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

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

$$= \langle 0 | O_f(0) e^{-Ht} O_i^\dagger(0) | 0 \rangle$$

Hamiltonian has a complete set of eigenstates

$$H|n\rangle = E_n|n\rangle$$

$$= \sum_n e^{-E_n t} \langle 0 | O_f(0) | n \rangle \langle n | O_i^\dagger(0) | 0 \rangle$$

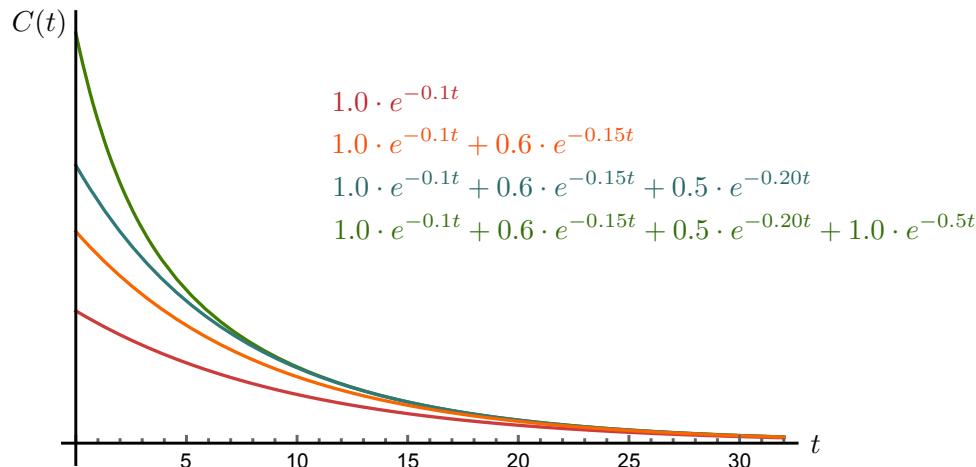
amplitude for  $O_i^\dagger$   
to ‘interpolate’ state  $|n\rangle$   
from the vacuum

$$1 = \sum_n |n\rangle\langle n|$$

(only discrete eigenstates?)

# time dependence of two point correlation functions

## diagonal correlation function

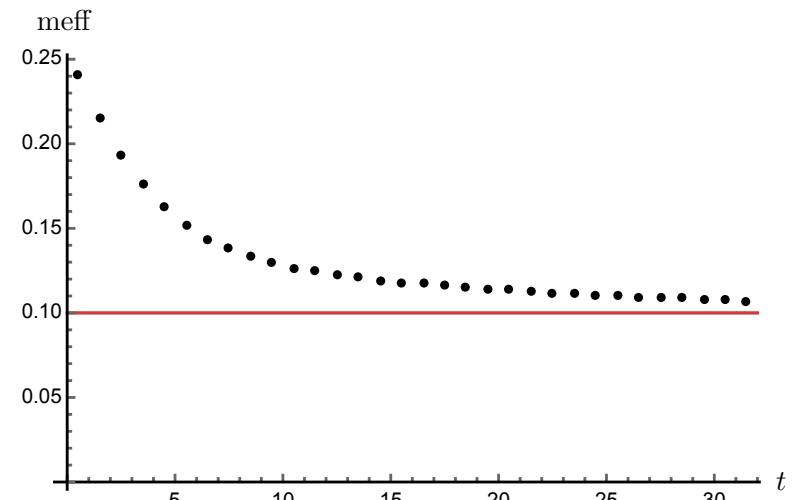
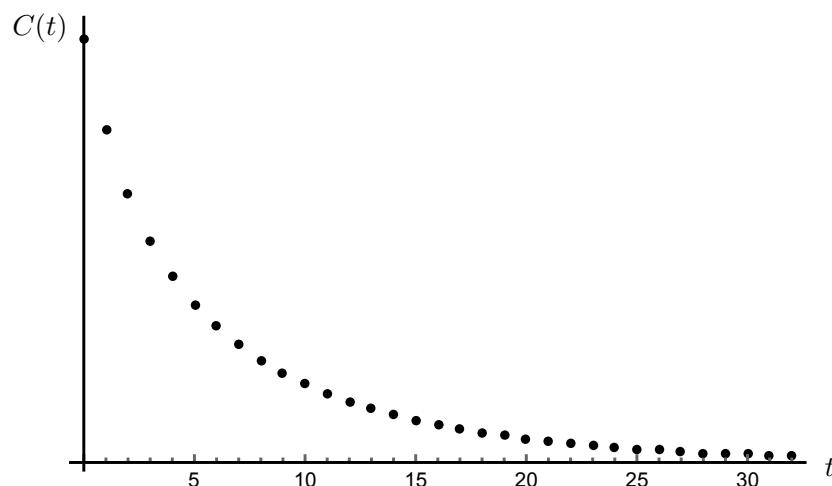


notice that as  $t \rightarrow \infty$

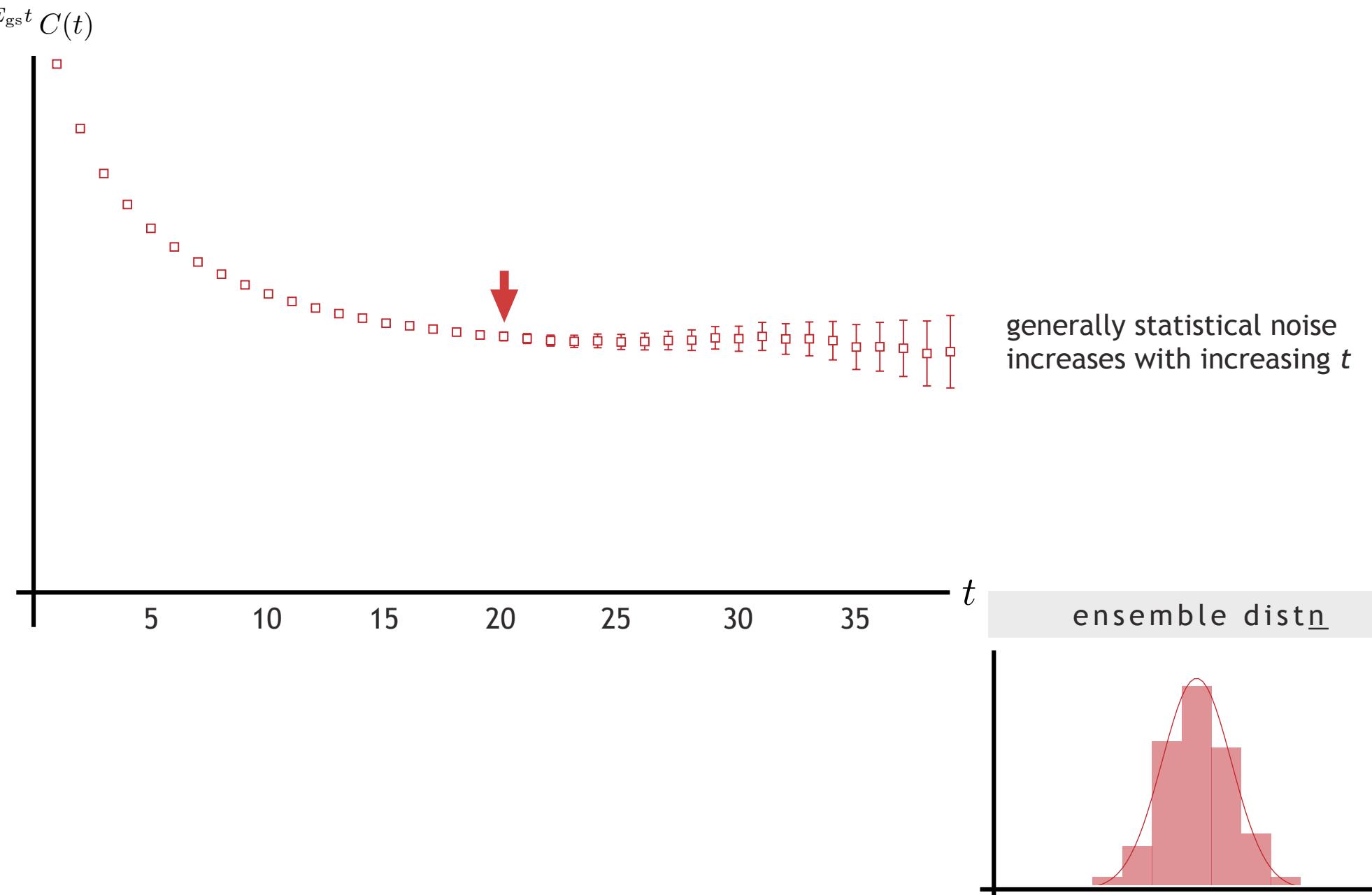
$$C(t) \rightarrow c \cdot e^{-E_{\text{gs}} t}$$

useful to define  
the ‘effective mass’

$$\log \left[ \frac{C(t)}{C(t+1)} \right]$$



# an actual lattice QCD two point correlation function



# noise growth – simplistic argument

at large times, the signal  $\langle O(t) O(0) \rangle \sim e^{-Mt}$  for lightest state with mass  $M$

the variance is the mean of the square  $\langle [O(t)O(t)] [O(0)O(0)] \rangle$

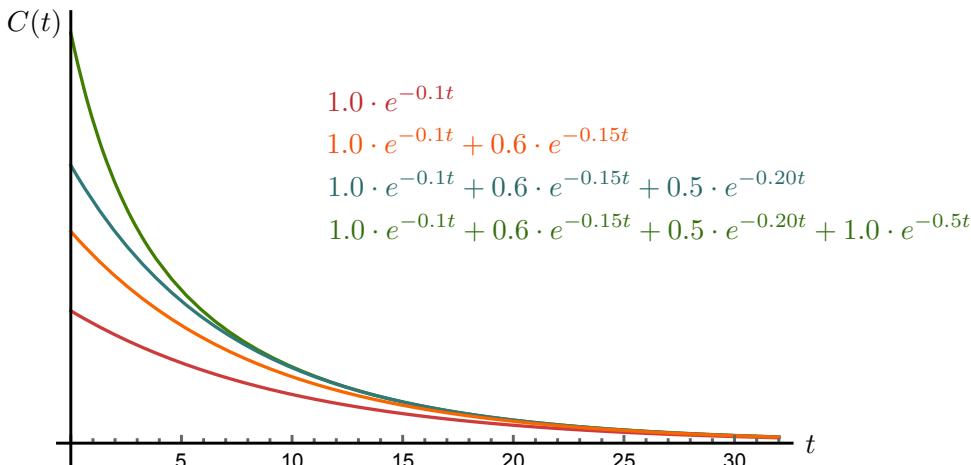
and the operator  $O \cdot O$  will have  
a  $0^+$  component which overlaps with  $\pi\pi$

$$\langle [O(t)O(t)] [O(0)O(0)] \rangle \sim e^{-2m_\pi t}$$

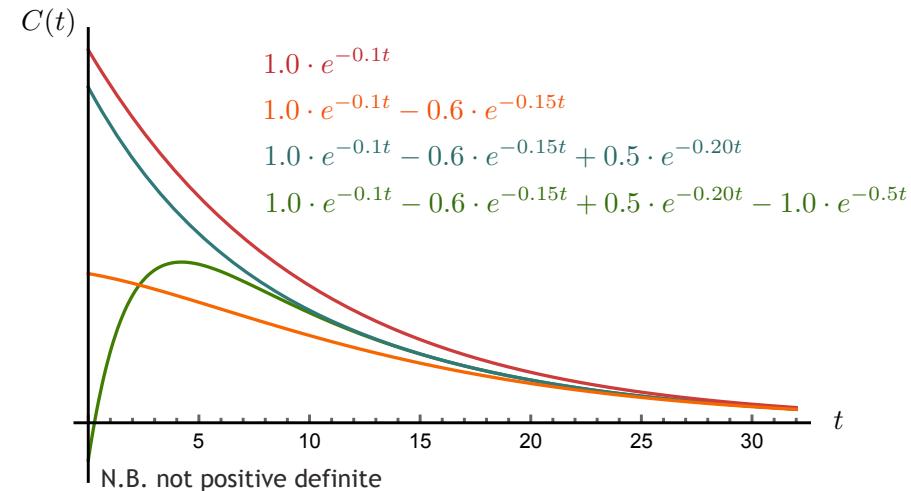
$$\Rightarrow \frac{\text{noise}}{\text{signal}} \sim e^{(M-m_\pi)t}$$

so for everything except pion correlators,  
expect the noise to grow with  $t$

## diagonal correlation function



## off-diagonal correlation function



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

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

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

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

how do we find these optimizing weights ?

# 'variational' approach

$$\Omega_{\mathfrak{n}}^\dagger = \sum_i v_i^{(\mathfrak{n})} O_i^\dagger \quad \Omega_{\mathfrak{n}}^\dagger |0\rangle = |\mathfrak{n}\rangle + \sum_{\mathfrak{m} \neq \mathfrak{n}} \epsilon_{\mathfrak{m}} |\mathfrak{m}\rangle \quad \text{with the } \epsilon_{\mathfrak{m}} \text{ as small as possible}$$

'optimal' correlation function

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

$$= \sum_{ij} v_i^* \langle 0 | O_i(t) O_j^\dagger(0) | 0 \rangle v_j = \sum_{ij} v_i^* C_{ij}(t) v_j \quad \text{by varying the } \mathbf{v}$$

can avoid the trivial minimum ( $\mathbf{v}_i=0$ ) 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

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

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

# generalized eigenvalue problem

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

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

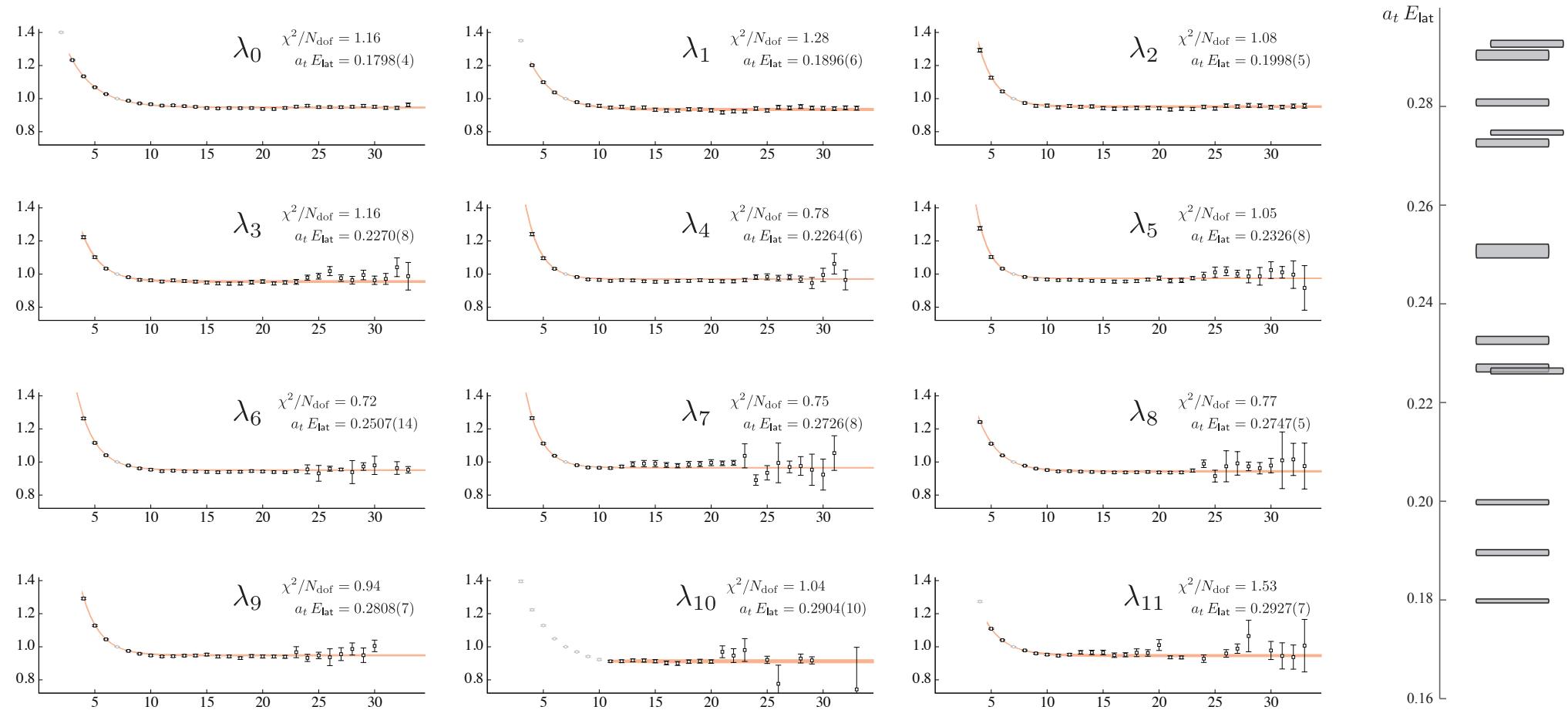
eigenvector orthogonality  $\mathbf{v}^{(\mathfrak{n})} \cdot \mathbf{C}(t_0) \cdot \mathbf{v}^{(\mathfrak{m})} = \delta_{\mathfrak{n},\mathfrak{m}}$

