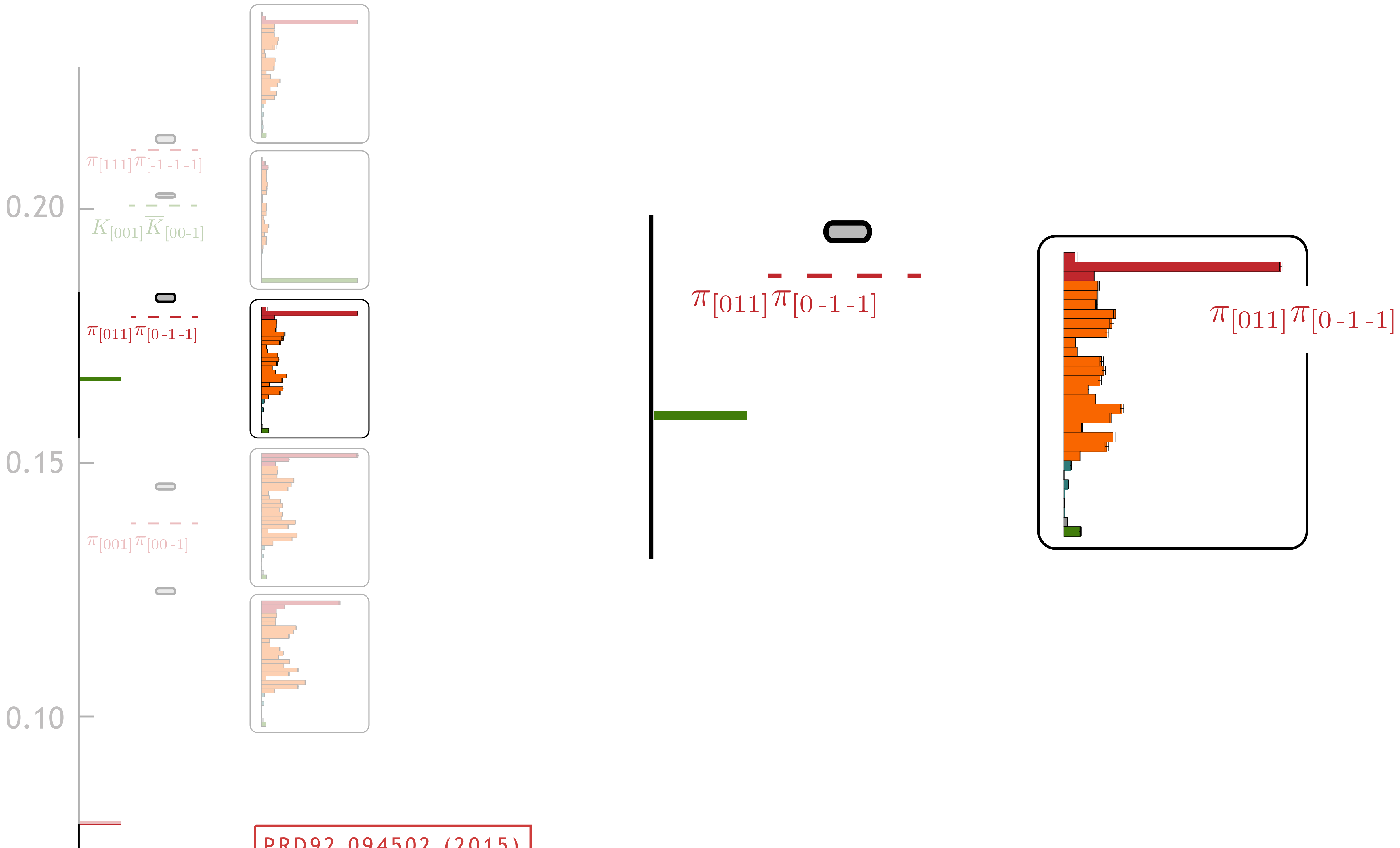

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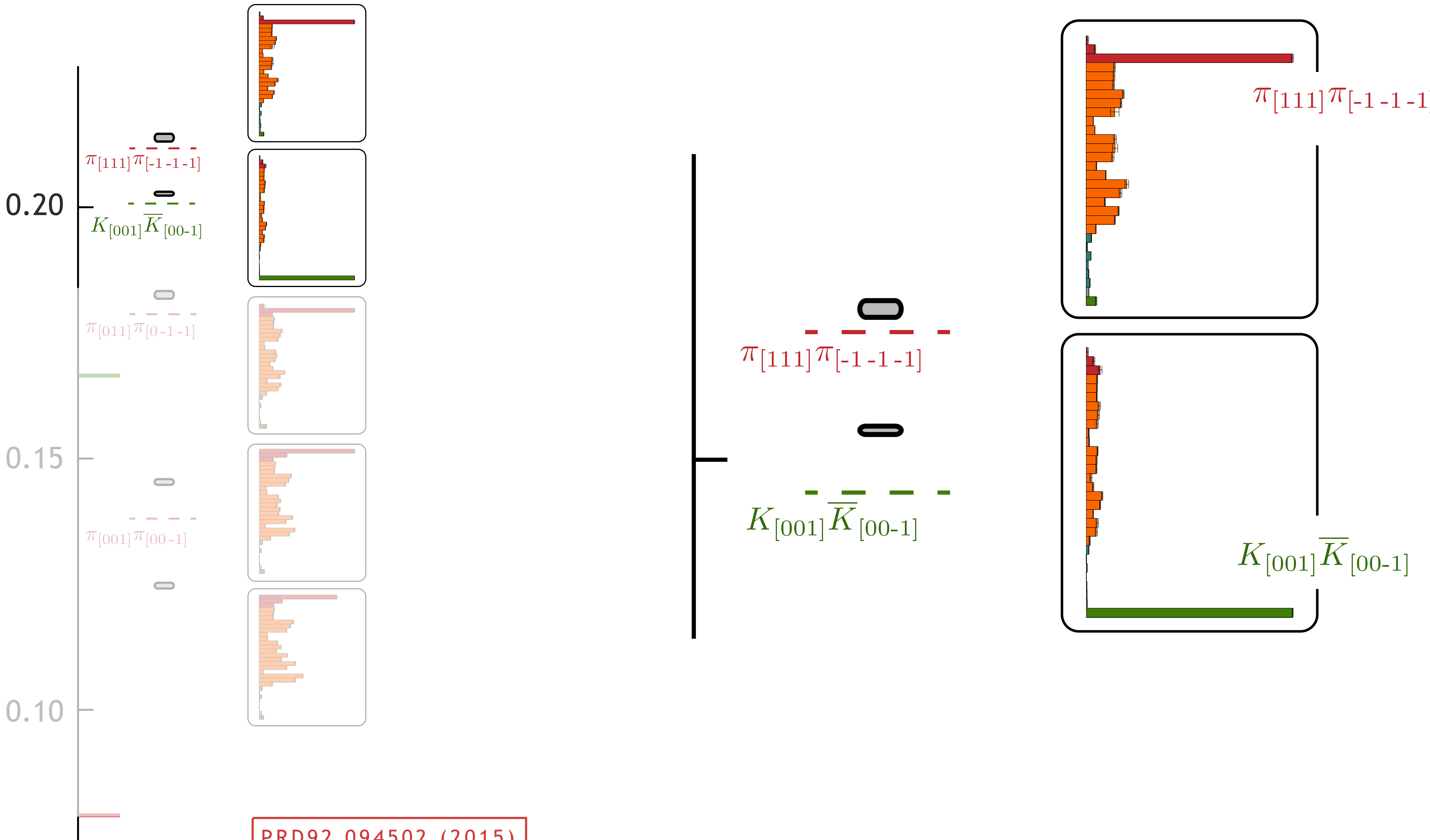
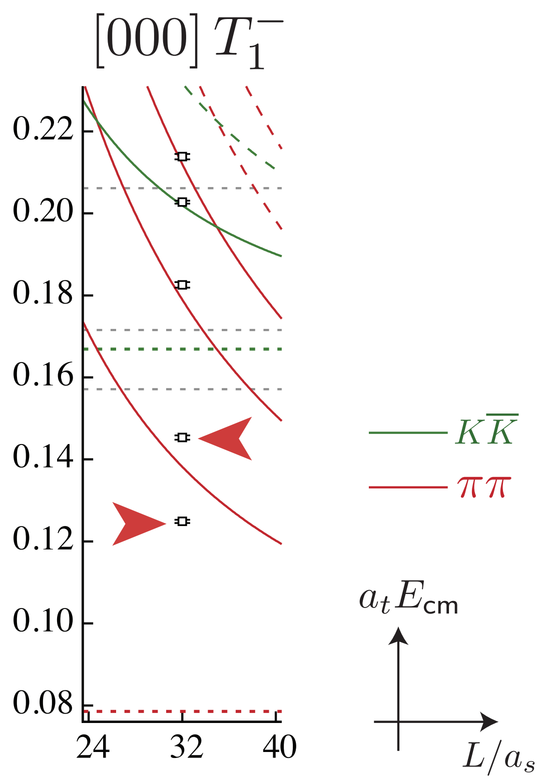


PRD92 094502 (2015)

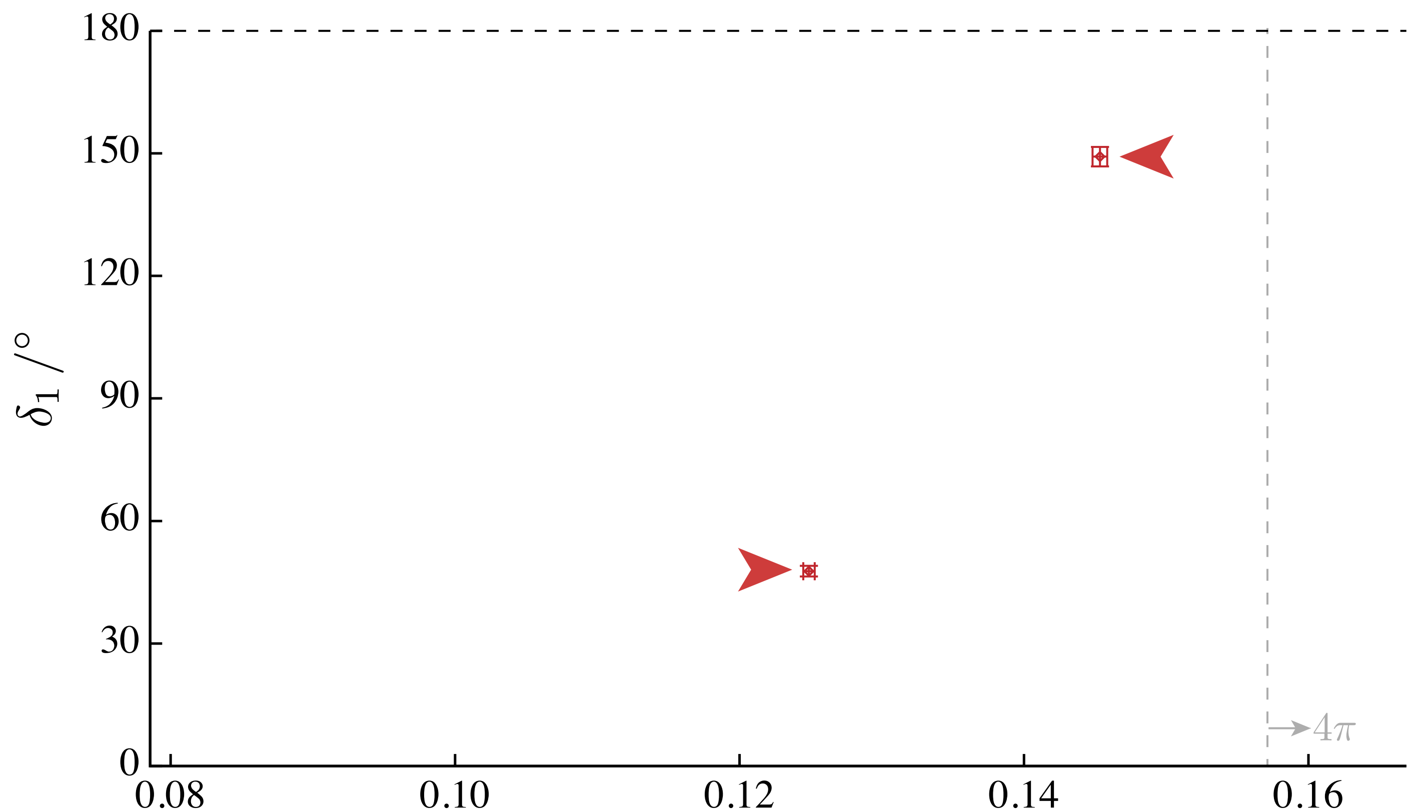
$m_\pi = 0.039$
$m_K = 0.083$ $L \sim 3.8$ fm

