Nuclear Physics from First Principles

Symmetries in Nuclei from Lattice QCD and Effective Theories

Thorsten Kurth and Evan Berkowitz for the Collaboration

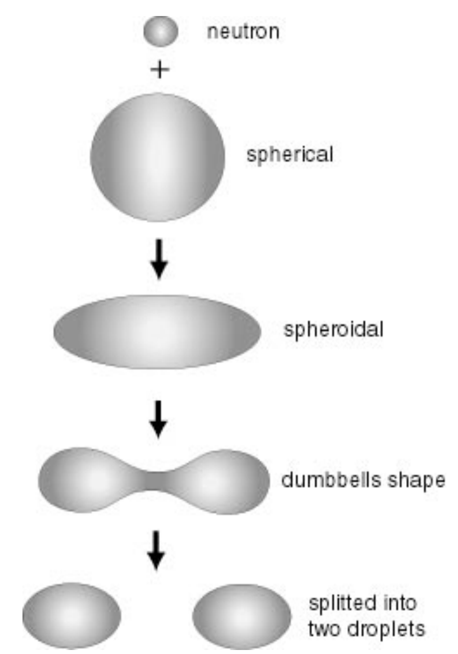
Team

- LLNL: Robert Falgout, Ron Soltz, Pavlos Vranas, Chris Schroeder, Evan Berkowitz, Enrico Rinaldi, Joe Wasem
- LBL/UCB: Wick Haxton, Thorsten Kurth, Ken McElvain, Mark Strother
- SDSU: Calvin Johnson
- nVidia: Michael Clark
- BNL: Sergey Syritsyn
- JLAB/W&M: André Walker-Loud
- JSC/Bonn University: Tom Luu

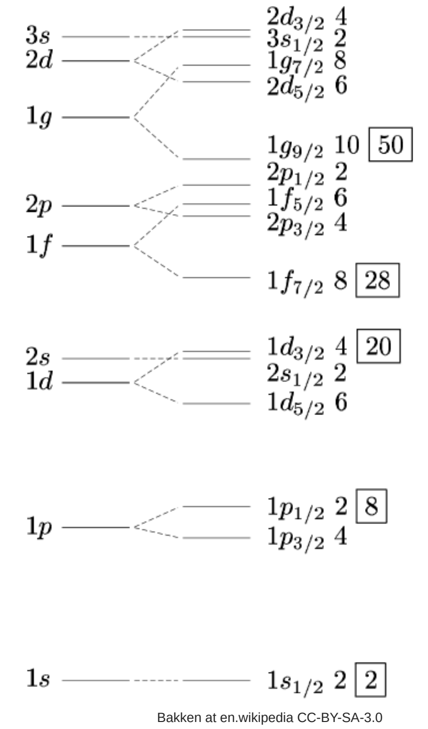
Motivation

- Historically, nuclear physics has relied on models.
- Nuclei are made of protons and neutrons, which in turn are made of quarks and gluons.
- We can use QCD to extract nucleon properties and interactions,
  - connecting model parameters to the Standard Model.
  - giving first-principles understanding.