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

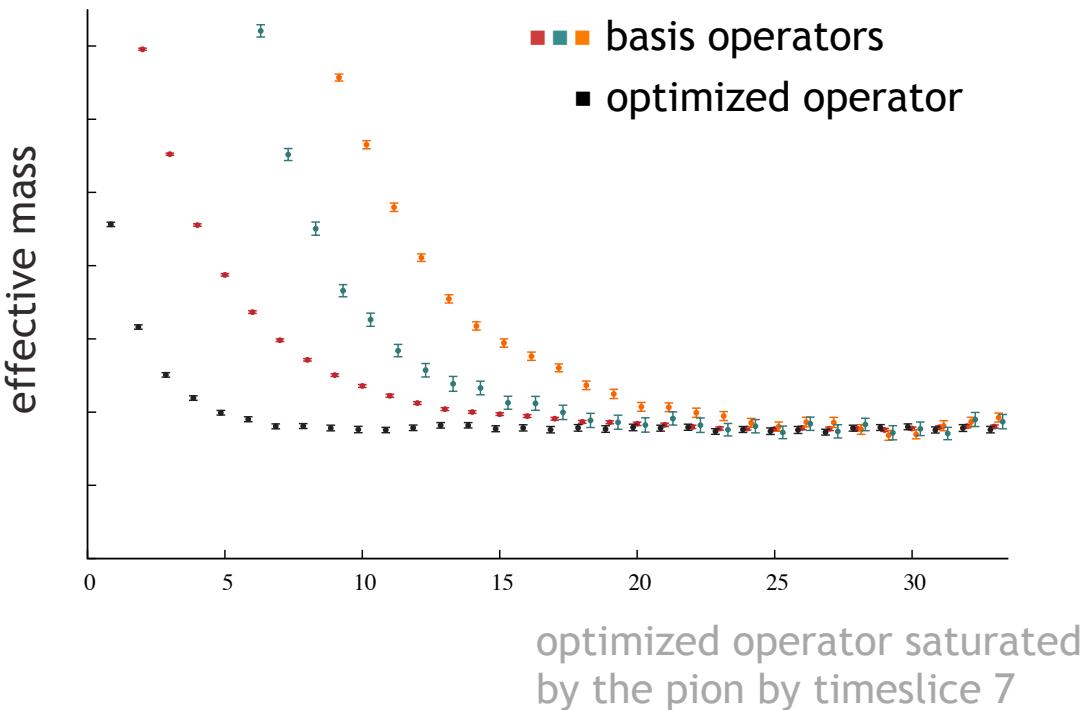


fitted with

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

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

## [000] $A_1$ diagonal correlators



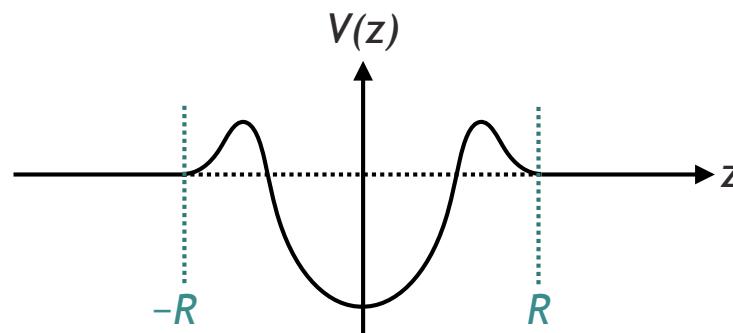
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ok, so it looks like we should be able to compute spectra, but we wanted **scattering amplitudes !**

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

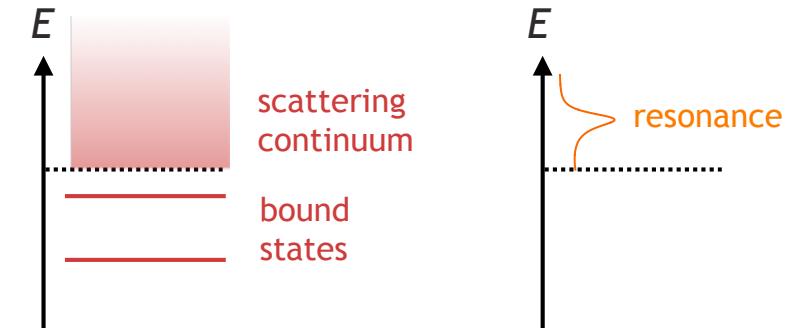
**spectra are discrete** in a finite volume – no scattering continuum ?

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



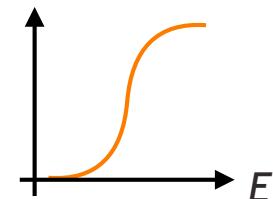
solve the Schrödinger equation

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



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

phase-shift



# 'scattering' in a finite-volume

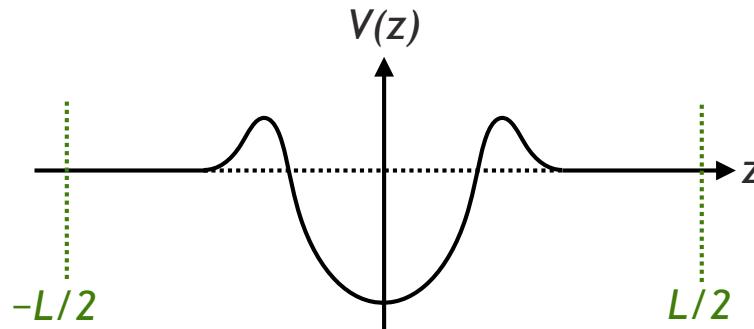
now put the system in a 'box' – periodic boundary condition at  $z = \pm L/2$

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

$$\begin{aligned}\psi(L/2) &= \psi(-L/2) \\ \frac{d\psi}{dz}(L/2) &= \frac{d\psi}{dz}(-L/2)\end{aligned}$$

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

Lüscher 1986

⋮

many subsequent works  
see the RMP for a complete list

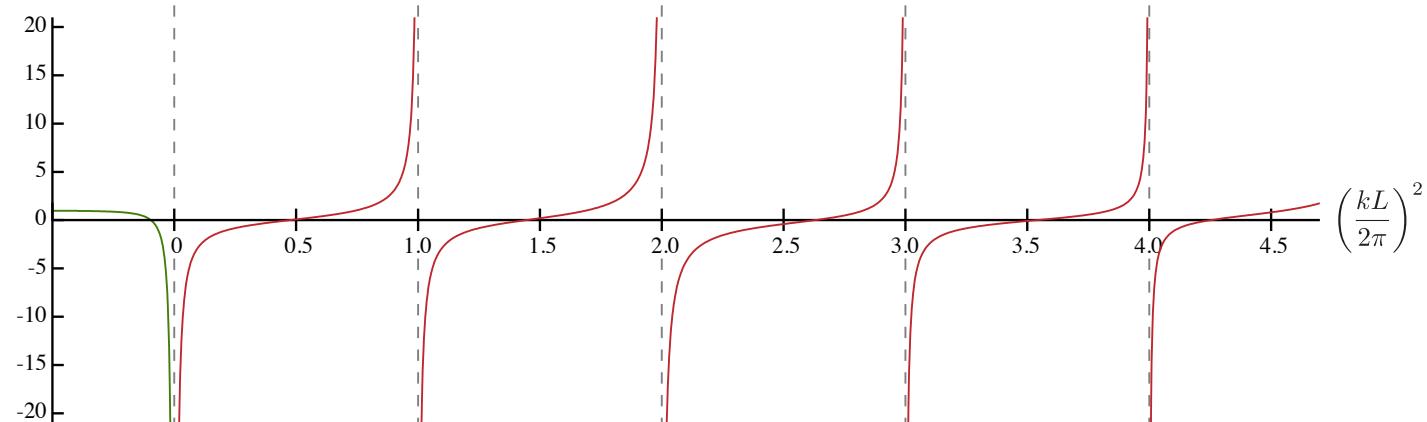
in the simplest case of  
a single partial wave  
being non-zero

will present some  
complications later ...

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

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

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



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

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

# finite-volume functions

$$\mathcal{M}_{\ell m, \ell' m'}(E, L) = \frac{1}{\pi^{3/2}} \sum_{\bar{\ell}, \bar{m}} \sqrt{\frac{(2\ell+1)(2\bar{\ell}+1)}{(2\ell'+1)}} \langle \ell m; \bar{\ell} \bar{m} | \ell' m' \rangle \langle \ell 0; \bar{\ell} 0 | \ell' 0 \rangle \left(\frac{2\pi}{kL}\right)^{\bar{\ell}+1} Z_{\bar{\ell} \bar{m}} \left(s \rightarrow 1; \left(\frac{kL}{2\pi}\right)^2\right)$$

Lüscher zeta function

$$Z_{\ell m} \left(s; \left(\frac{kL}{2\pi}\right)^2\right) = \sum_{\mathbf{n}} \frac{|\mathbf{n}|^\ell Y_{\ell m}(\hat{\mathbf{n}})}{\left[|\mathbf{n}|^2 - \left(\frac{kL}{2\pi}\right)^2\right]^s}$$

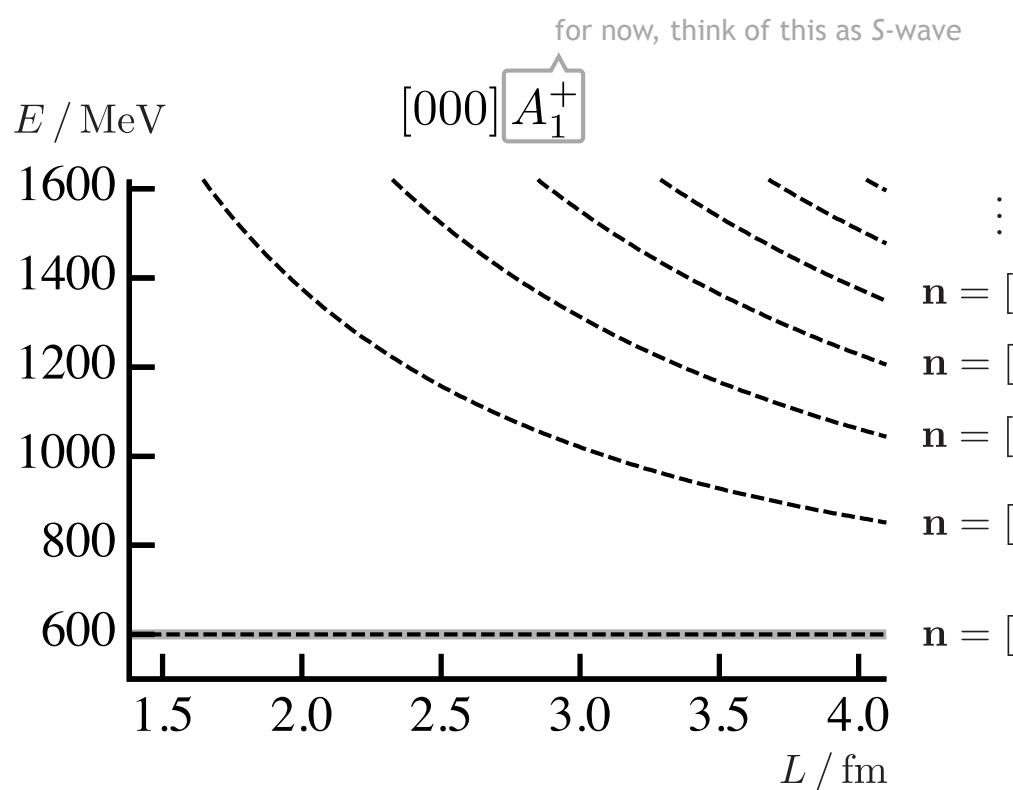
$$\mathbf{n} = [n_x, n_y, n_z]$$

e.g.  $\mathcal{M}_{00,00} = \frac{1}{\pi} \frac{1}{kL} \lim_{s \rightarrow 1^+} \sum_{\mathbf{n}} \frac{1}{\left[|\mathbf{n}|^2 - \left(\frac{kL}{2\pi}\right)^2\right]^s}$

will have a divergence at each  $k^2 = \left(\frac{2\pi}{L} |\mathbf{n}|\right)^2$

i.e. at the non-interacting energies

# no interaction



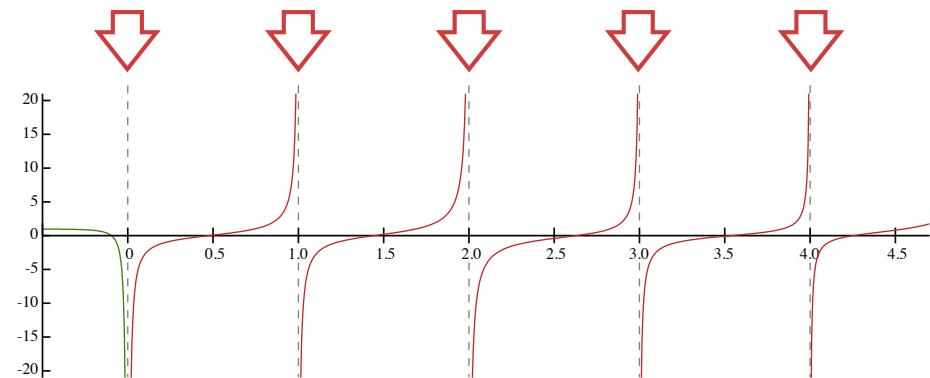
scattering particles  $m = 300 \text{ MeV}$