$\pi\pi$ I=1 J^P=1⁻ scattering

m_π ~ 236 MeV

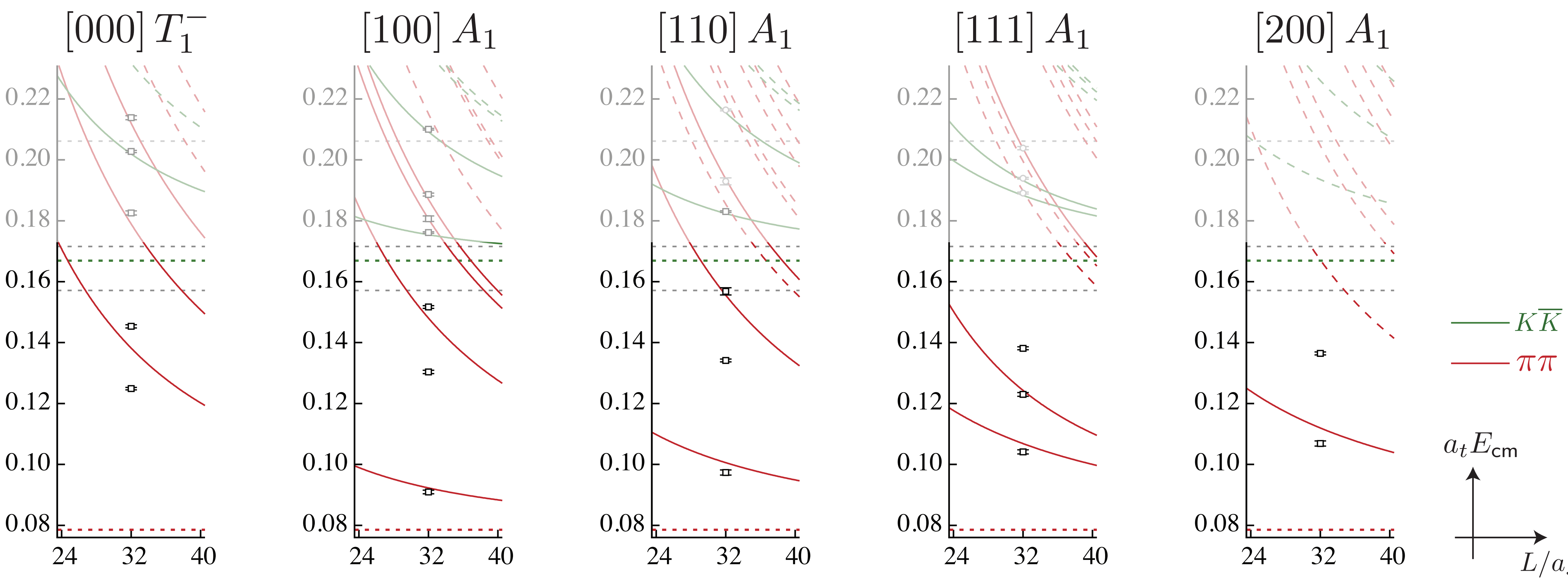


$$t(E) = \frac{1}{\rho(E)} e^{i\delta(E)} \sin\delta(E)$$



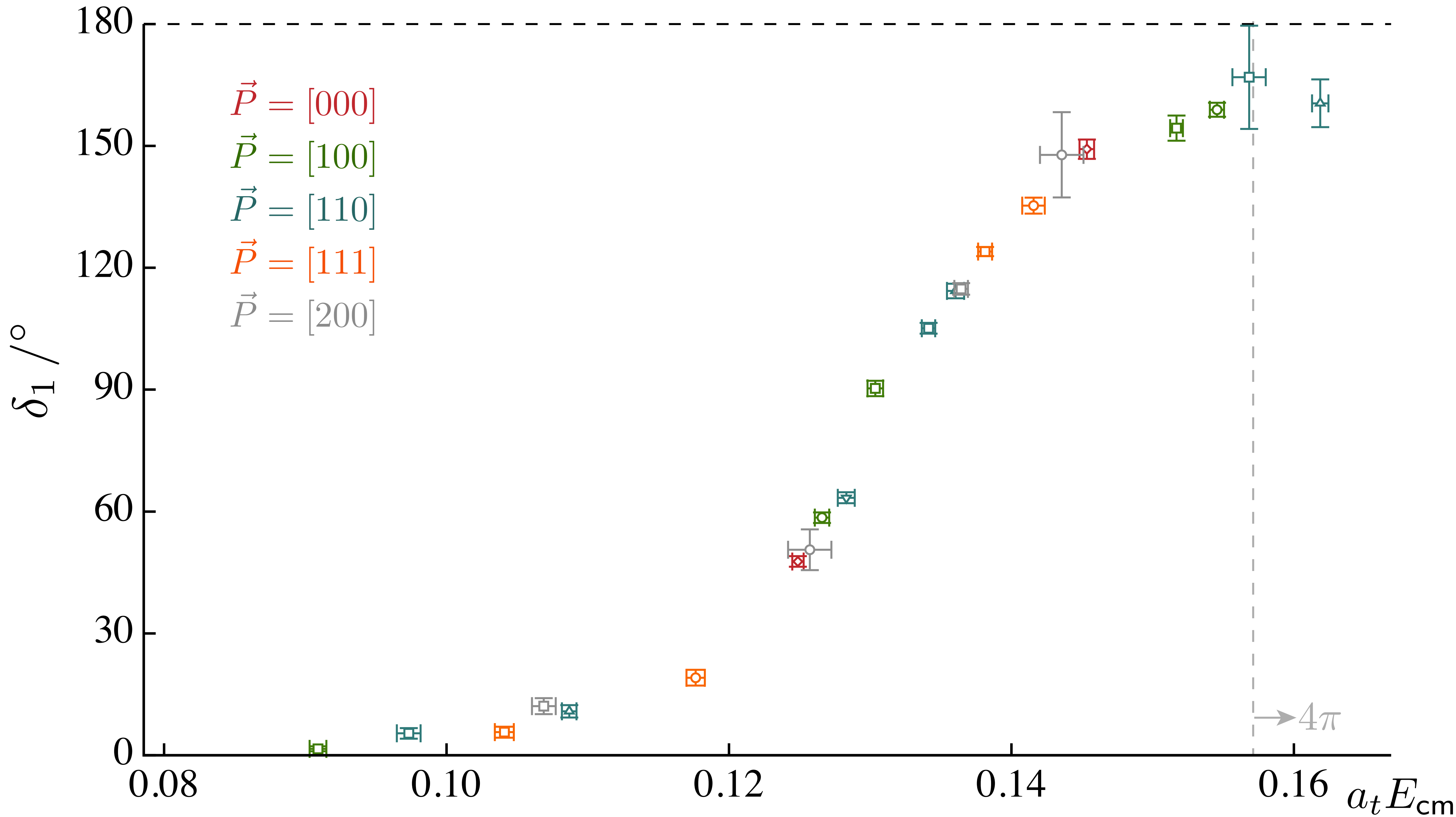
m_π = 0.039
m_K = 0.083
L ~ 3.8 fm

… and in moving frames …



m_π = 0.039
m_K = 0.083

L ~ 3.8 fm



$m_\pi = 0.039$
$m_K = 0.083$
L ~ 3.8 fm

… looks like a classic resonance signal …

what happens if we vary the operator basis ?

$m_\pi = 0.039$
$m_K = 0.083$
$L \sim 3.8$ fm

‘single-meson’-like versus ‘meson-meson’-like ?

volume dependence !

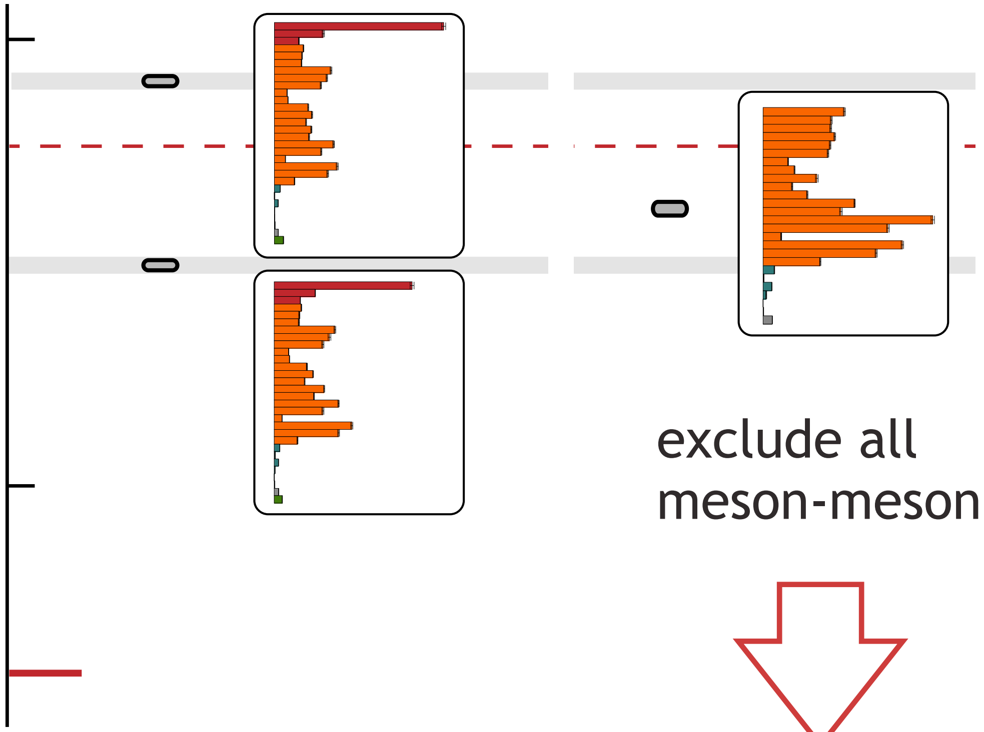
‘meson-meson’-like $\sum_{\mathbf{x}} e^{i\mathbf{p}\cdot\mathbf{x}}\, \bar{\psi}_{\mathbf{x}}\mathbf{\Gamma}\psi_{\mathbf{x}} \sum_{\mathbf{y}} e^{i\mathbf{q}\cdot\mathbf{y}}\, \bar{\psi}_{\mathbf{y}}\mathbf{\Gamma}'\psi_{\mathbf{y}}$ samples the whole volume of the lattice

