

Developments in 2-baryon LQCD calculations

Evan Berkowitz

Institut für Kernphysik

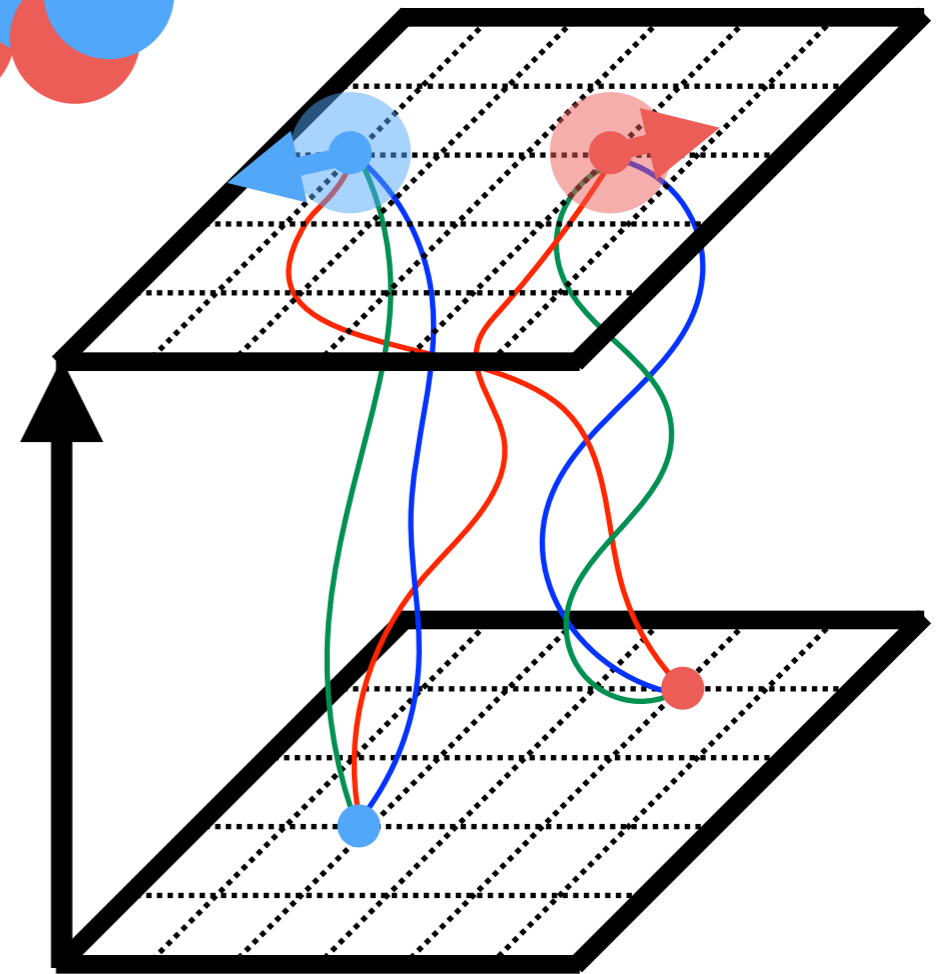
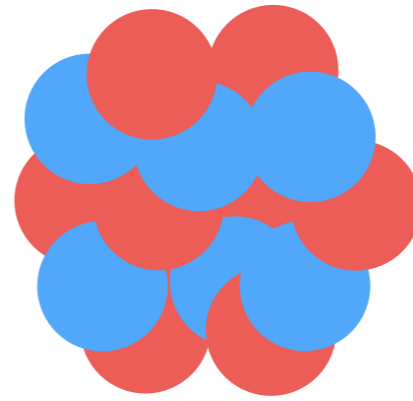
Institute for Advanced Simulation

Forschungszentrum Jülich

08 July 2017

0vββ / INT-17-67w

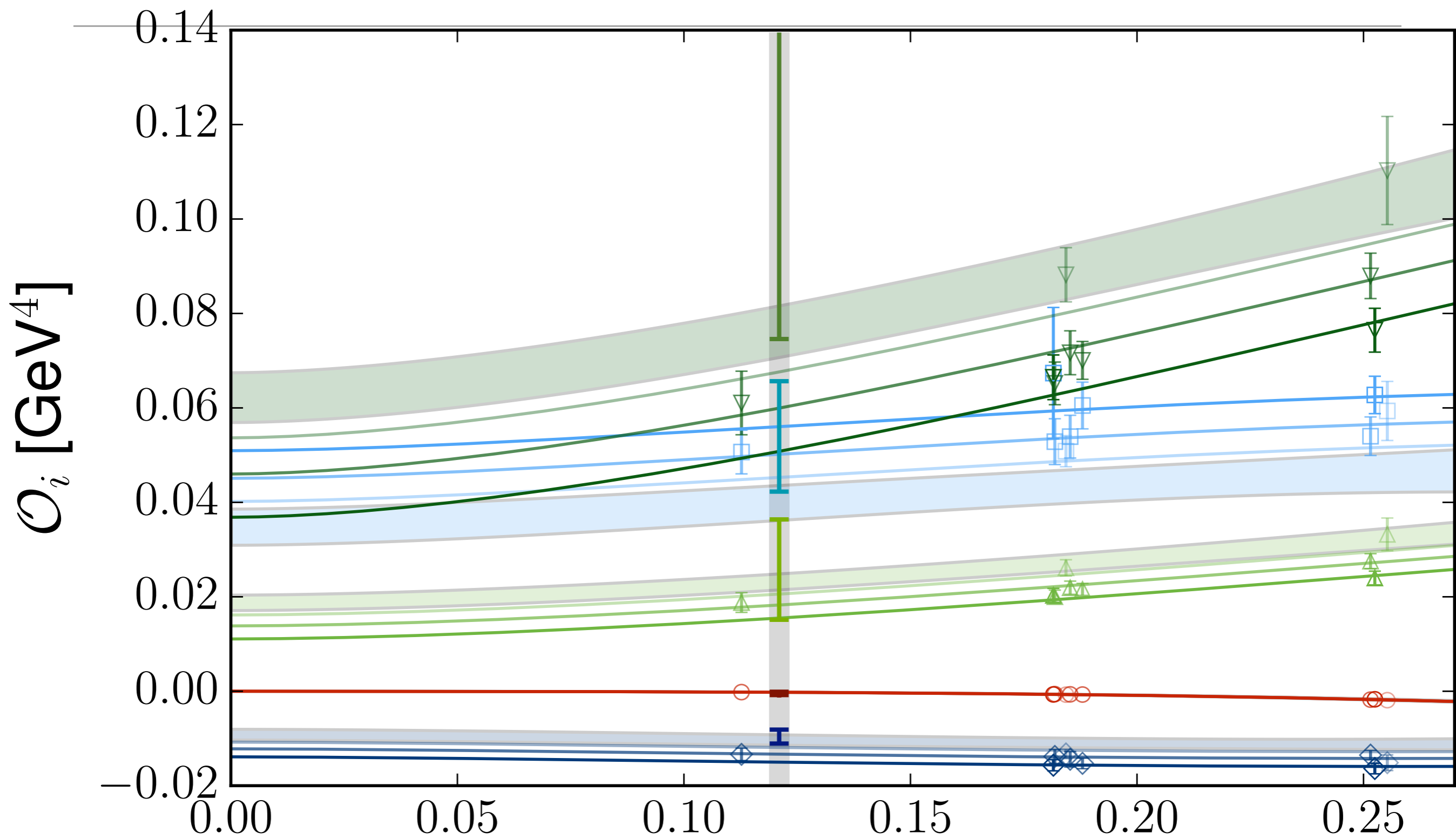
Seattle, Washington



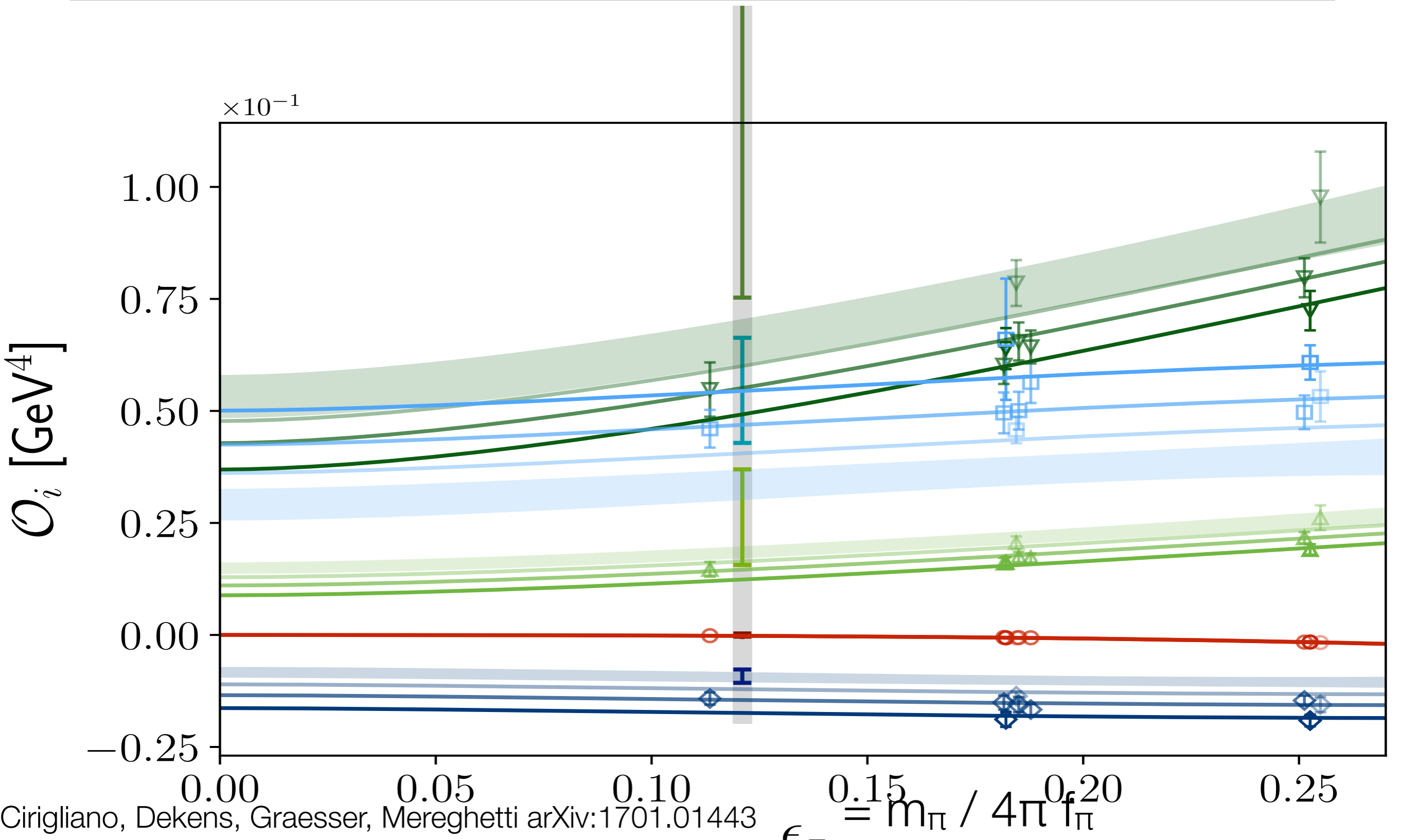
CS

CS

Preliminary Short-distance $0\nu\beta\beta$ w/o Renormalization

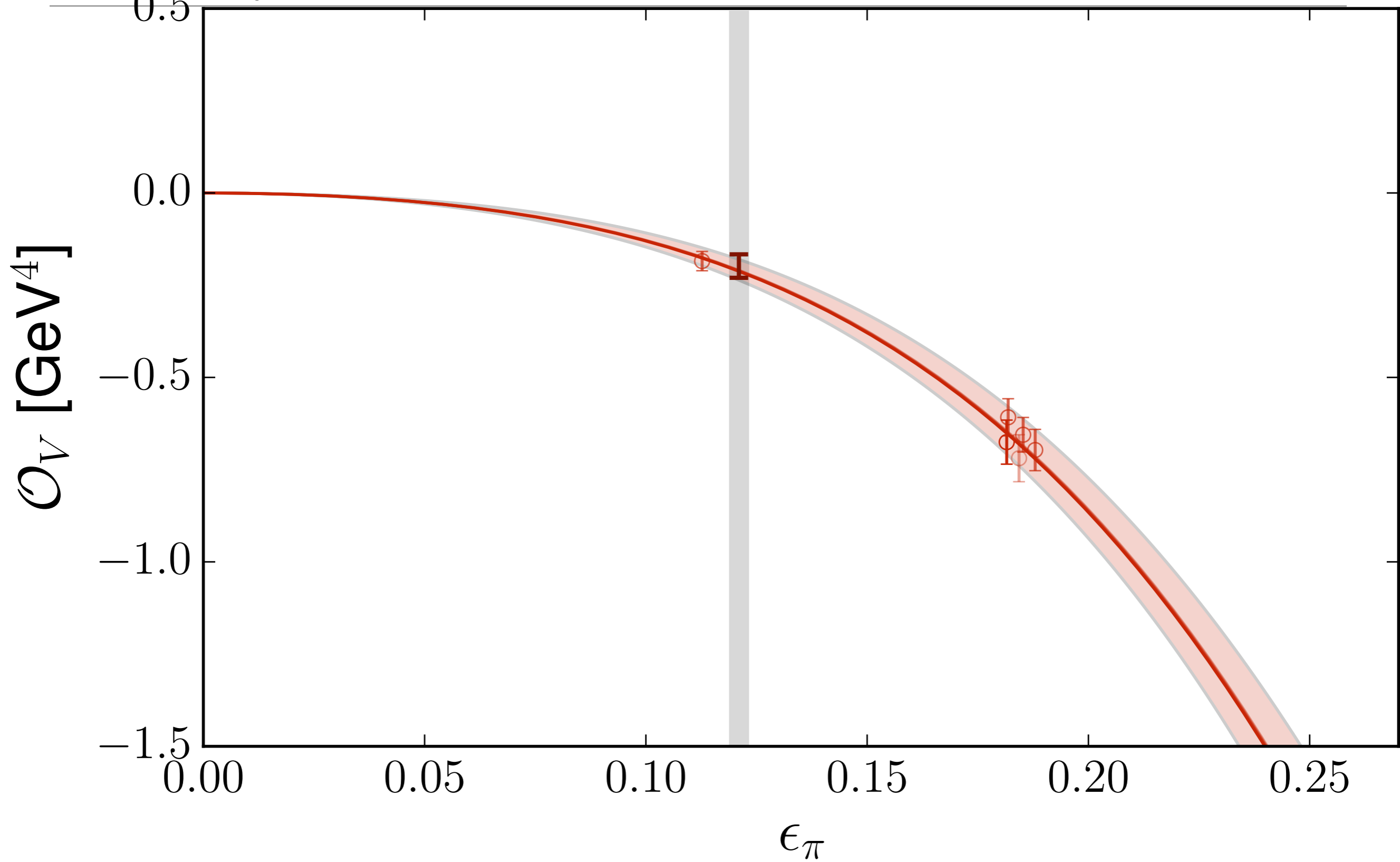


Preliminary Short-distance $0\nu\beta\beta$ w Renormalization

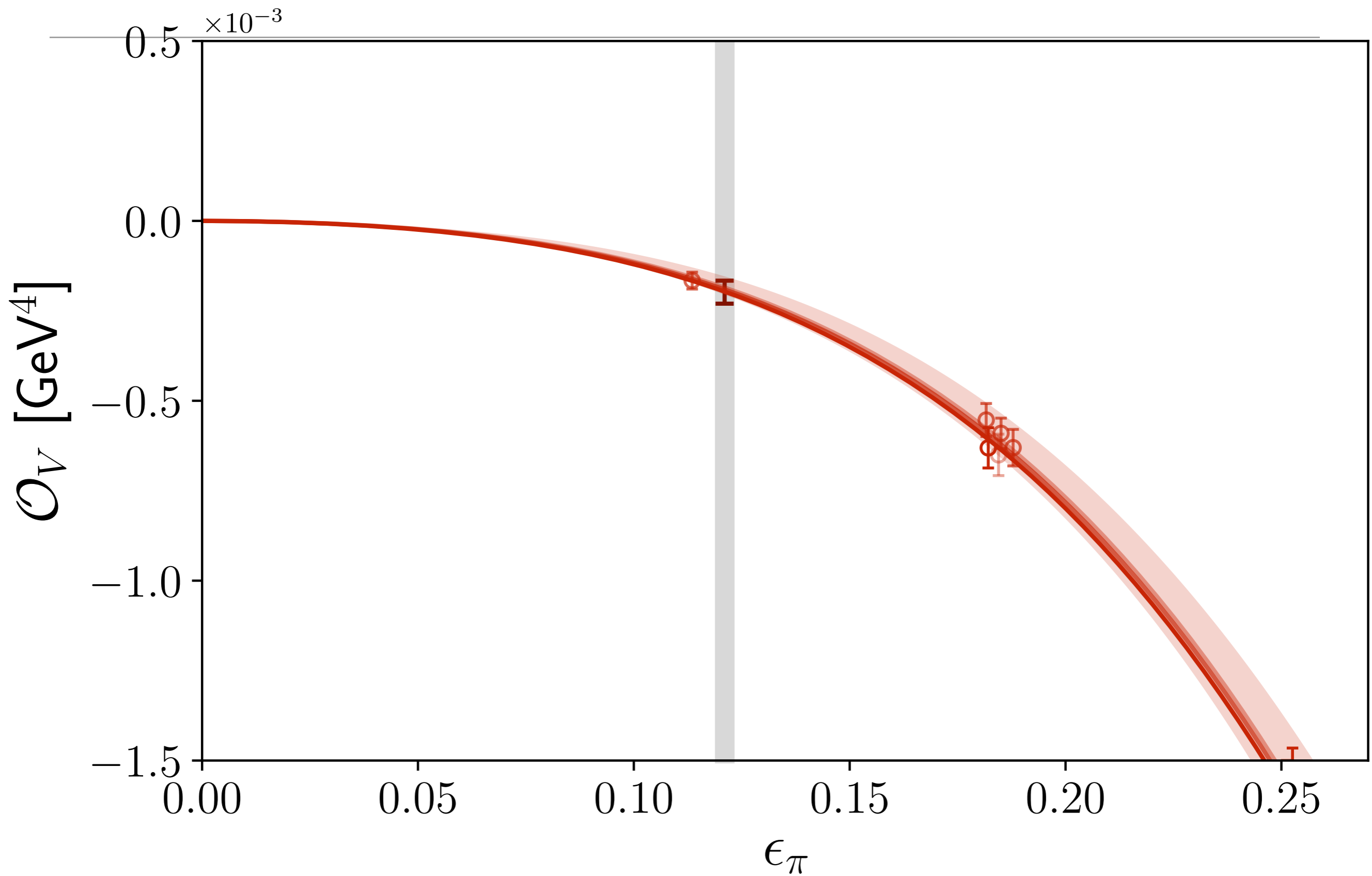


Before

0.5×10^{-3}



After



Outline

- Cubic Irreps / Considerations for cubic volume
 - Sinks and Sources: computational reuse
- Single nucleon improvement in NN calculations

New Methods



Generally Applicable



Improved Systematics



Computationally Affordable

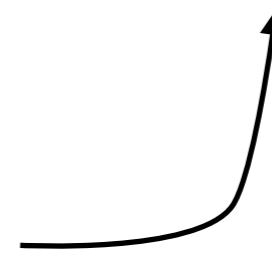
Lüscher Formalism

$$\det \left[(\mathcal{M}^\infty)^{-1} + \delta\mathcal{G}^V \right] = 0$$

Infinite volume
scattering amplitudes

finite volume spectrum
+ boundary conditions

Lattice calculation



Subduction

HadSpec 1004.4930

Isospin 0

Isospin 1

Partial wave	Irreps	Partial wave	Irreps
1P_1	T_1^-	1S_0	A_1^+
$^3S_1, ^3D_1$	T_1^+	3P_0	A_1^-
3D_2	$E^+ \oplus T_2^+$	3P_1	T_1^-
3D_3	$A_2^+ \oplus T_1^+ \oplus T_2^+$	$^3P_2, ^3F_2$	$E^- \oplus T_2^-$
1F_3	$A_2^- \oplus T_1^- \oplus T_2^-$	1D_2	$E^+ \oplus T_2^+$
		3F_3	$A_2^- \oplus T_1^- \oplus T_2^-$
		3F_4	$A_1^- \oplus E^- \oplus T_1^- \oplus T_2^-$

unphysical mixing

Some states only couple to particular sources.

Two-Nucleon Spectrum

- Spectrum given by effective mass of (schematic) NN correlator:

$$\left\langle \Omega \left| \mathcal{O}_{\Lambda' \mu', I m_I}^{[J' \ell' S']} (t) \mathcal{O}_{\Lambda \mu, I m_I}^{[J \ell S]} (0) \right| \Omega \right\rangle$$

$\delta \mathcal{G}^V$



- Sink

$$\mathcal{O}_{J m_J I m_I; S \ell} (t, |\mathbf{k}|) = \sum \text{Clebsch-Gordans} \sum_{R \in \mathcal{O}_h} Y_{\ell m_\ell} (\widehat{R\mathbf{k}}) N_{m_{s_1}}^{m_{I_1}} (t, R\mathbf{k}) N_{m_{s_2}}^{m_{I_2}} (t, -R\mathbf{k})$$

- Source

$$\mathcal{O}_{J m_J I m_I; S \ell} (t, \mathbf{x}, \Delta \mathbf{x}) = \sum \text{Clebsch-Gordans} \sum_{R \in \mathcal{O}_h} Y_{\ell m_\ell} (\widehat{R\Delta \mathbf{x}}) N_{m_{s_1}}^{m_{I_1}} (t, \mathbf{x}) N_{m_{s_2}}^{m_{I_2}} (t, \mathbf{x} + R\Delta \mathbf{x})$$

- Box breaks rotational symmetry \rightarrow spectrum falls into irreps of \mathcal{O}_h , not $\text{SO}(3)$.