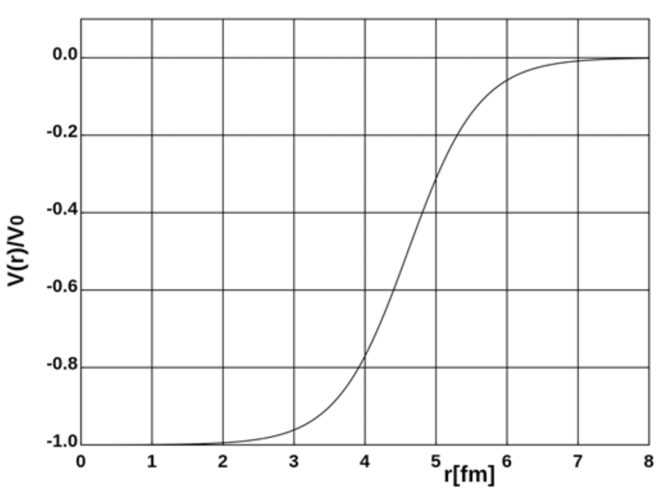
Liquid Drop



Shell



Mean Field Potentials

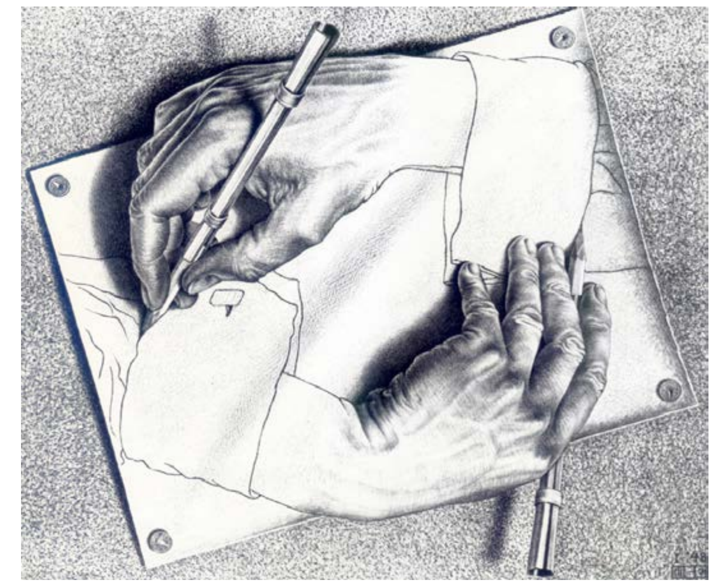


QCD

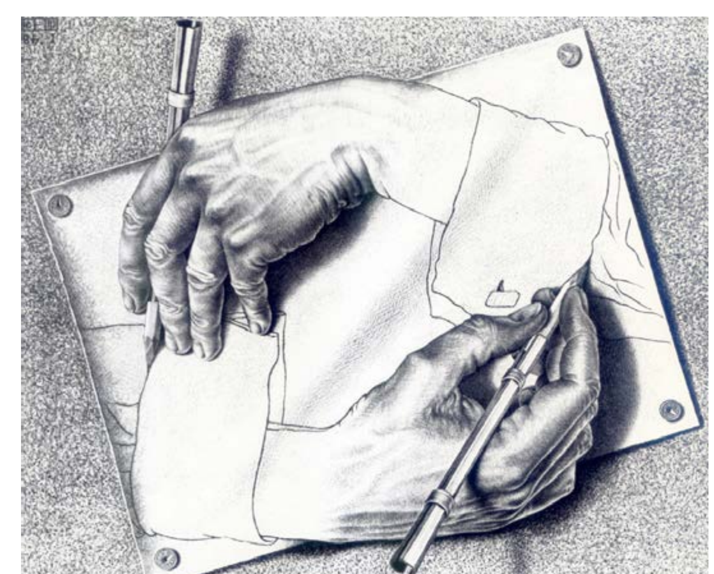
$$\mathcal{L} = \bar{\psi}(i\not{D} + m)\psi - \frac{1}{4}\mathrm{Tr}(F^2)$$

Nuclei as Laboratories

- There are observables that are *hard to measure experimentally.*
- Nuclei provide a low-energy environment where high-precision “experiments” happen all the time.
- Can test many-body physics.
- Hadronic electroweak neutral current responsible for parity violation (PV) is the least constrained observable in the SM.
  - Weak interaction is $\sim G_F F_\pi^2 = \mathcal{O}(10^{-7})$ compared to strong interaction $\sim \mathcal{O}(1)$.
  - Nuclear data show *enhanced* isoscalar and *suppressed* isovector PV.



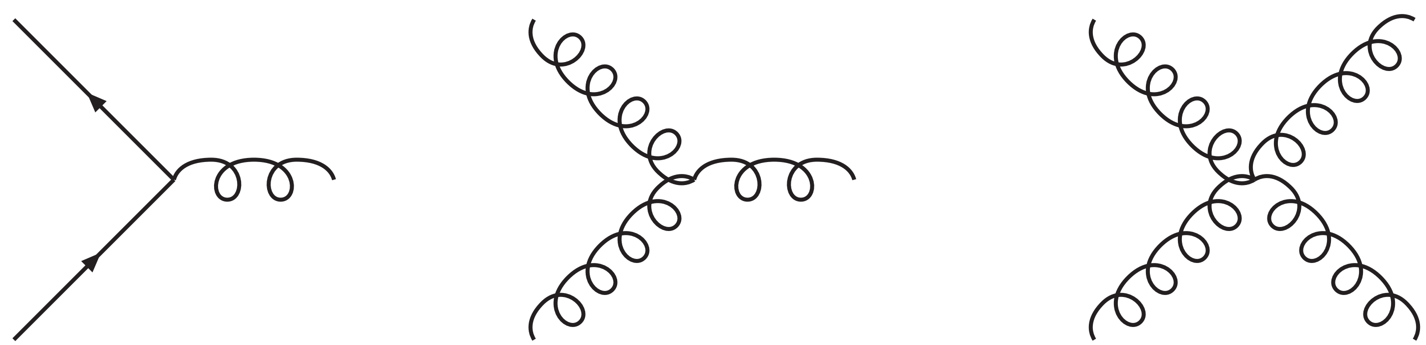
PV $\neq$ Vꟼ



What is QCD?

- Quantum Chromodynamics is the fundamental theory of strong/nuclear interactions (fusion, fission, α-decay, …)