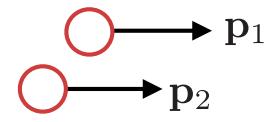
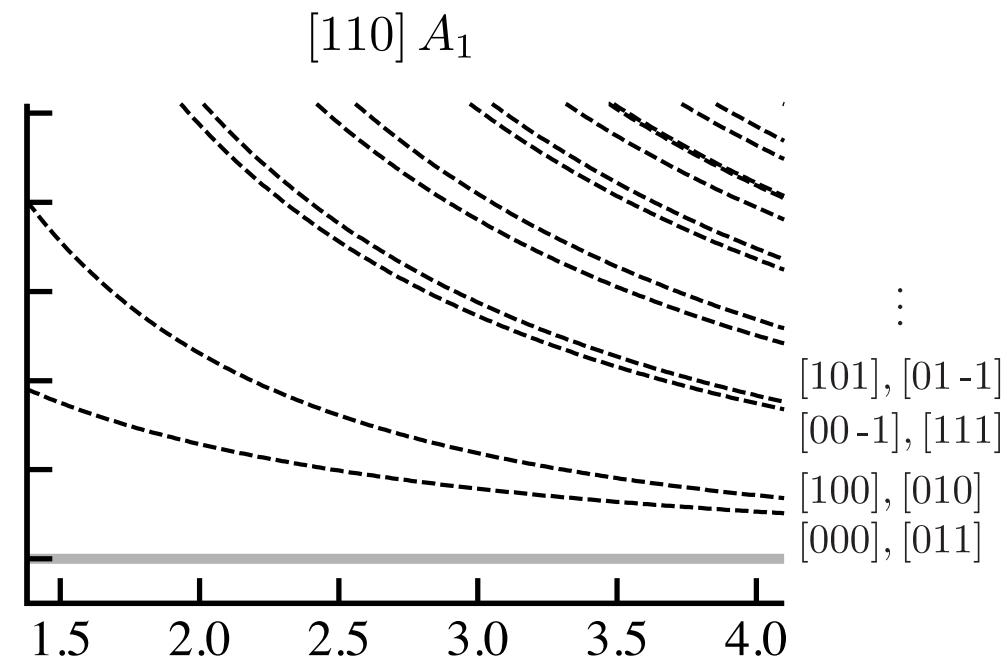
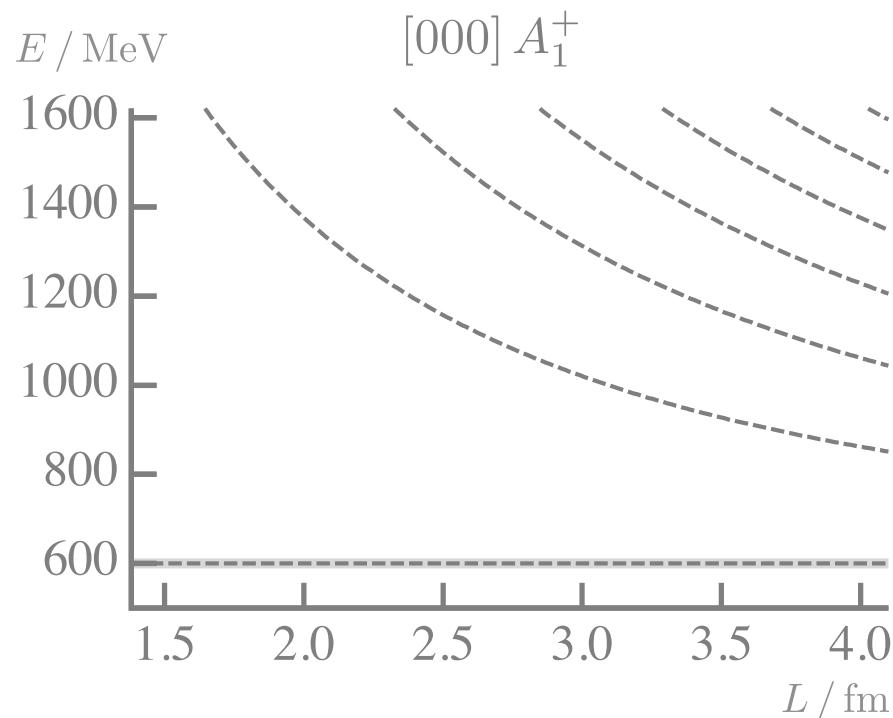
$$E_{ni} = 2\sqrt{m^2 + \mathbf{p}^2}$$

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

$$\cot \delta(E) = \mathcal{M}(E(L), L) \quad \delta \rightarrow 0, \cot \delta \rightarrow \infty$$



divergences correspond to non-interacting energies



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

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

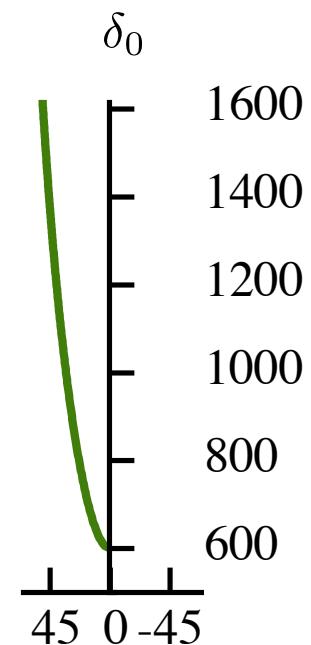
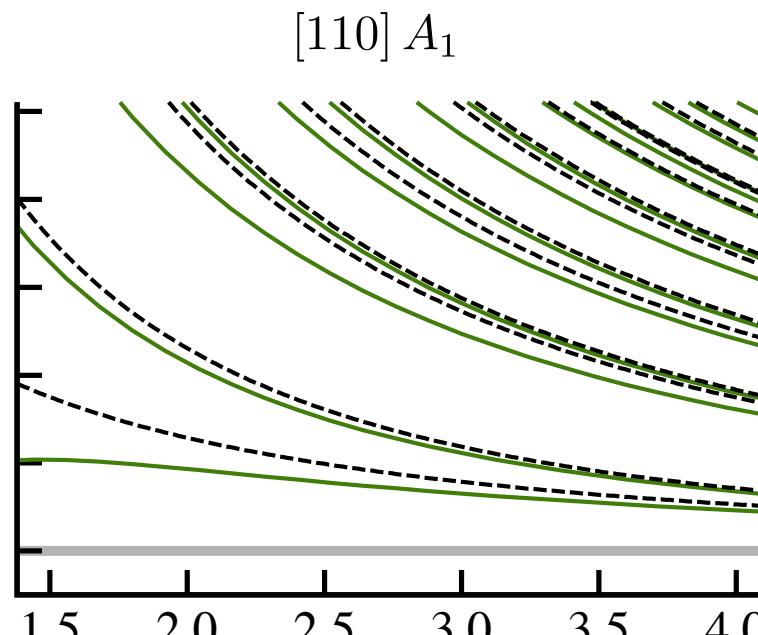
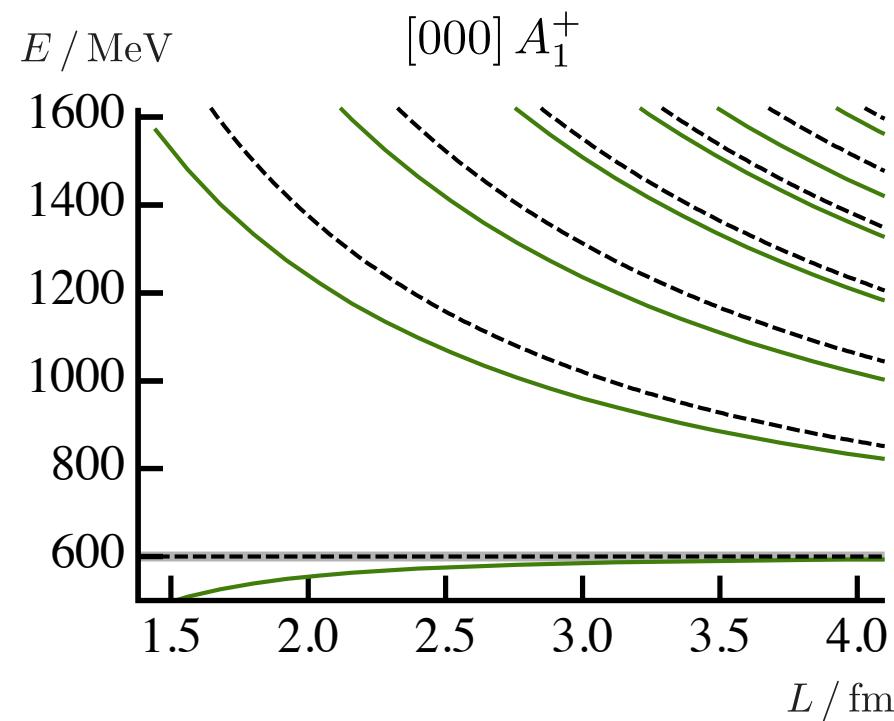
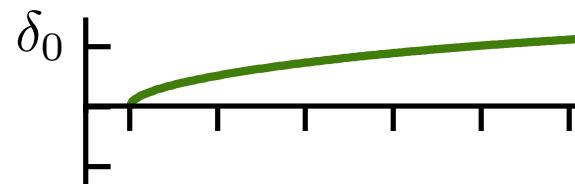
$$\mathbf{P} = \frac{2\pi}{L}\mathbf{n}$$

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

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

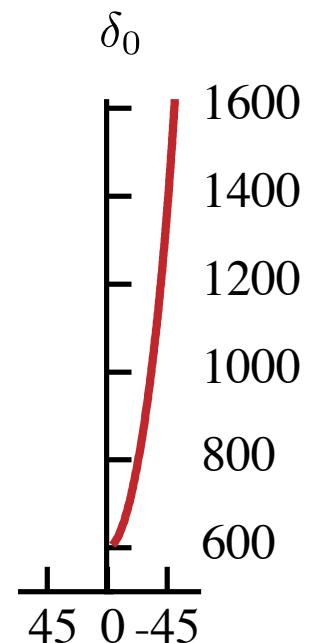
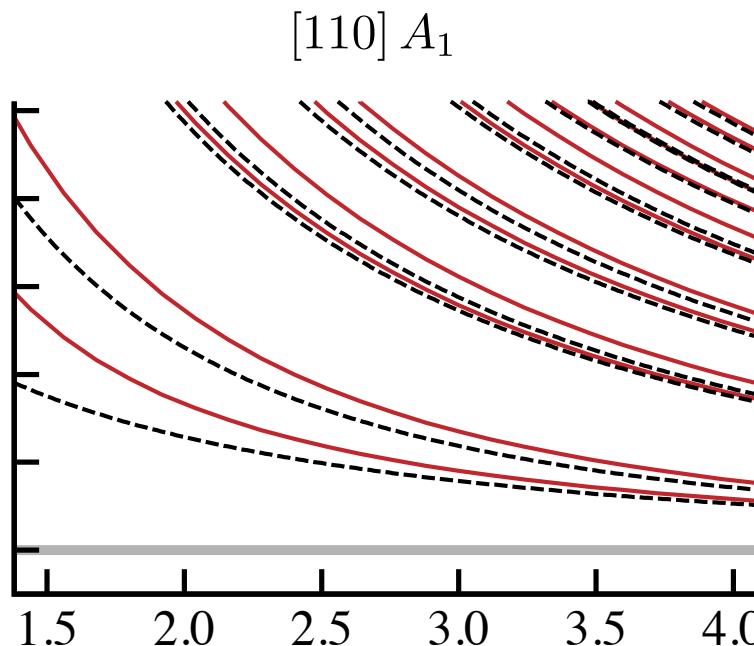
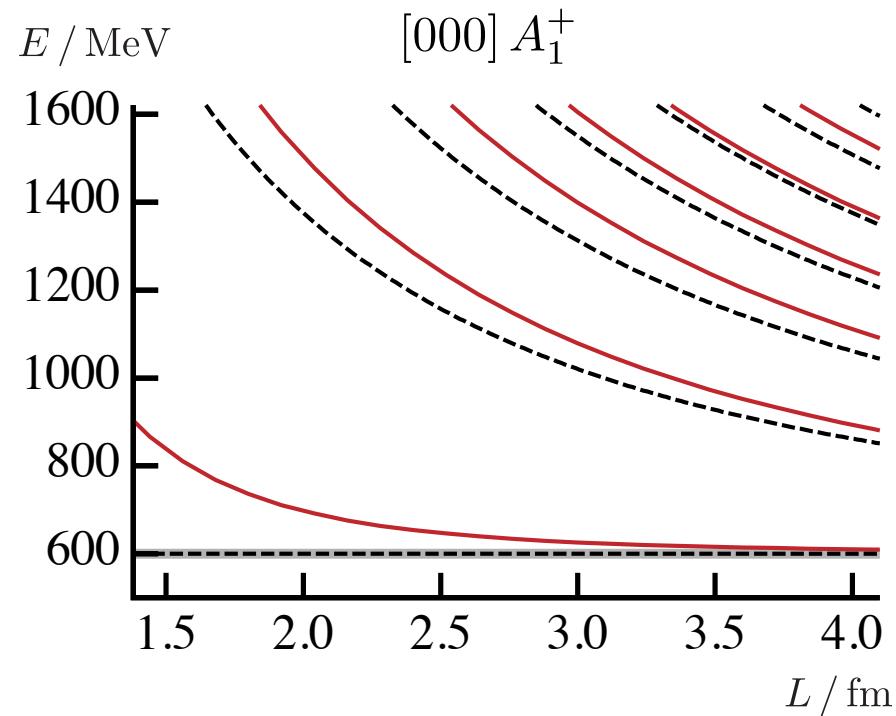
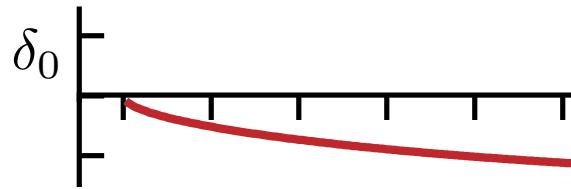
# weak attraction

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



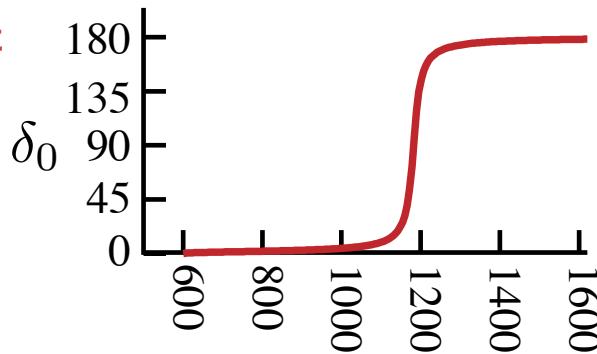
# weak repulsion

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



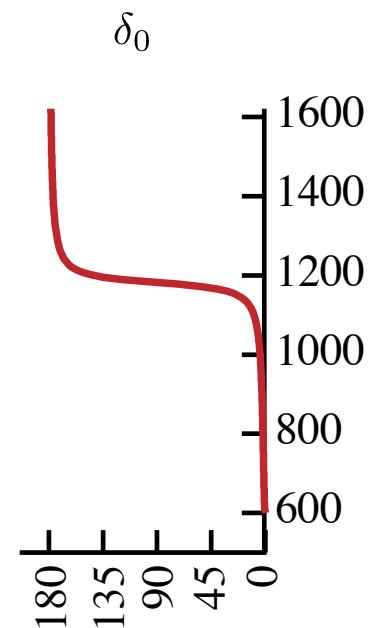
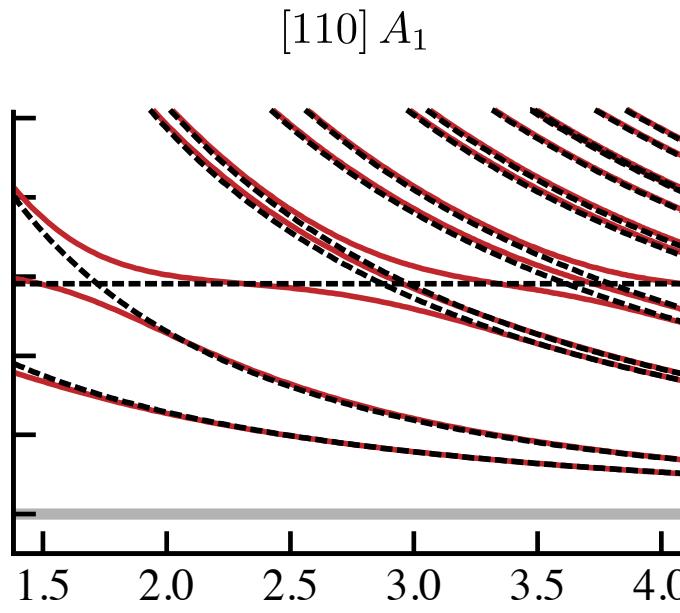
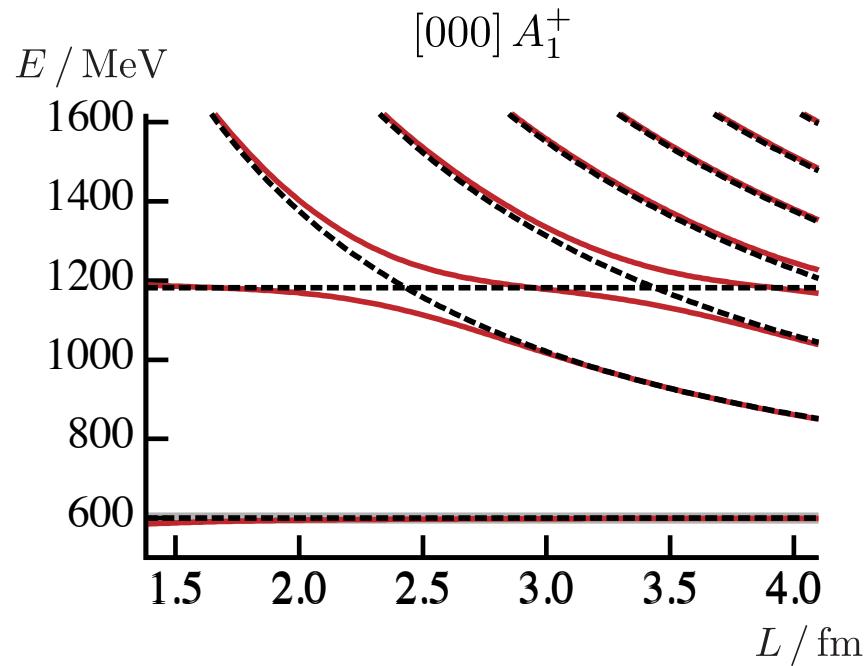
# an elastic resonance