‘single-meson’-like $\sum_{\mathbf{x}} e^{i\mathbf{P}\cdot\mathbf{x}}\, \bar{\psi}_{\mathbf{x}}\mathbf{\Gamma}\psi_{\mathbf{x}}$ samples a single point (translated)

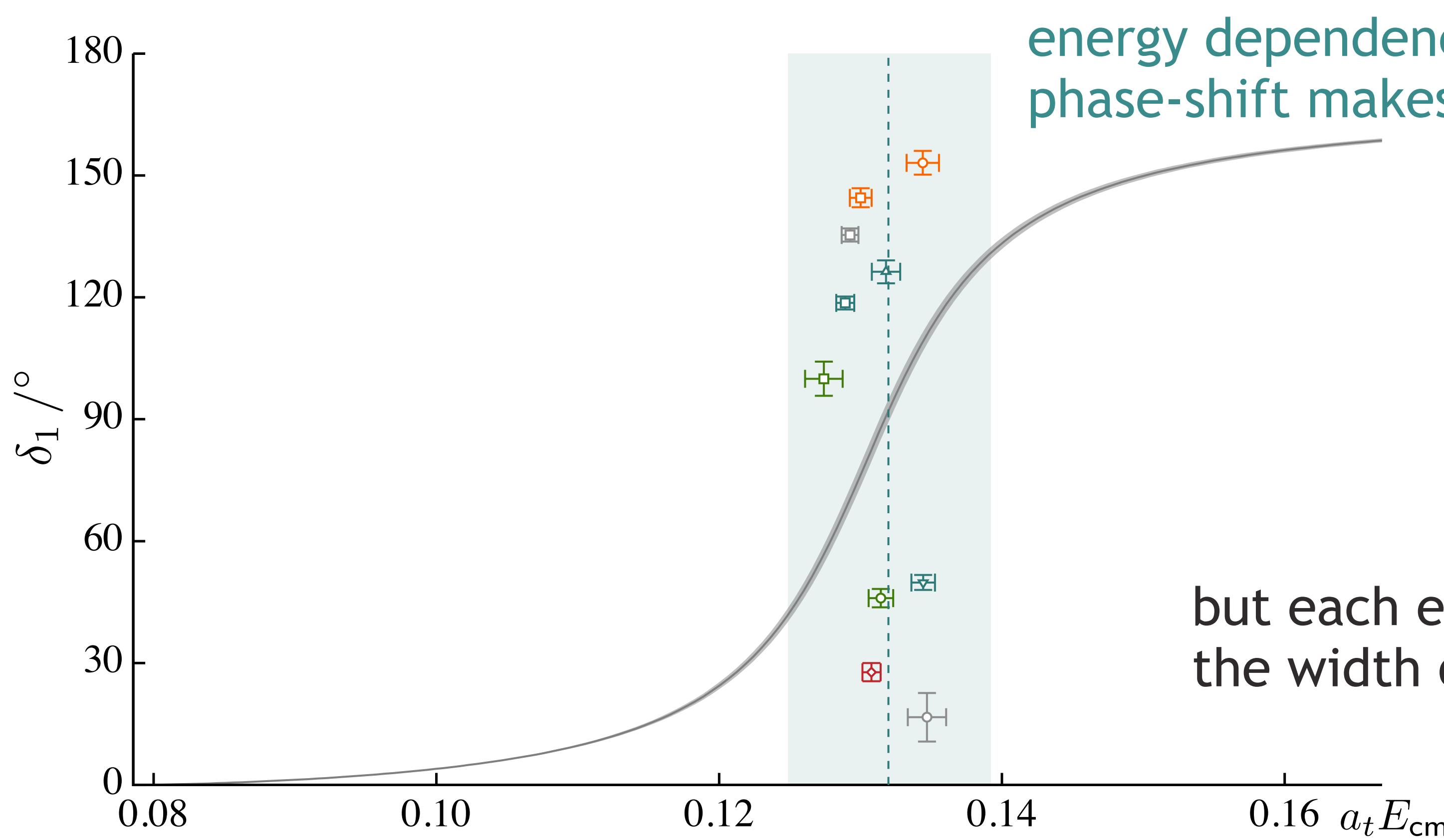
so: ‘looks-like’ = ‘has the same volume sampling as’

interesting side note:
tetraquark operators won’t work well for interpolating meson-meson components — wrong volume sampling

how bad is it really to get the wrong energies ?



exclude all
meson-meson



energy dependence of the
phase-shift makes no sense

but each energy within
the width of the resonance … ?

some technical stuff — ‘meson-meson’-like operators

what actually goes into a ‘$\pi\pi$’-like operator ?

one option for construction is to use products of single-meson operators in lattice irreps

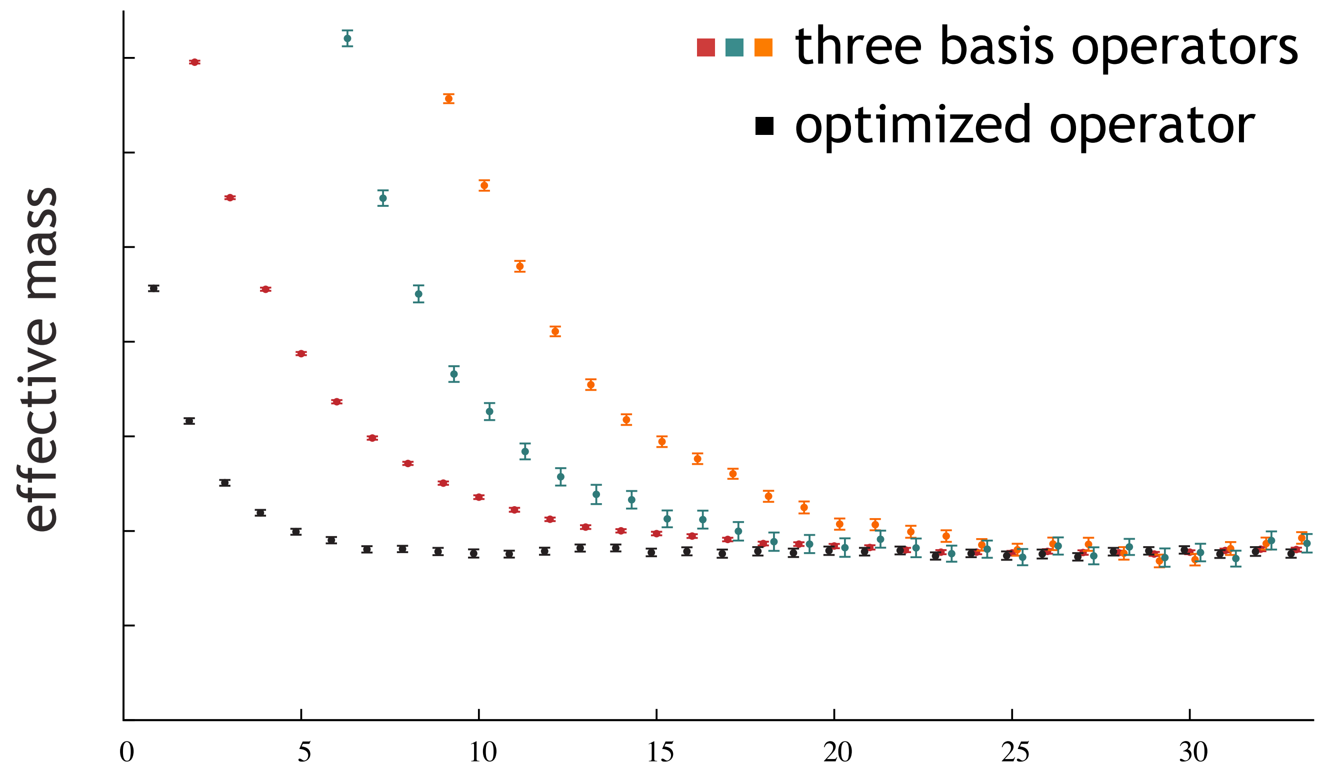
$$\sum_{\substack{\hat{\mathbf{p}}_1,\hat{\mathbf{p}}_2 \\ \mathbf{p}_1+\mathbf{p}_2=\mathbf{P}}} C_{\Lambda_1\otimes\Lambda_2\to\Lambda}\left(\hat{\mathbf{p}}_1,\hat{\mathbf{p}}_2\right)\pi(\mathbf{p}_1;\Lambda_1)\,\pi(\mathbf{p}_2;\Lambda_2)$$

‘lattice’ Clebsch-Gordan coefficients

some group theory to work them out

then each single-meson operator can be the **variationally optimized** one for that ***p***, *Λ*