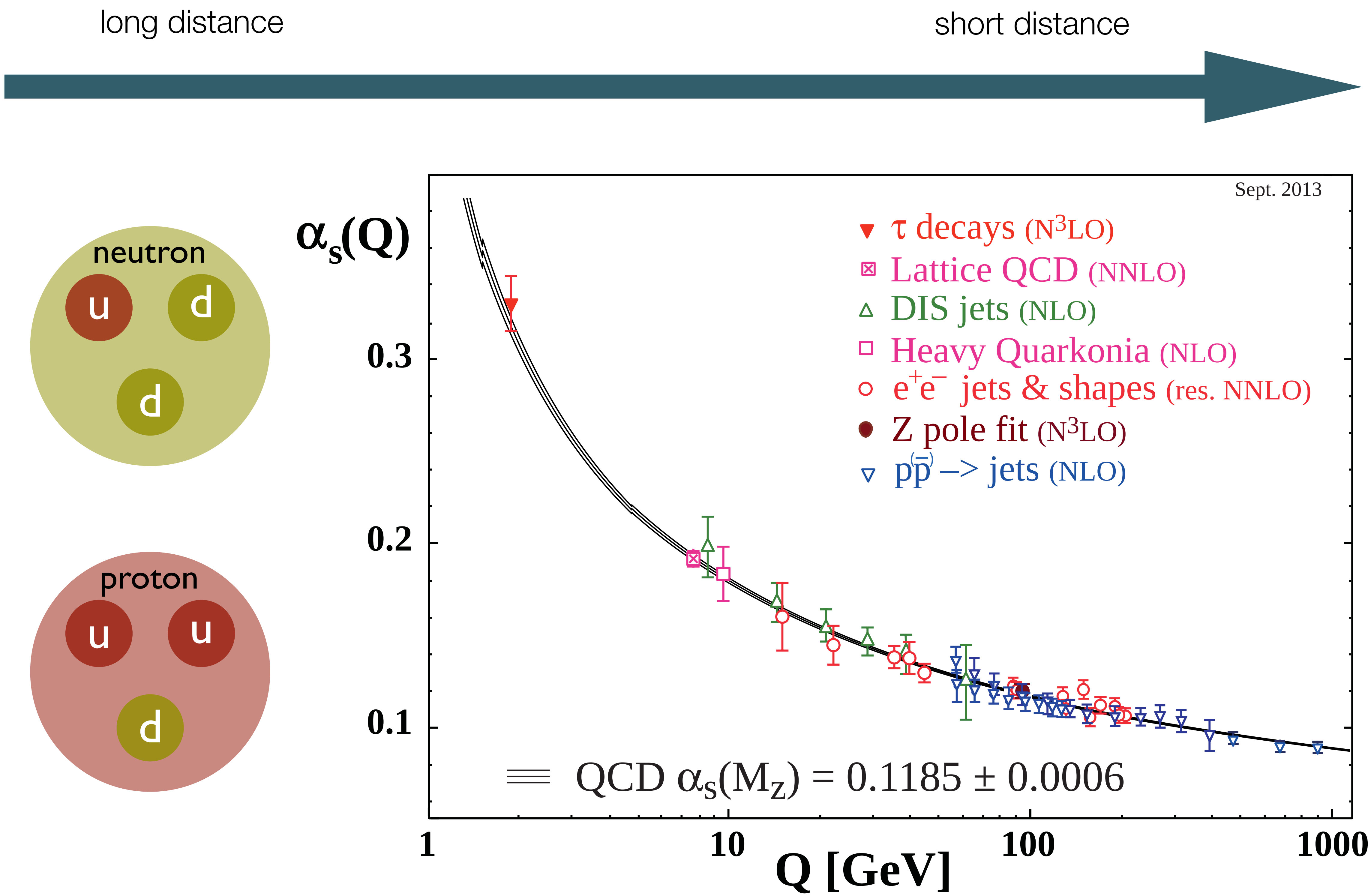
- QCD describes interactions between Quarks and Gluons



g $\qquad$ g $\qquad$ g^2

Quark-Gluon coupling (QED-like) $\qquad$ Gluon self-interaction

- QCD features confinement (small energies) and asymptotic freedom (large energies)



long distance
short distance
neutron
u
d
d
proton
u
u
d
Sept. 2013
αs(Q)
τ decays (N3LO)
Lattice QCD (NNLO)
DIS jets (NLO)
Heavy Quarkonia (NLO)
e+e− jets & shapes (res. NNLO)
Z pole fit (N3LO)
pp(−) –> jets (NLO)
0.3
0.2
0.1
QCD αs(MZ) = 0.1185 ± 0.0006
1
10
100
1000
Q [GeV]

How to solve QCD?

- QCD is described by infinite dimensional integrals

$$Z_E = \int \mathrm{D}U_\mu \, \mathrm{D}\psi \, \mathrm{D}\bar{\psi} \, \exp\left(-S_g[U] - \int_{\mathbb{R}^4} \mathrm{d}^4x \, \bar{\psi}(x) D[U] \psi(x)\right)$$