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



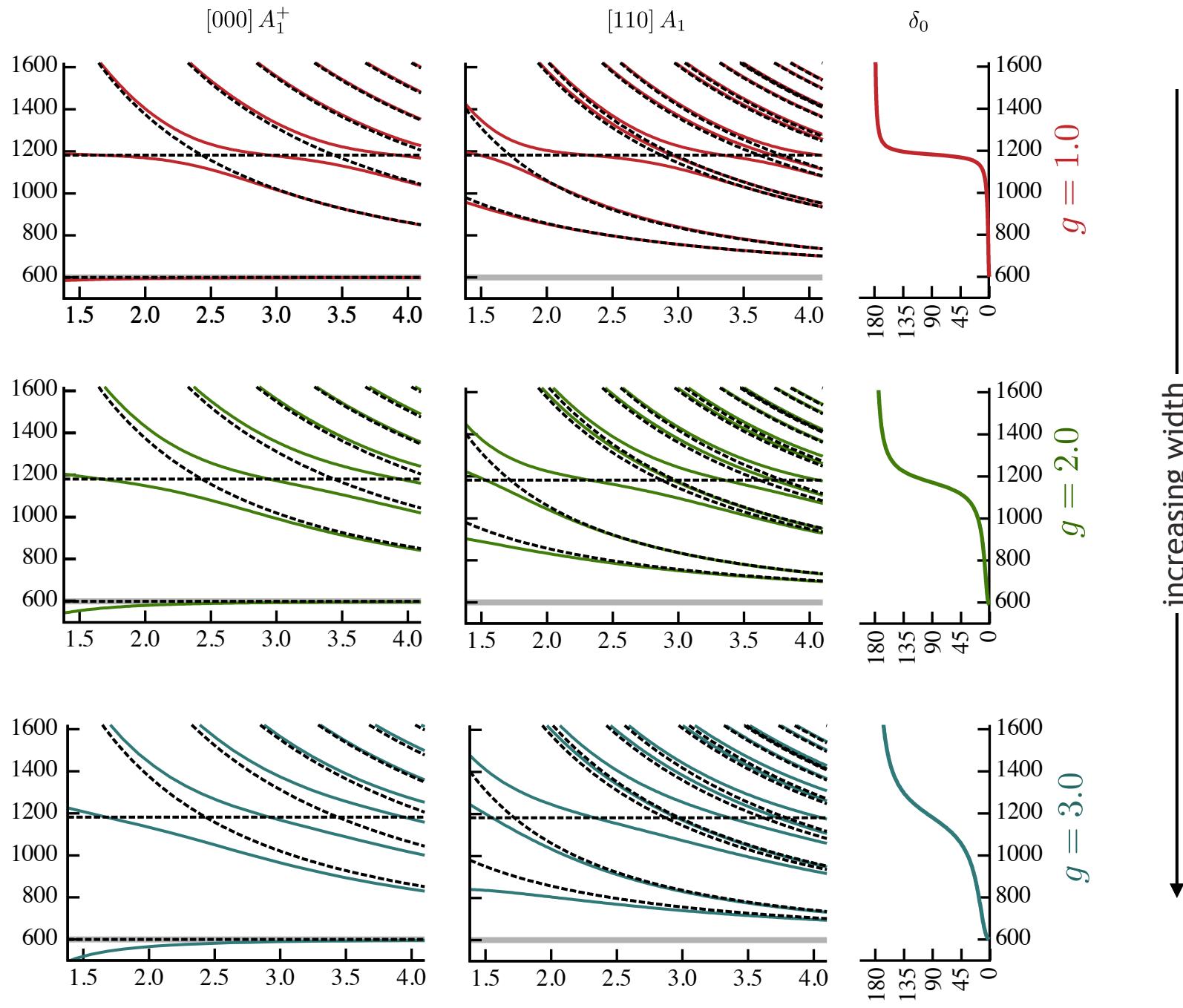
$$\tan \delta = \frac{E \Gamma(E)}{m_R^2 - E^2}$$

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



note the **avoided level crossings**

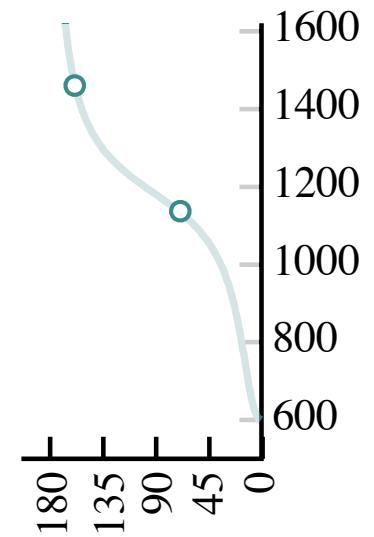
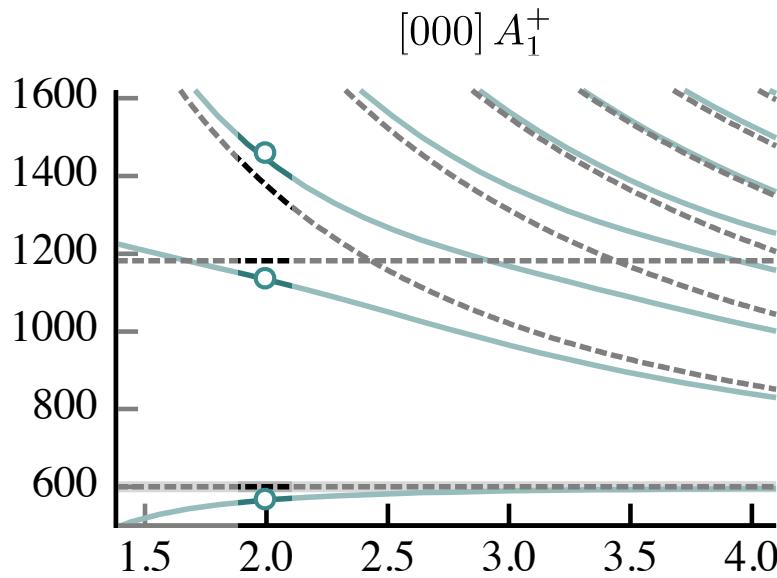
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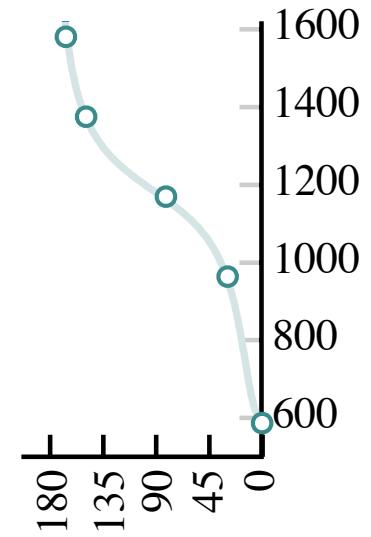
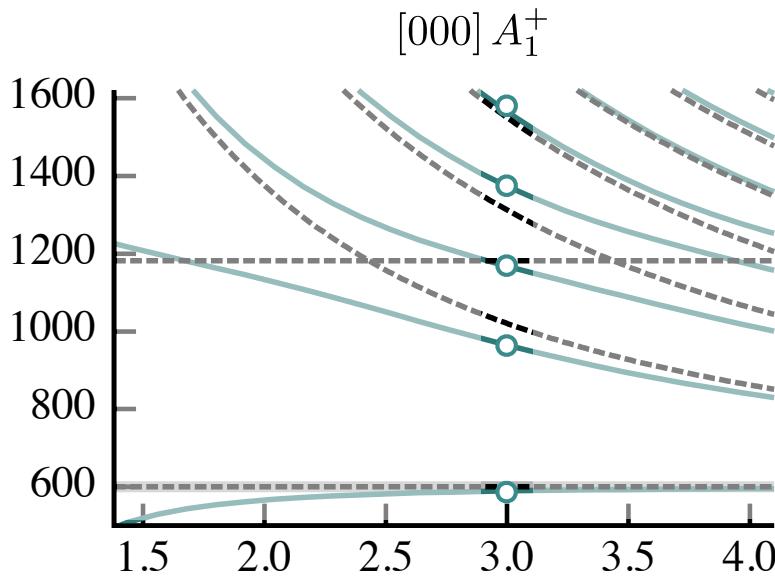
# an elastic resonance – finite-volume mapping

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



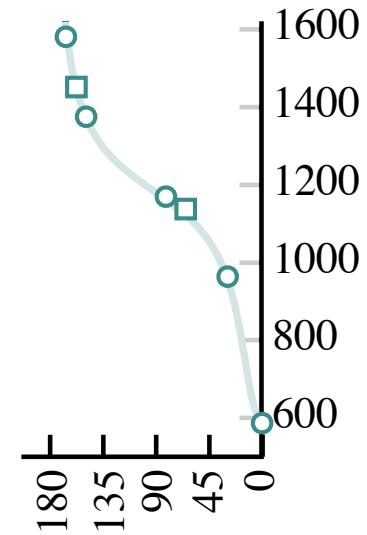
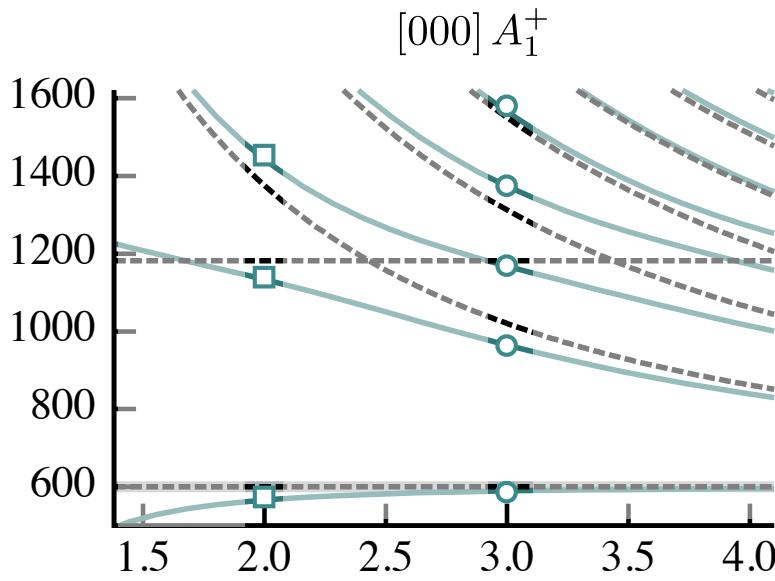
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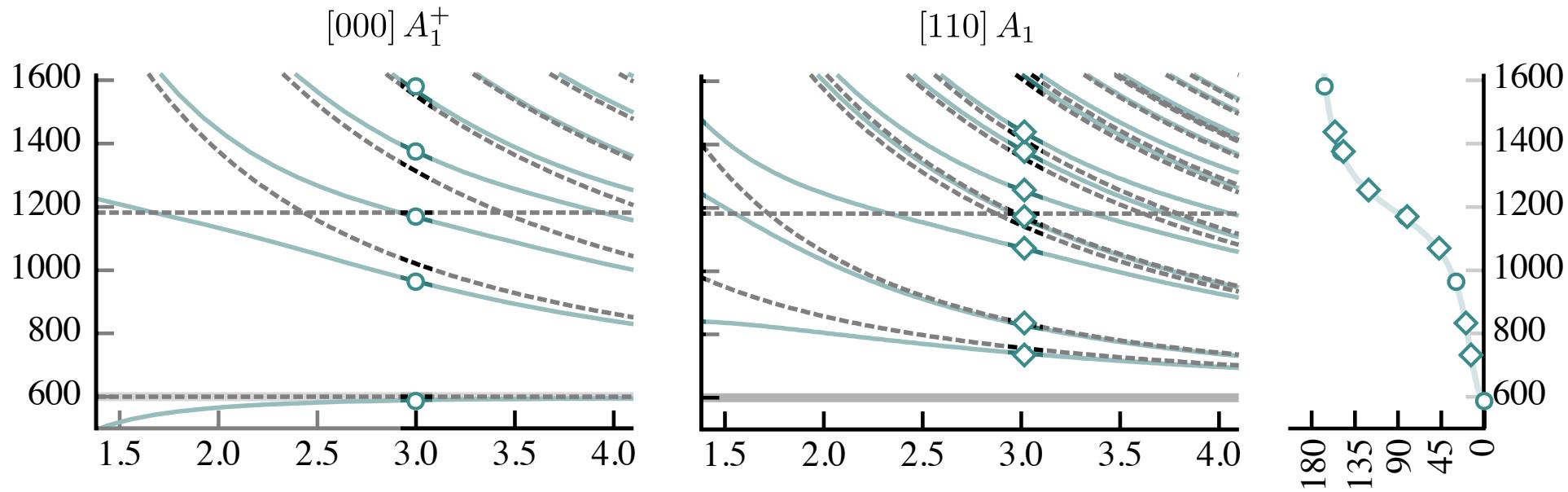
# an elastic resonance – finite-volume mapping

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



more volumes give more information,  
but each new volume is a completely new lattice calculation  
and hence very computationally costly

# an elastic resonance – finite-volume mapping



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

**subduction**  $|\Lambda, \rho\rangle = \sum_m S_{J,m}^{\Lambda,\rho} |J, m\rangle$

for non-zero momentum it's even worse

– in continuum have **little group**, those rotations which don't change  $p$

$\Rightarrow$  label by **helicity**

can subduce helicity states into irreps of the reduced cubic symmetry

PRD85 014507 (2012)

# some annoying technical stuff – breaking of rotational symmetry

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

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

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

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

features all  $\ell$  subduced into irrep  $\Lambda$

$n$  = embedding of  $\ell$  into  $\Lambda$

e.g. [000]  $A_1$

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

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

# 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

$\Gamma$  = Dirac gamma  
+ gauge-covariant derivatives

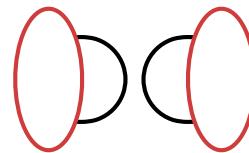
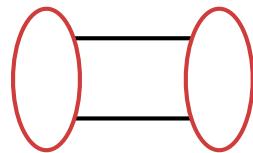
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Wick  
contractions



‘annihilation’  
required for isospin=0

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

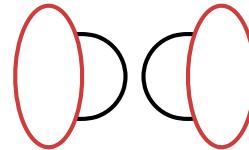
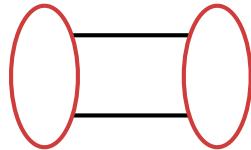
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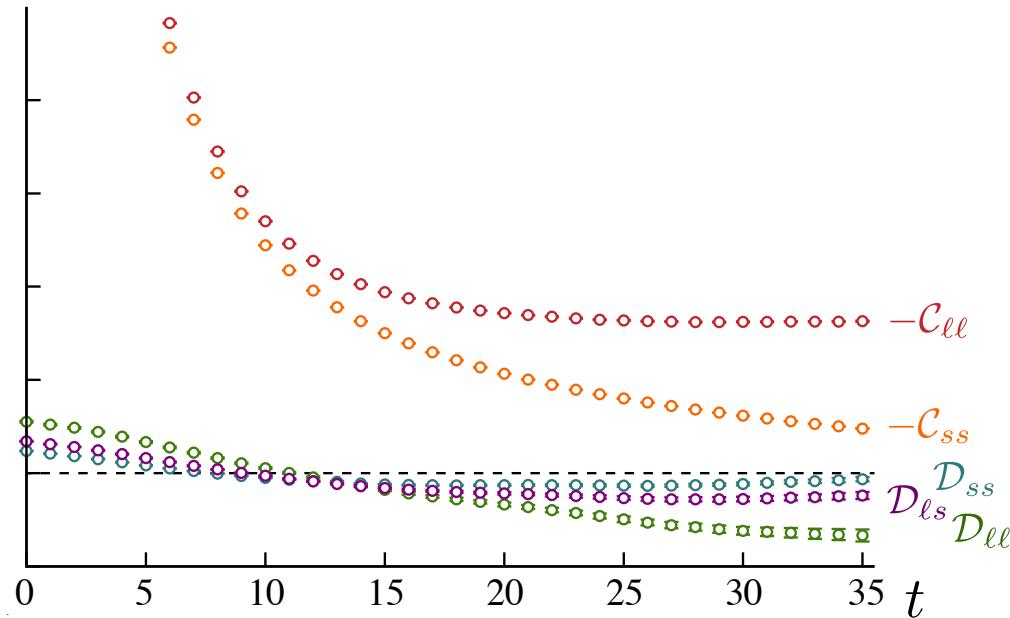
Wick  
contractions



‘annihilation’  
required for isospin=0

quark propagation from  $t$  to  $t$   
 $\Rightarrow$  matrix inversions on many  $t$

an isospin=0 correlation function



turns out this is not enough ...