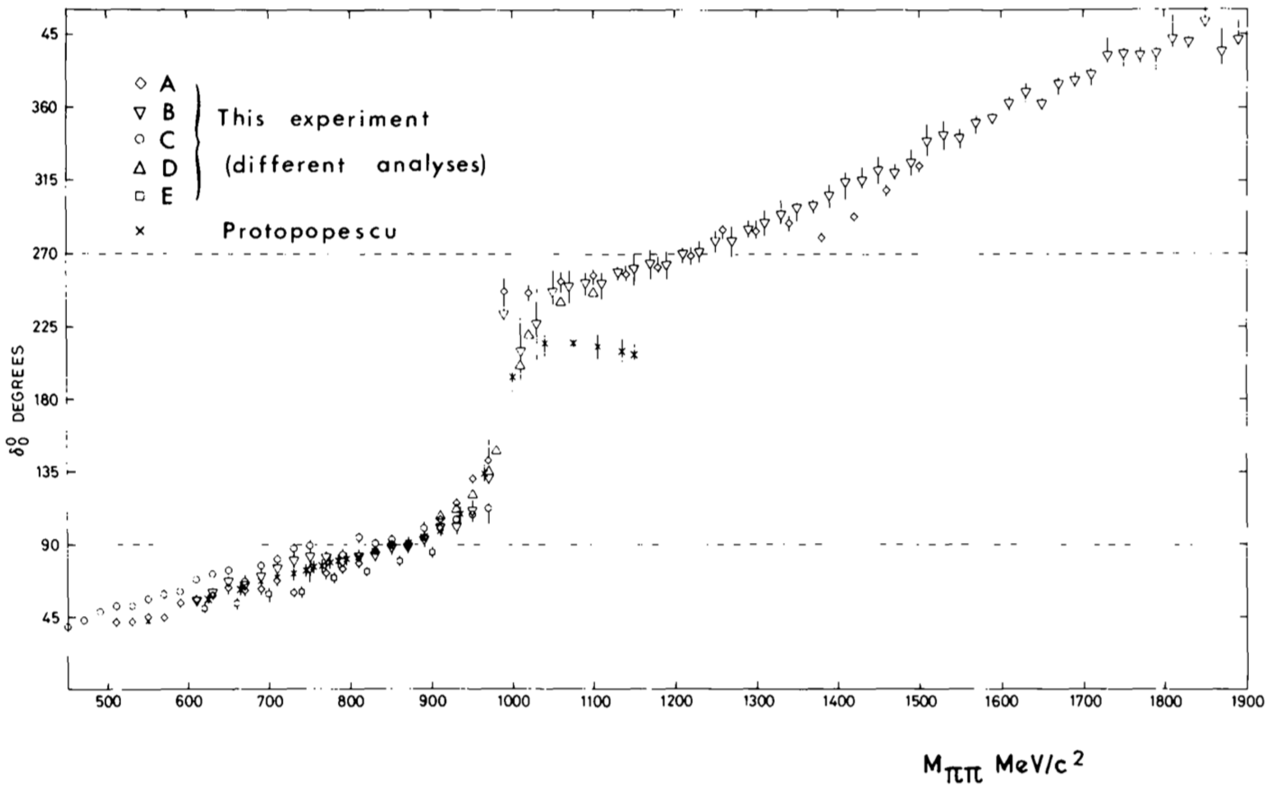
[000] A_1^+ diagonal correlators



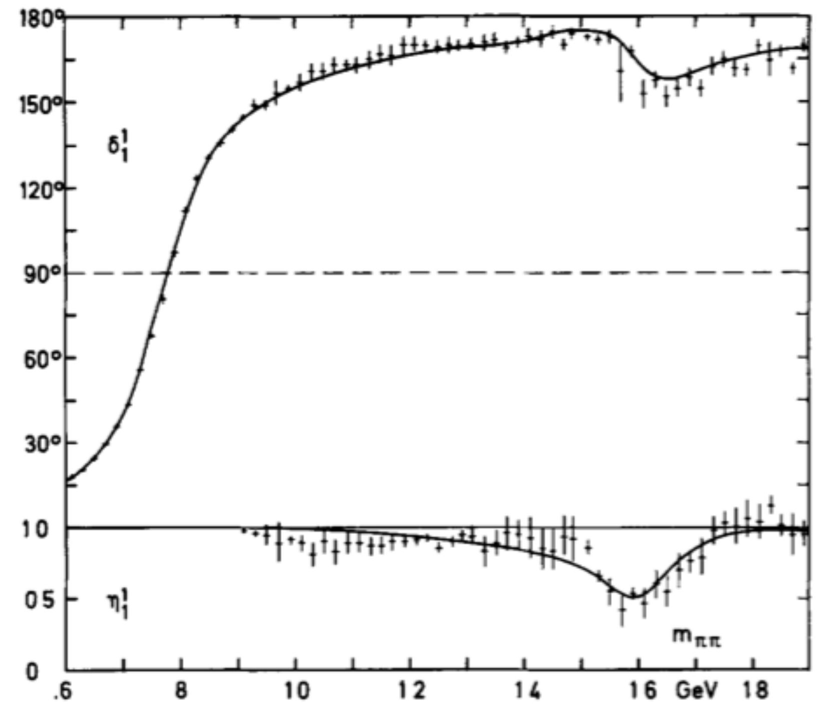
optimized operator saturated by the pion by timeslice 7

the "simplest" case: $\pi\pi$ elastic scattering

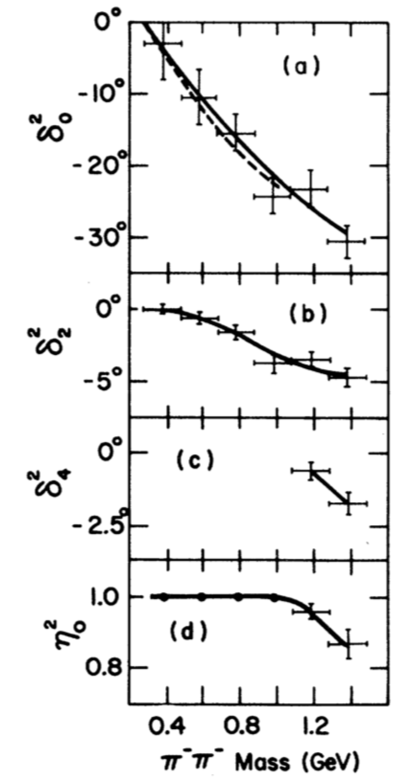
isospin=0



isospin=1



isospin=2



a first target: can a **first-principles QCD** calculation lead to these kinds of behaviour ?

a next target: can we understand these behaviours in terms of **resonances** ?

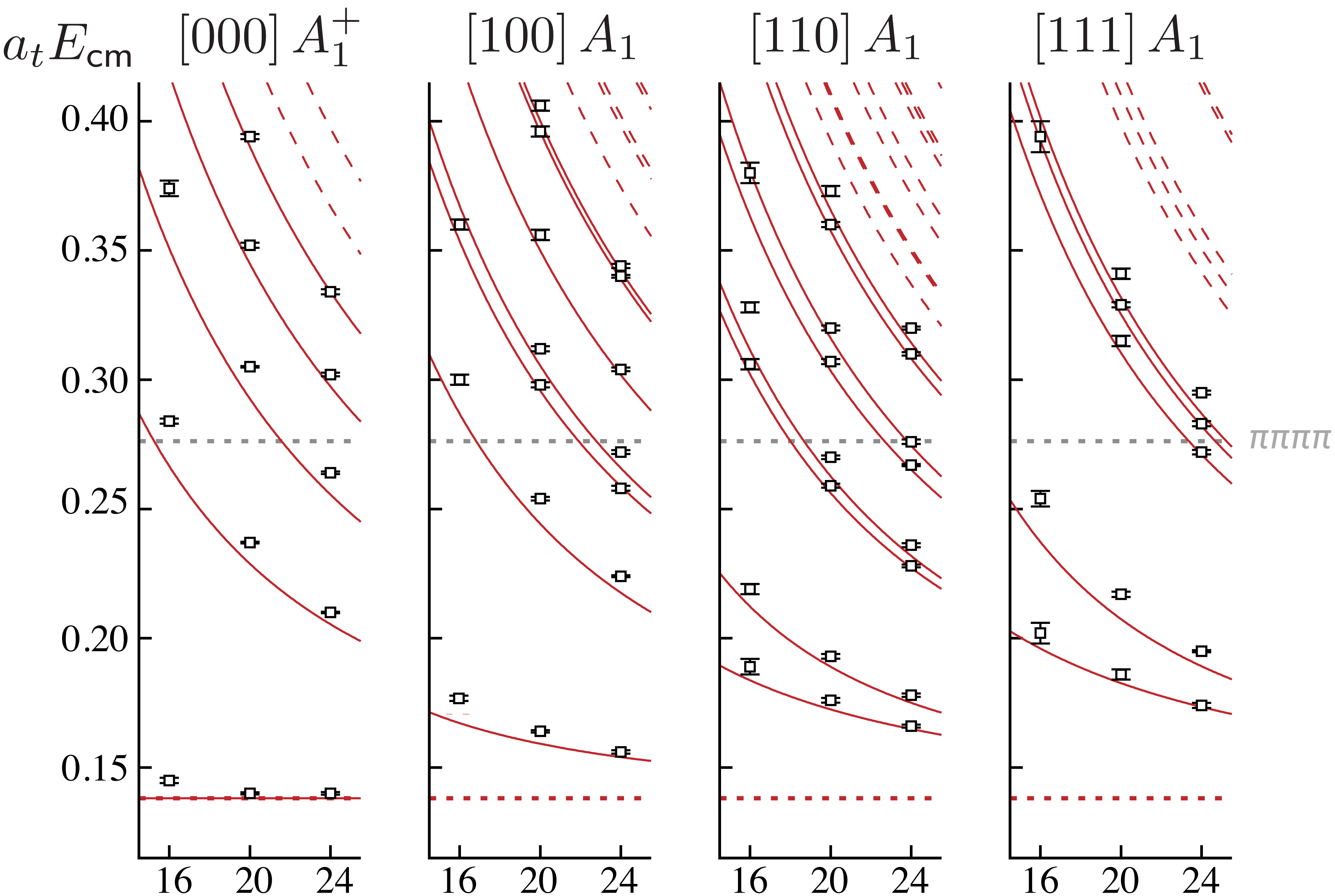
an ultimate target: can we understand the **quark-gluon make-up** of these resonances ?

$\pi\pi$ isospin=2 — m_π~391 MeV

PRD86 034031 (2012)

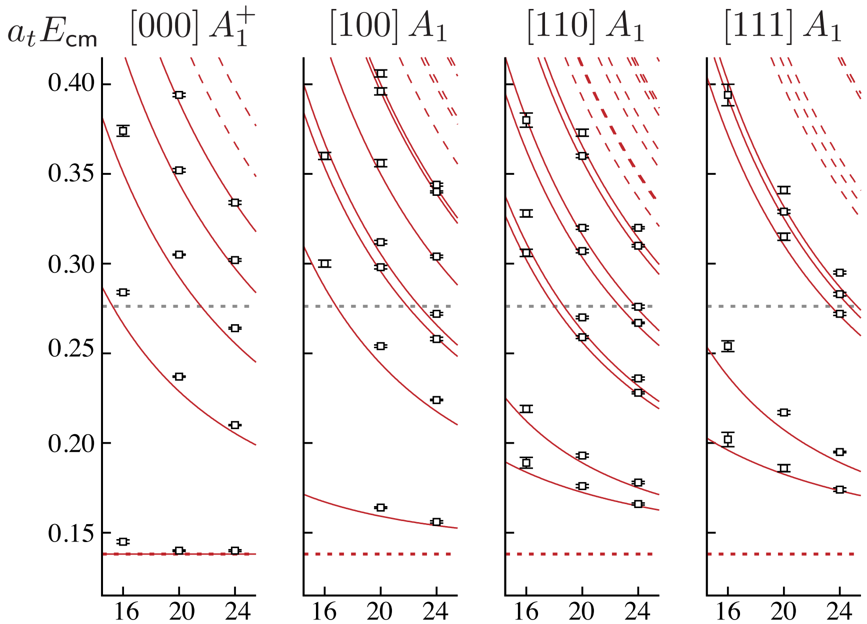
[basis of $\pi\pi$-like operators only]