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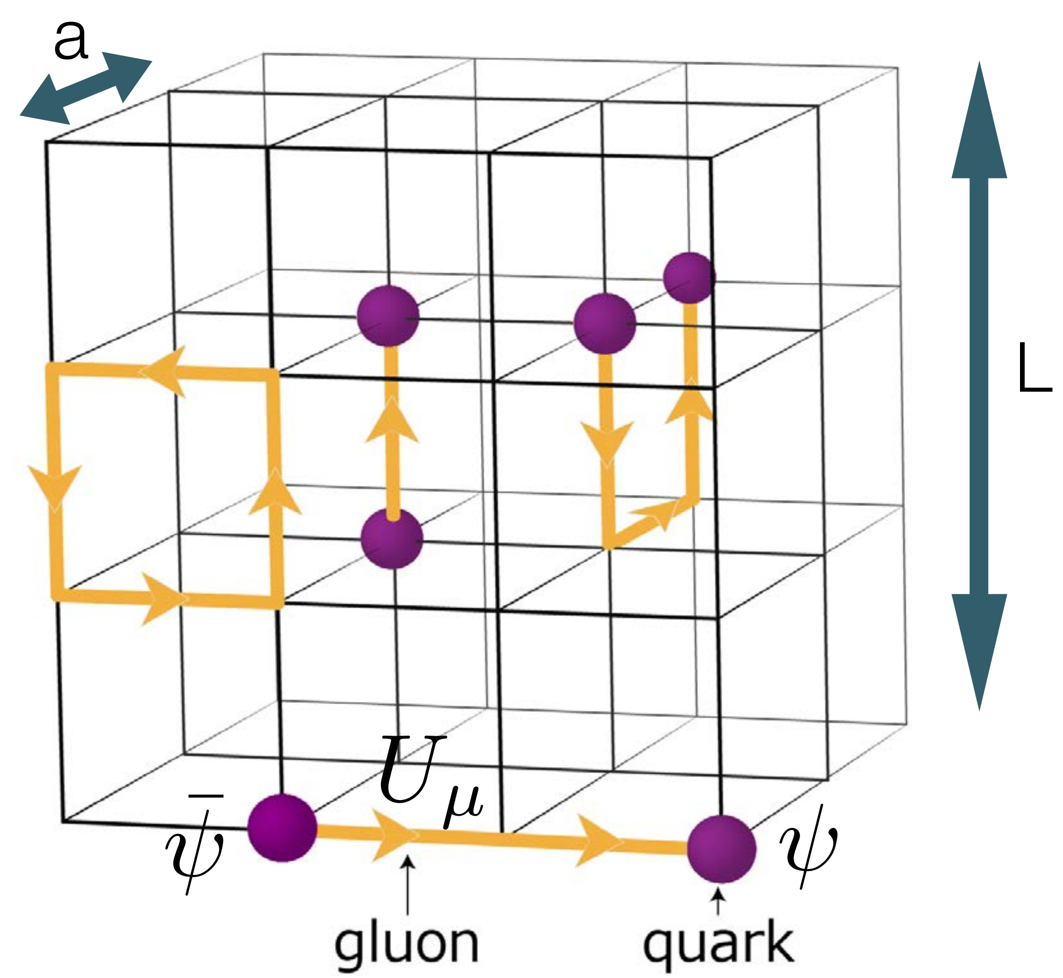

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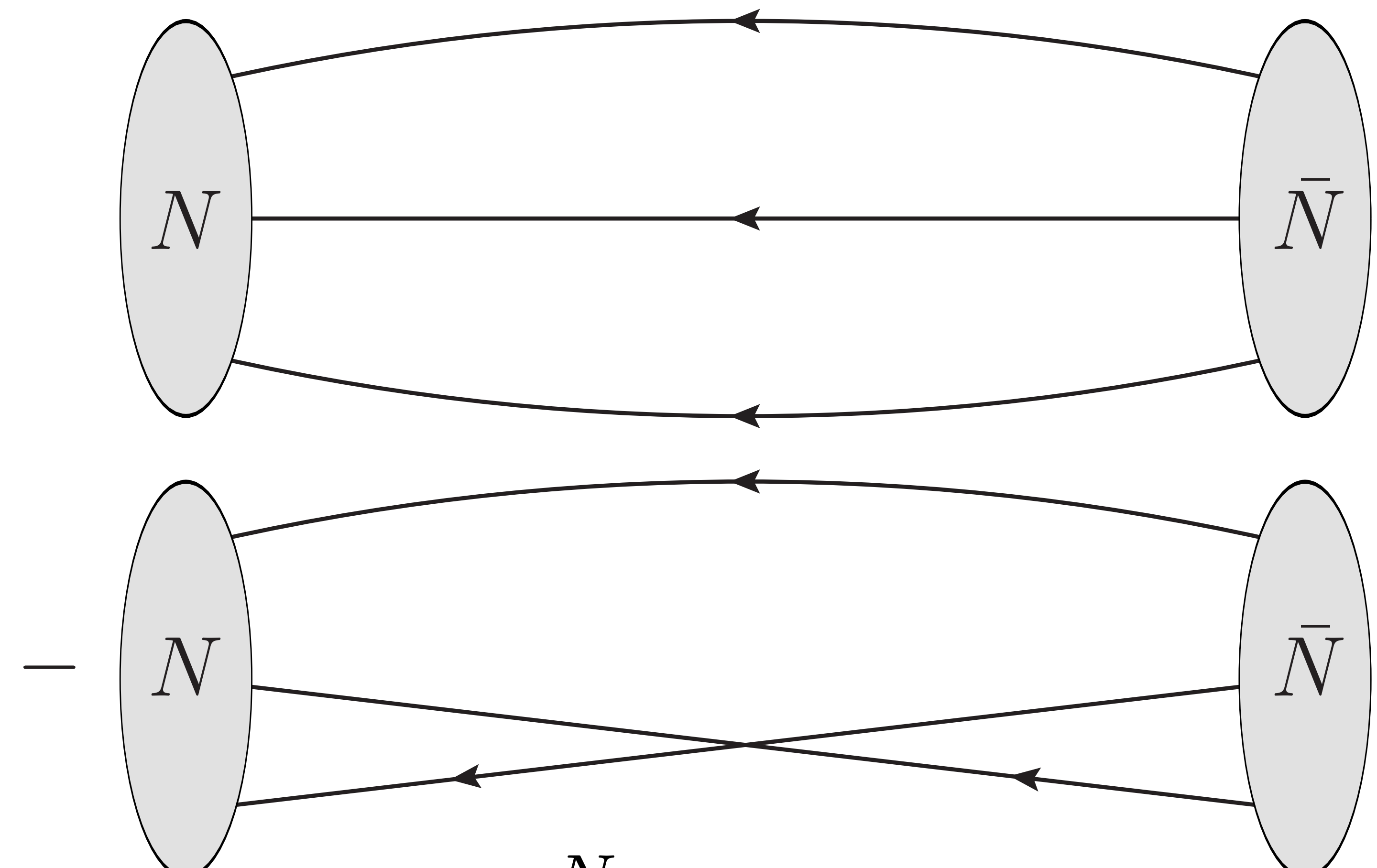