# meson operators

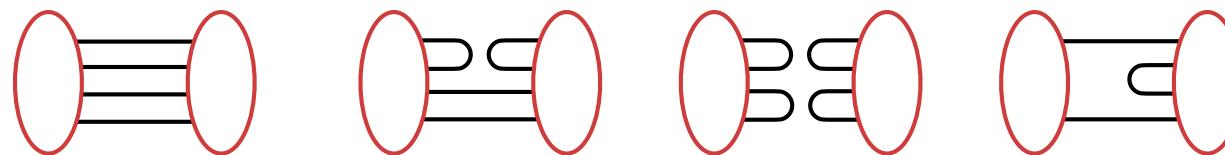
easiest constructions with meson quantum numbers – fermion bilinears  $\bar{\psi}\Gamma\psi$

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

e.g. ‘local’ tetraquark operators  $\bar{\psi}_x \bar{\psi}_x \psi_x \psi_x$

e.g. ‘meson-meson’-like operators  $\sum_x e^{i\mathbf{p} \cdot \mathbf{x}} \bar{\psi}_x \Gamma \psi_x \sum_y e^{i\mathbf{q} \cdot \mathbf{y}} \bar{\psi}_y \Gamma' \psi_y$

schematic  
Wick  
contractions



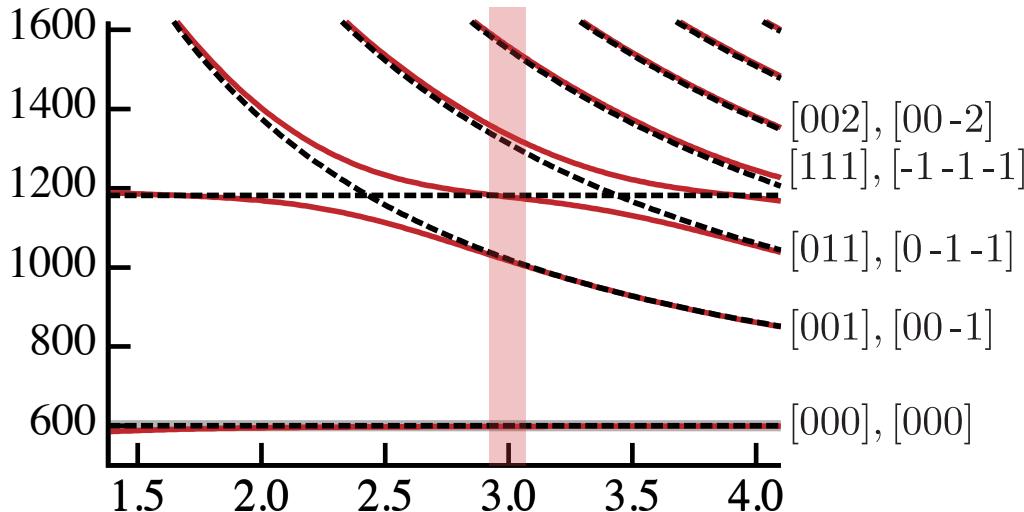
‘annihilation’  
generally  
required

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]

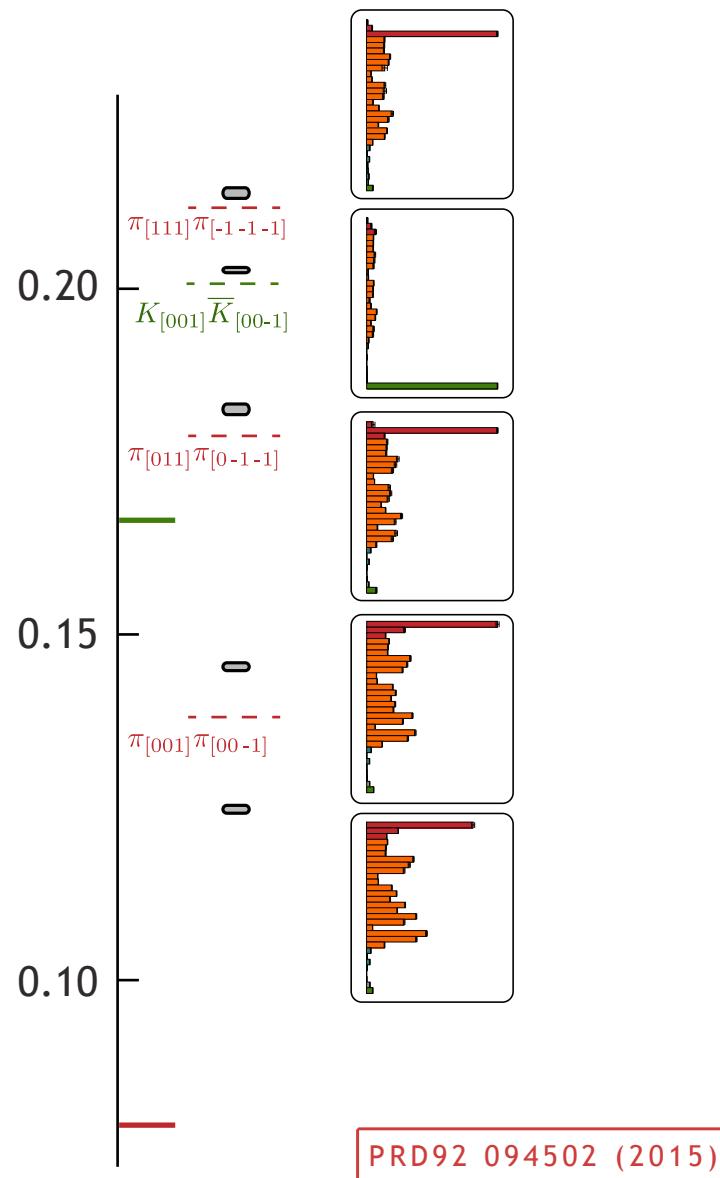
‘look like’ the expected  
meson-meson basis states

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

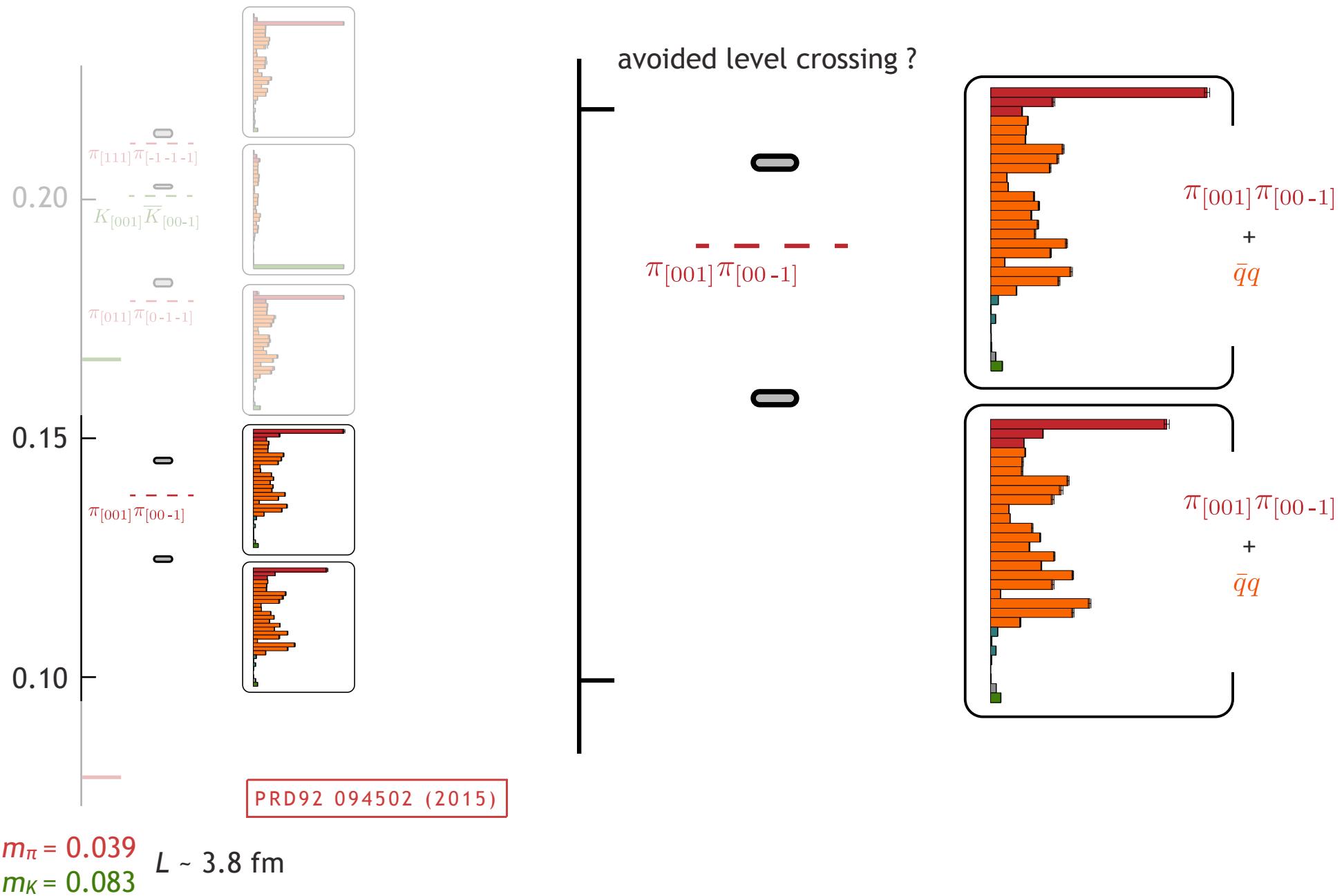
variational analysis of  $30 \times 30$  correlation matrix:  $3 \times \pi\pi$ ,  $26 \times \bar{\psi}\Gamma\psi$ ,  $1 \times K\bar{K}$



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

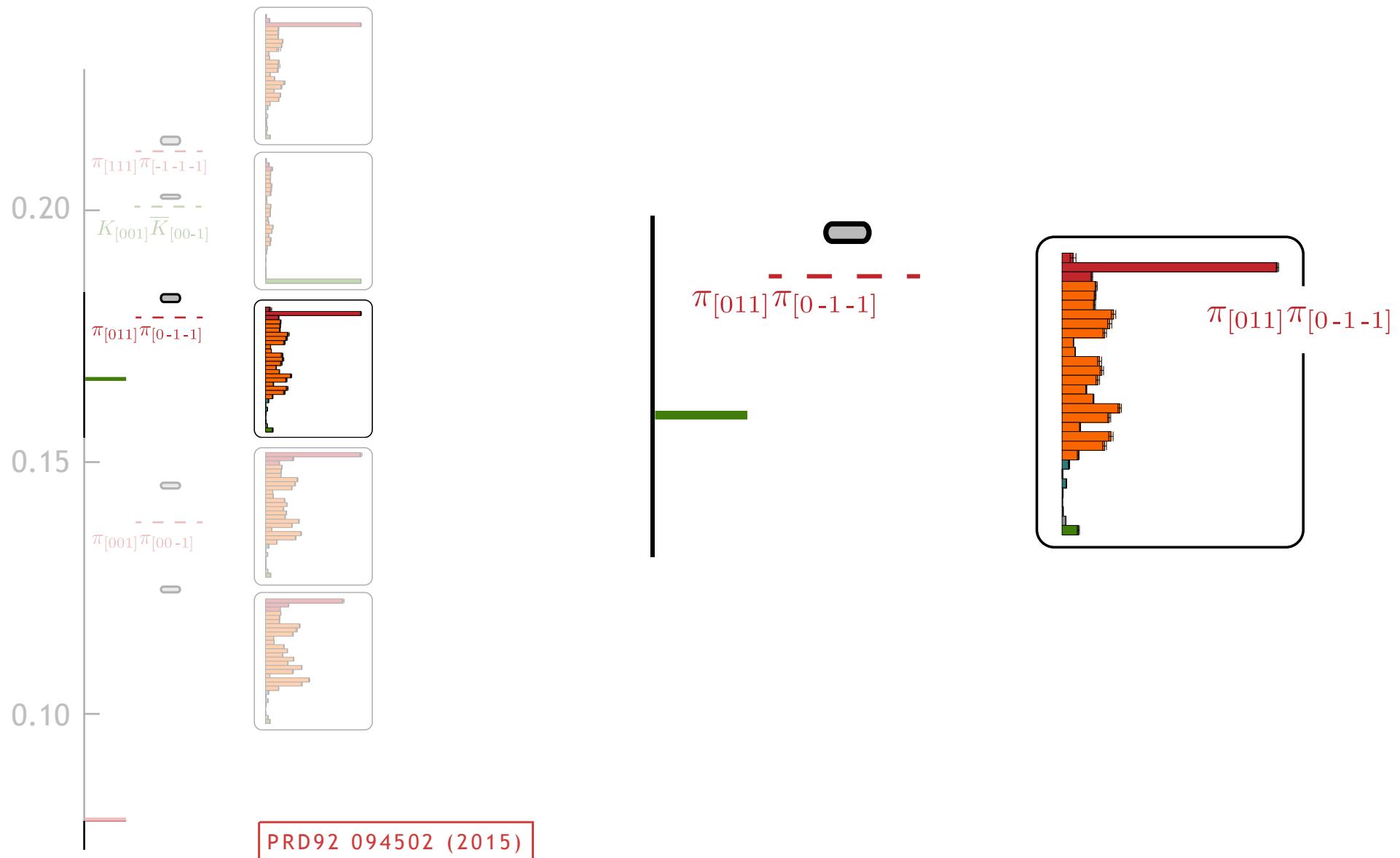
# isospin=1 $T_1^-$ irrep spectrum

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# isospin=1 $T_1^-$ irrep spectrum