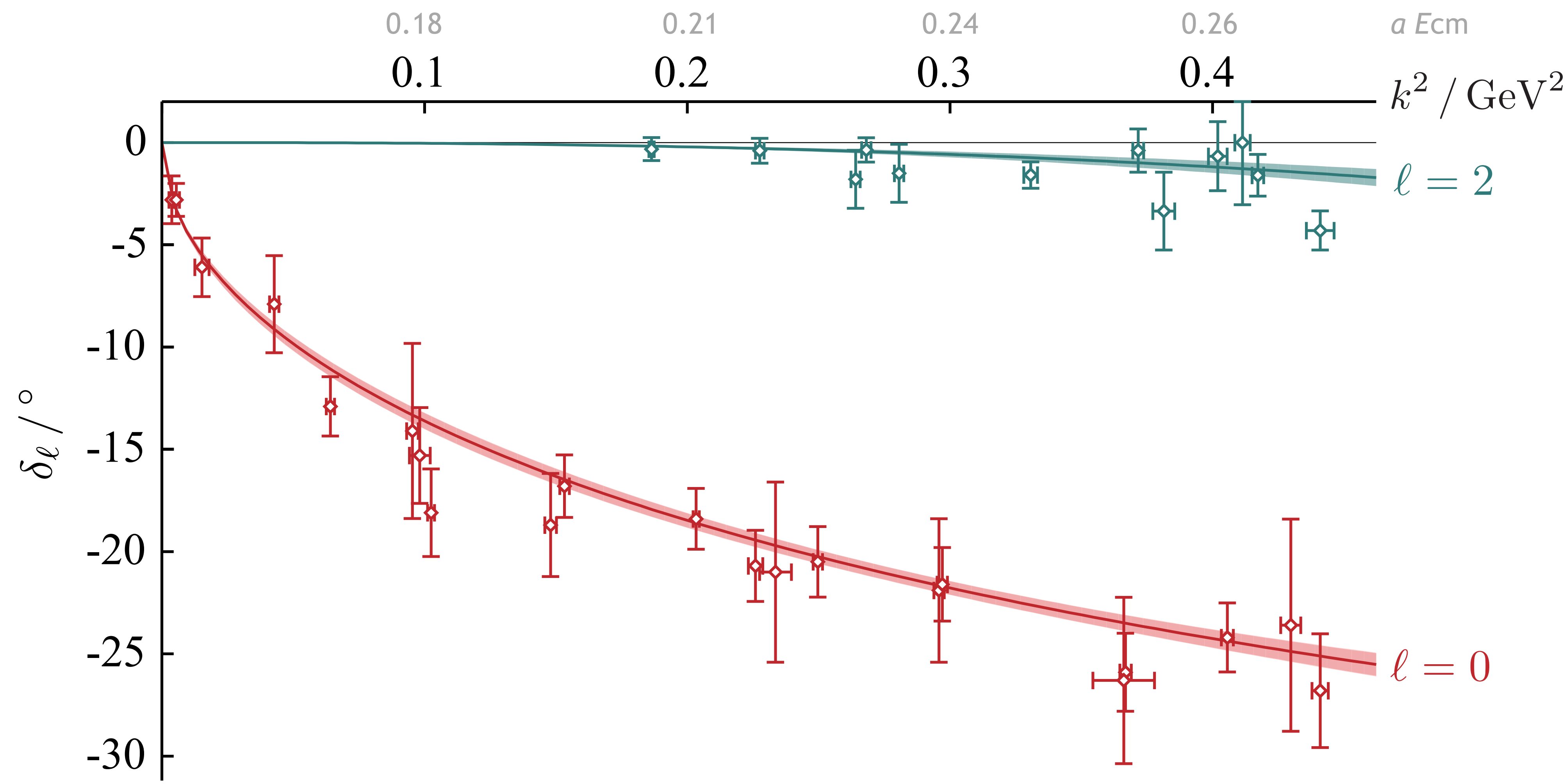
[computed in three volumes]

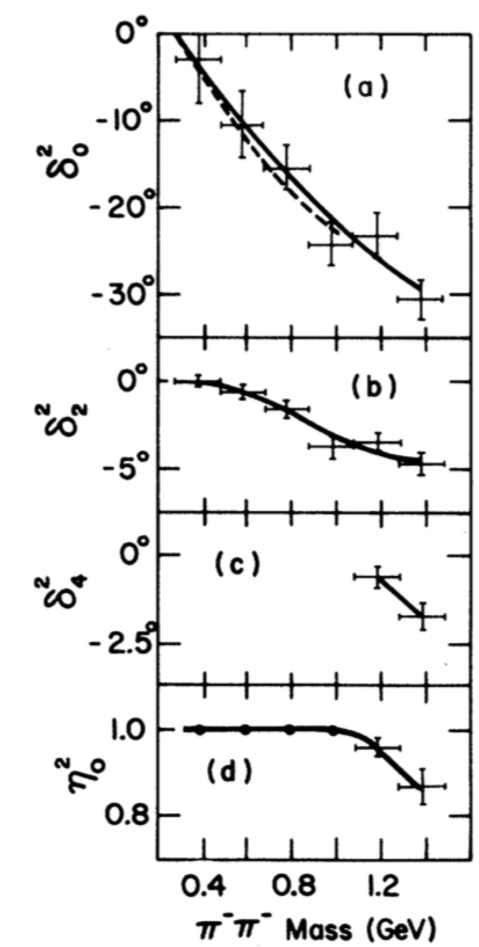


& spectra in irreps with lowest ℓ=2 (not shown here)