$$\langle \mathcal{O} \rangle \approx \frac{1}{N} \sum_{n=1}^{N} \mathcal{O}[U_n, D[U_n]^{-1}]$$

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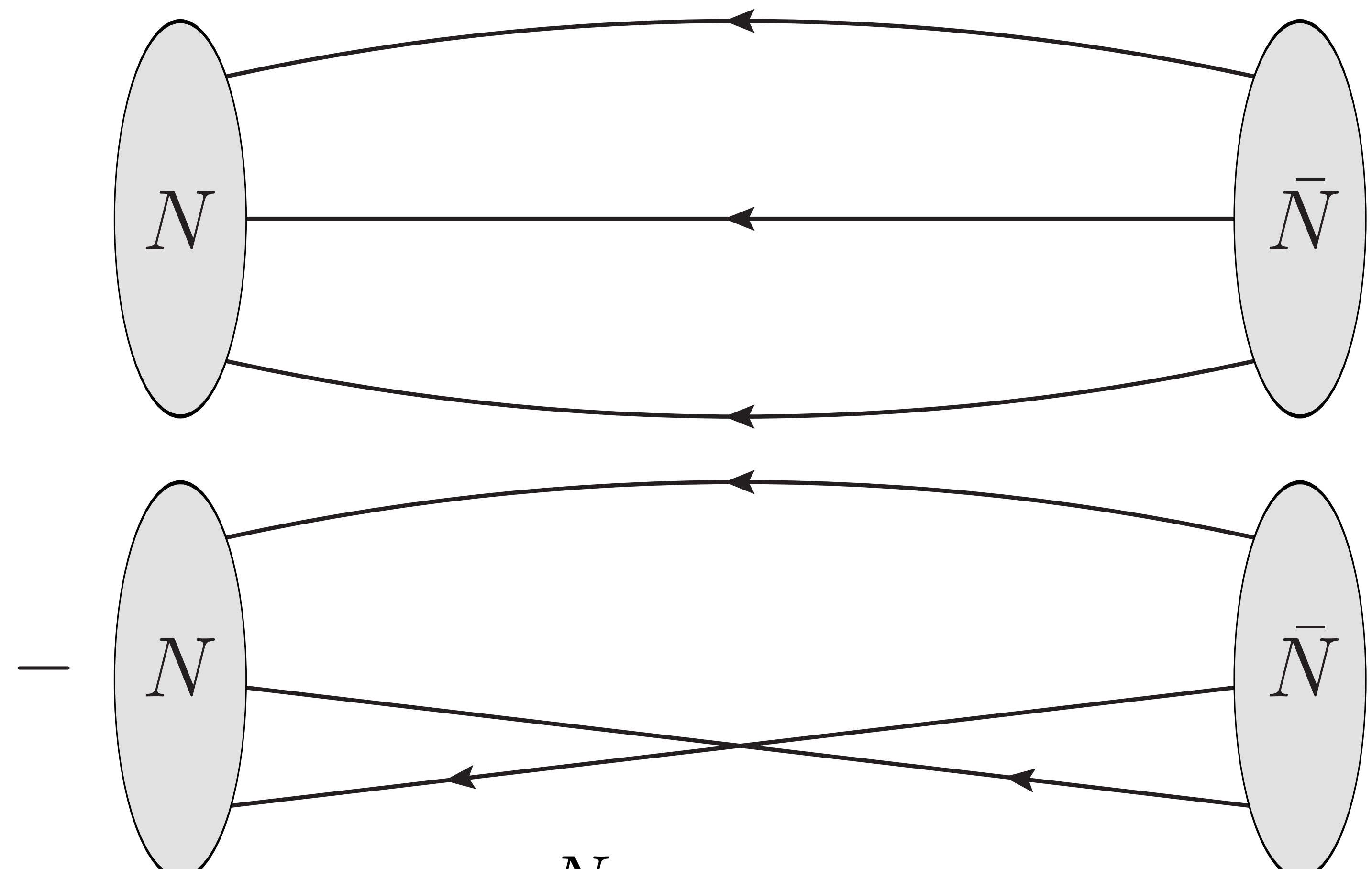

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- but: $t_{CPU} \sim a^{-5}$

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$$= \int \mathrm{D}U_\mu \, \mathrm{D}\phi \, \mathrm{D}\phi^\dagger \, \exp\left(-S_g[U] - \int_{\mathbb{R}^4} \mathrm{d}^4x \, \phi^\dagger(x) D[U]^{-\frac{1}{2}} \phi(x)\right)$$

expensive matrix inversions

$$S(x,y) = \overbrace{\psi(x)\bar{\psi}}(y) = D[U]^{-1}(x,y)$$

How to solve QCD?