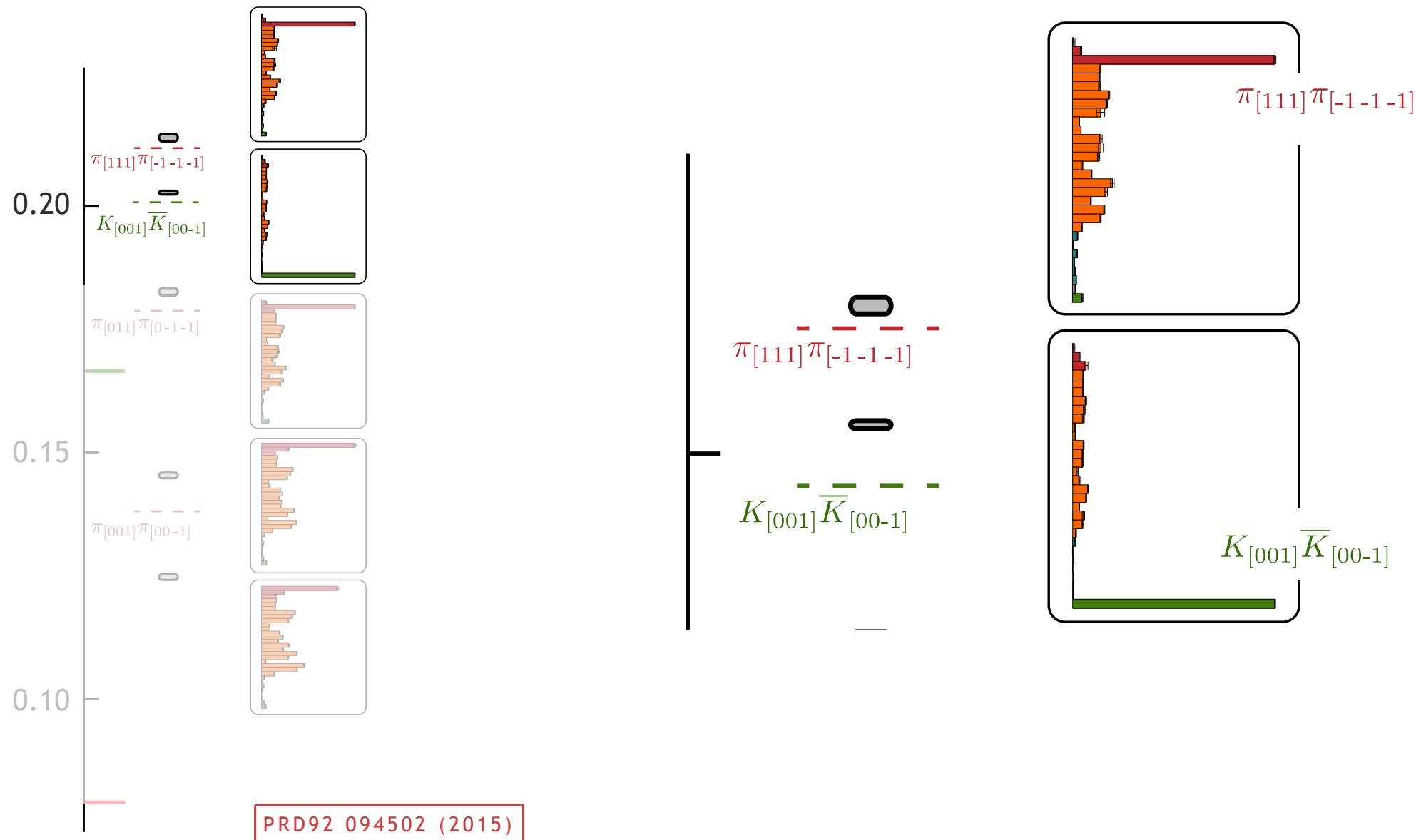
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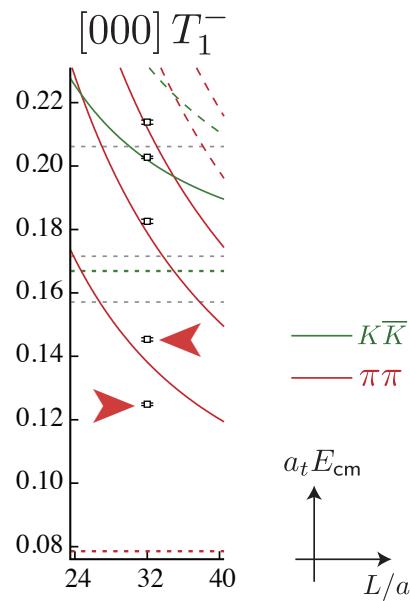
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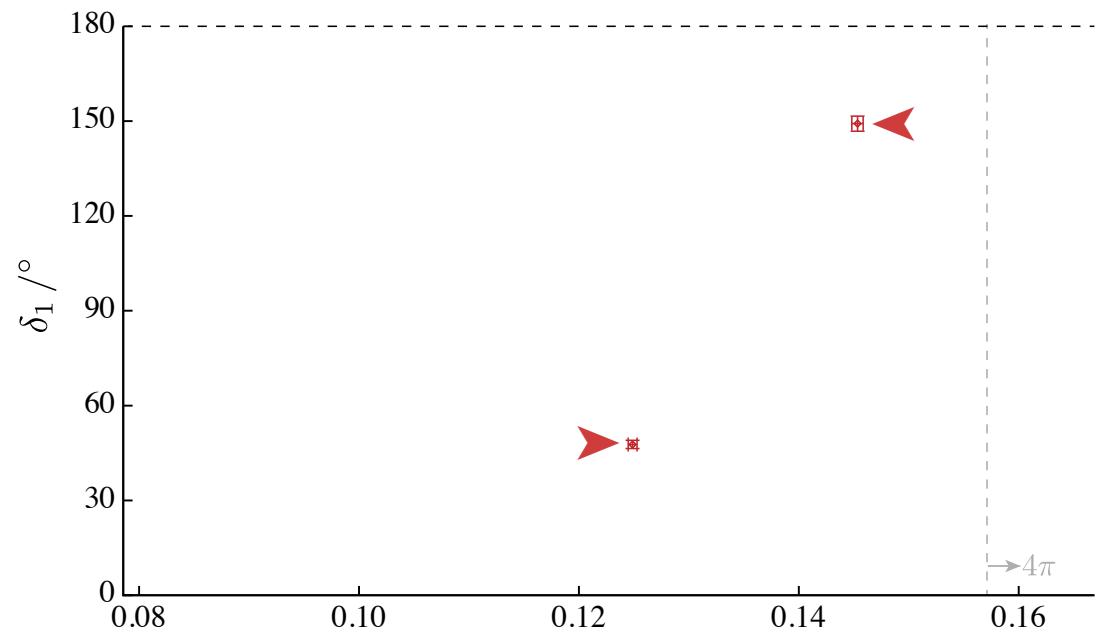


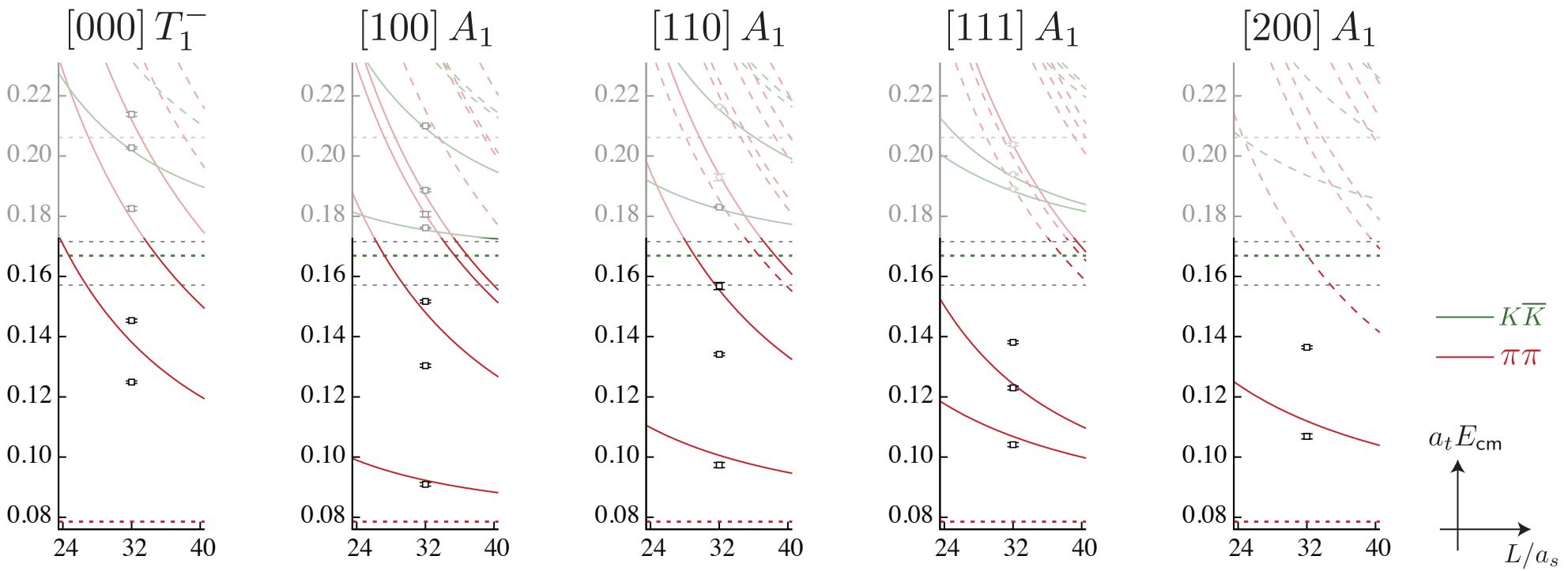
$m_\pi = 0.039$     $L \sim 3.8$  fm  
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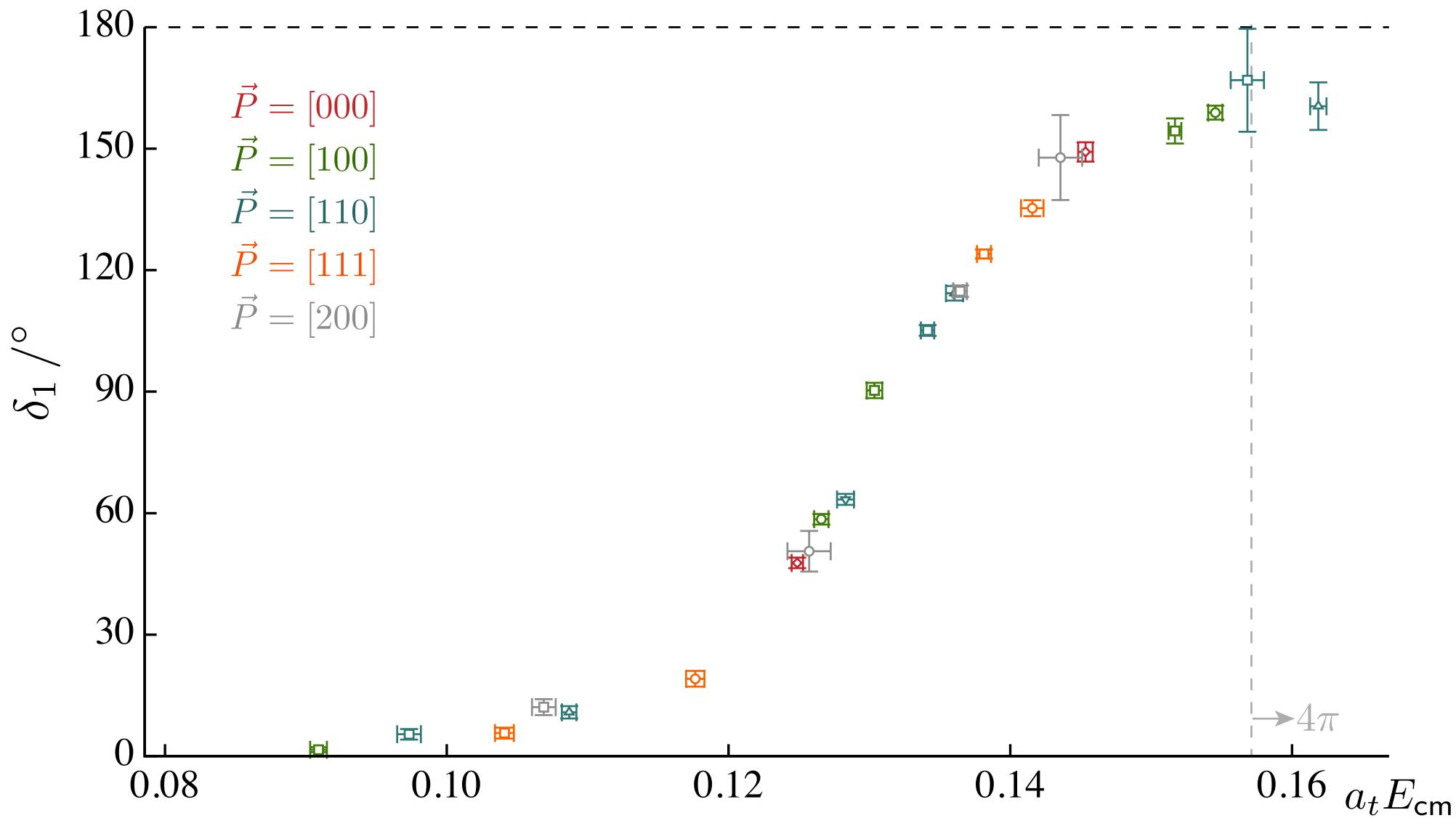
$$t(E) = \frac{1}{\rho(E)} e^{i\delta(E)} \sin \delta(E)$$

$m_\pi = 0.039$     $L \sim 3.8$  fm  
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$m_\pi = 0.039$     $L \sim 3.8$  fm  
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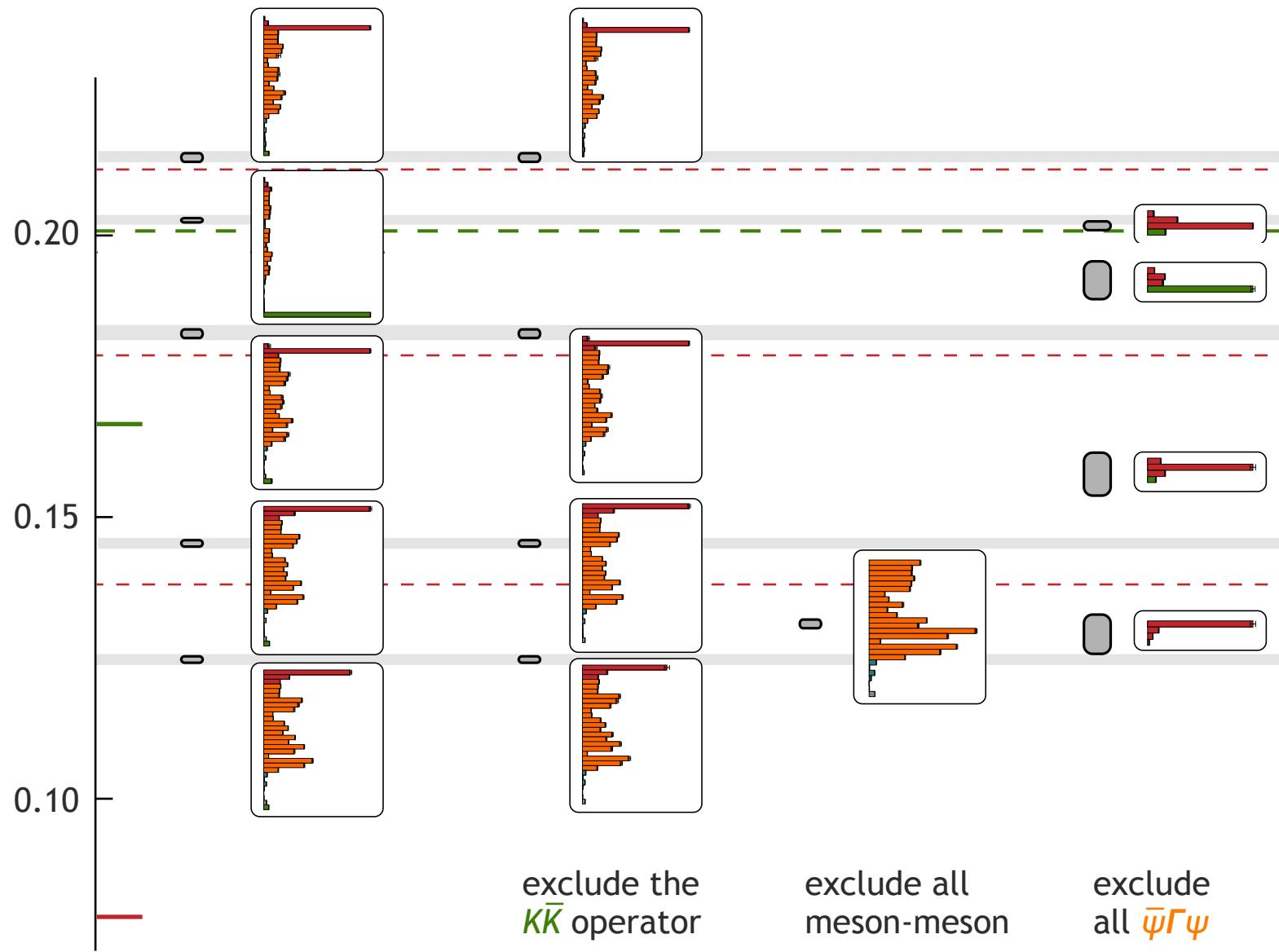
... looks like a classic resonance signal ...