$\pi\pi$ isospin=2 — m_π~391 MeV



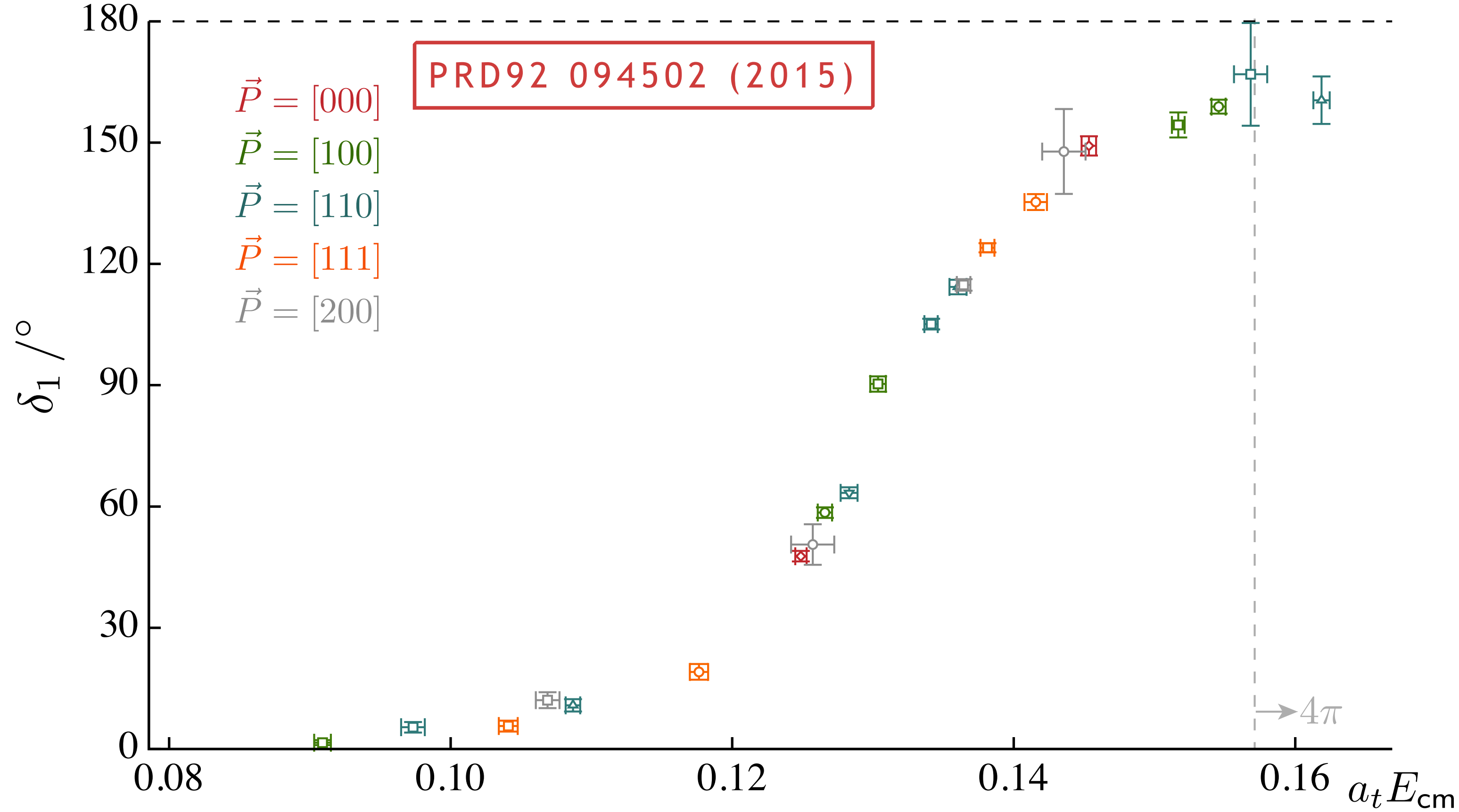




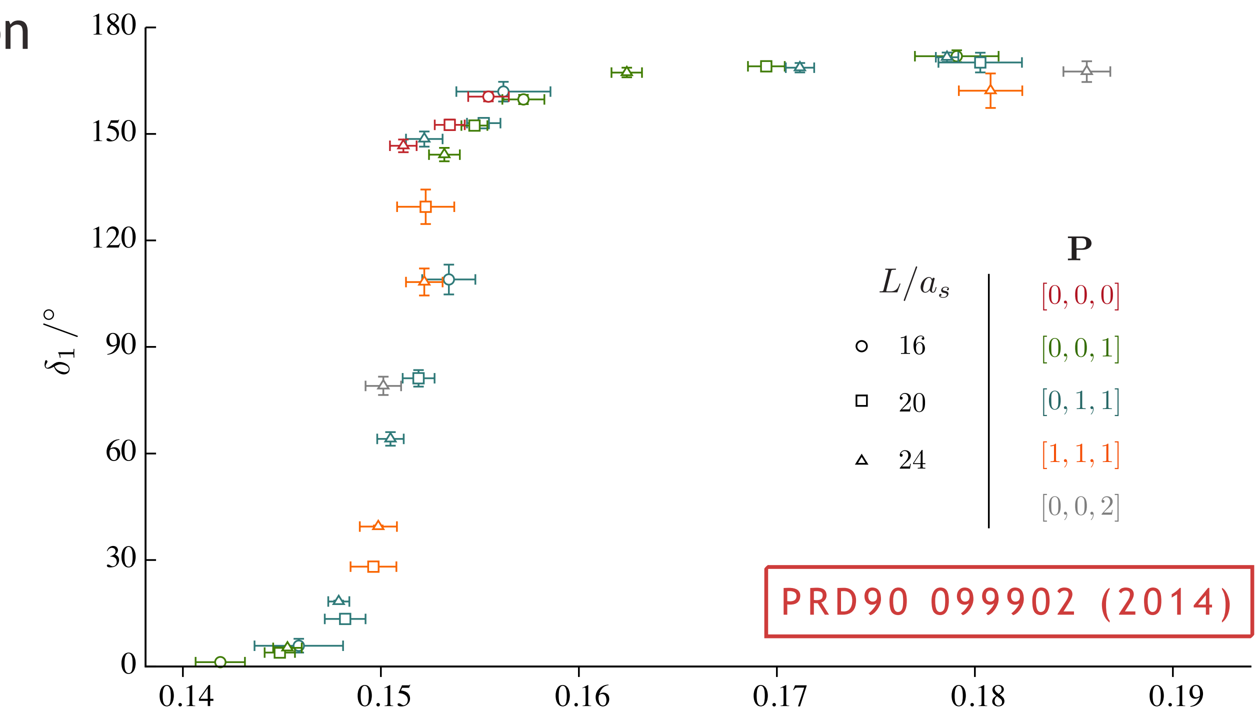
Cohen 1972

ππ isospin=1 — m_π~236 MeV, m_π~391 MeV

you saw this earlier …



and a similar calculation at a heavier pion mass



ππ isospin=1 — m_π~236 MeV, m_π~391 MeV

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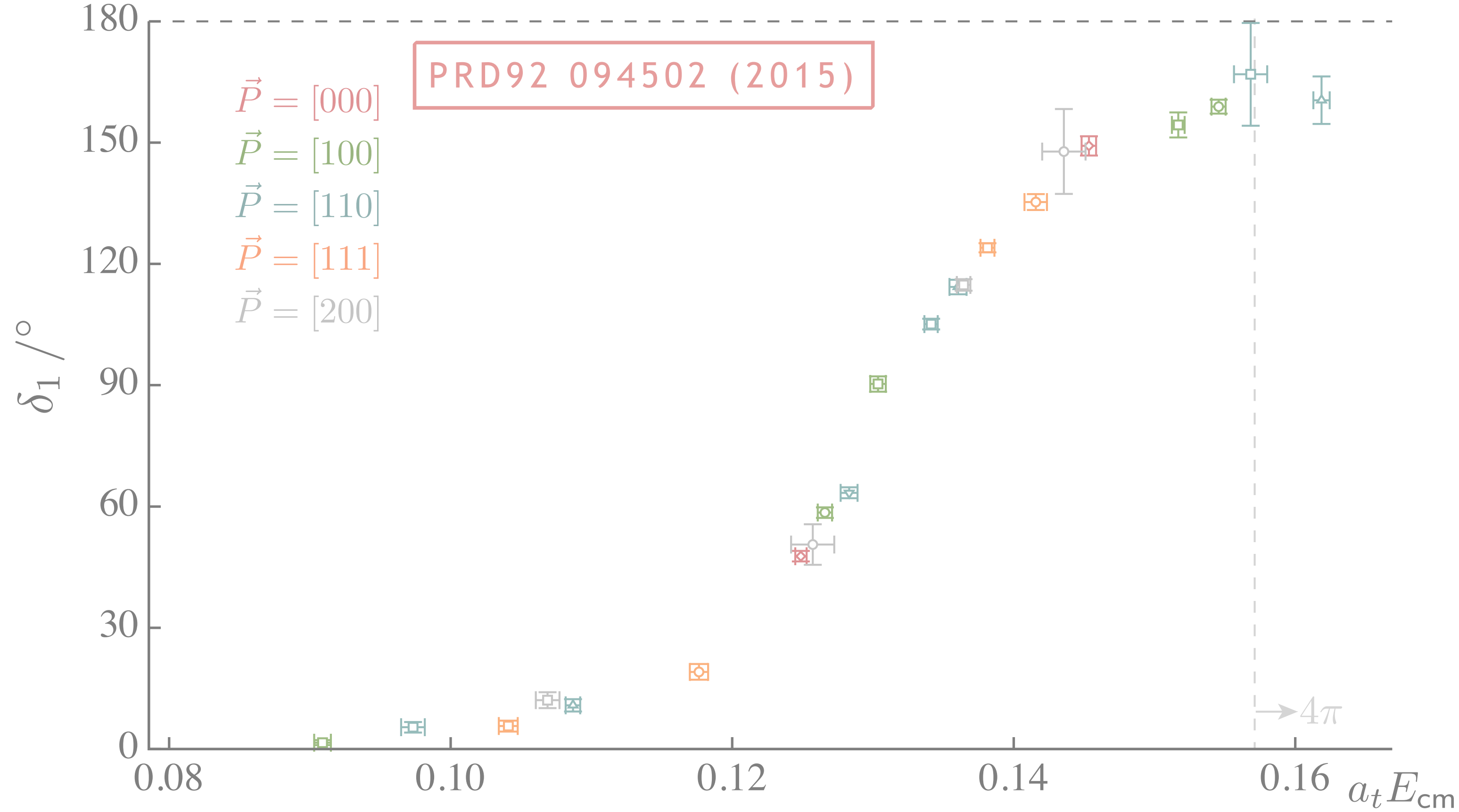
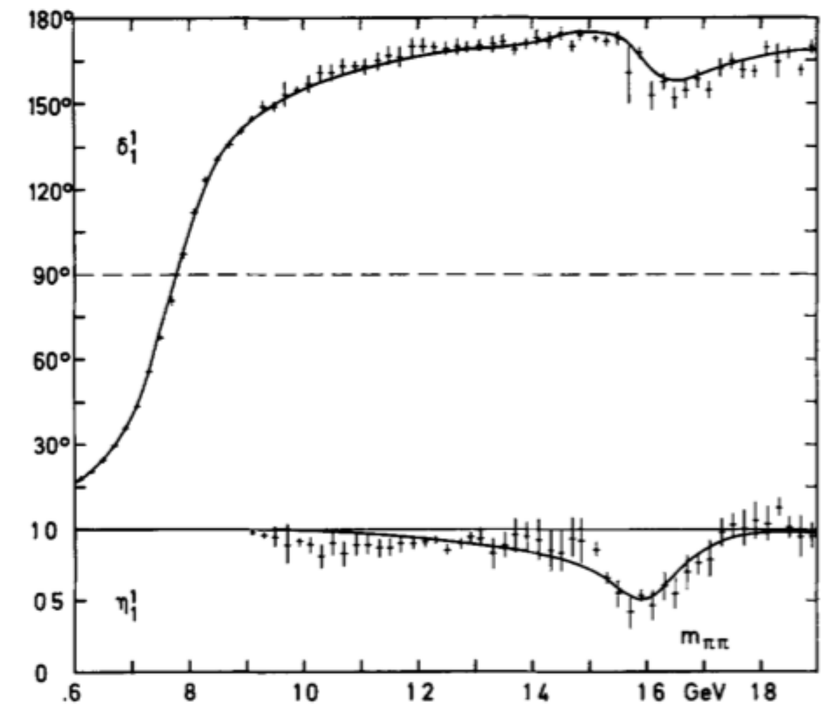
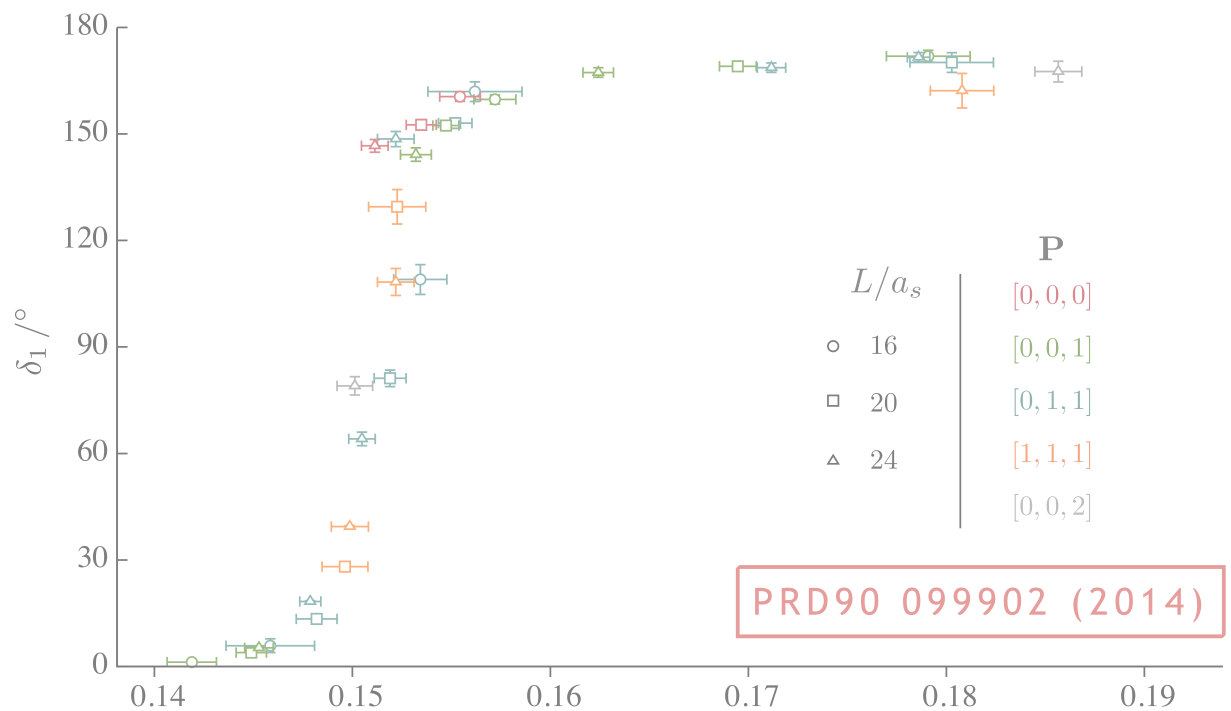




Hyams 1973

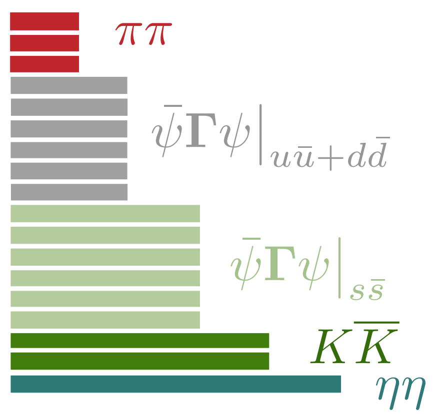
and a similar calculation at a heavier pion mass



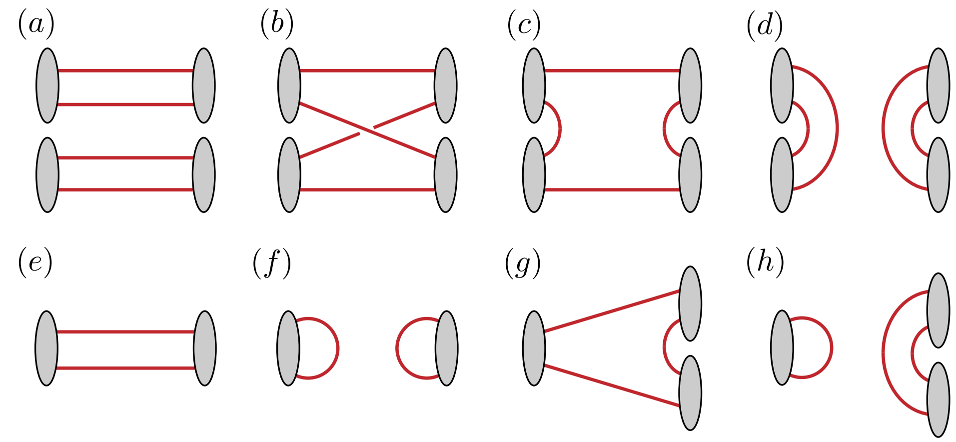
ππ isospin=0

this is the hardest one by far ...