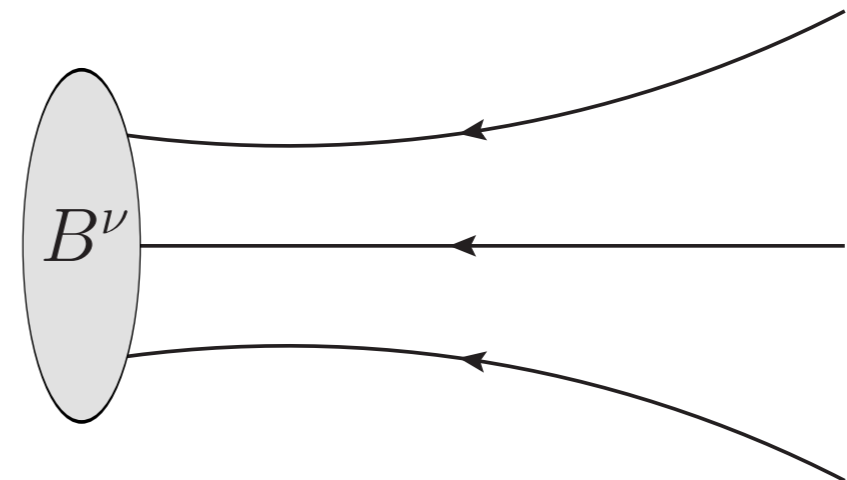
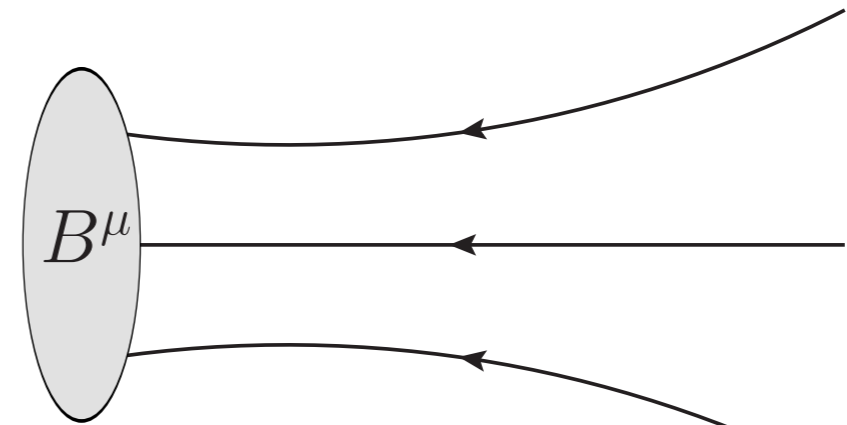
- Subduction

$$\mathcal{O}_{\Lambda \mu, I m_I}^{[J \ell S]} (t, |\mathbf{k}|) = \sum_{m_J} [\text{CG}_\Lambda^J]_{\mu, m_J} \mathcal{O}_{J m_J I m_I; S \ell} (t, |\mathbf{k}|)$$

HPC

Doi & Endres 1205.0585, Detmold & Orginos 1207.1452

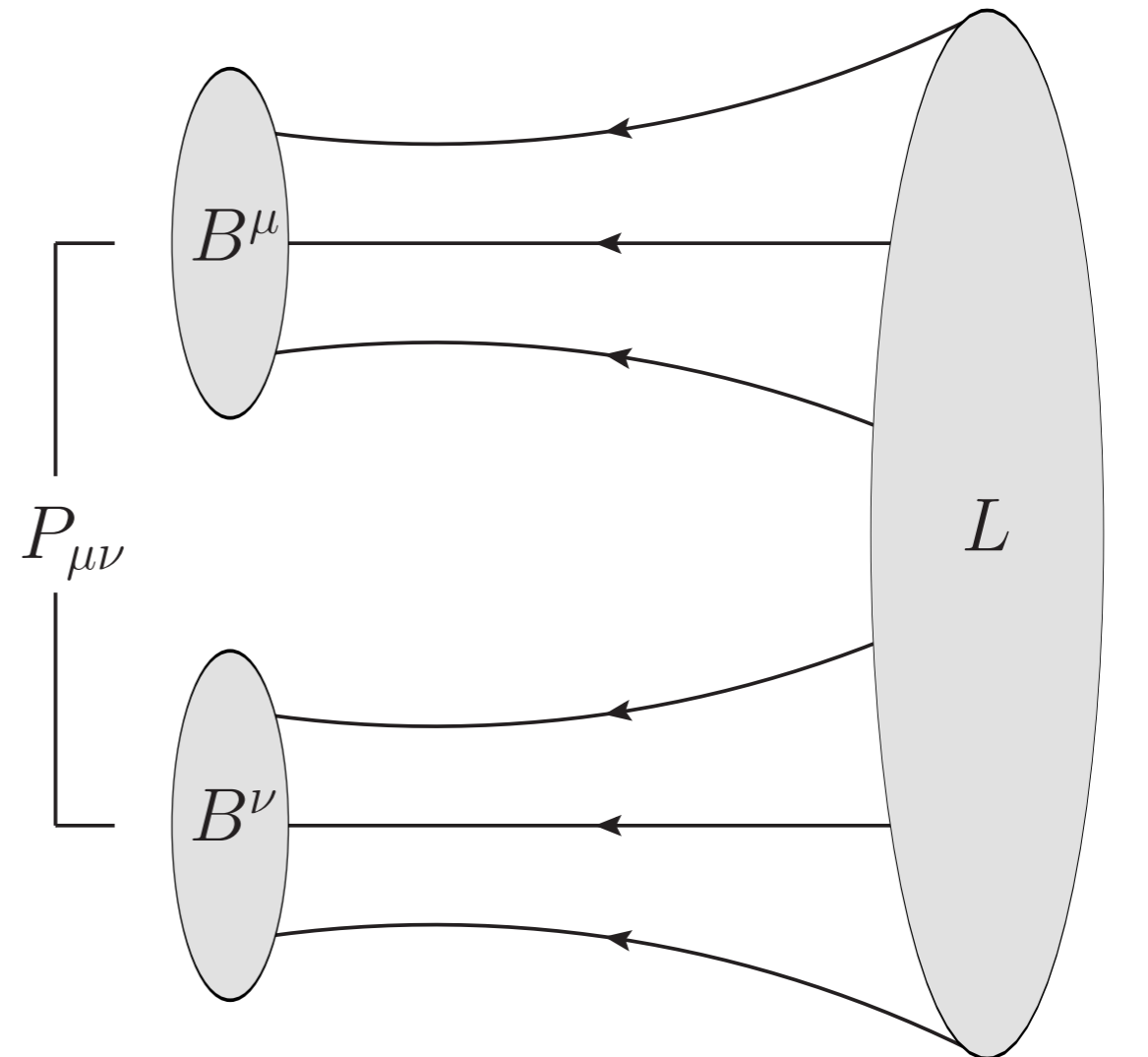
- Use baryon blocks
- Use sparse tensor contraction to take advantage of sparsity of L
- For each **source displacement $R\Delta x$** , store (sink-side) **full-volume** correlator for each $S'm's S_m s l_m l$



HPC

Doi & Endres 1205.0585, Detmold & Orginos 1207.1452

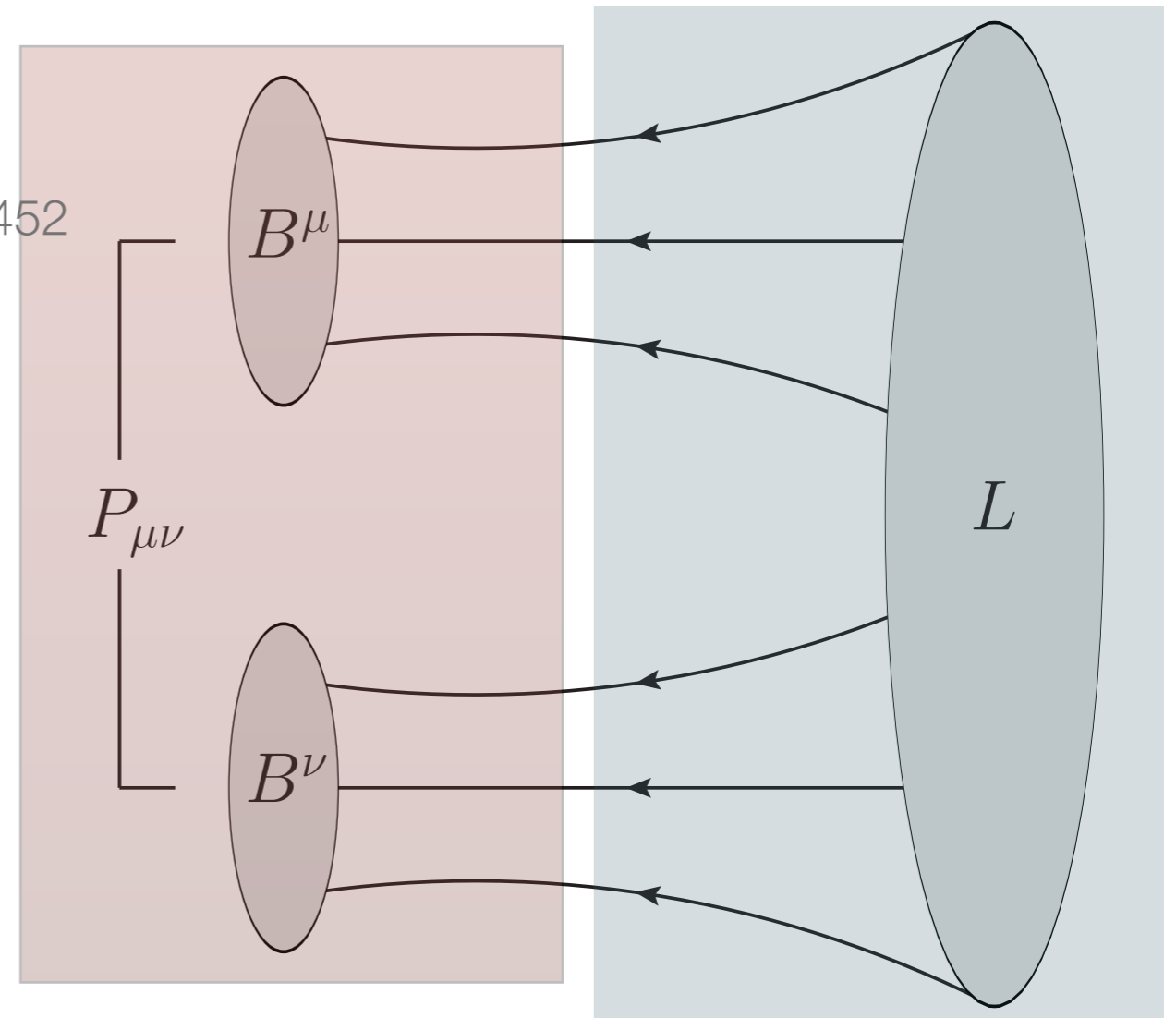
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HPC

Doi & Endres 1205.0585, Detmold & Orginos 1207.1452

- Use baryon blocks
- Use sparse tensor contraction to take advantage of sparsity of L
- For each **source displacement $R\Delta x$** , store (sink-side) **full-volume** correlator for each $S'm's Sm_s Im_I$



momentum space
full volume

position space
single displacements

all ← point x
all ← point x+RΔx

$$C_{Im_I}^{S'm'_s Sm_s}(\mathbf{k}', t' - t, R\Delta \mathbf{x}) =$$

$$\sum_{\mathbf{x}} \langle \Omega | \left(N_{i'}^{\mu'}(t', \mathbf{k}') P_{\mu'\nu'}^{S'm'_s} T_{Im_I}^{i'j'} N_{j'}^{\nu'}(t', -\mathbf{k}') \right) \left(\bar{N}_i^\mu(t, \mathbf{x}) P_{\mu\nu}^{Sm_s} T_{Im_I}^{ij} \bar{N}_j^\nu(t, \mathbf{x} + R\Delta \mathbf{x}) \right) | \Omega \rangle$$

Sample with
Sobol sequence

Projectors

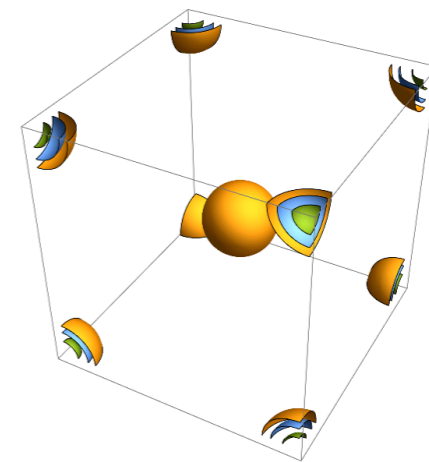
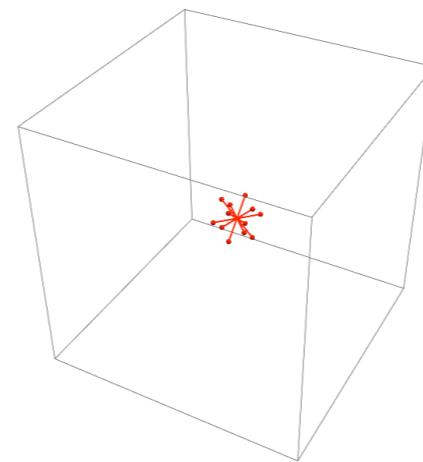
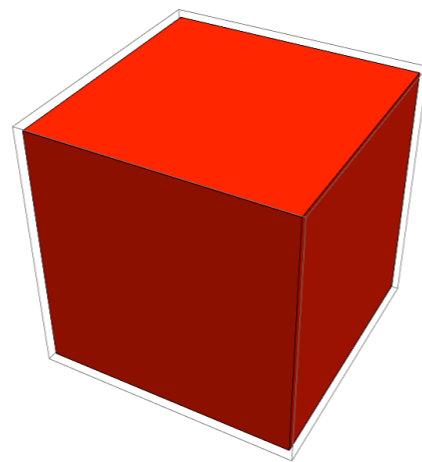
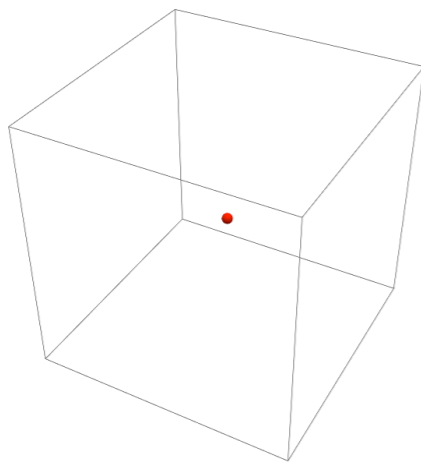
Sinks

Luu & Savage 1101.3347

- Project to eigenstates of a noninteracting theory in a box.
- Full volume information \rightarrow exactly project to any desired irrep

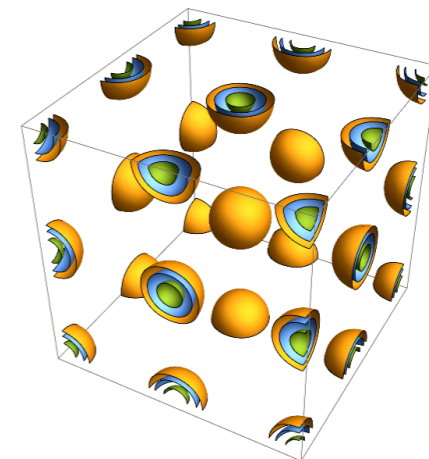
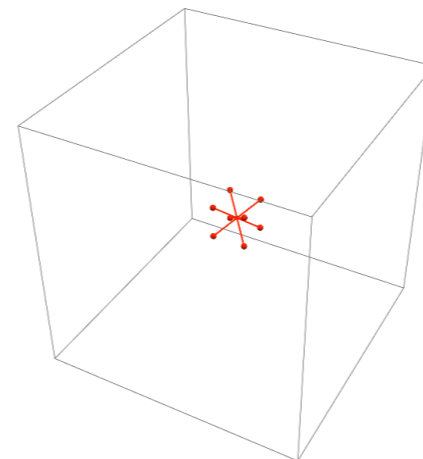
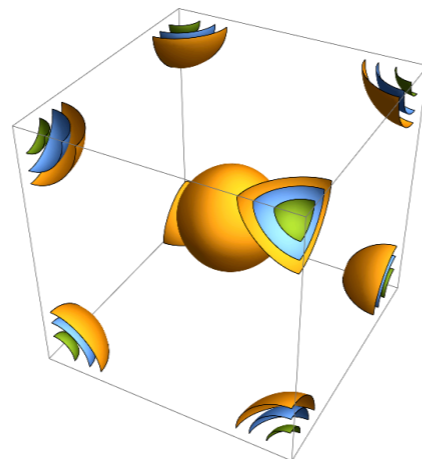
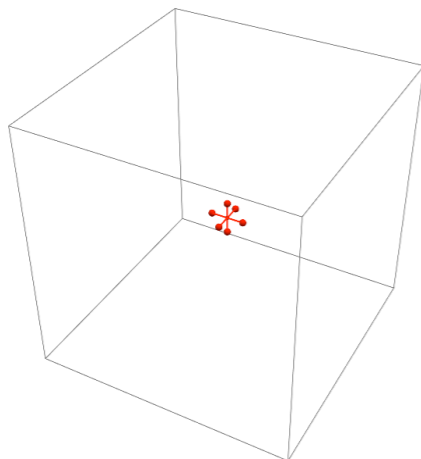
A_1^+

$n^2=0$



$n^2=2$

$n^2=1$



$n^2=3$

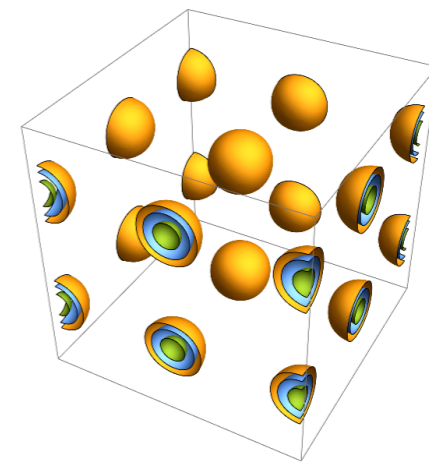
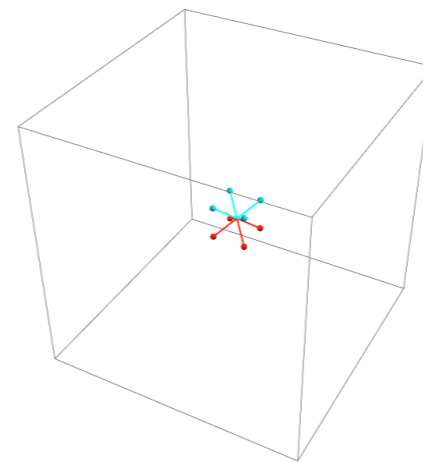
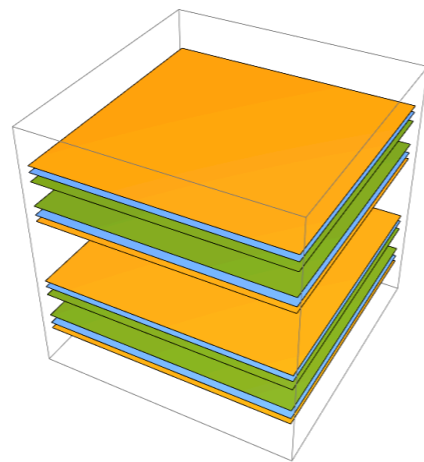
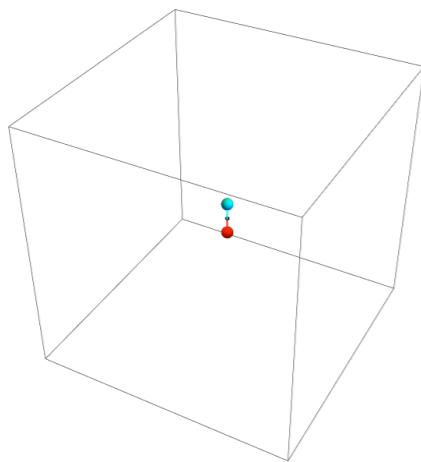
Sinks