# what happens if we vary the operator basis ?

PRD92 094502 (2015)

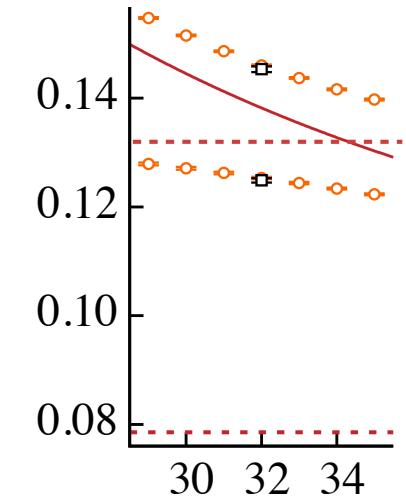
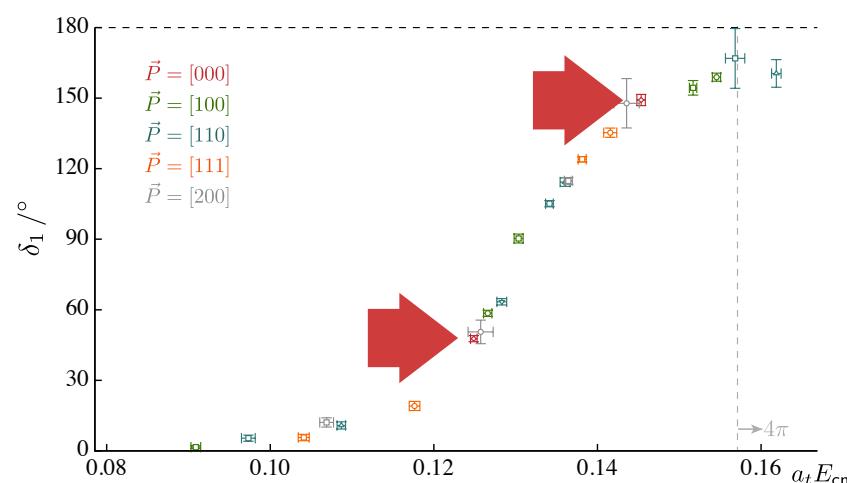
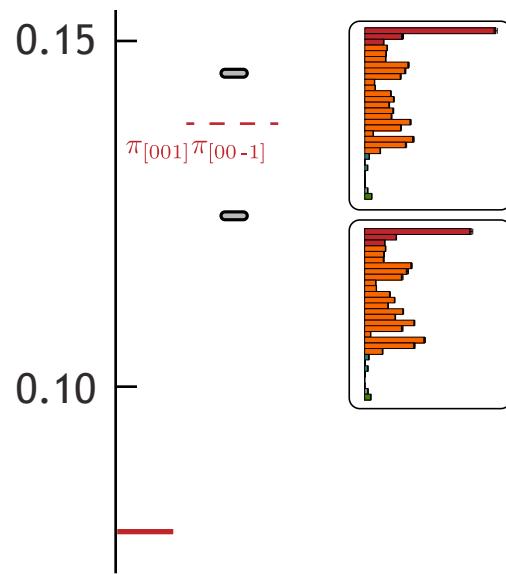
86



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

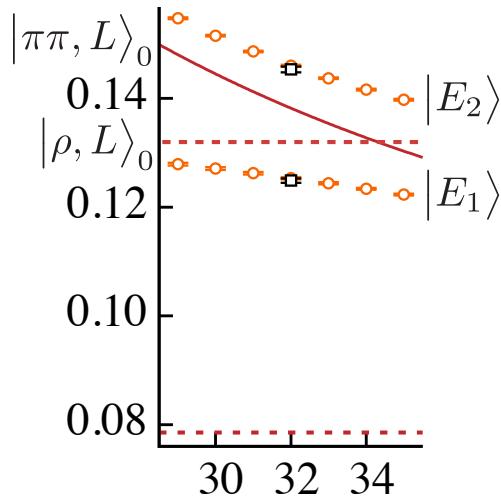
# what's happening here ?

focus on the lowest two states



an avoided level crossing

# what's happening here ?



think about this as a **two-state problem**

imagine we could turn off the coupling so  
a ‘bound-state’ and a ‘meson-meson’ state were eigenstates

$$|\rho, L\rangle_0$$

$$|\pi\pi, L\rangle_0$$

with the coupling turned on, the eigenstates are admixtures

$$|E_1\rangle = \cos \theta |\rho, L\rangle_0 + \sin \theta |\pi\pi, L\rangle_0$$

$$|E_2\rangle = -\sin \theta |\rho, L\rangle_0 + \cos \theta |\pi\pi, L\rangle_0$$

with operators that ‘look-like’  $|\rho, L\rangle_0$  and  $|\pi\pi, L\rangle_0$  in the basis, the variational method separates  $|E_1\rangle, |E_2\rangle$

$$\begin{pmatrix} C_{\rho,\rho}(t) & C_{\rho,\pi\pi}(t) \\ C_{\pi\pi,\rho}(t) & C_{\pi\pi,\pi\pi}(t) \end{pmatrix} = \begin{pmatrix} Z_\rho & 0 \\ 0 & Z_{\pi\pi} \end{pmatrix} \cdot \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \cdot \begin{pmatrix} e^{-E_1 t} & 0 \\ 0 & e^{-E_2 t} \end{pmatrix} \cdot \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \cdot \begin{pmatrix} Z_\rho & 0 \\ 0 & Z_{\pi\pi} \end{pmatrix}$$

$$\mathcal{O}_\rho |0\rangle = Z_\rho |\rho, L\rangle_0 + \epsilon |\pi\pi, L\rangle_0$$

$$\mathcal{O}_{\pi\pi} |0\rangle = Z_{\pi\pi} |\pi\pi, L\rangle_0 + \epsilon |\rho, L\rangle_0$$

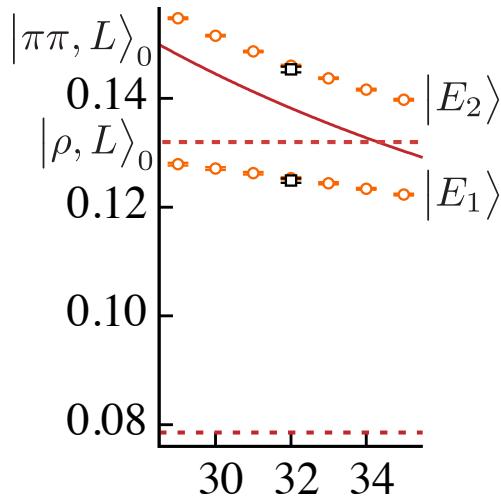
GEVP eigenvectors will find the rotation

and the principal correlators

$$\lambda_1(t) \sim e^{-E_1 t}$$

$$\lambda_2(t) \sim e^{-E_2 t}$$

# what's happening here ?



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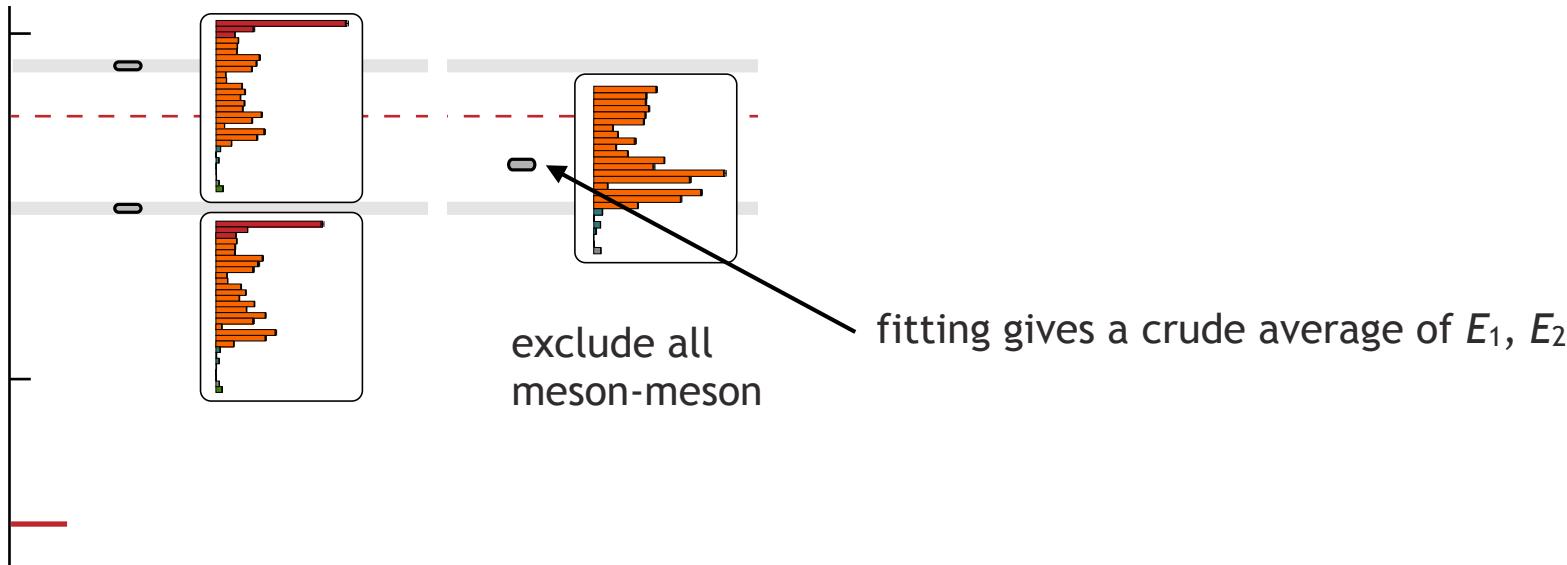
now suppose we used only the  $\mathcal{O}_\rho$  operators

then  $C(t) \propto \cos^2 \theta e^{-E_1 t} + \sin^2 \theta e^{-E_2 t}$  and there'll be two energies present ...

... and they're very hard to separate

# what's happening here ?

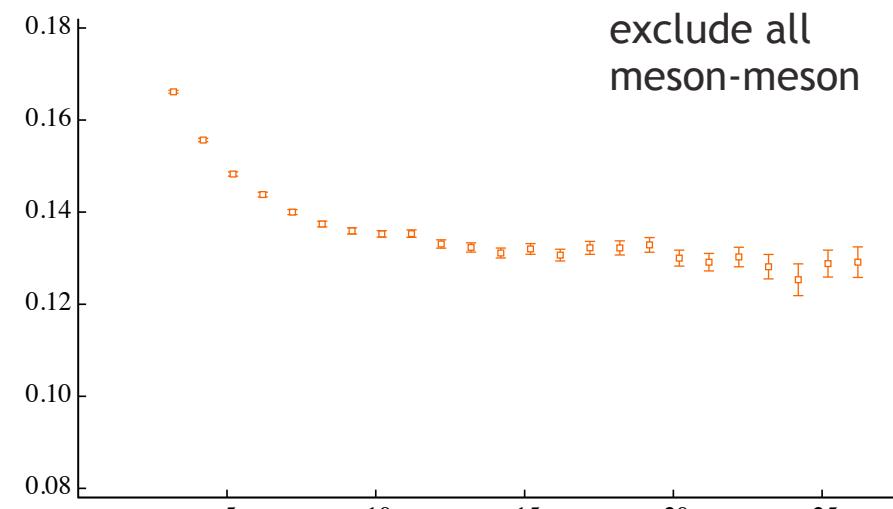
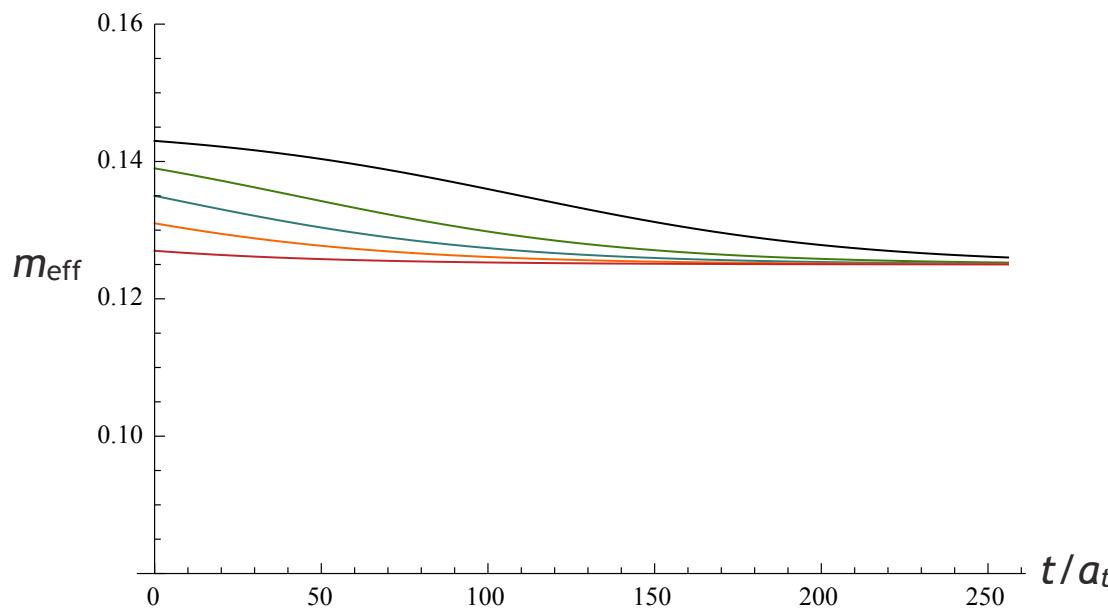
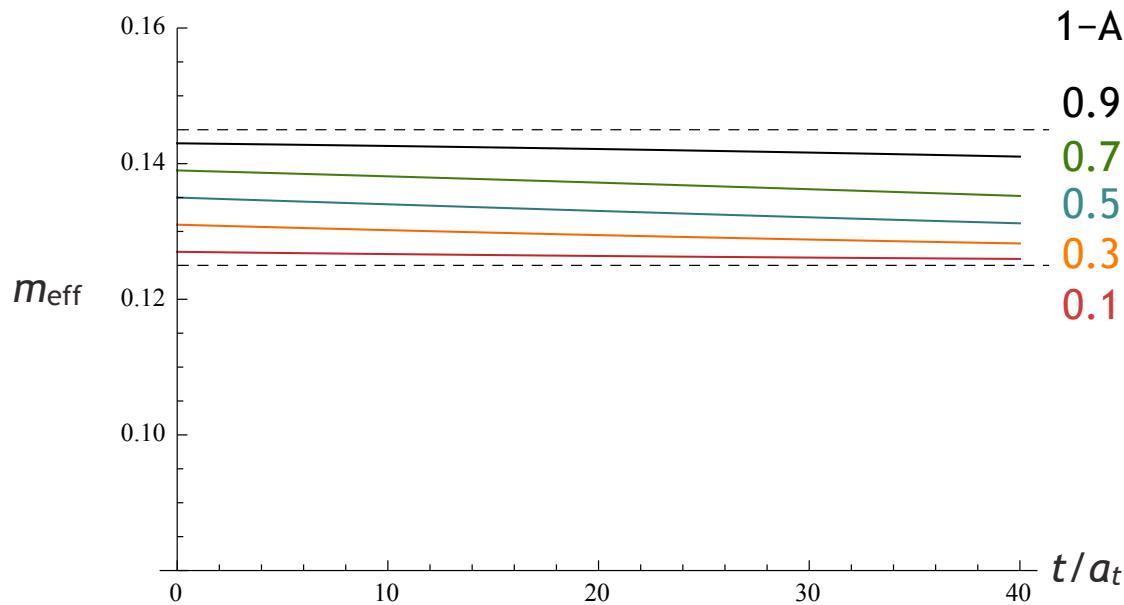
it looks like this is what's happening