operator basis



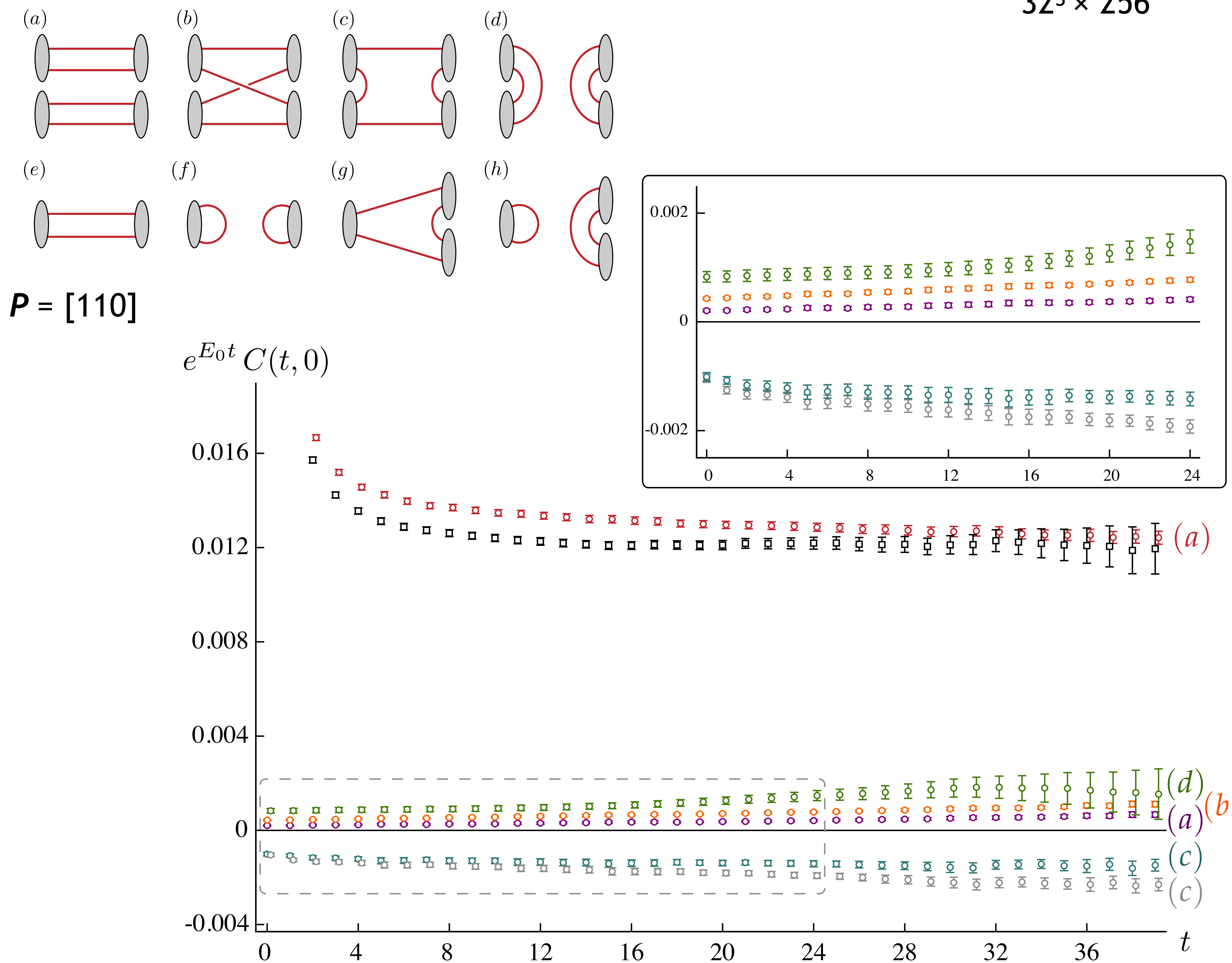
Wick diagrams



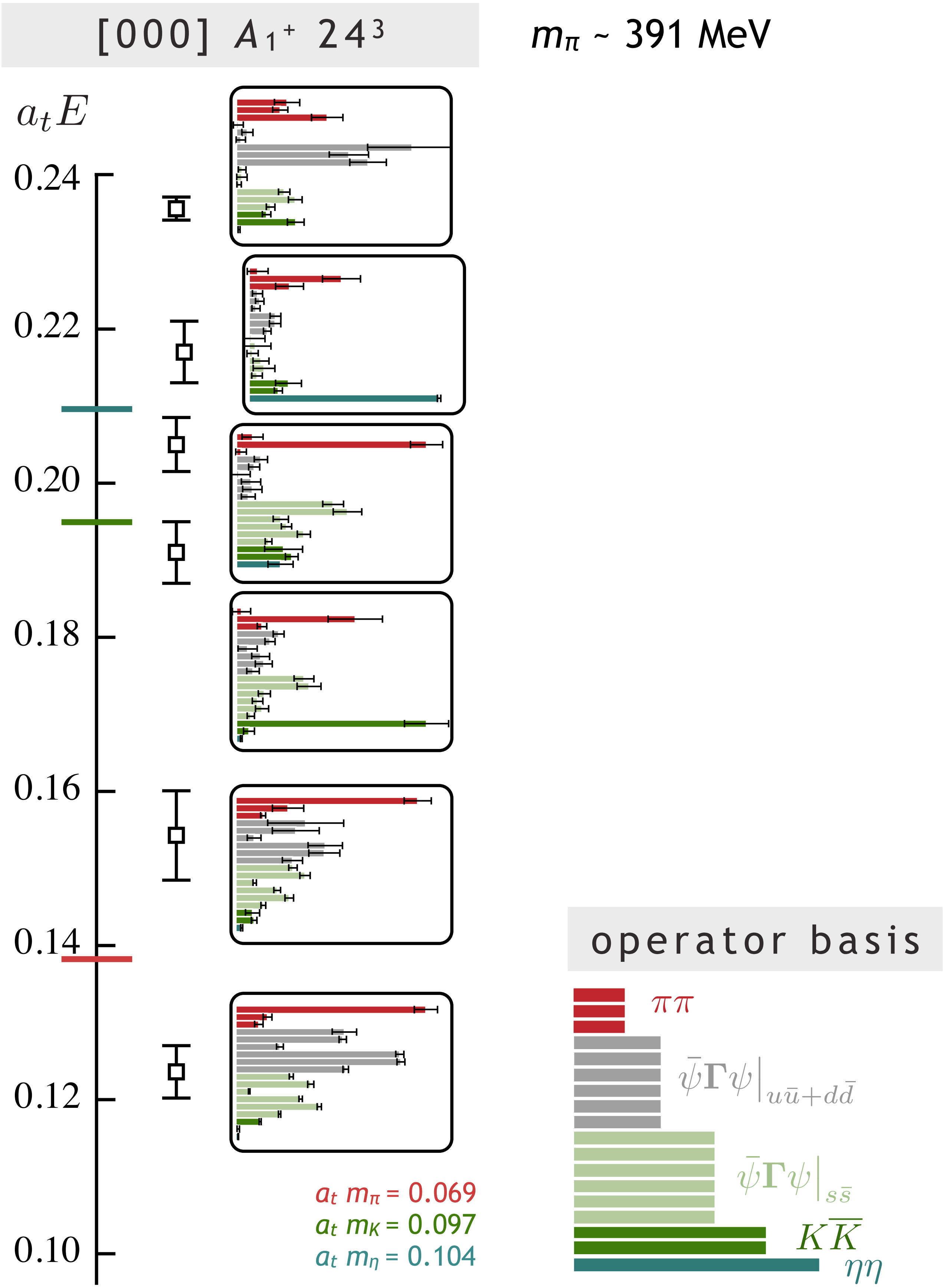
$\pi\pi$ isospin=0

a single entry of the correlation matrix — $\pi\pi$-like operator :