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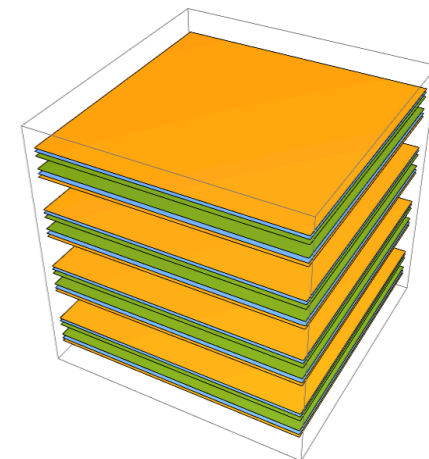
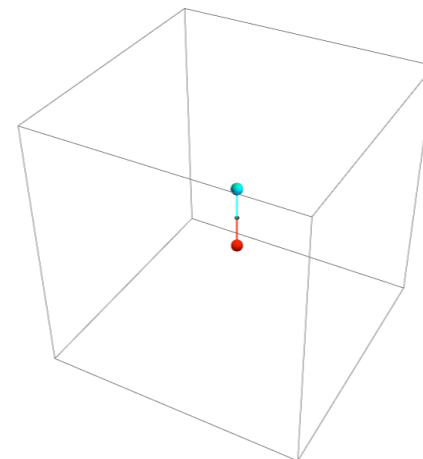
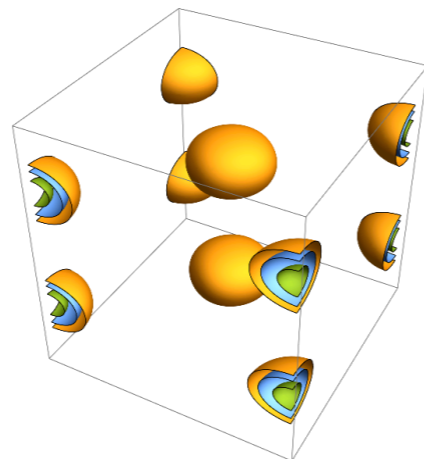
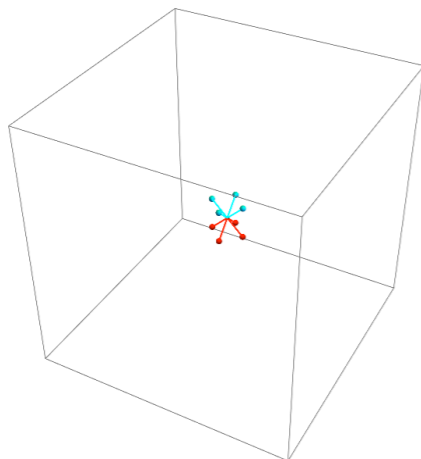
T_1^-

$n^2=1$



$n^2=3$

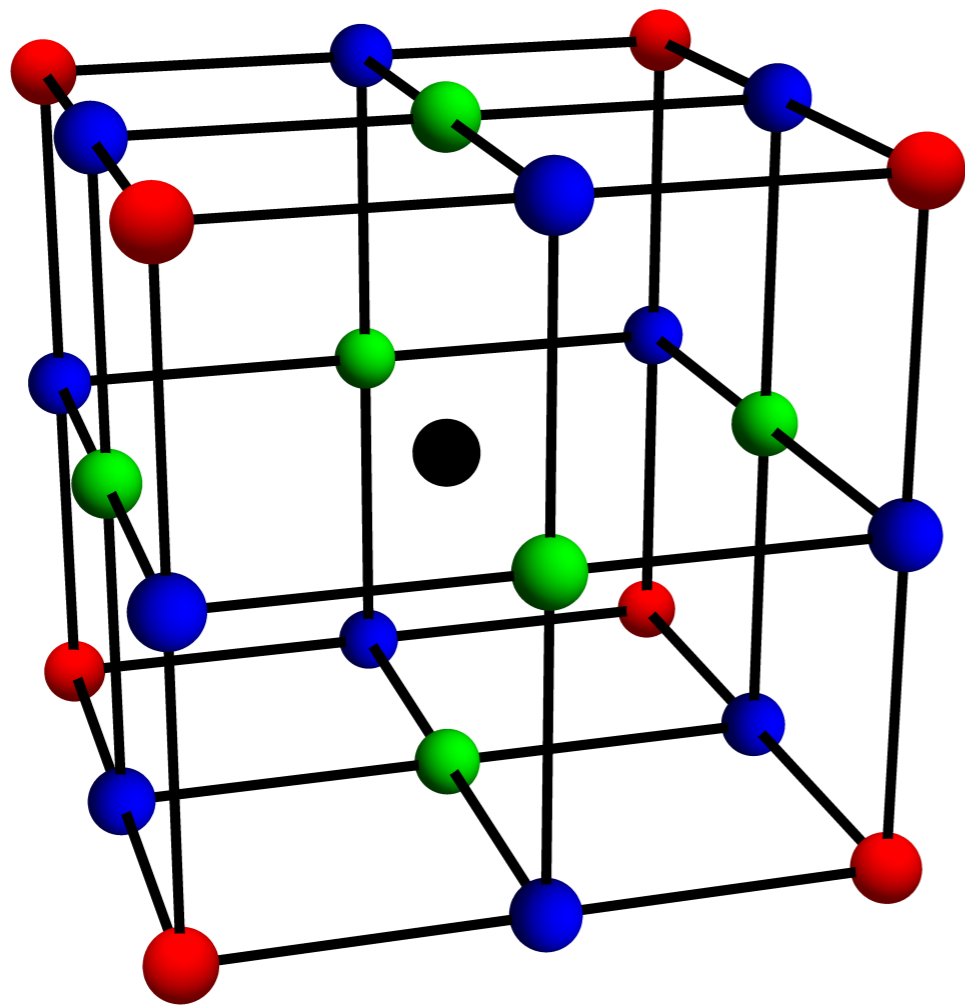
$n^2=2$



$n^2=4$

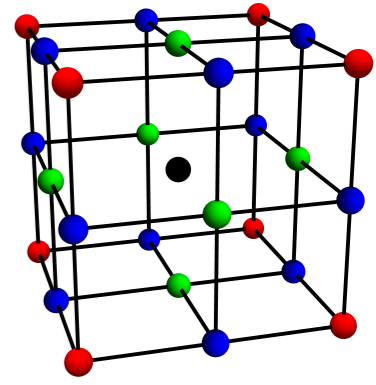
Sources

- Exact projection source-side requires spatial-volume-to-all propagators.
- Pick displacements

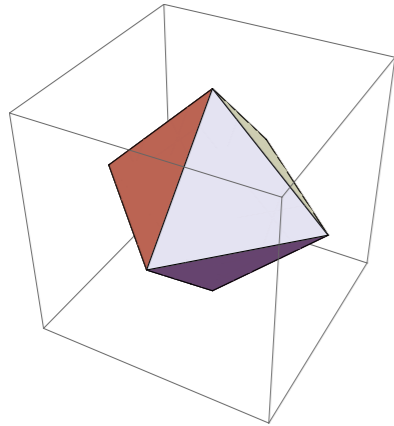


description	$\Delta x \propto$	count
local	(0,0,0)	1
face	(0,0,1)	6
edge	(0,1,1)	12
corner	(1,1,1)	8

Sources

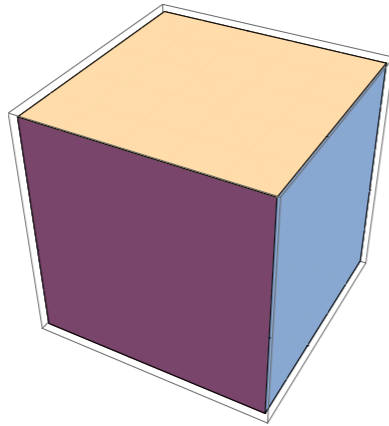


Octahedron
Vertices: 6



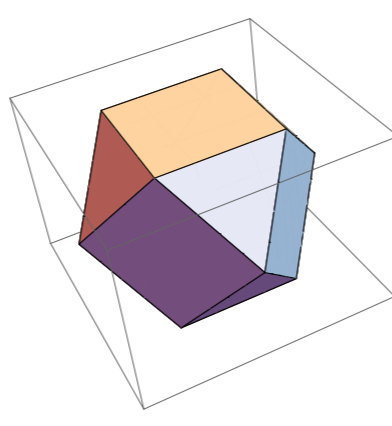
(0,0,1)

Cube
Vertices: 8



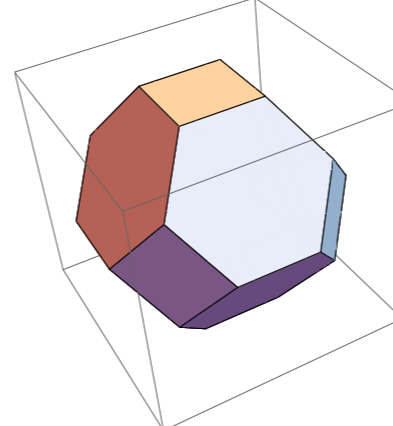
(1,1,1)

Cuboctahedron
Vertices: 12



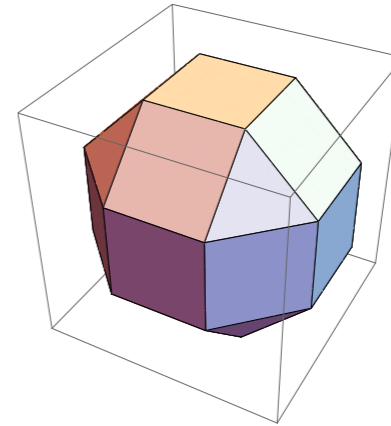
(0,1,1)

TruncatedOctahedron
Vertices: 24



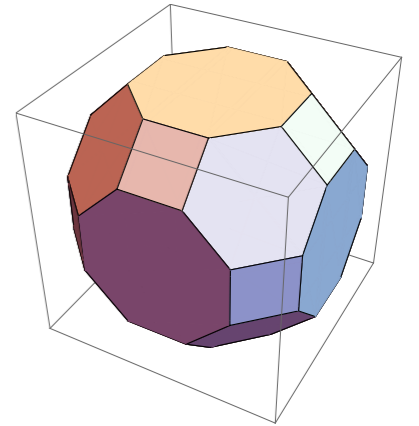
(0,1,2)

SmallRhombicuboctahedron
Vertices: 24



(1,1,2)

GreatRhombicuboctahedron
Vertices: 48



(1,2,3)

Solids generated by $O_h \leftrightarrow$ Irreps of O_h

face

octahedron

6

edge

cuboctahedron

12

corner

cube

8

knight's move

truncated octahedron

24

more complicated

small rhombicuboctahedron

24

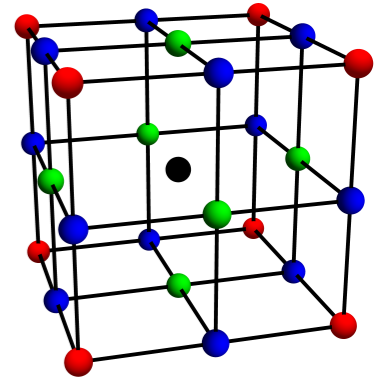
more complicated

great rhombicuboctahedron

48

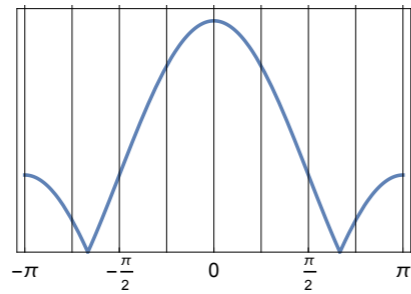
Too expensive.

Source Overlap

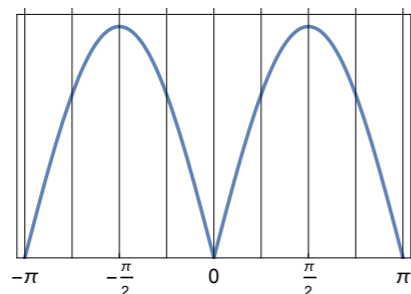


Project Luu & Savage momentum sources to **faces** as a function of $\pi\Delta x/L$

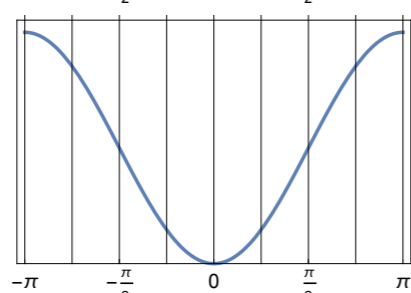
S



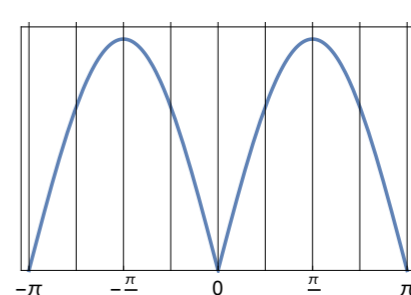
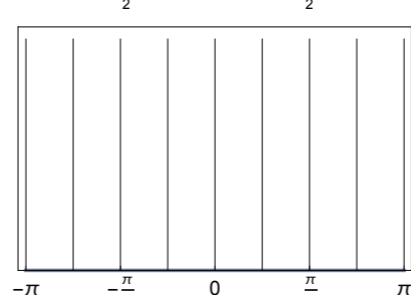
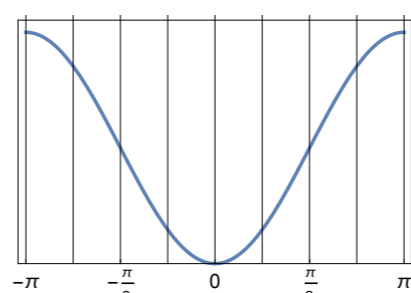
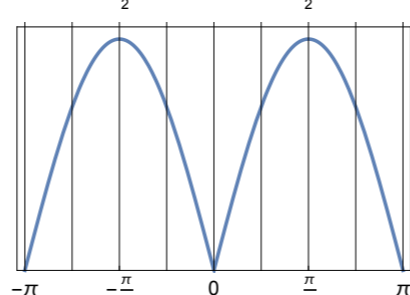
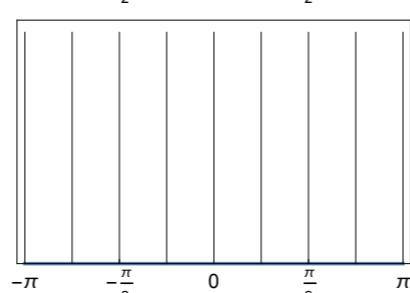
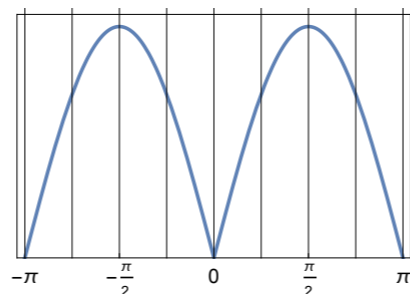
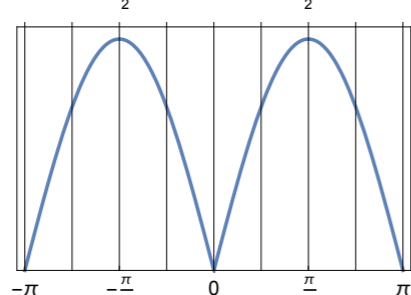
P



D



F



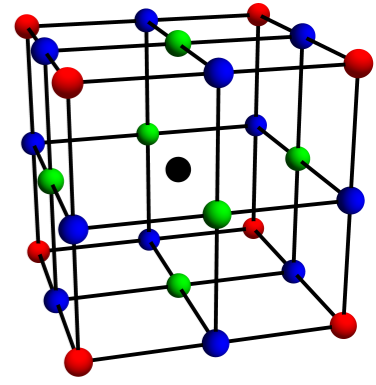
$m_L=0$

$m_L=1$

$m_L=2$

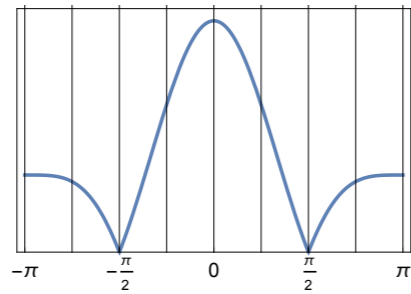
$m_L=3$

Source Overlap

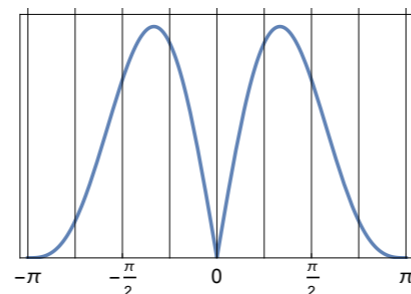
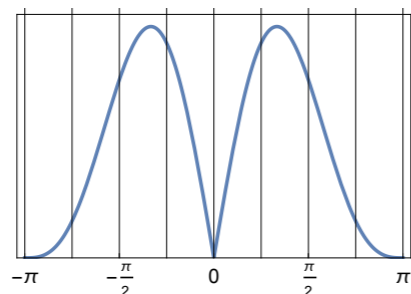


Project Luu & Savage momentum sources to **edges** as a function of $\pi\Delta x/L$

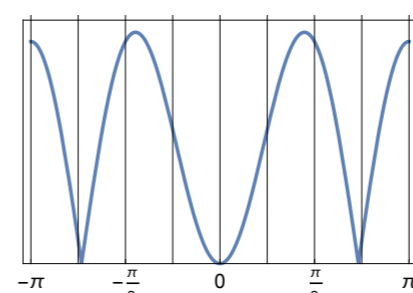
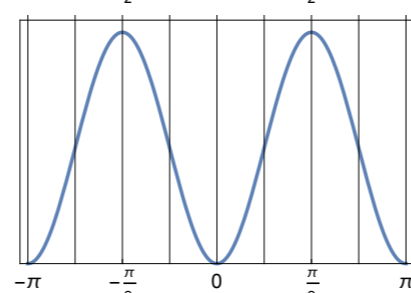
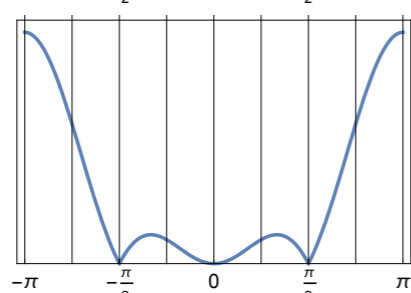
S



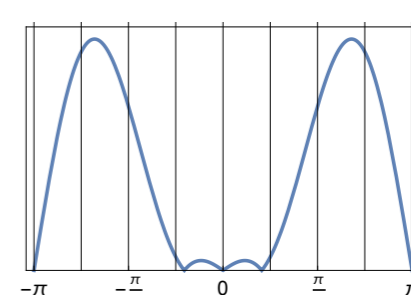
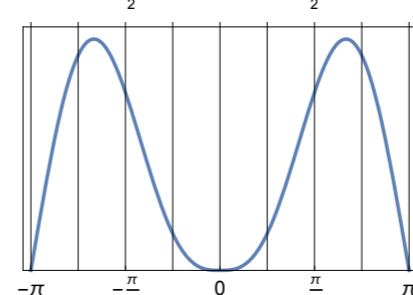
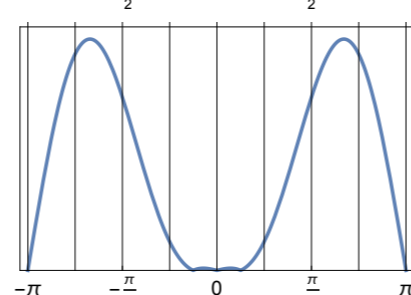
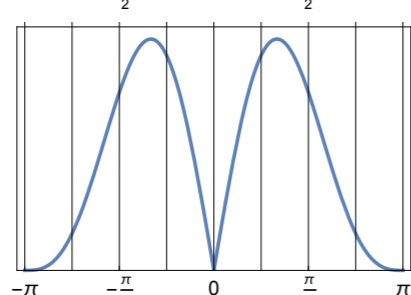
P



D



F



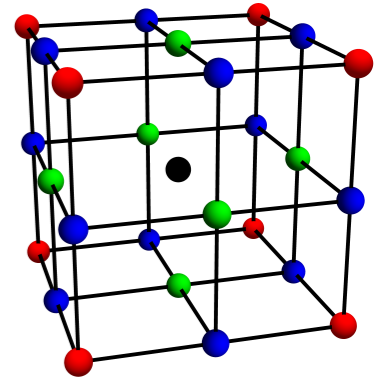
$m_L=0$

$m_L=1$

$m_L=2$

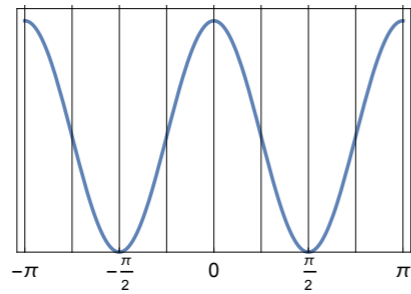
$m_L=3$

Source Overlap

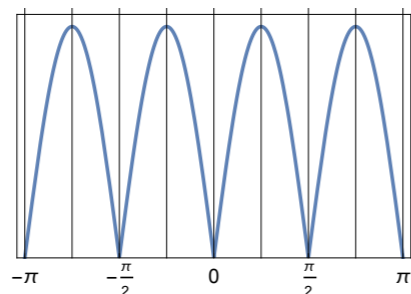


Project Luu & Savage momentum sources to **corner** as a function of $\pi\Delta x/L$