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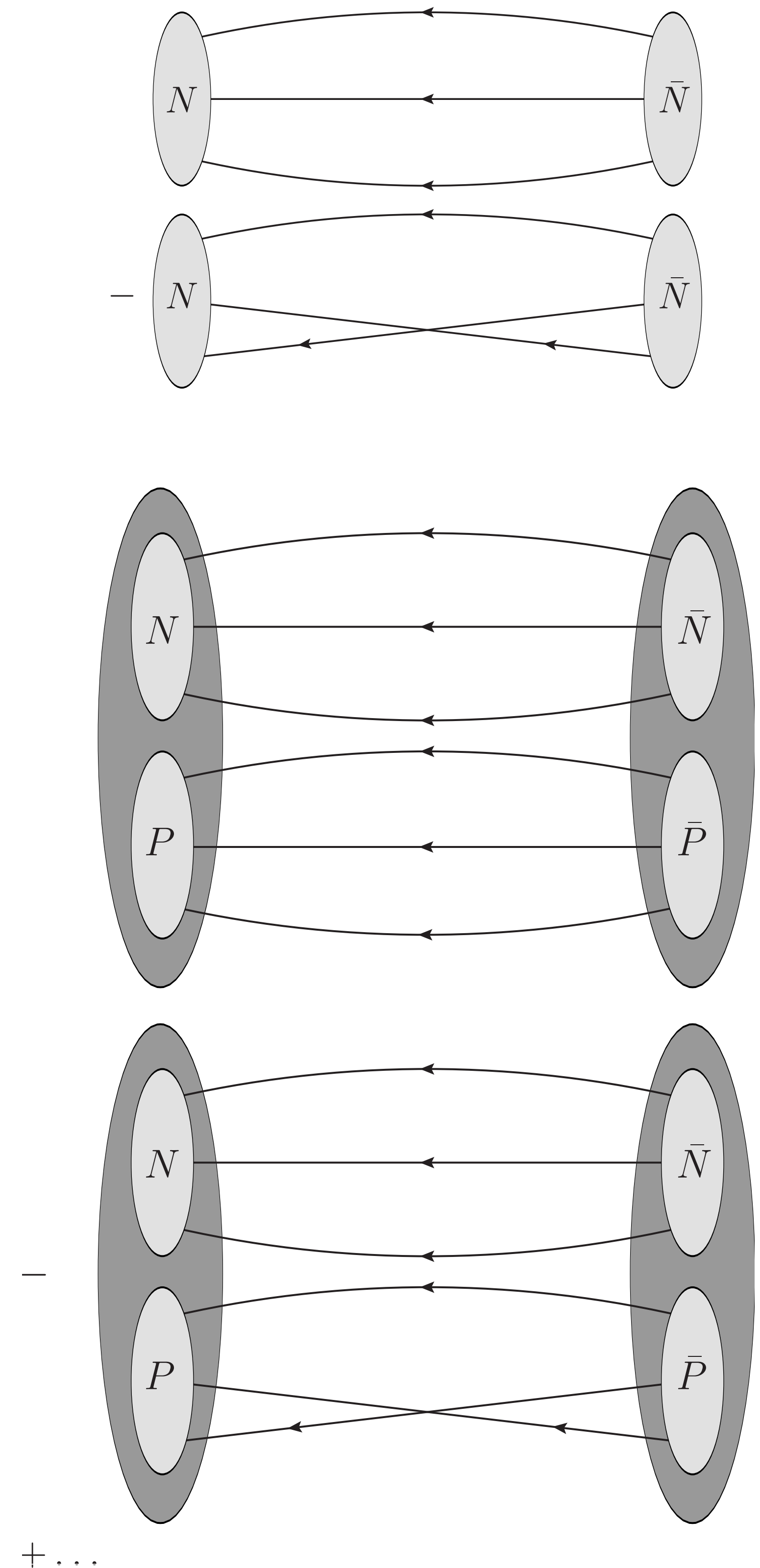
- generate configurations and extract observables
- perform limit $a \to 0$, $L \to \infty$ to recover continuum QCD
- but: $t_{CPU} \sim a^{-5}$
- big computers needed