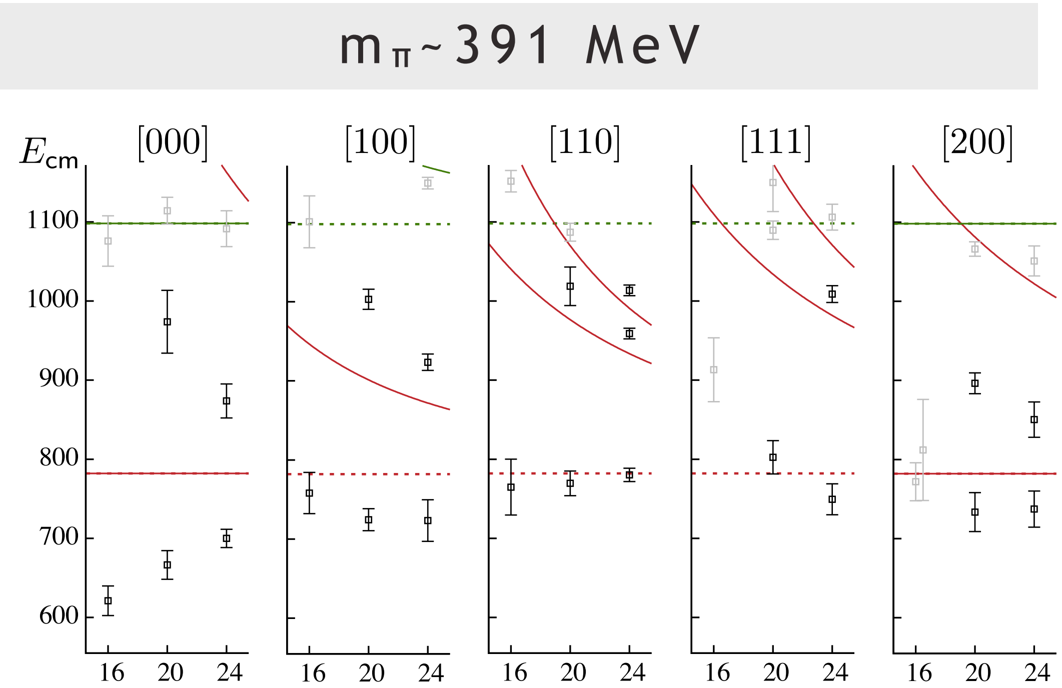
$m_\pi \sim 236$ MeV
$32^3 \times 256$



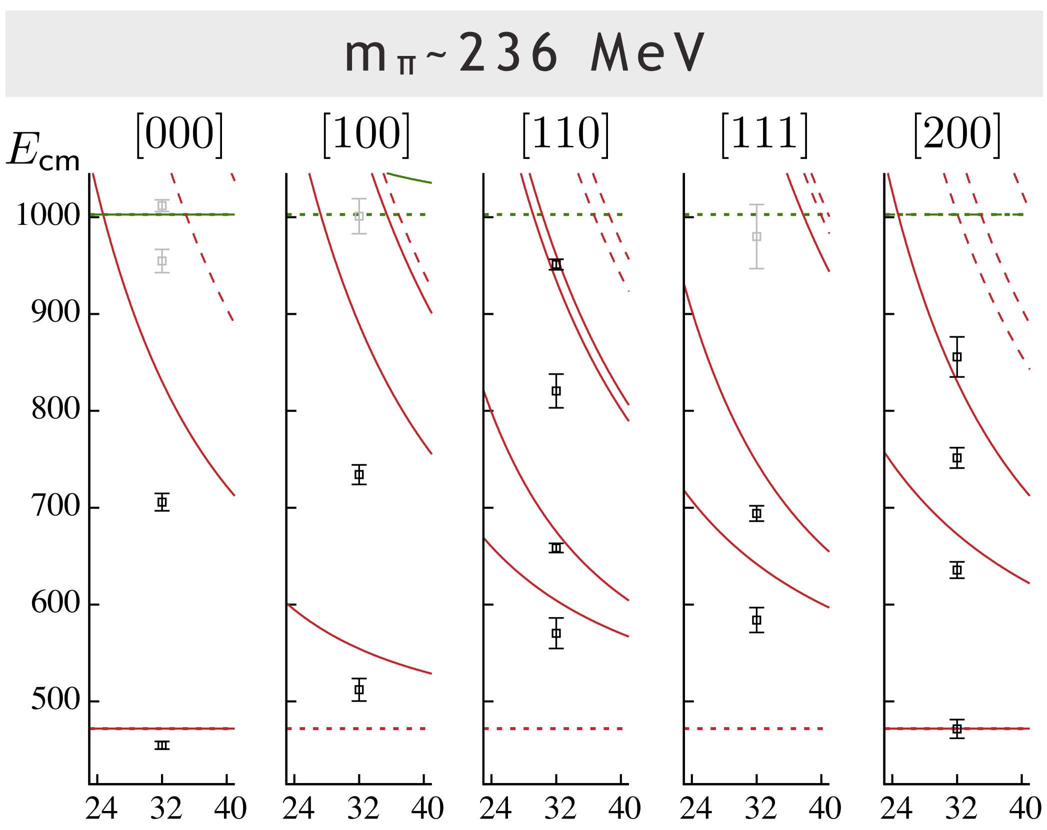
$\pi\pi$ isospin=0



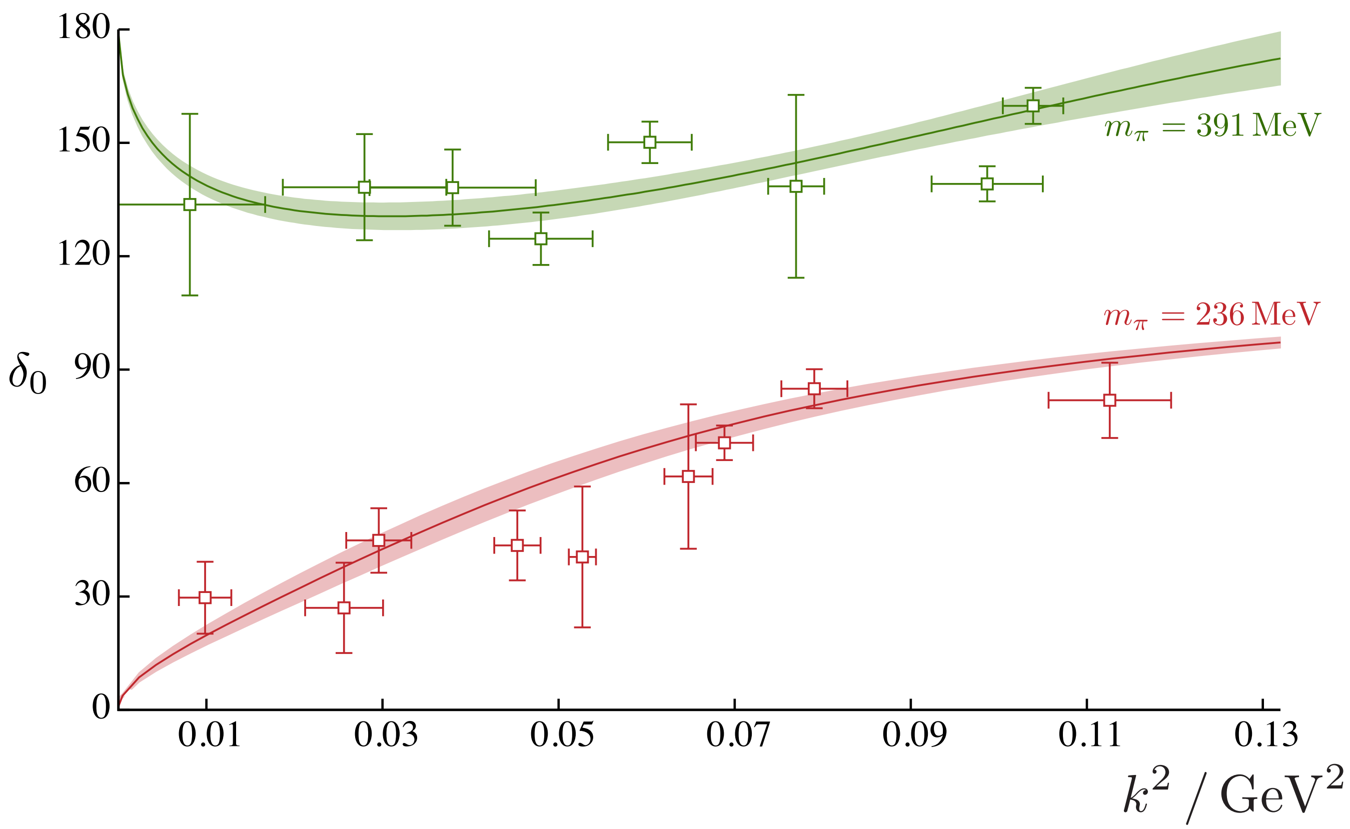
ππ isospin=0



mπ~391 MeV
E_cm
[000]
[100]
[110]
[111]
[200]
1100
1000
900
800
700
600
16
20
24

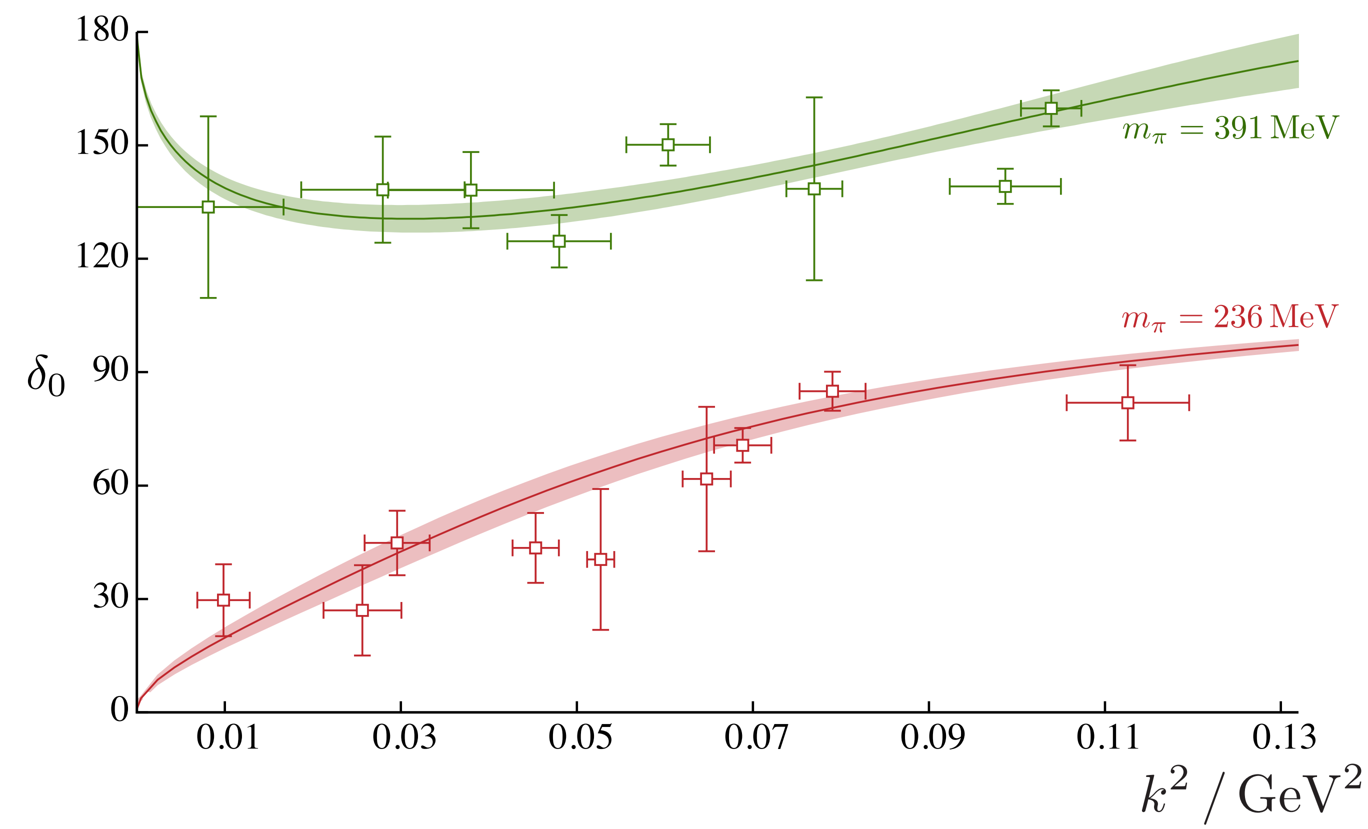


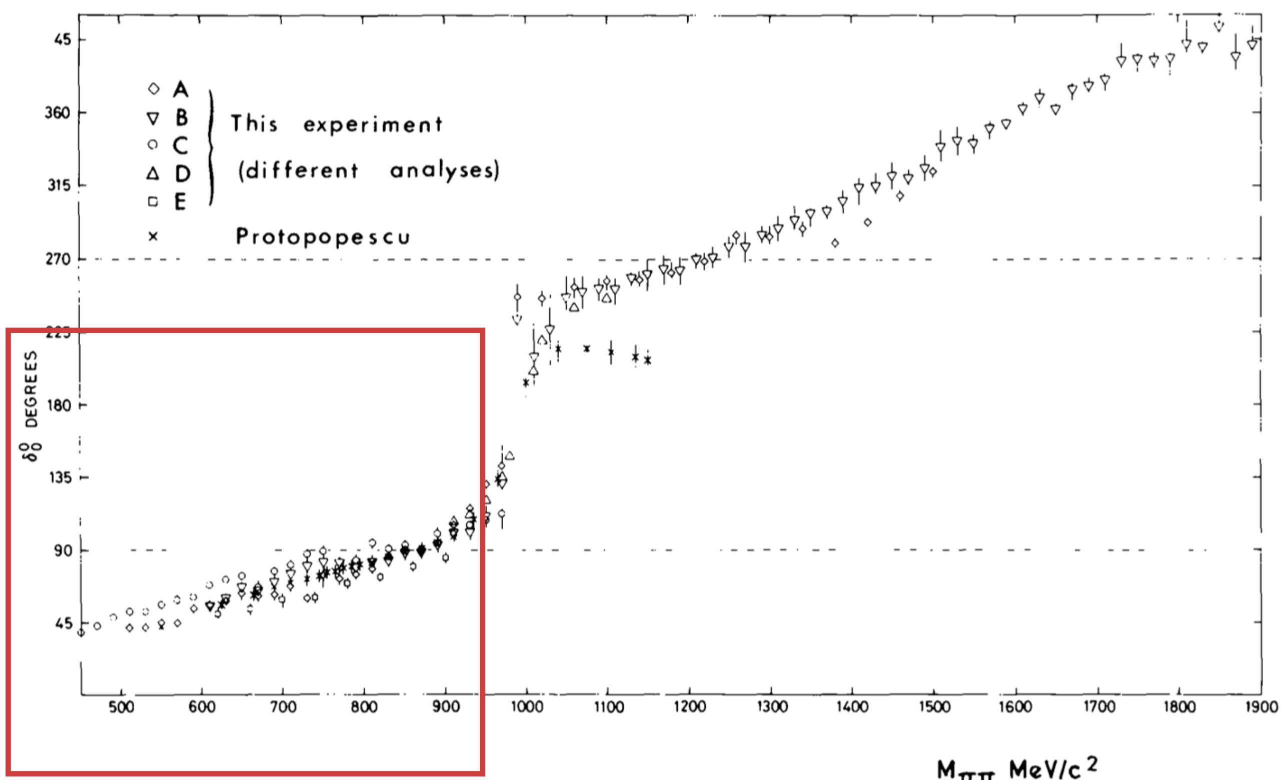
mπ~236 MeV
E_cm
[000]
[100]
[110]
[111]
[200]
1000
900
800
700
600
500
24
32
40



δ0
180
150
120
90
60
30
0
0.01
0.03
0.05
0.07
0.09
0.11
0.13
k² / GeV²
mπ = 391 MeV
mπ = 236 MeV

$\pi\pi$ isospin=0





Grayer 1974