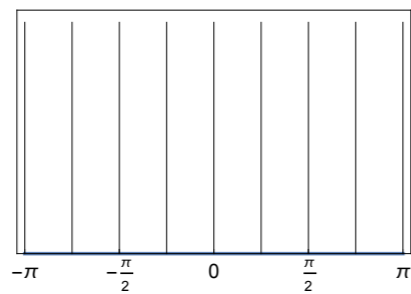
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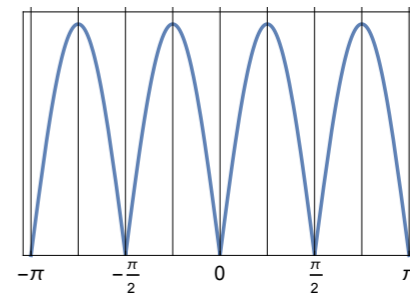
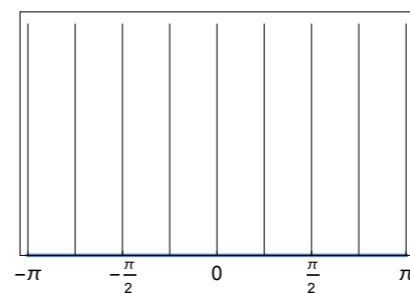
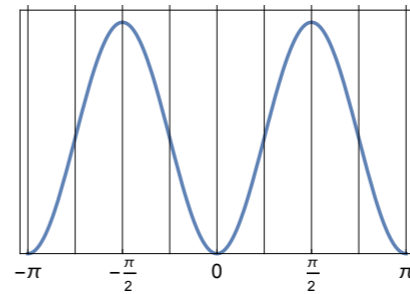
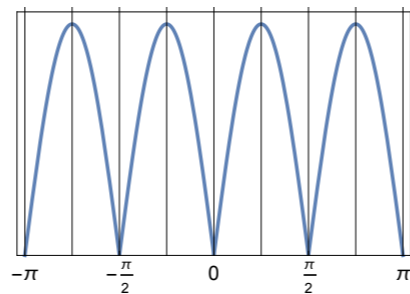
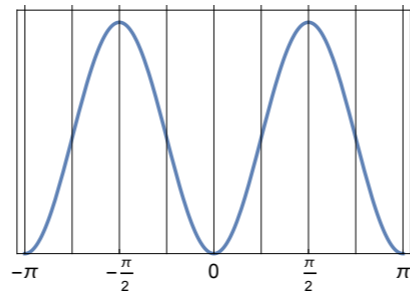
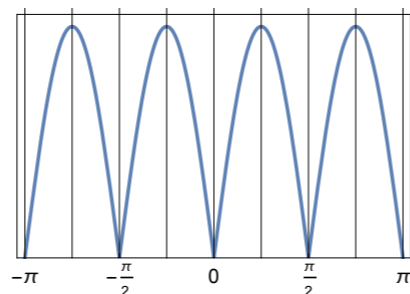
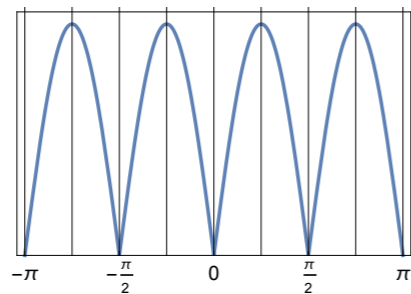
P



D



F



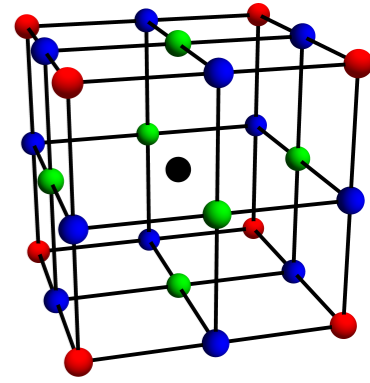
$m_L=0$

$m_L=1$

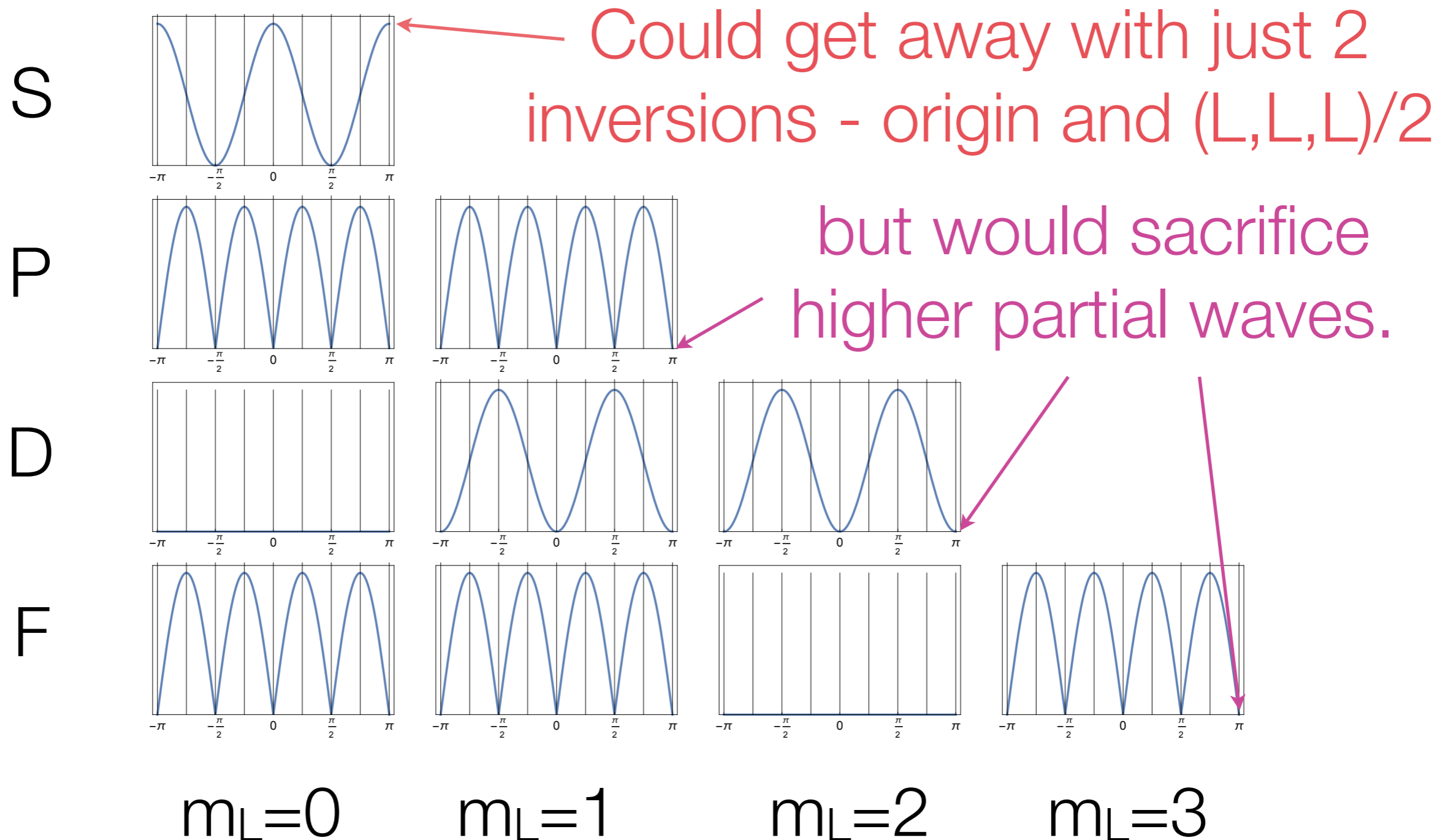
$m_L=2$

$m_L=3$

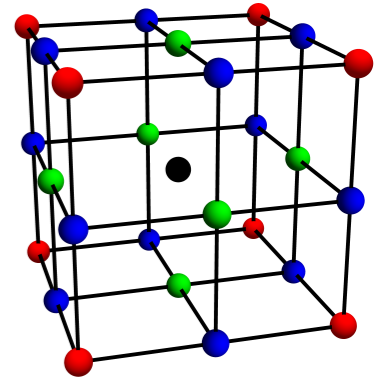
Source Overlap



Project Luu & Savage momentum sources to **corner** as a function of $\pi\Delta x/L$

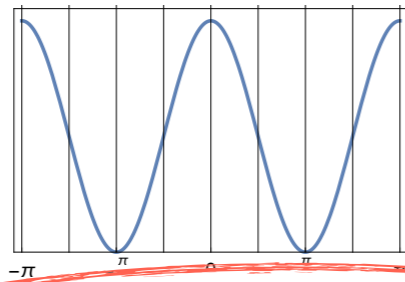


Source Overlap



Project Luu & Savage momentum sources to **corner** as a function of $\pi\Delta x/L$

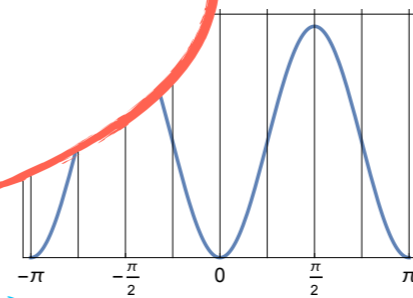
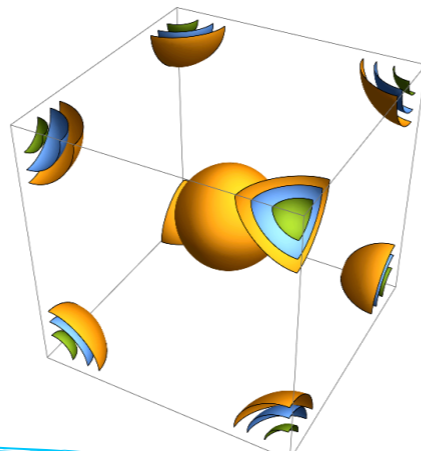
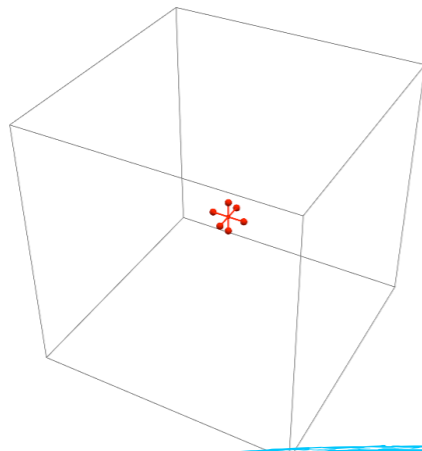
S



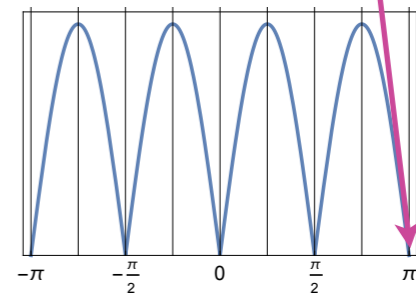
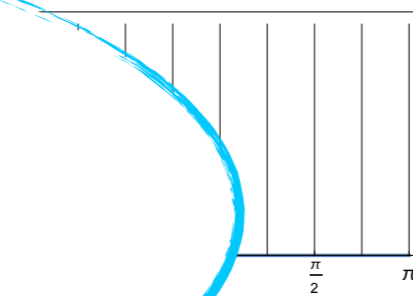
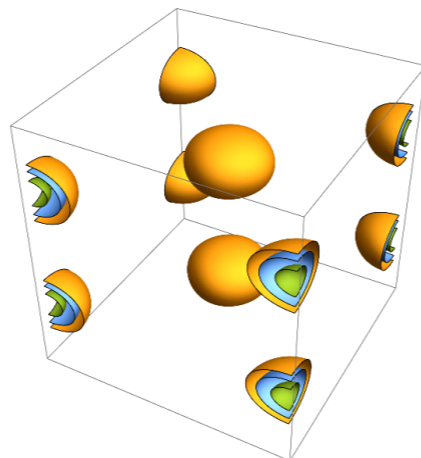
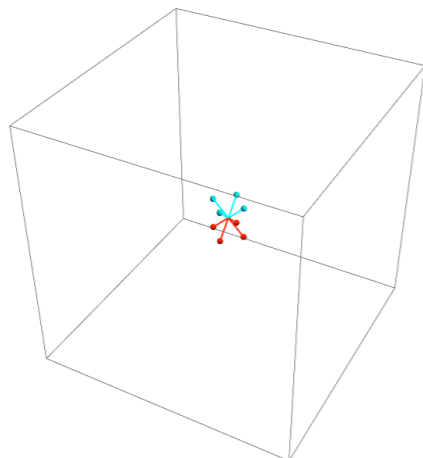
Could get away with just 2
inversions - origin and $(L,L,L)/2$

but would sacrifice
higher partial waves.

A_1^+
 $n^2=1$



T_1^-
 $n^2=2$

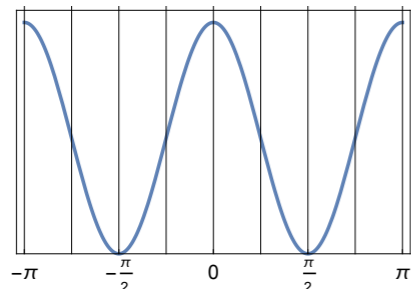


$m_L=2$

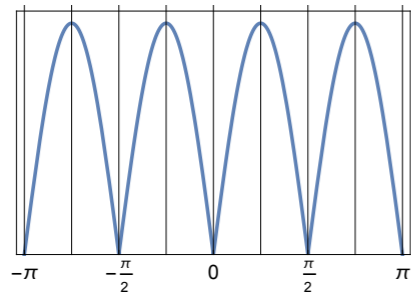
$m_L=3$

Propagator Reuse

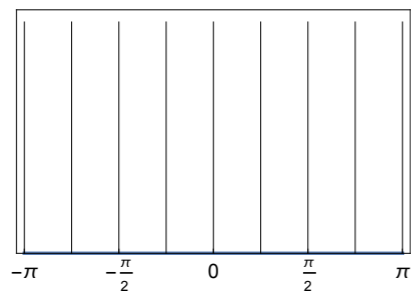
S



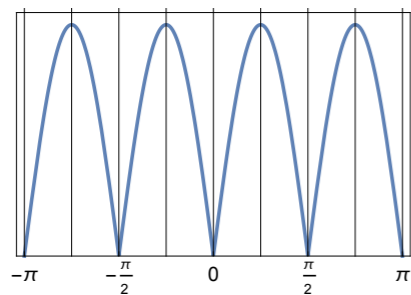
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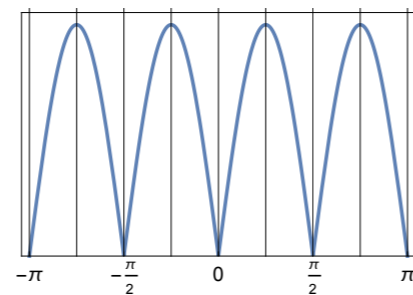
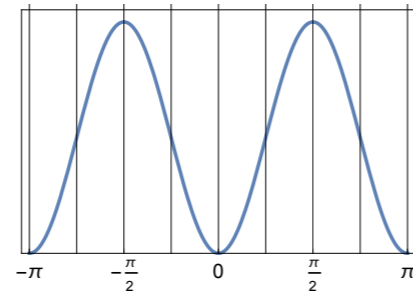
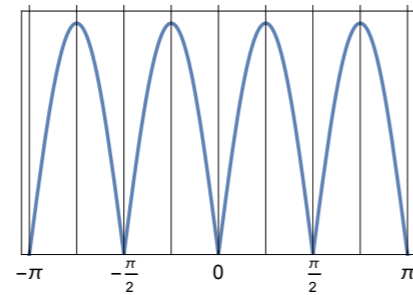
D



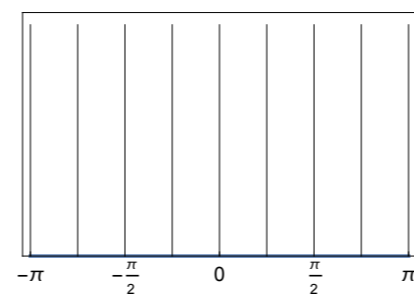
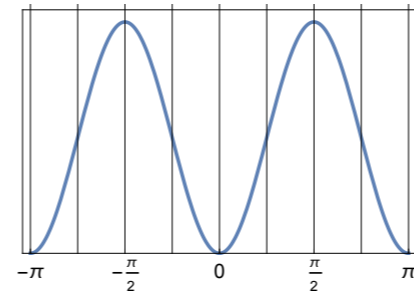
F