Nuclear Physics from Bottom Up

- compute multi-nucleon correlation functions



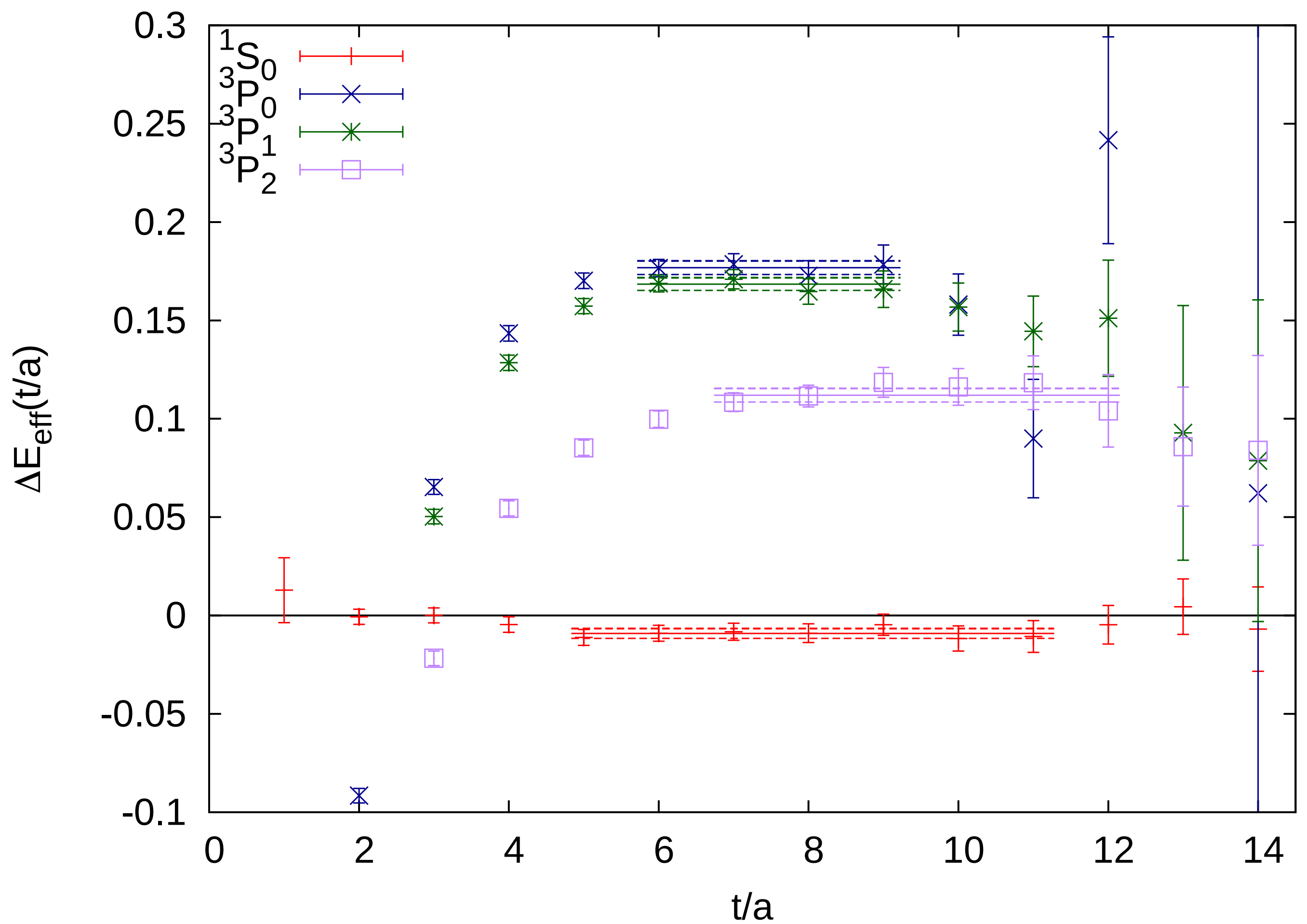
single Nucleon
2!1!=2

deuteron
3!3!=36

He$_3$-scattering 5!4!=2880

Nuclear Physics from Bottom Up

- compute multi-nucleon correlation functions
- measure energy difference between interacting and non-interacting system



$$\Delta E^{\Gamma}_{\mathrm{eff}}(t) = \frac{1}{2}\log\left(\frac{C^{\Gamma}_{NN}(t-1)}{C^{\Gamma}_{NN}(t+1)}\frac{C^{2}_{N}(t+1)}{C^{2}_{N}(t-1)}\right)$$

Nuclear Physics from Bottom Up

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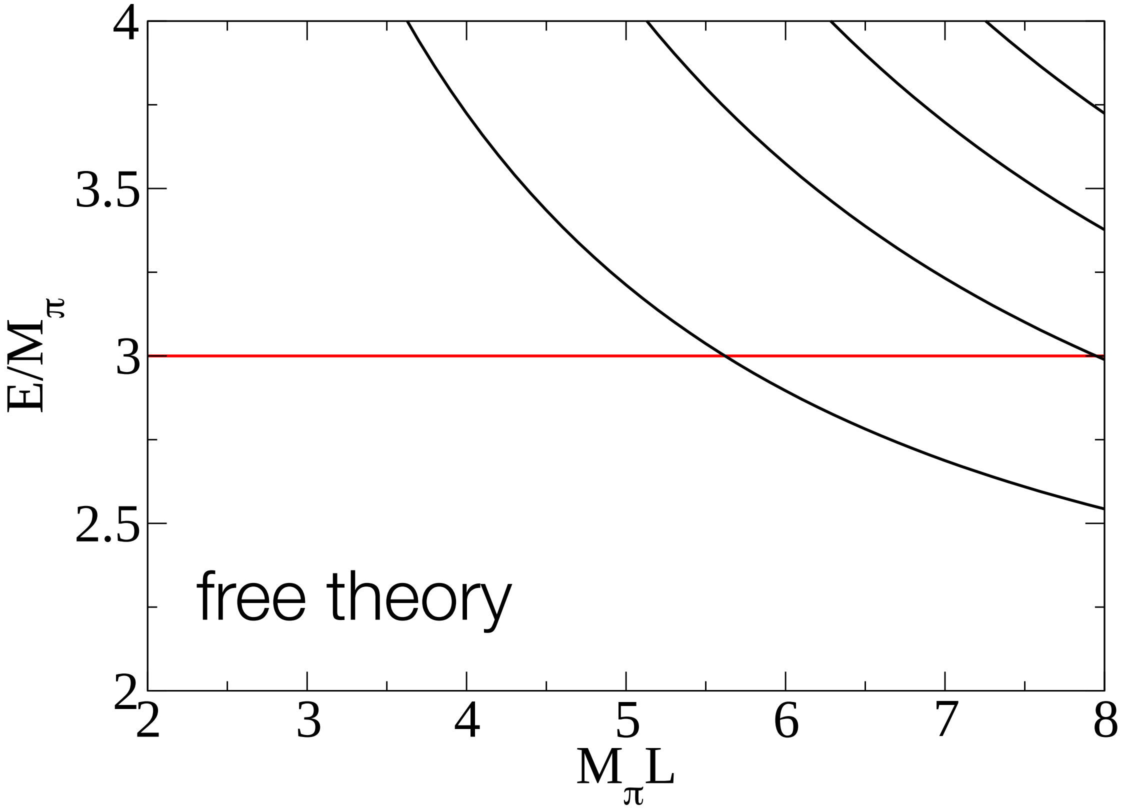
- use Lüscher's finite volume formula to relate measured energies to phase shifts δ(k)