# two-state admixture

$$C(t) = A e^{-0.125 t/a_t} + (1 - A) e^{-0.145 t/a_t}$$

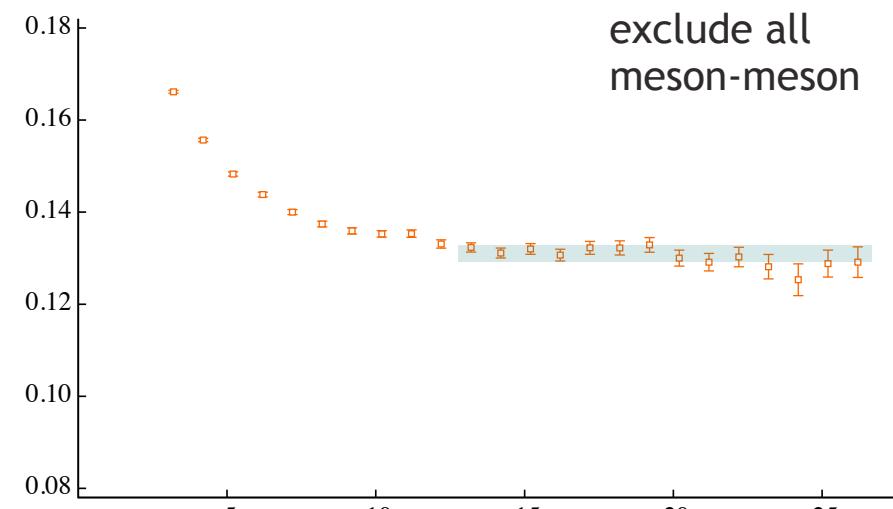
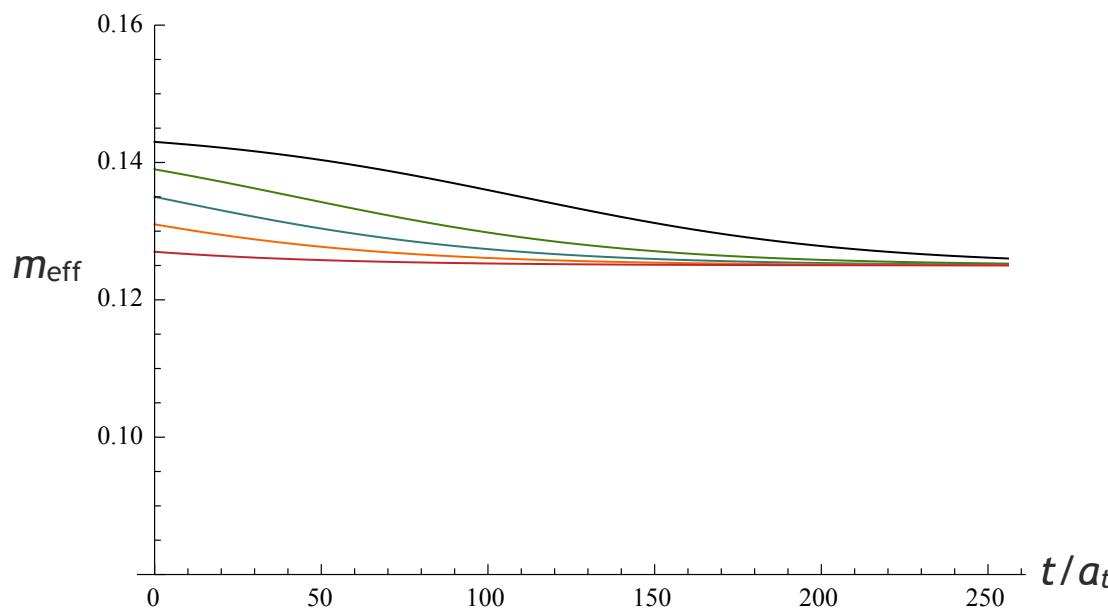
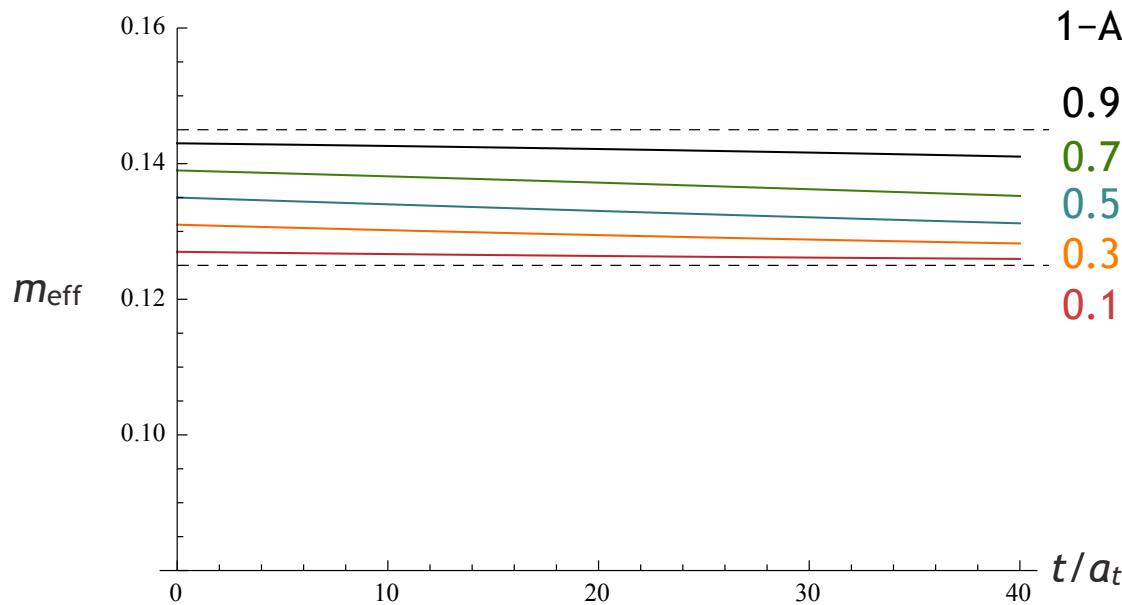
X



# two-state admixture

$$C(t) = A e^{-0.125 t/a_t} + (1 - A) e^{-0.145 t/a_t}$$

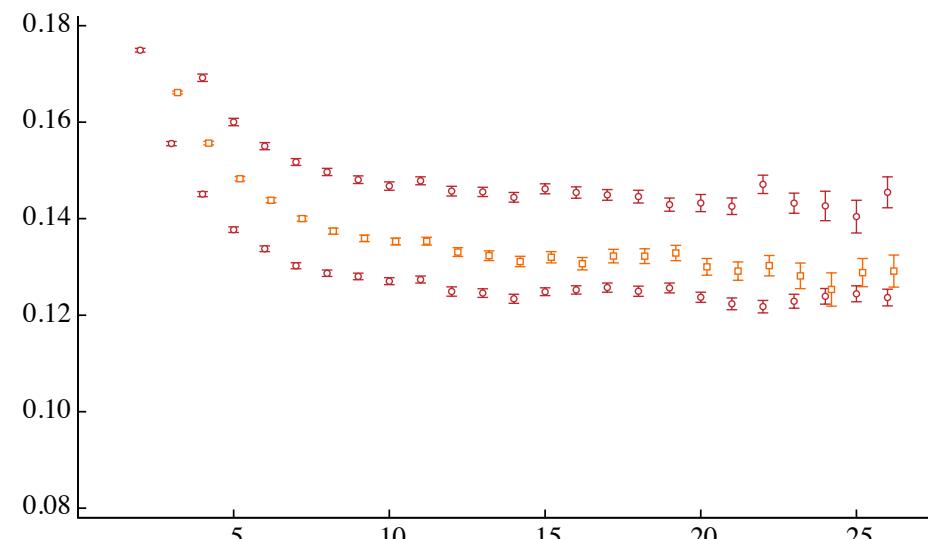
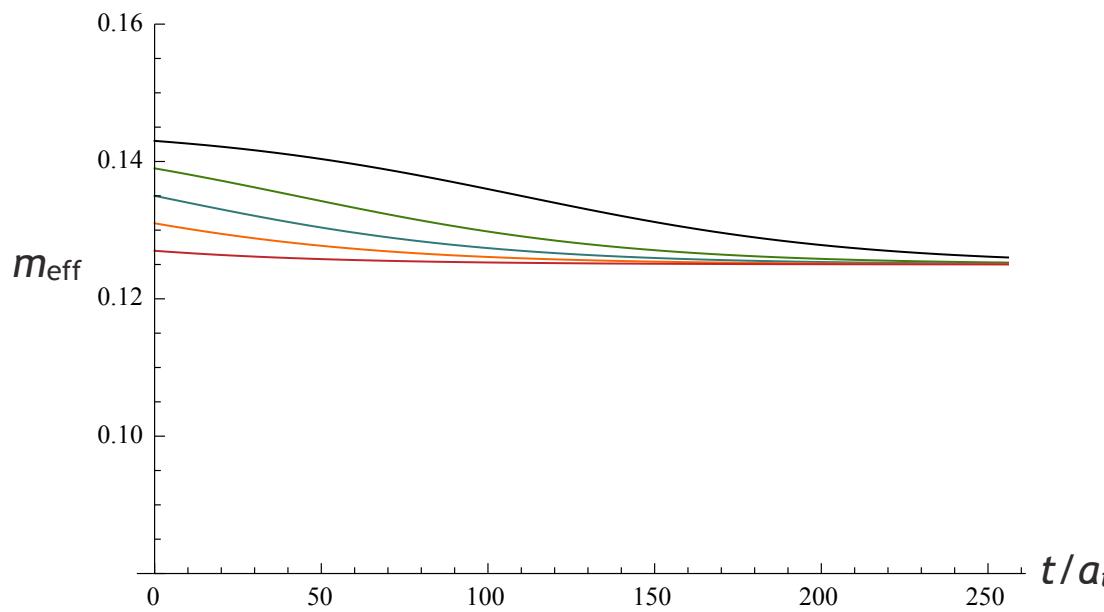
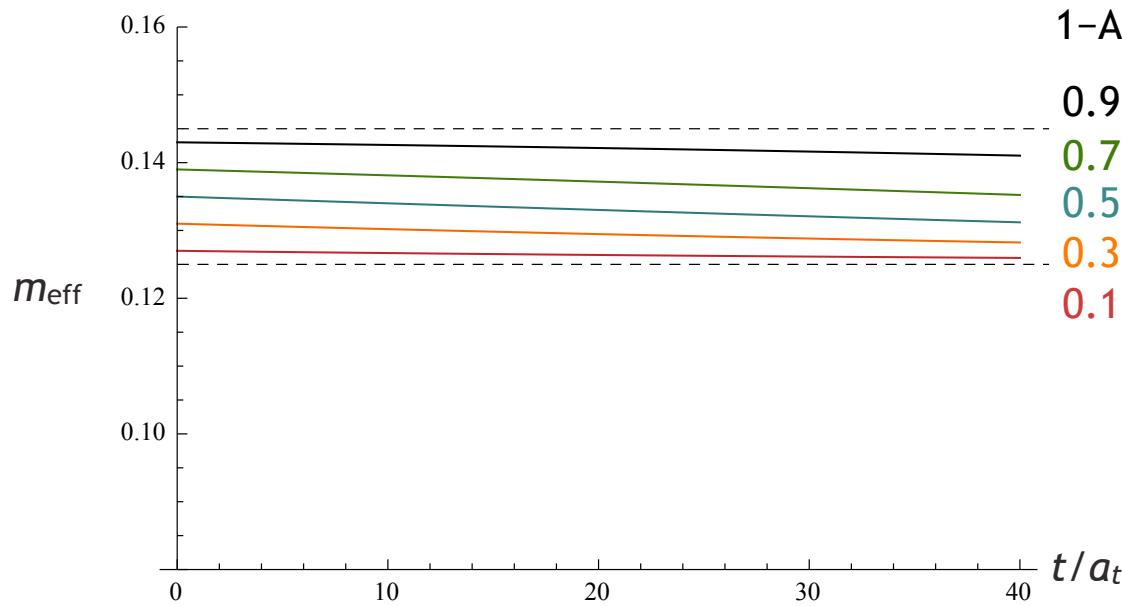
X



# two-state admixture

$$C(t) = A e^{-0.125 t/a_t} + (1 - A) e^{-0.145 t/a_t}$$

X



volume dependence !

‘meson-meson’-like  $\sum_x e^{i\mathbf{P} \cdot \mathbf{x}} \bar{\psi}_x \Gamma \psi_x \sum_y e^{i\mathbf{q} \cdot \mathbf{y}} \bar{\psi}_y \Gamma' \psi_y$  samples the whole volume of the lattice

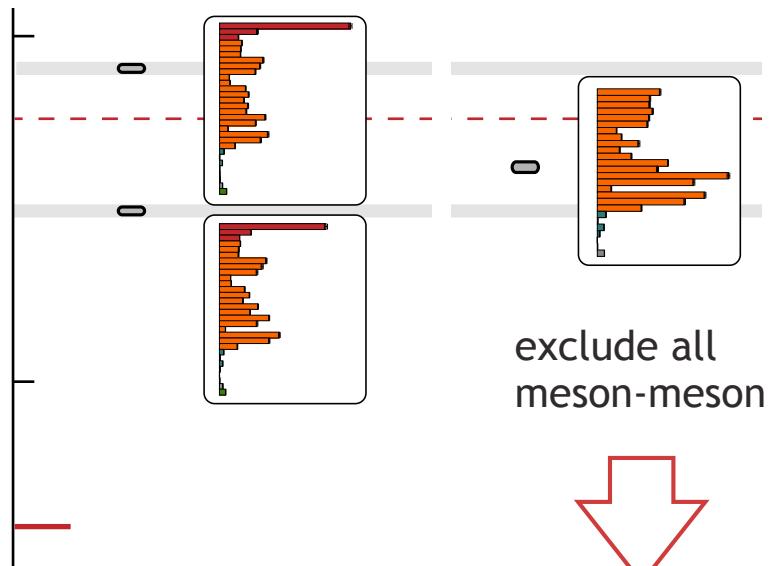
‘single-meson’-like  $\sum_x e^{i\mathbf{P} \cdot \mathbf{x}} \bar{\psi}_x \Gamma \psi_x$  samples a single point (translated)

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

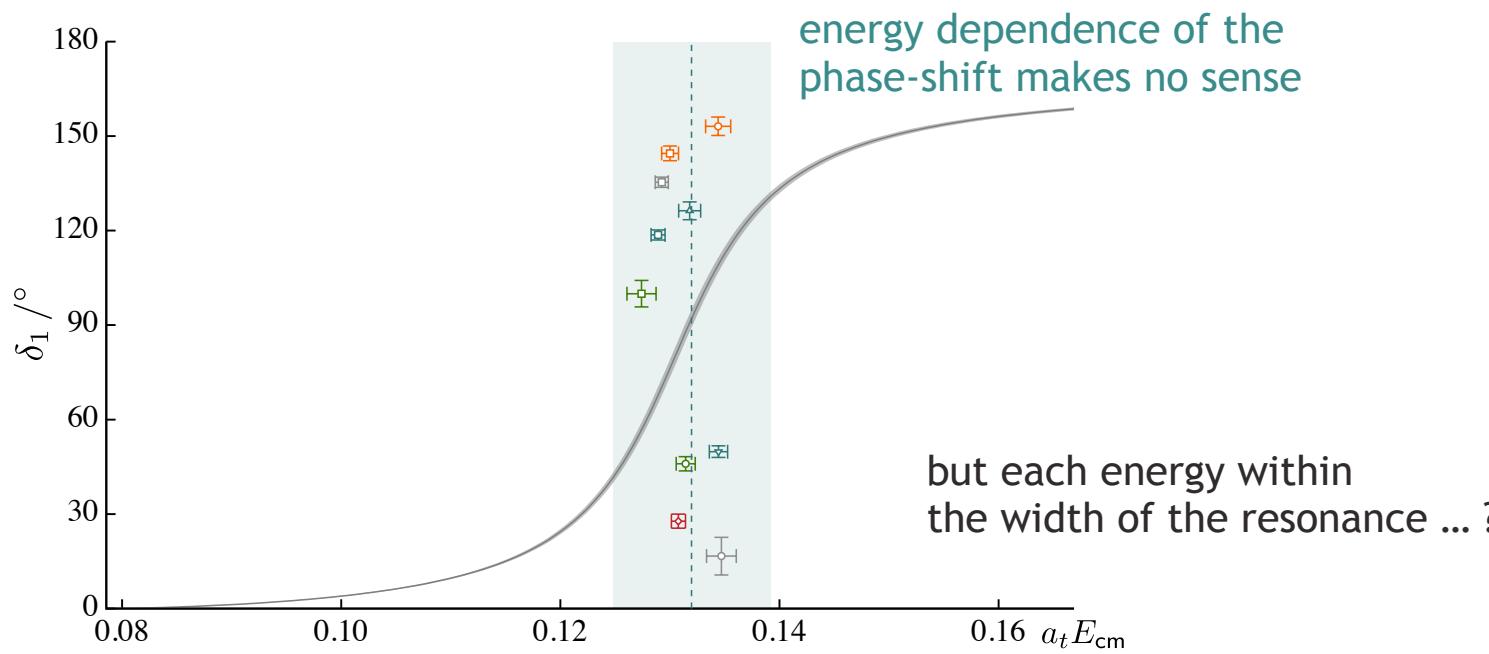
interesting side note:

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

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

‘lattice’ Clebsch-Gordan coefficients

some group theory to work them out

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