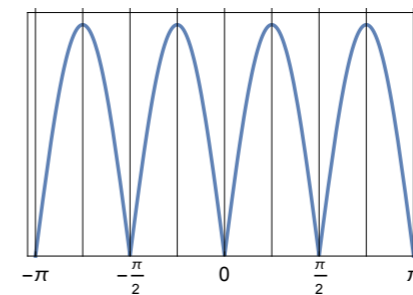
$m_L=0$



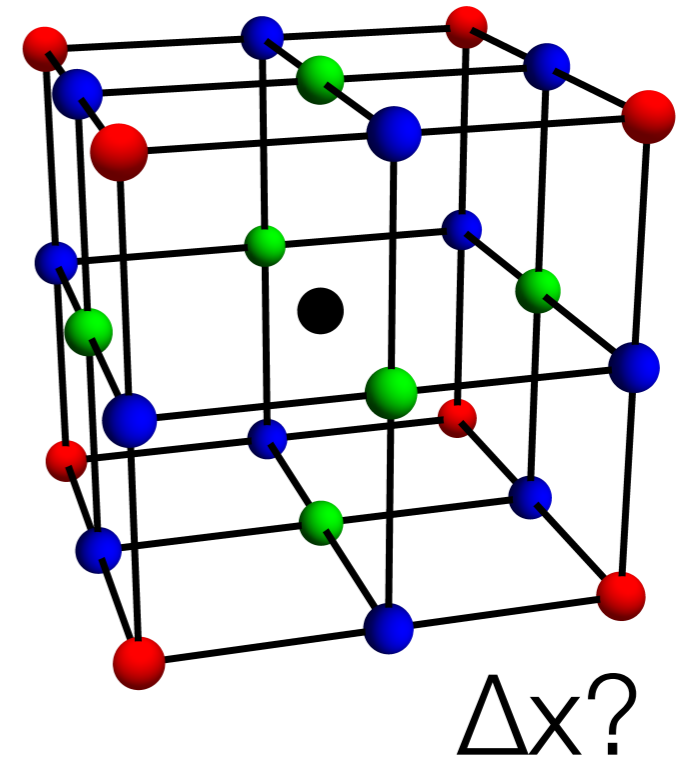
$m_L=1$



$m_L=2$



$m_L=3$



Propagator Reuse

$$0 = (0,0,0)$$

$$A = (L,L,L)/2$$

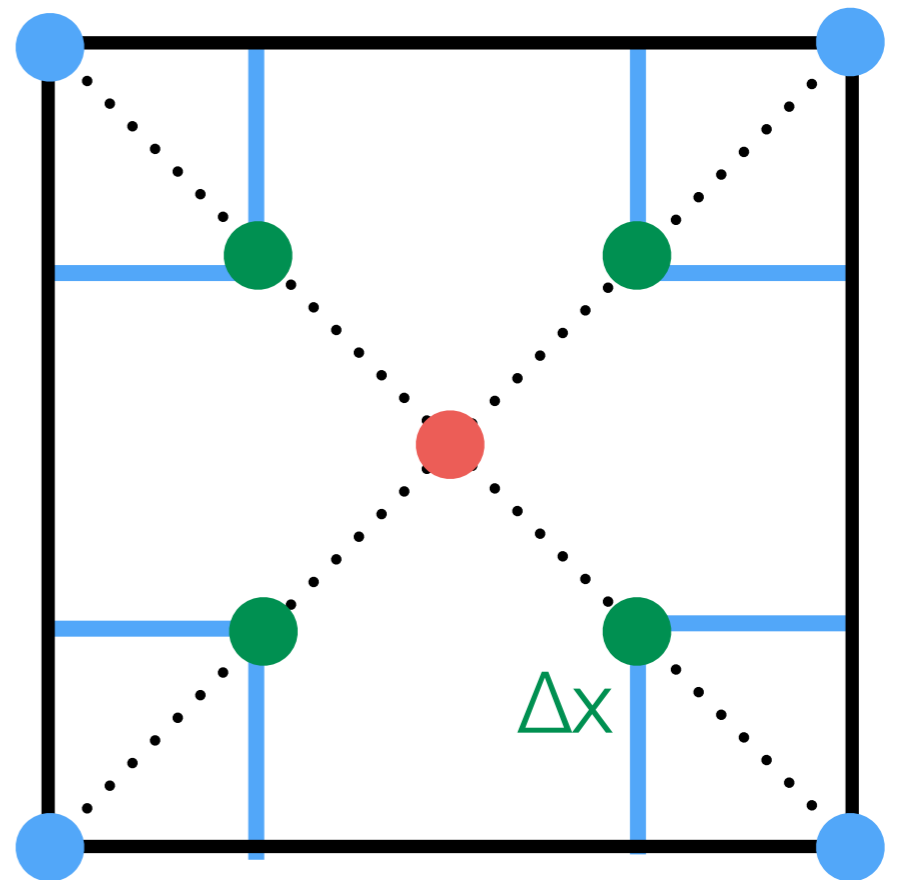
$$C = (\pm 1, \pm 1, \pm 1) \Delta x$$

10 local sources

+1 maximally displaced

+1 corner(Δx) around 0

+1 corner($L/2 - \Delta x$) around A



Propagator Reuse

$$0 = (0,0,0)$$

$$A = (L,L,L)/2$$

$$C = (\pm 1, \pm 1, \pm 1) \Delta x$$

10 local sources

+1 *maximally displaced*

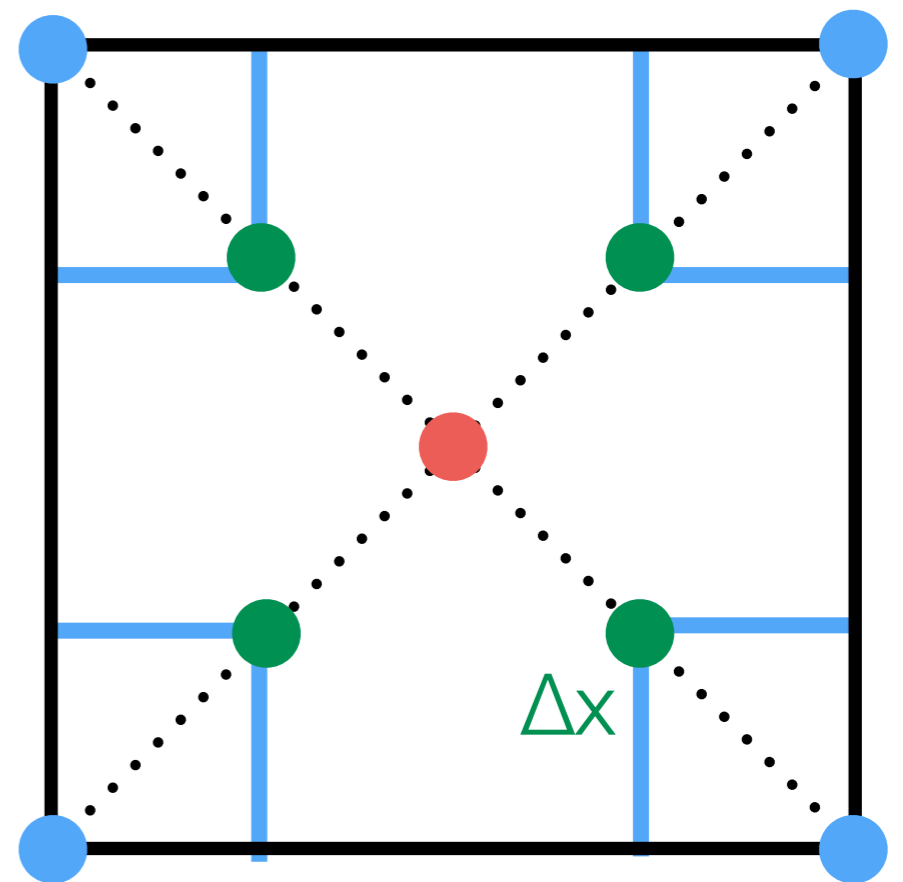
+1 *corner*(Δx) around 0

+1 *corner*($L/2 - \Delta x$) around A

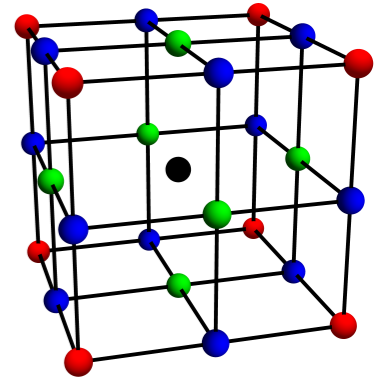
+1/2 *corner*($2\Delta x$) from C

+2 *faces*($2\Delta x$) from C

+1 *edges*($2\Delta x$) from C

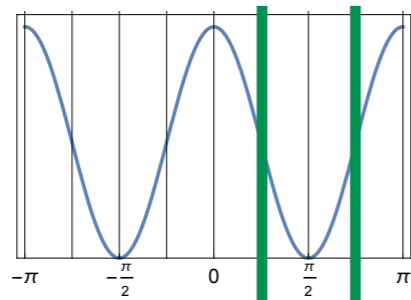


Magic Choice: $\Delta x = L/8 (\equiv 3L/8)$

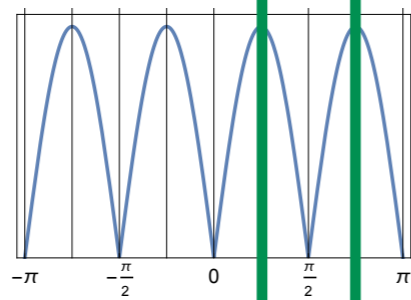


corner

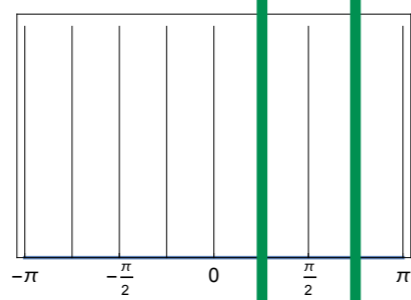
S



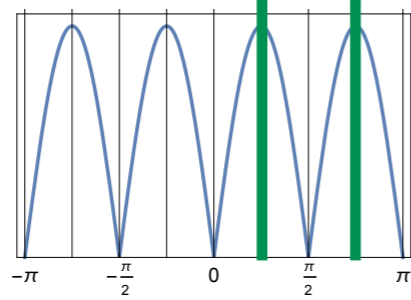
P



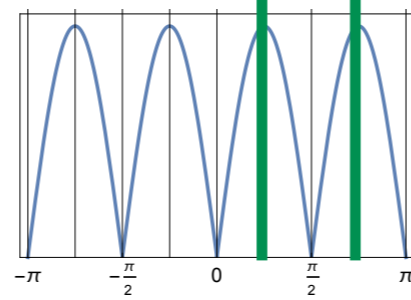
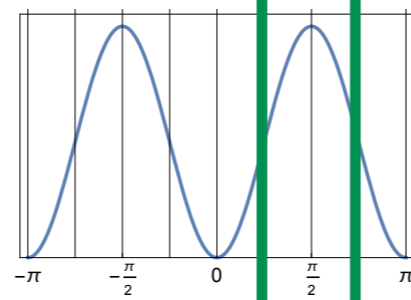
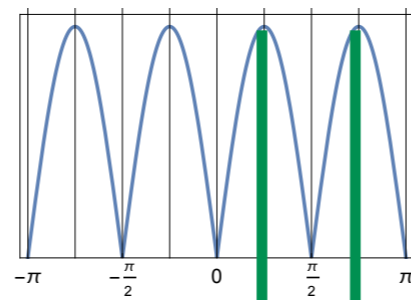
D



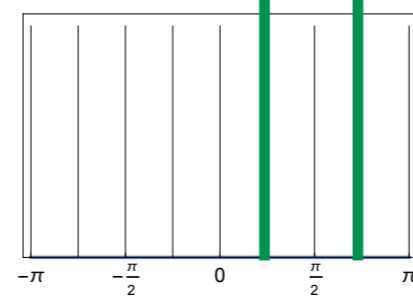
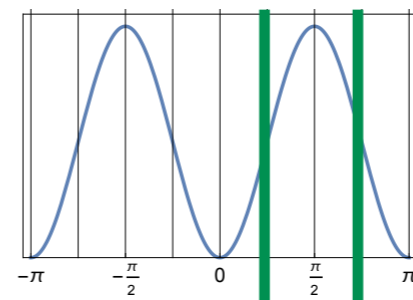
F



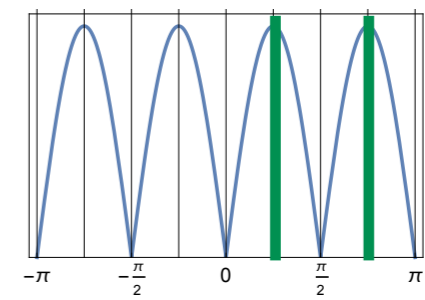
$m_L=0$



$m_L=1$

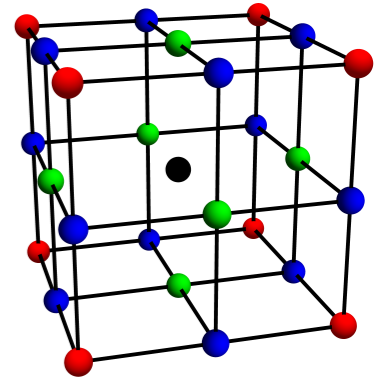


$m_L=2$



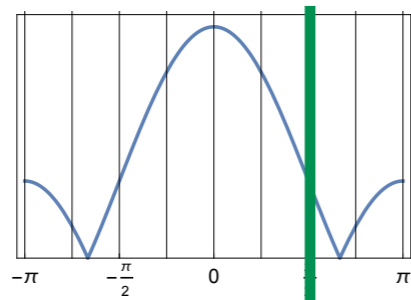
$m_L=3$

Magic Choice: $\Delta x = L/8 \ (\equiv 3L/8)$

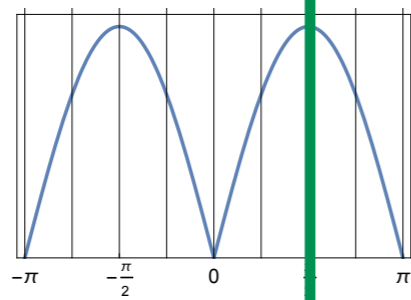


faces

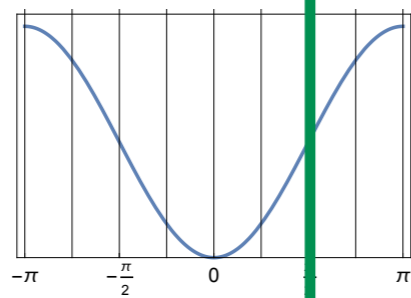
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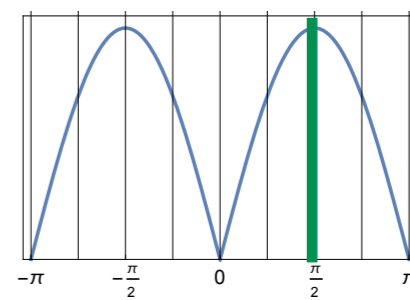
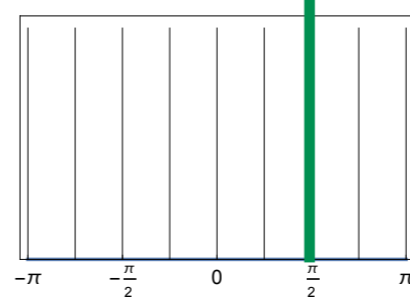
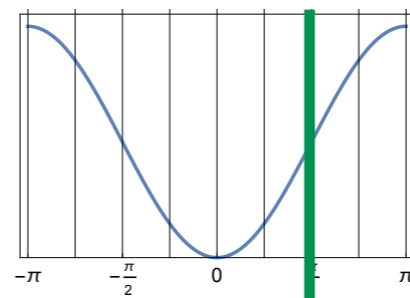
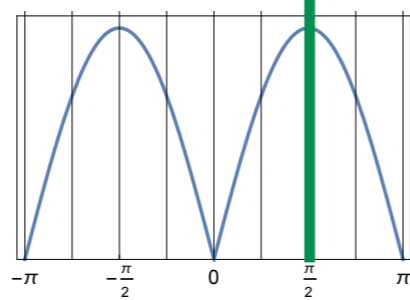
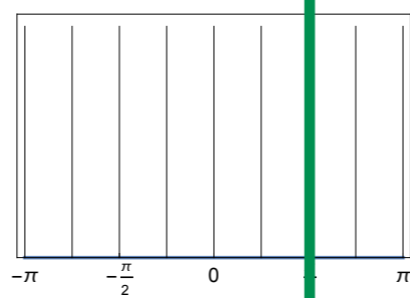
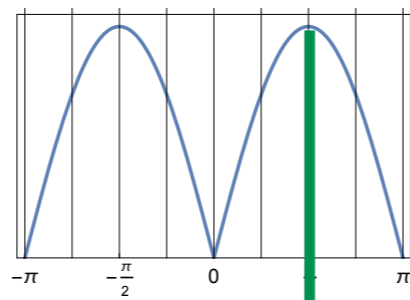
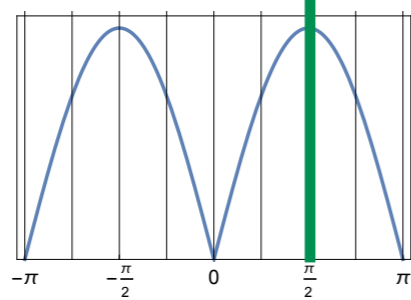
P



D



F



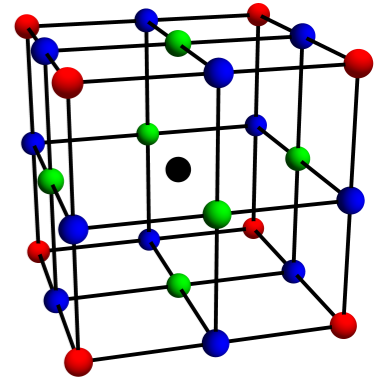
$m_L=0$

$m_L=1$

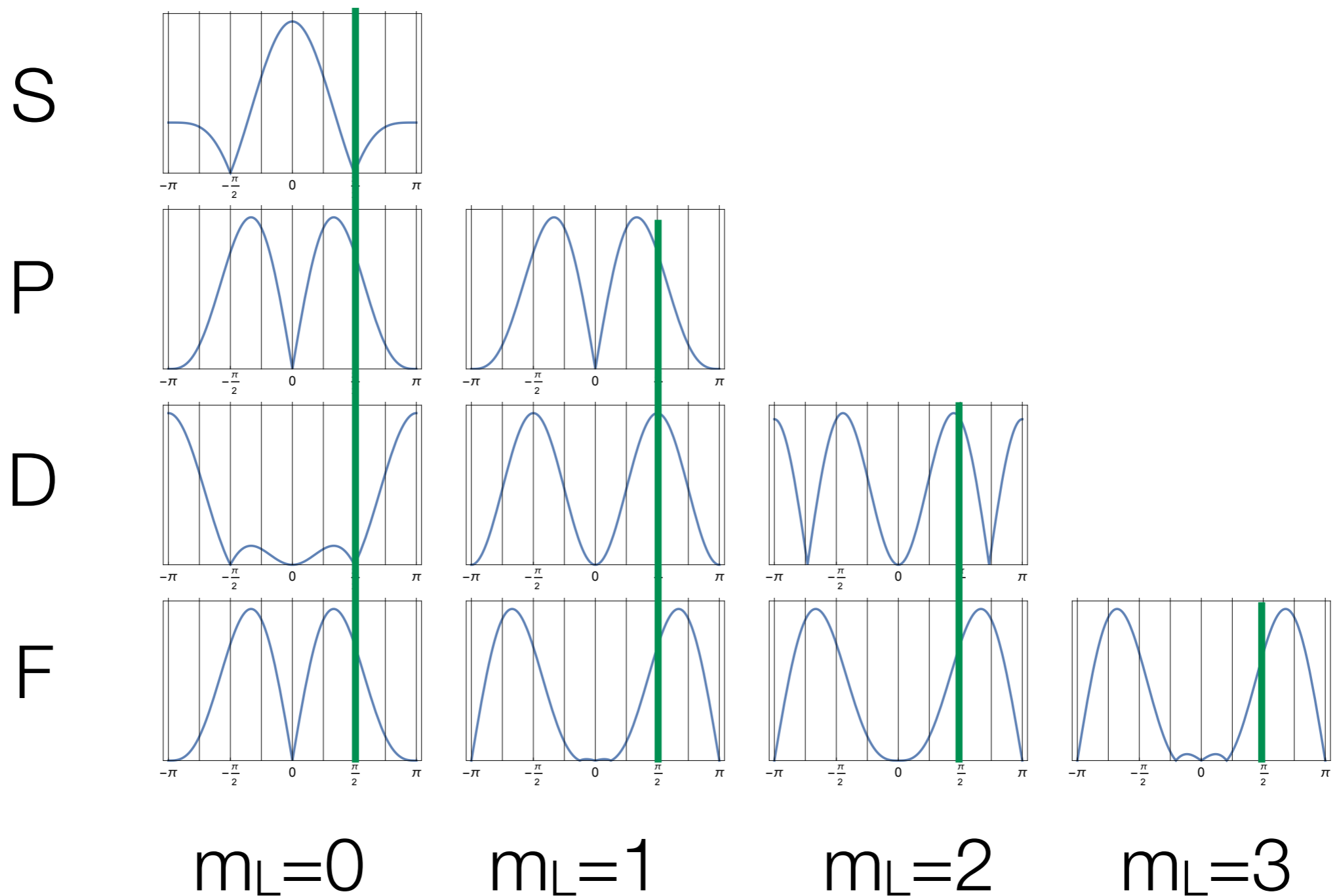
$m_L=2$

$m_L=3$

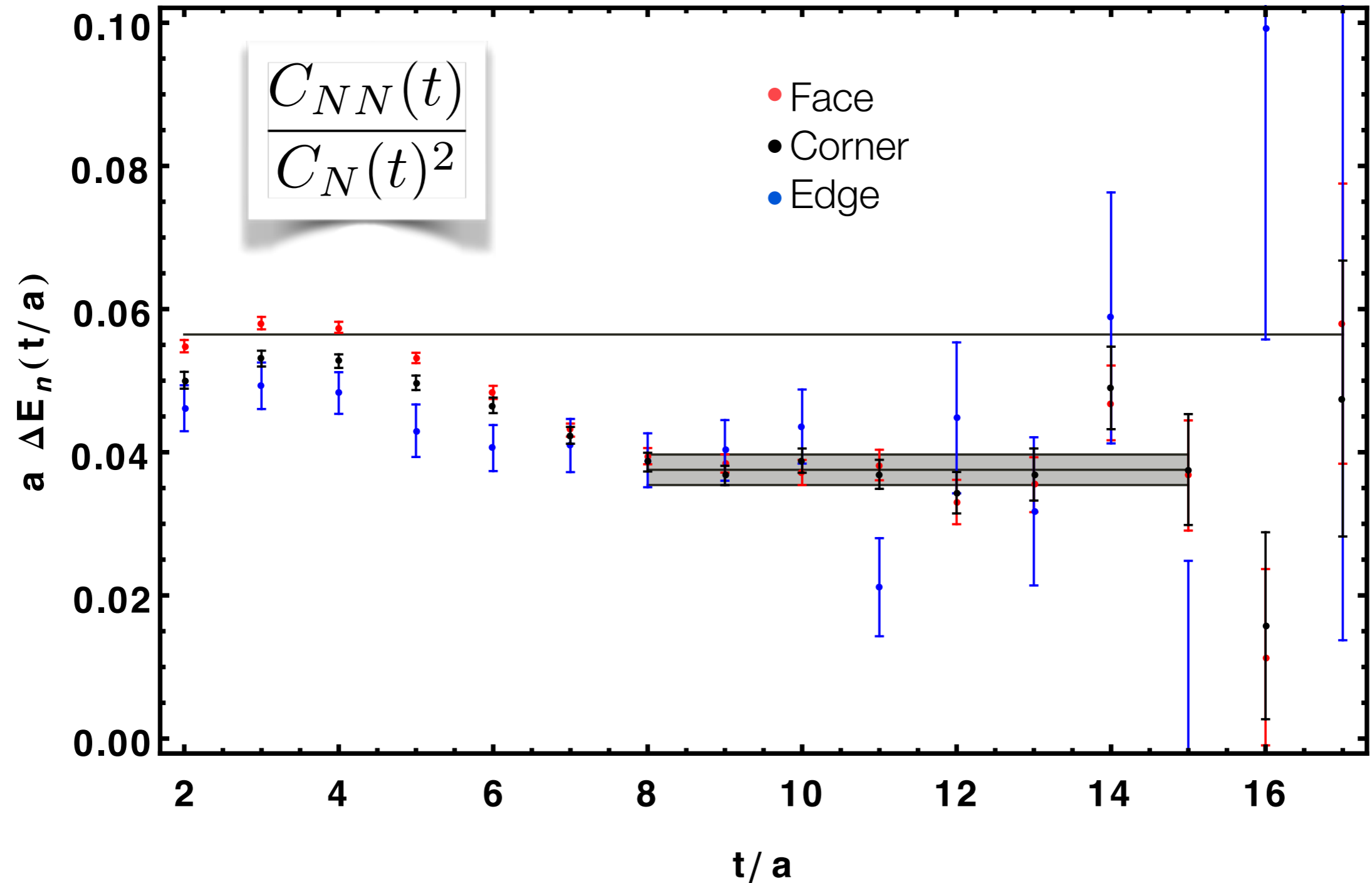
Magic Choice: $\Delta x = L/8 (\equiv 3L/8)$



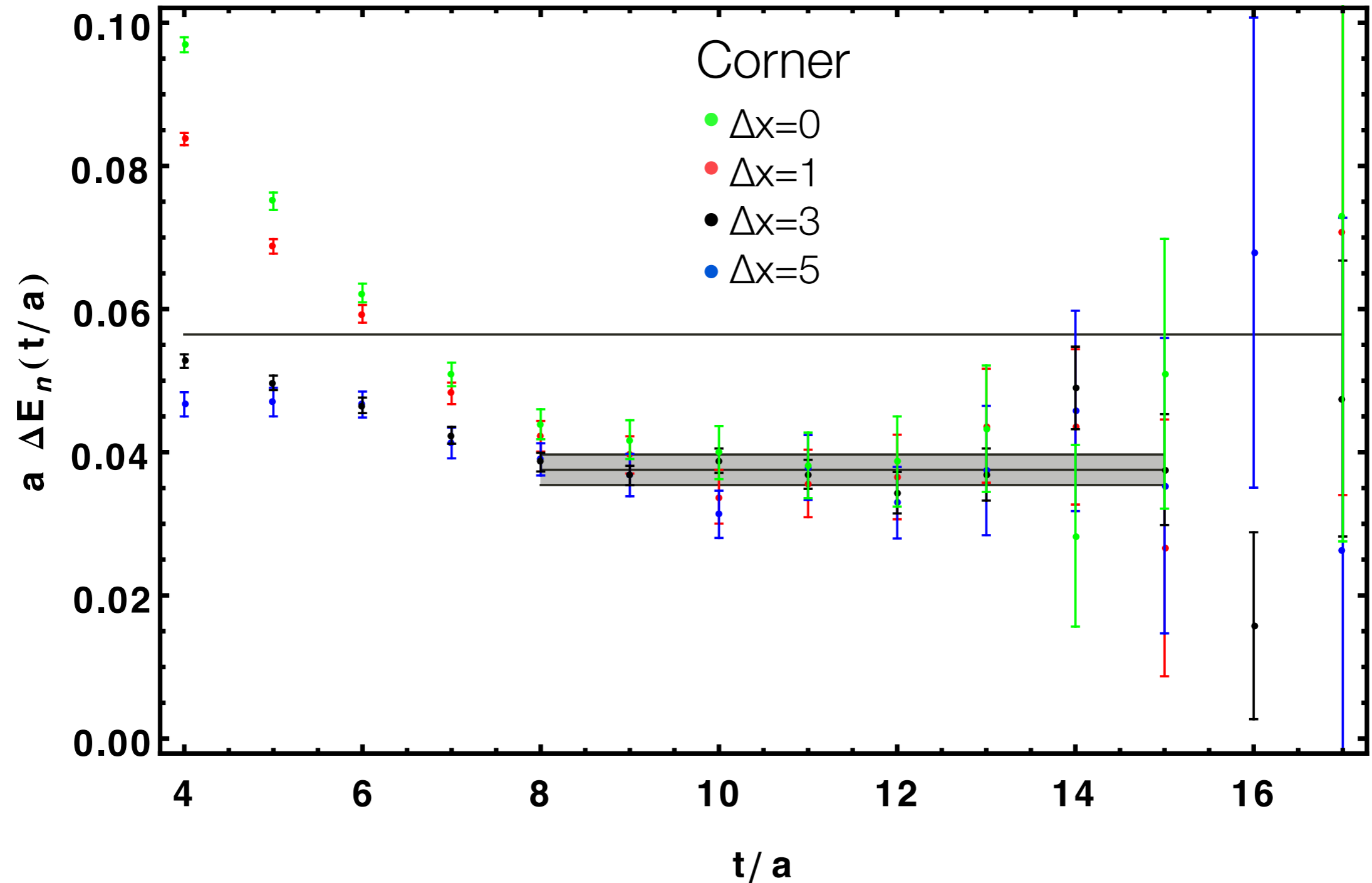
edges



Different sources give same plateau A_1^+ , $\Delta x=3$

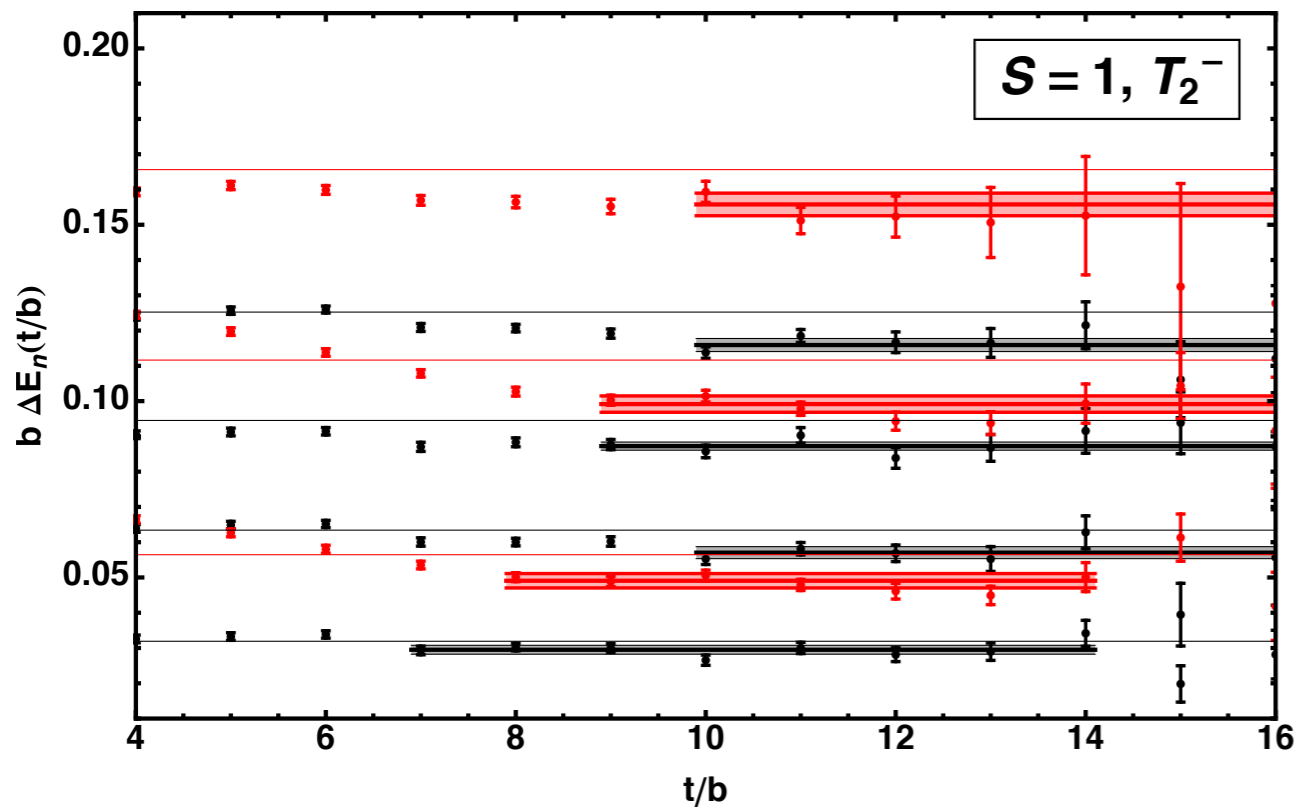


Different displacements give same plateau A_1^+



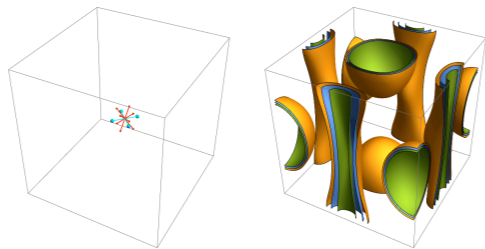
Clean separation of momentum shells

- $L=24$
- $L=32$

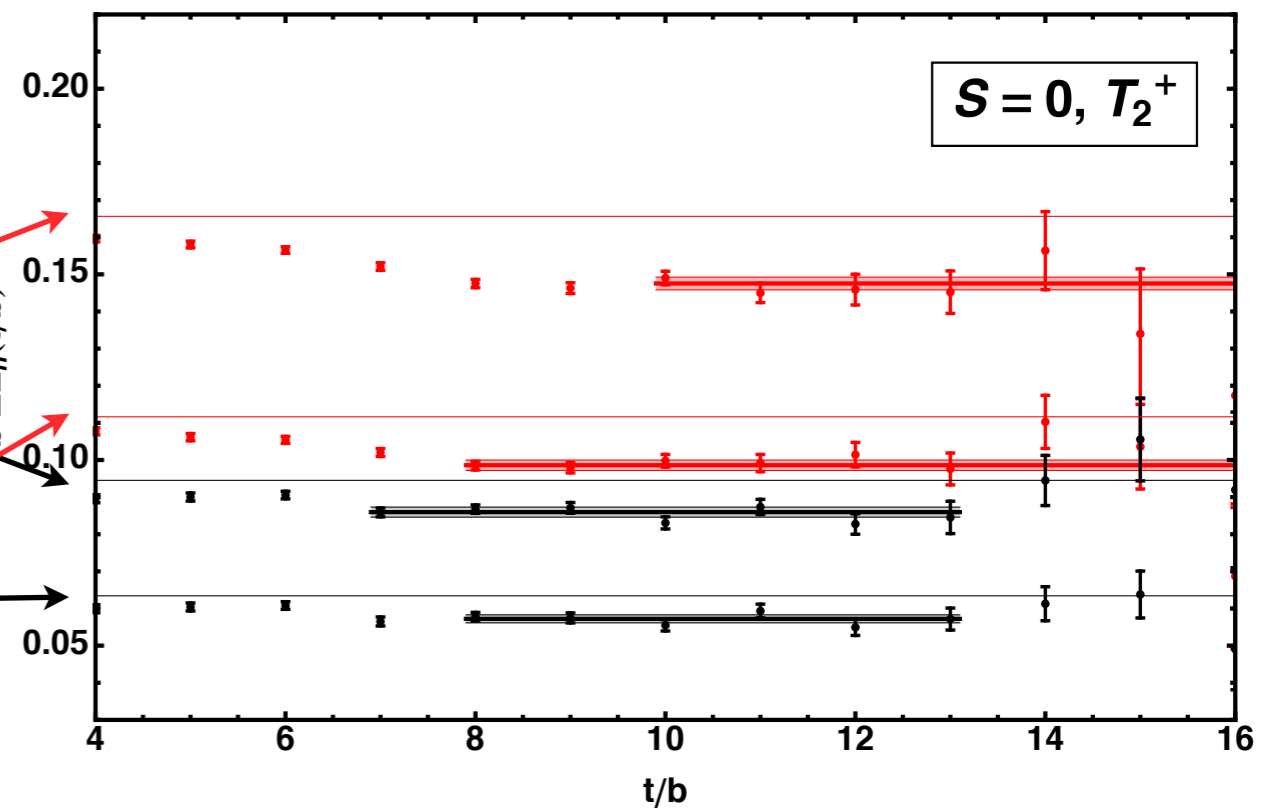
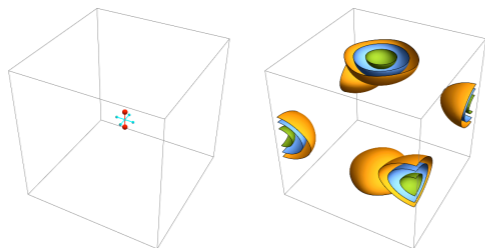


$\Delta E \rightarrow$ Lüscher

$n^2=2$



$n^2=1$



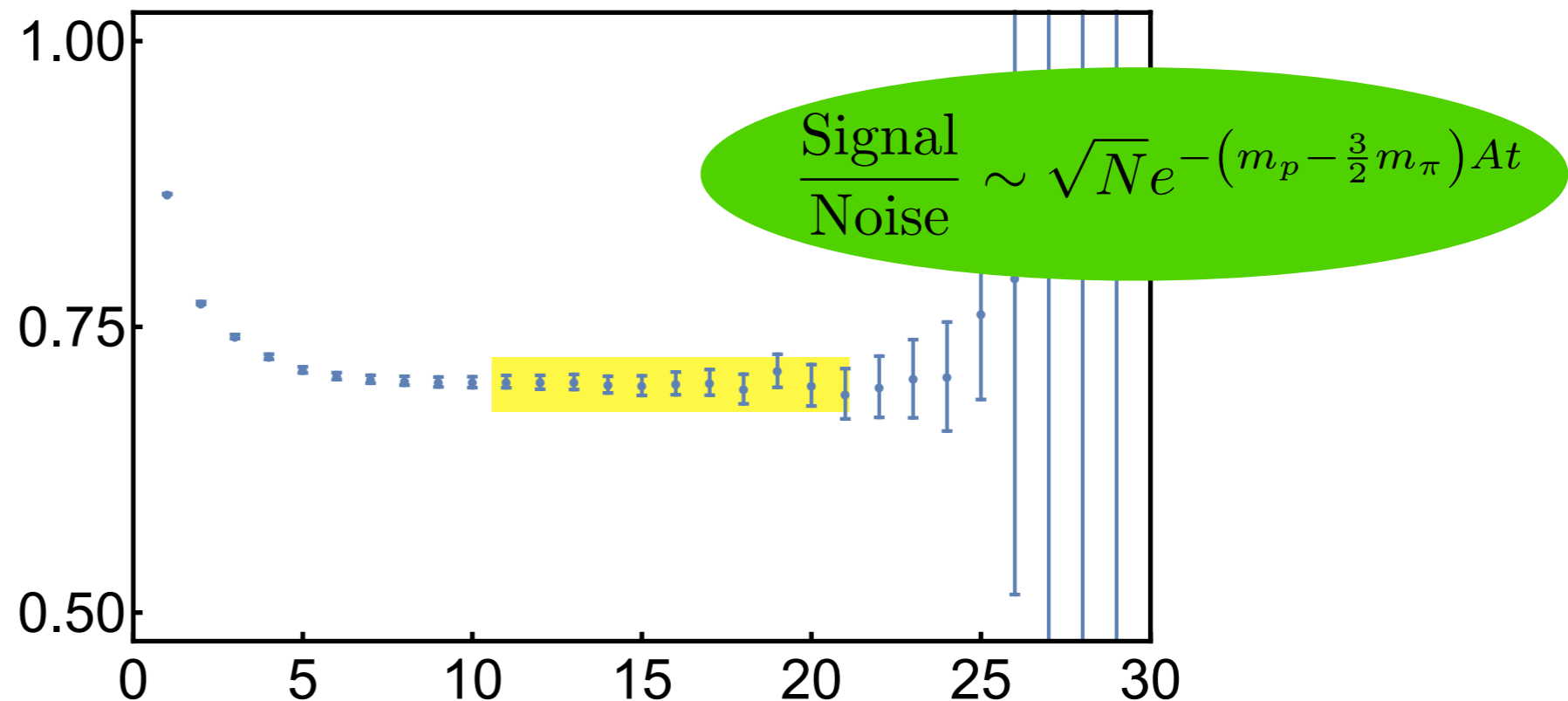
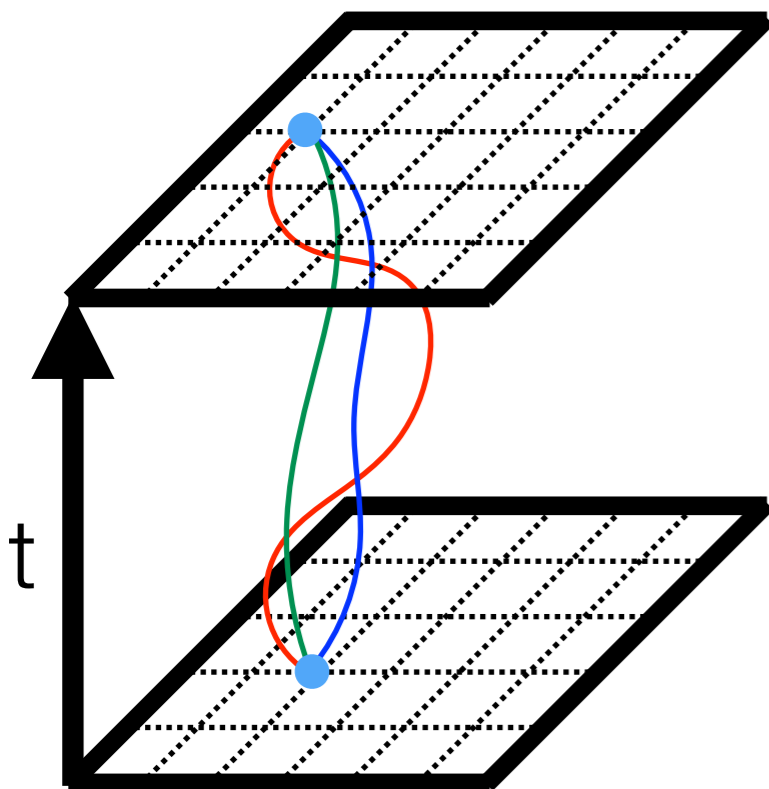
Correlation Functions and Effective Masses

$$C(t) = \langle \mathcal{O}(t) \mathcal{O}^\dagger(0) \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}U \mathcal{O}(t) \mathcal{O}^\dagger(0) e^{-S[\bar{\psi}, \psi, U]}$$

$$= \sum_k \langle \Omega | \mathcal{O} | k \rangle \langle k | \mathcal{O}^\dagger | \Omega \rangle e^{-E_k t}$$

Effective mass

$$E_0 = \lim_{t \rightarrow \infty} -\partial_t \log C(t)$$



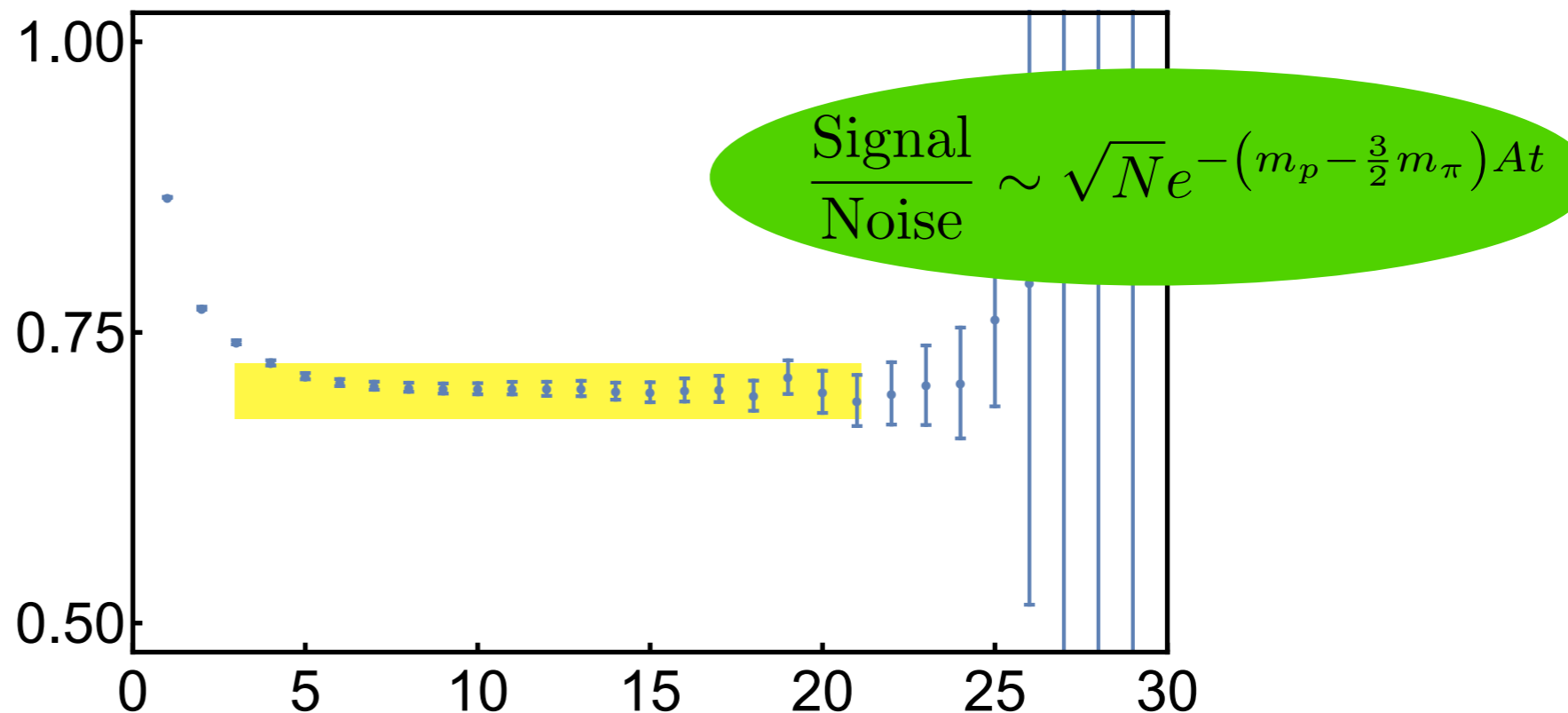
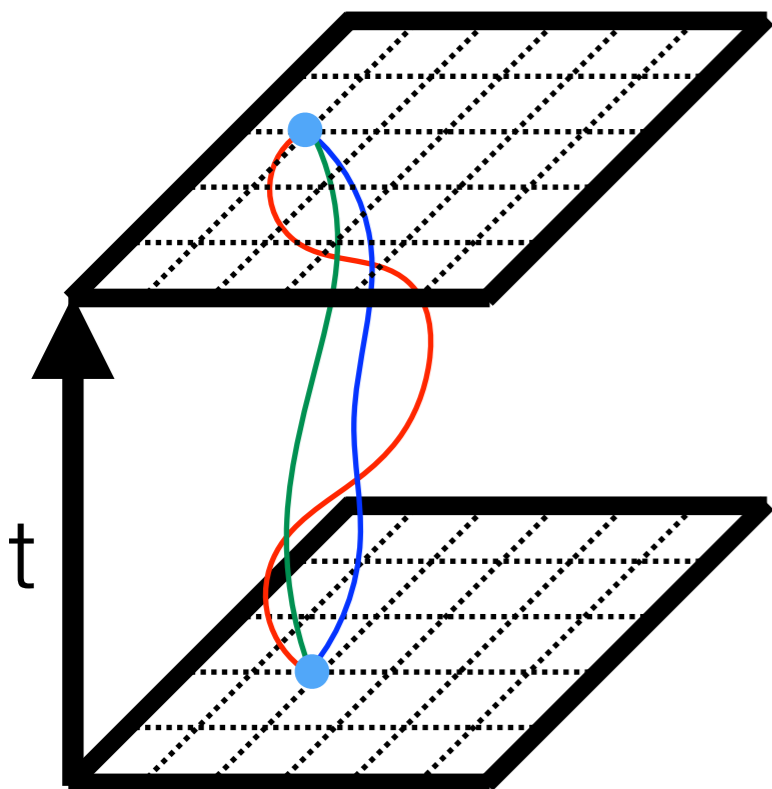
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Effective mass

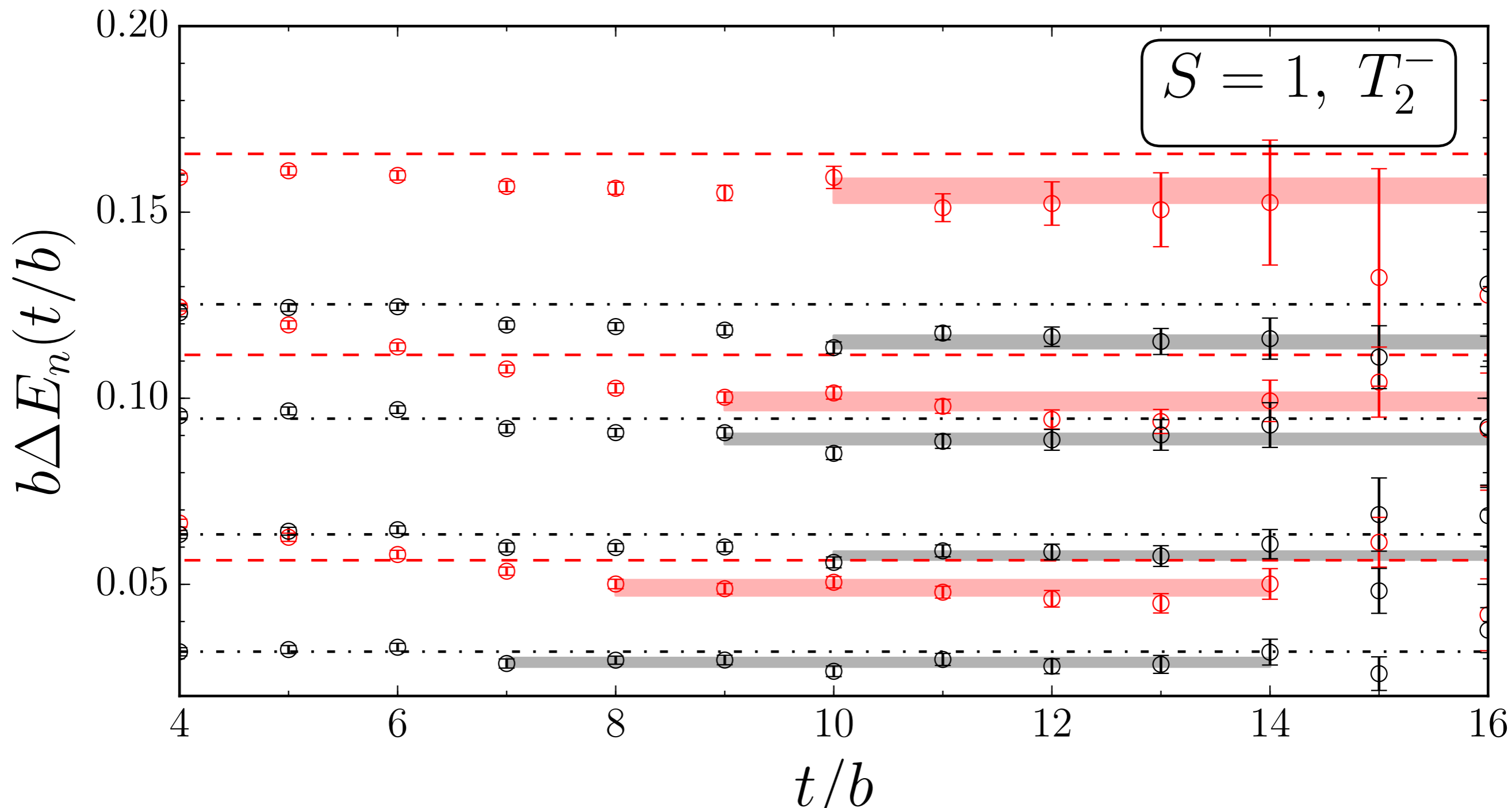
$$E_0 = \lim_{t \rightarrow \infty} -\partial_t \log C(t)$$



Fitting the Ratio

CalLat 1508.00886 Phys.Lett. B765 (2017) 285-292

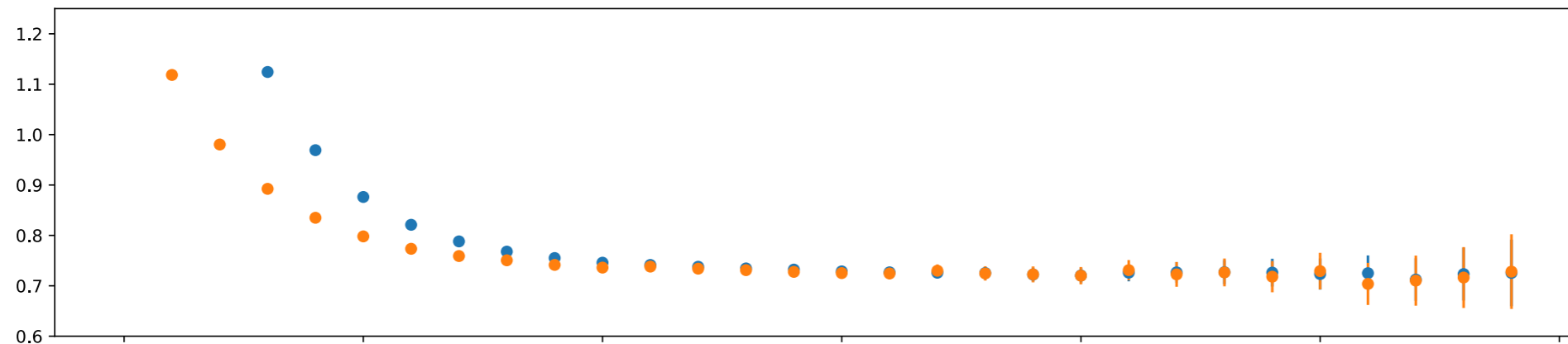
$$E_{\text{interaction}} = \lim_{t \rightarrow \infty} \frac{C_{NN}(t)}{C_N(t)^2}$$



Individual correlators

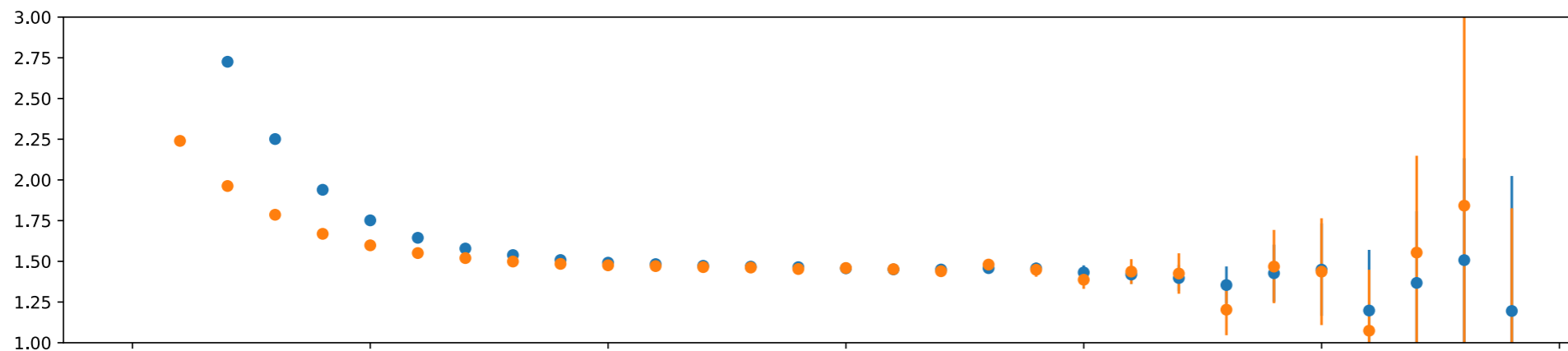
$m_\pi \sim 700$ MeV
gauss source

N

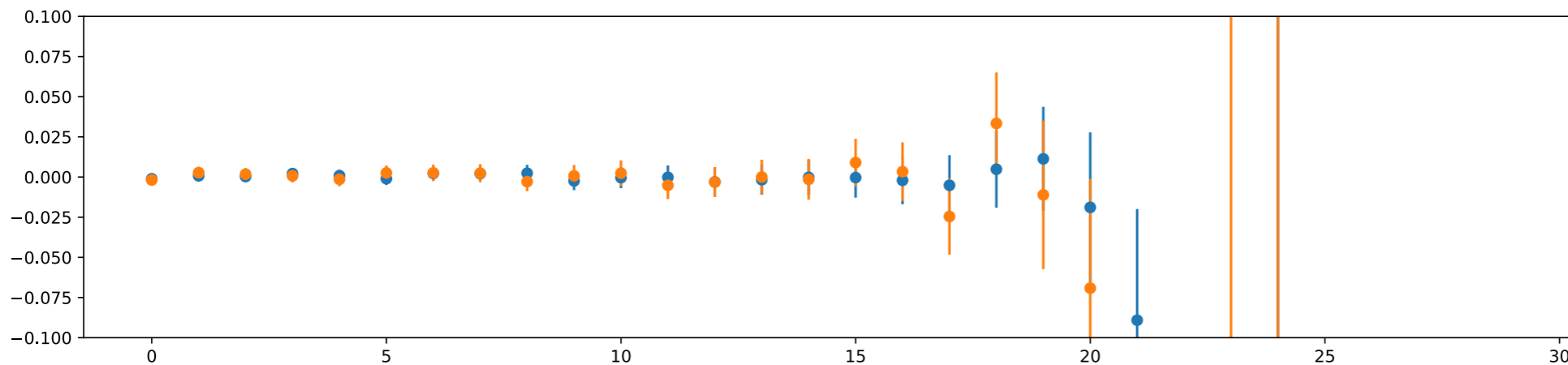


point sink
gauss sink

NN



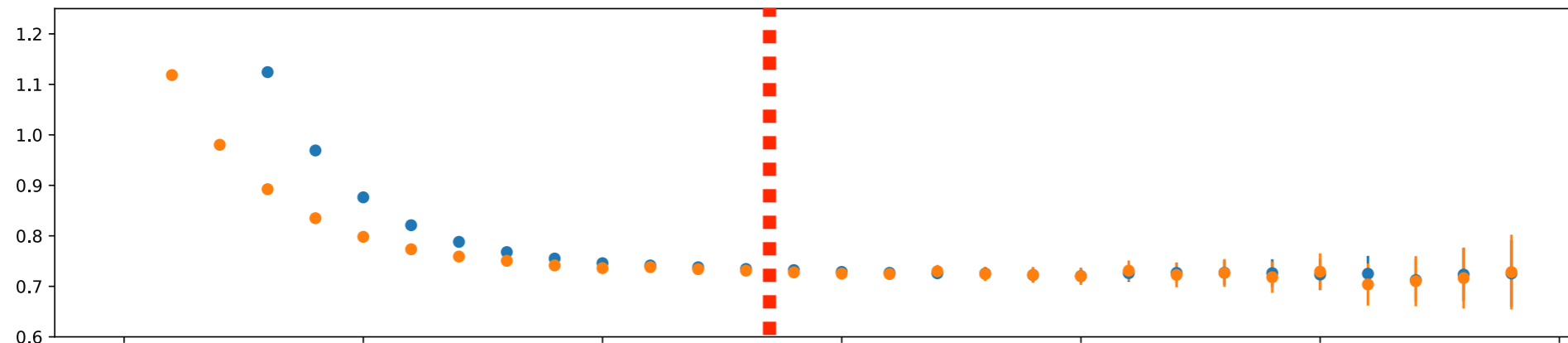
ratio



Individual correlators

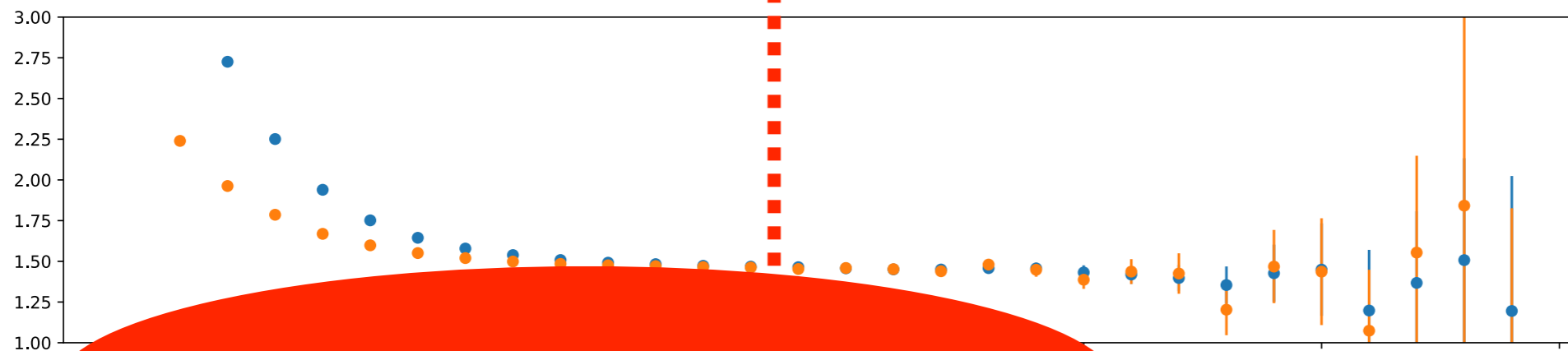
$m_\pi \sim 700$ MeV
gauss source

N



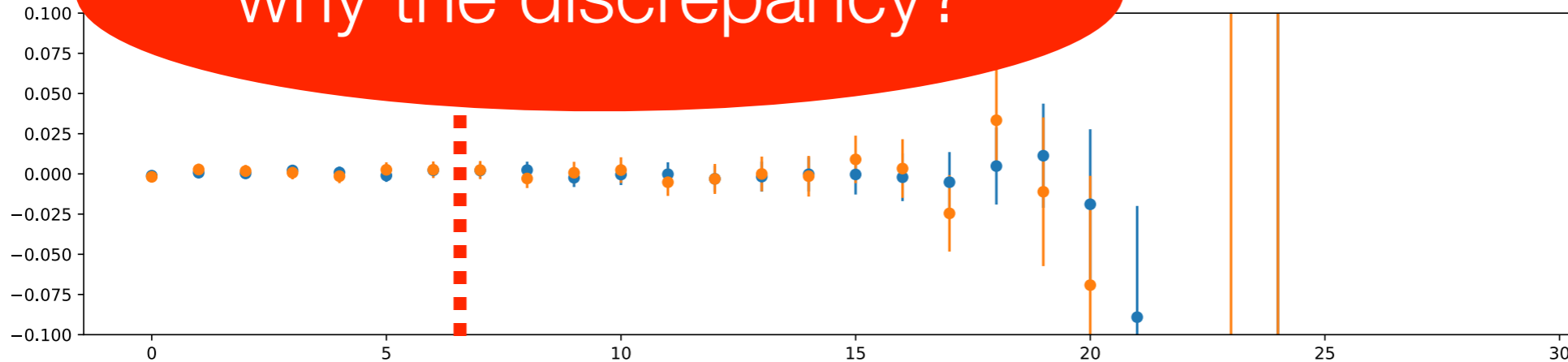
point sink
gauss sink

NN



why the discrepancy?

ratio

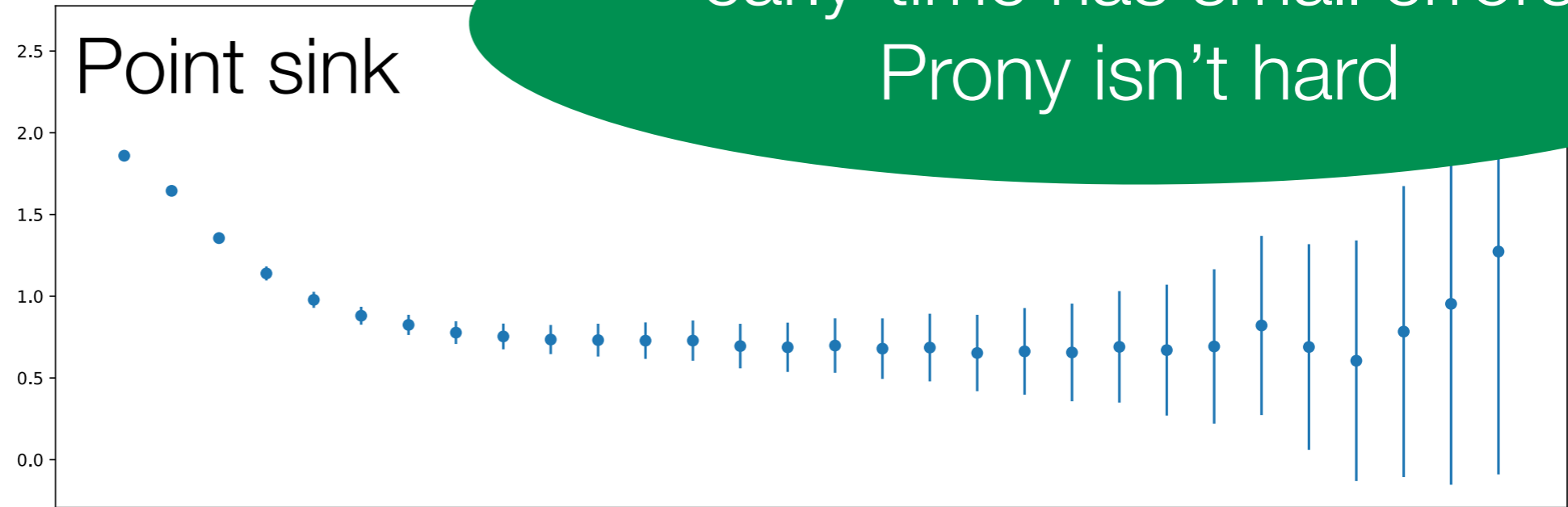
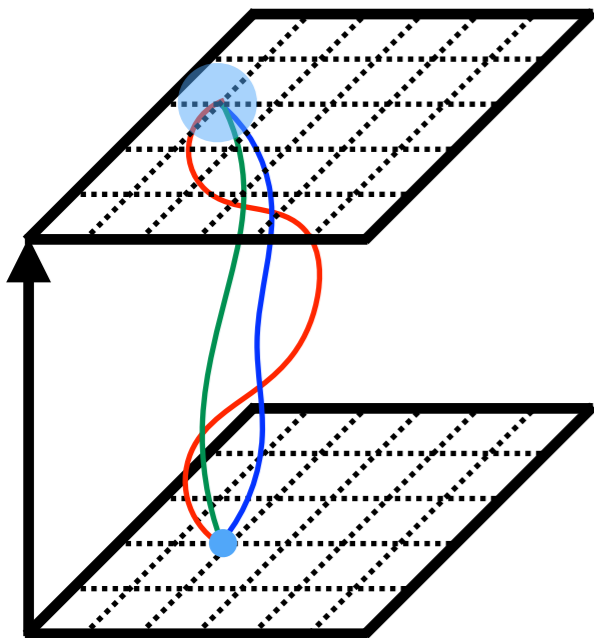
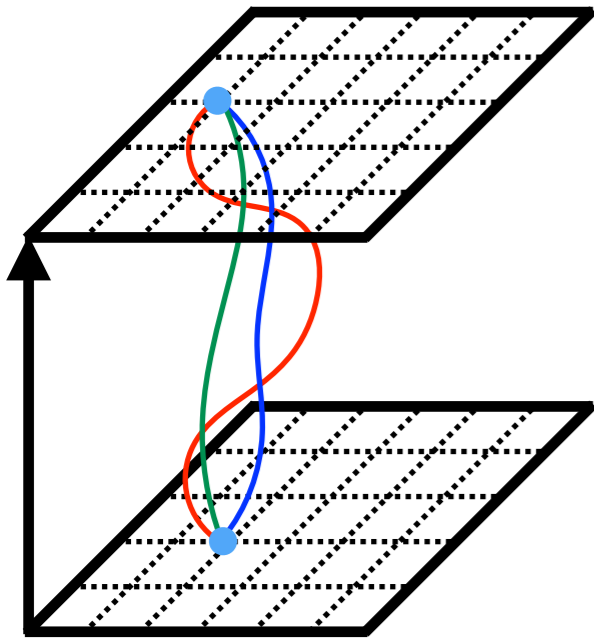


Suspicious coincidence

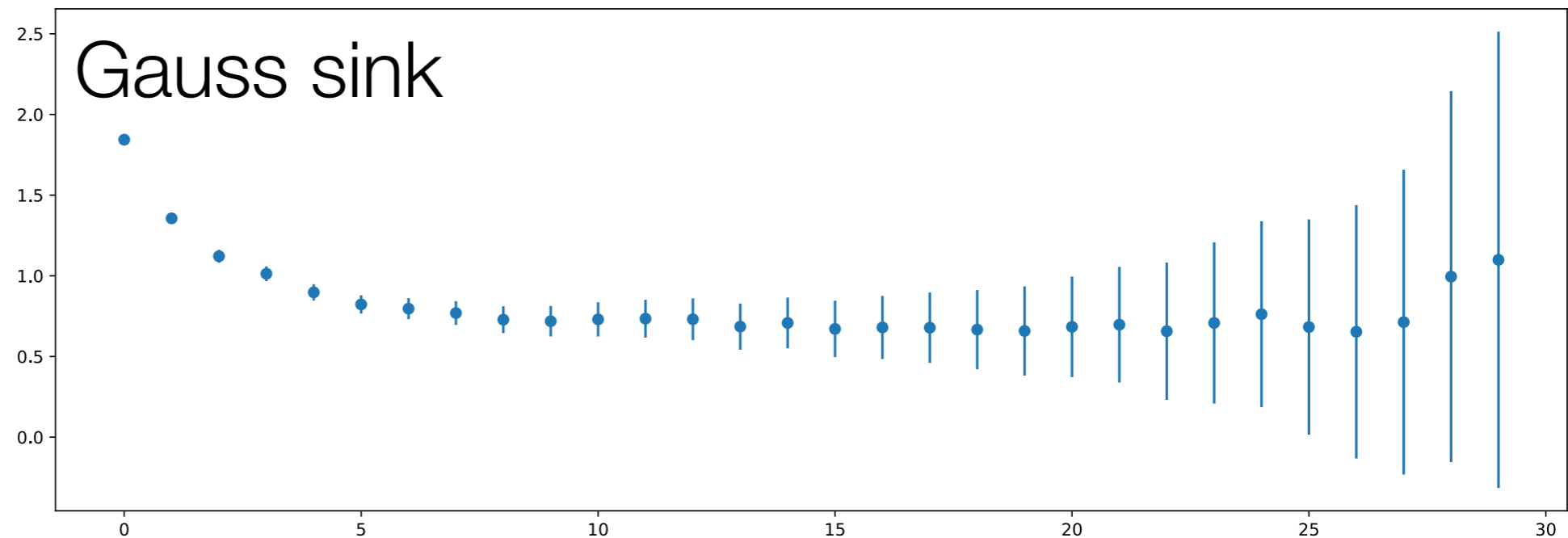
- Ratio does better than is really justified
- Ratio plateau starts way earlier than N or NN plateaus
- Matrix Prony on multiple NN signals doesn't help much

NN excited states are mostly single-nucleon excitations?

Single Nucleon Operator

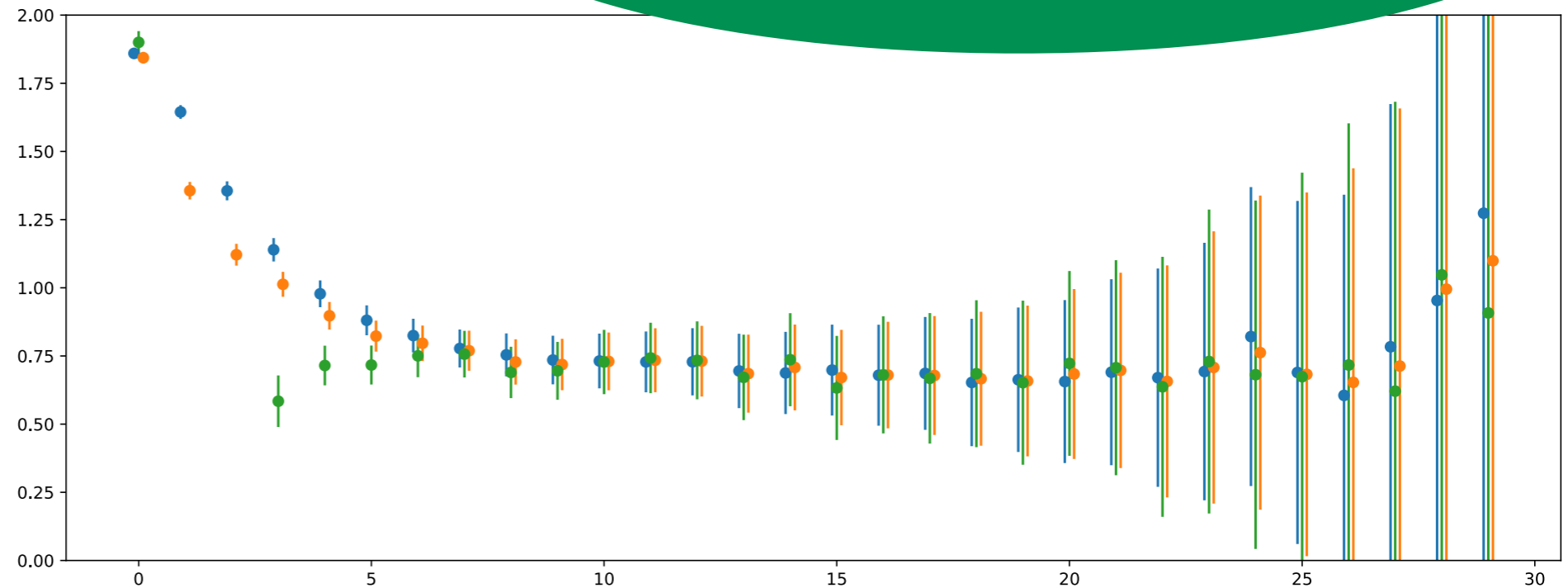
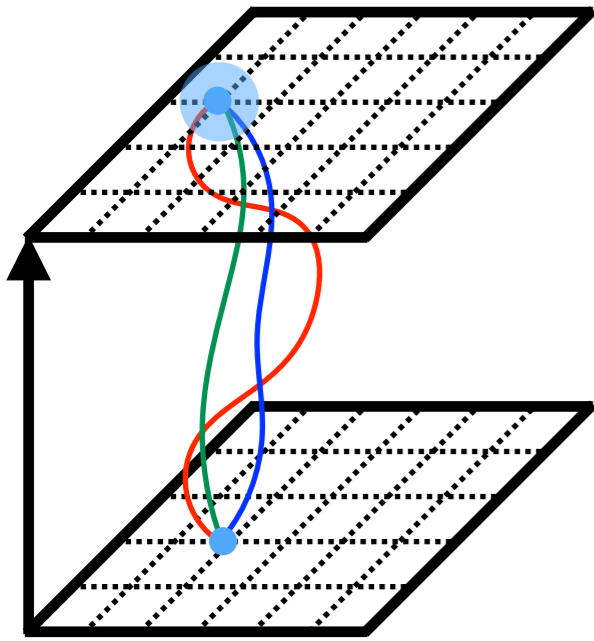


early-time has small errors
Prony isn't hard



Single Nucleon Operator

LC lengthens N plateau
from $t \sim 10$ to $t \sim 5$



- Determining linear combination doesn't require large statistics
- No additional inversions.
- One (or more) smearing + single-nucleon contraction

This is NOT the same as linear combinations of NN

Beane et al. (NPLQCD) 0905.0466

$$NN^{(pt)} = N^{(pt)} N^{(pt)}$$

$$NN^{(smr)} = N^{(smr)} N^{(smr)}$$

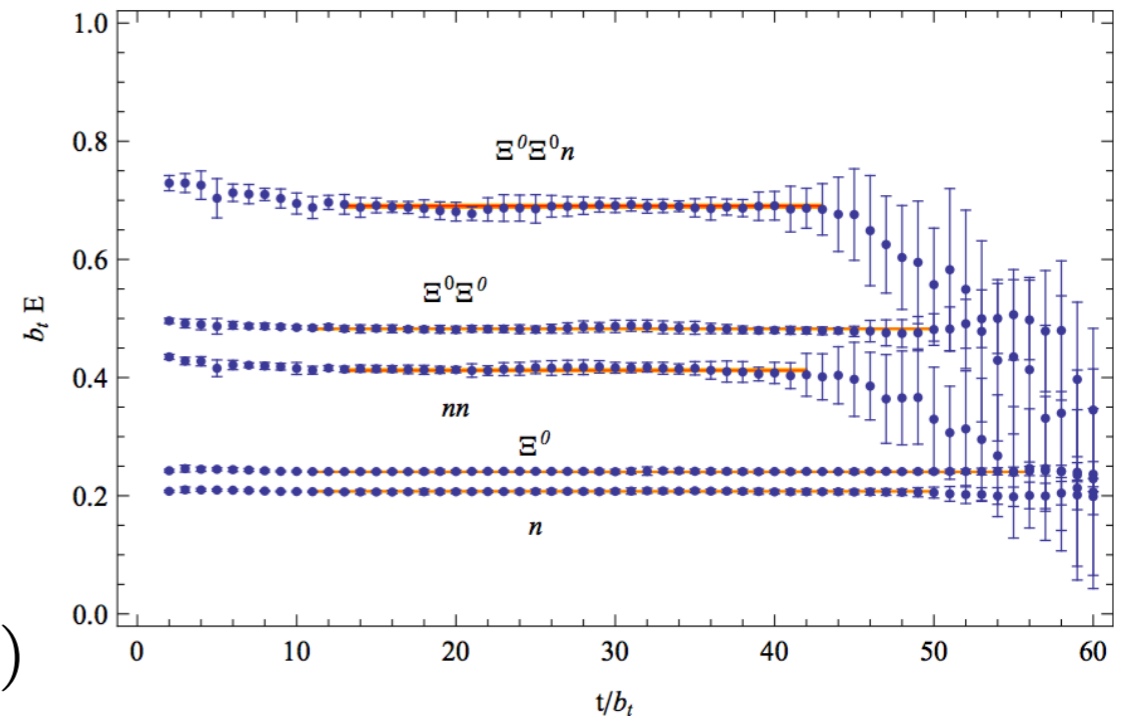
$$\text{Prony}(NN) = \alpha NN^{(pt)} + \beta NN^{(smr)}$$

$$= \alpha N^{(pt)} N^{(pt)} + \beta N^{(smr)} N^{(smr)}$$

$$NN^{(LC)} = N^{(LC)} N^{(LC)}$$

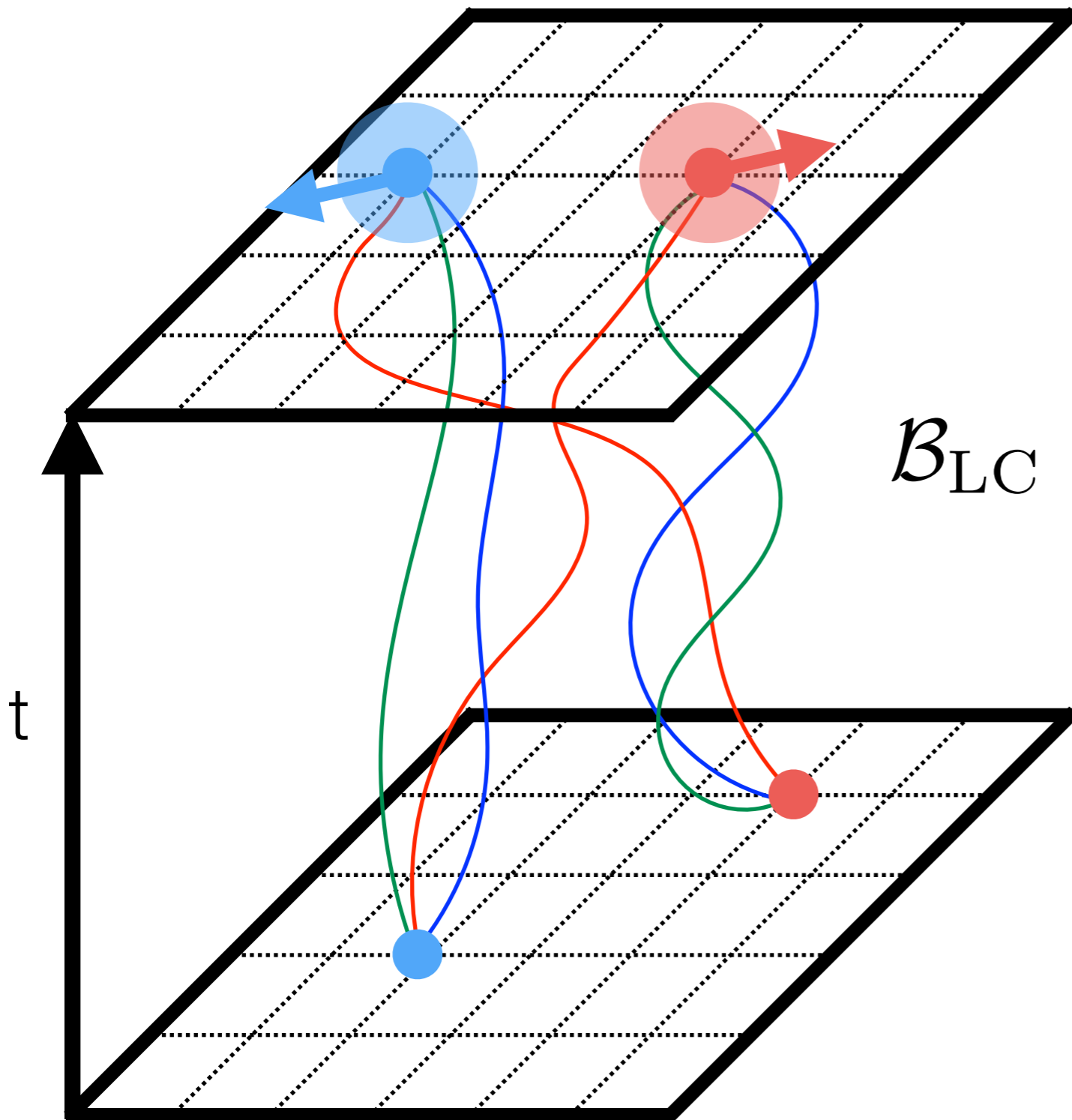
$$= (\gamma N^{(pt)} + \delta N^{(smr)}) (\gamma N^{(pt)} + \delta N^{(smr)})$$

difference is
cross terms



Easy to Incorporate into Baryon Blocks

Doi & Endres 1205.0585, Detmold & Orginos 1207.1452



multiple calls to
baryon block
construction routine

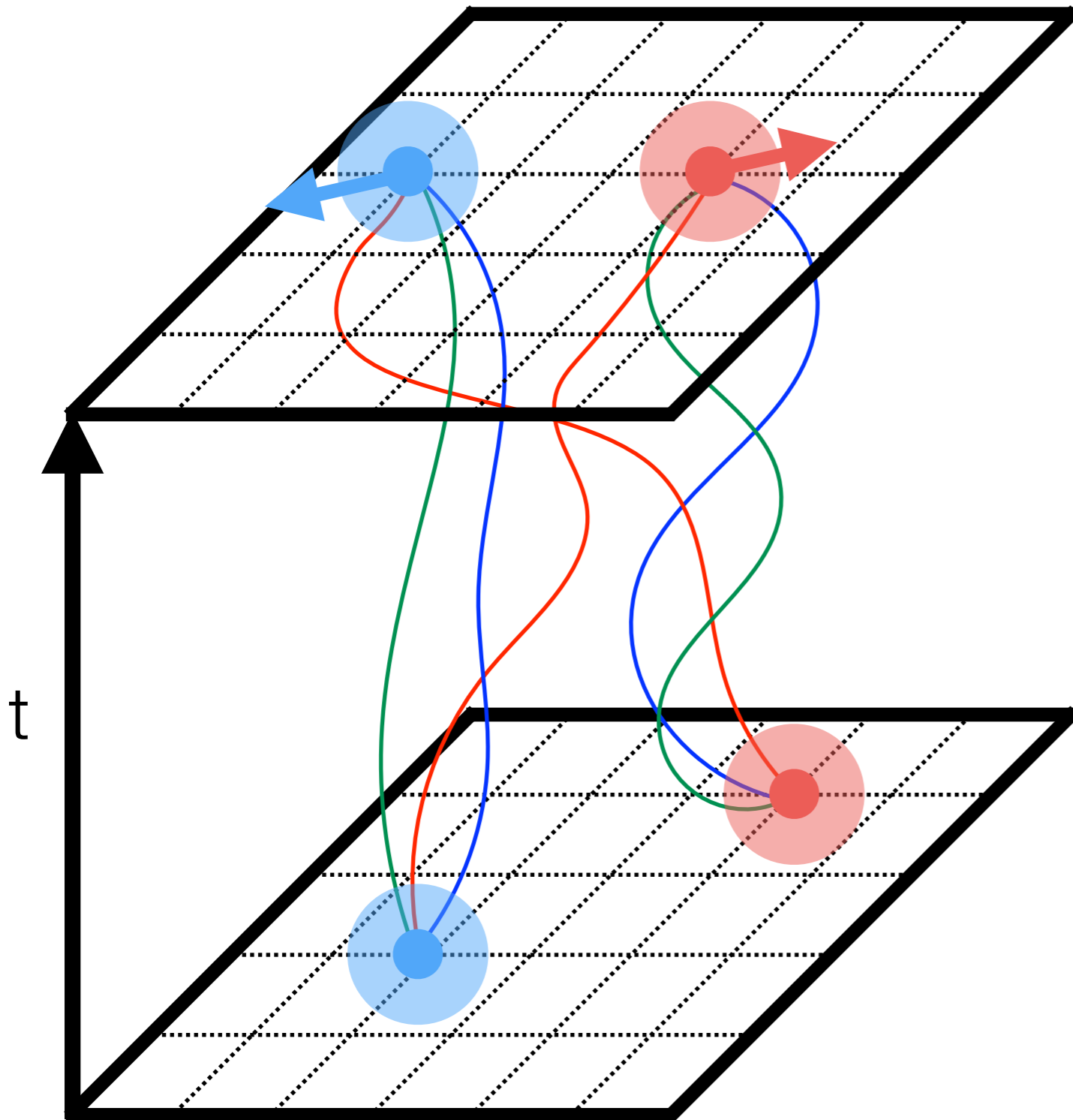
$$\mathcal{B}_{\text{LC}} = \sum_j c_j \mathcal{B}(\text{smearing}_j(S))$$

can be other baryon operators, too
e.g. HadSpec quark-displaced ops

same calls to tensor
contraction routine

$$C_{\text{LC}} = C(\mathcal{B}_{\text{LC}})$$

Source Improvement?



Tuning the 'whole proton' requires additional inversions

Adjusting quark sources is feasible but nonlinear

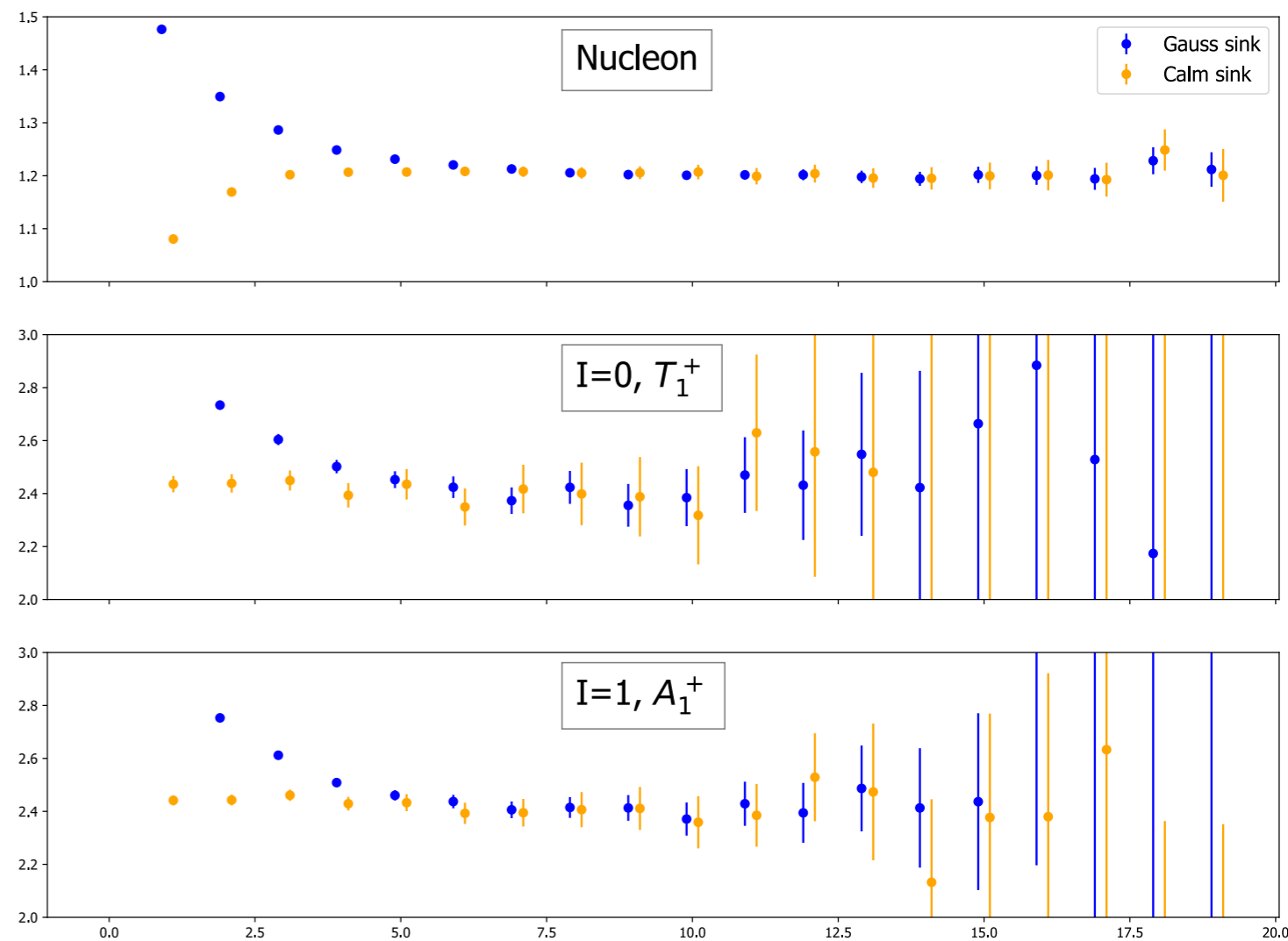
so far, unneeded



Defenestrated multi-nucleon Operators?

In preparation

- Easy to code
- Easy to tune
- Marginal additional cost (no extra inversions)
- Works even better on spatially displaced NN sources
1508.00886
- Don't fight the noise
But you still could!
eg. Wagman & Savage [1704.07356](#)
- Substantially longer plateaus for not much more work.



Defenestrated multi-nucleon Operators?

In preparation

- Ex-post-facto justification for fitting ratio?
- Plateau crisis? NN Prony or excited-state analysis should settle the issue
- Important single-N inelastic excited states in NN signal
- Not baryon (or QCD) specific, quite generally applicable
1706.06494 / C. Körber 22 June 16:20
- Can be used in matrix element calculations etc.