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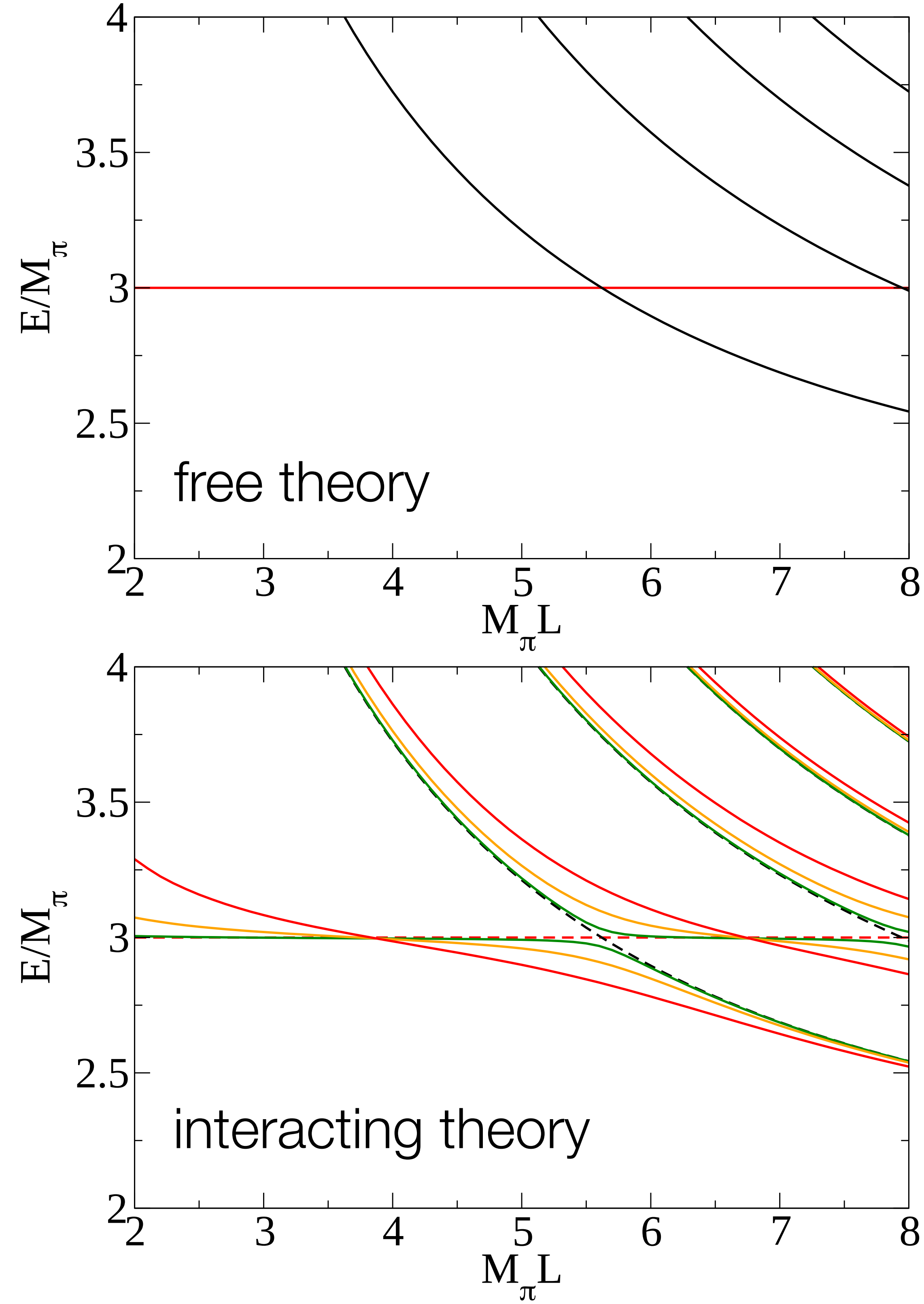

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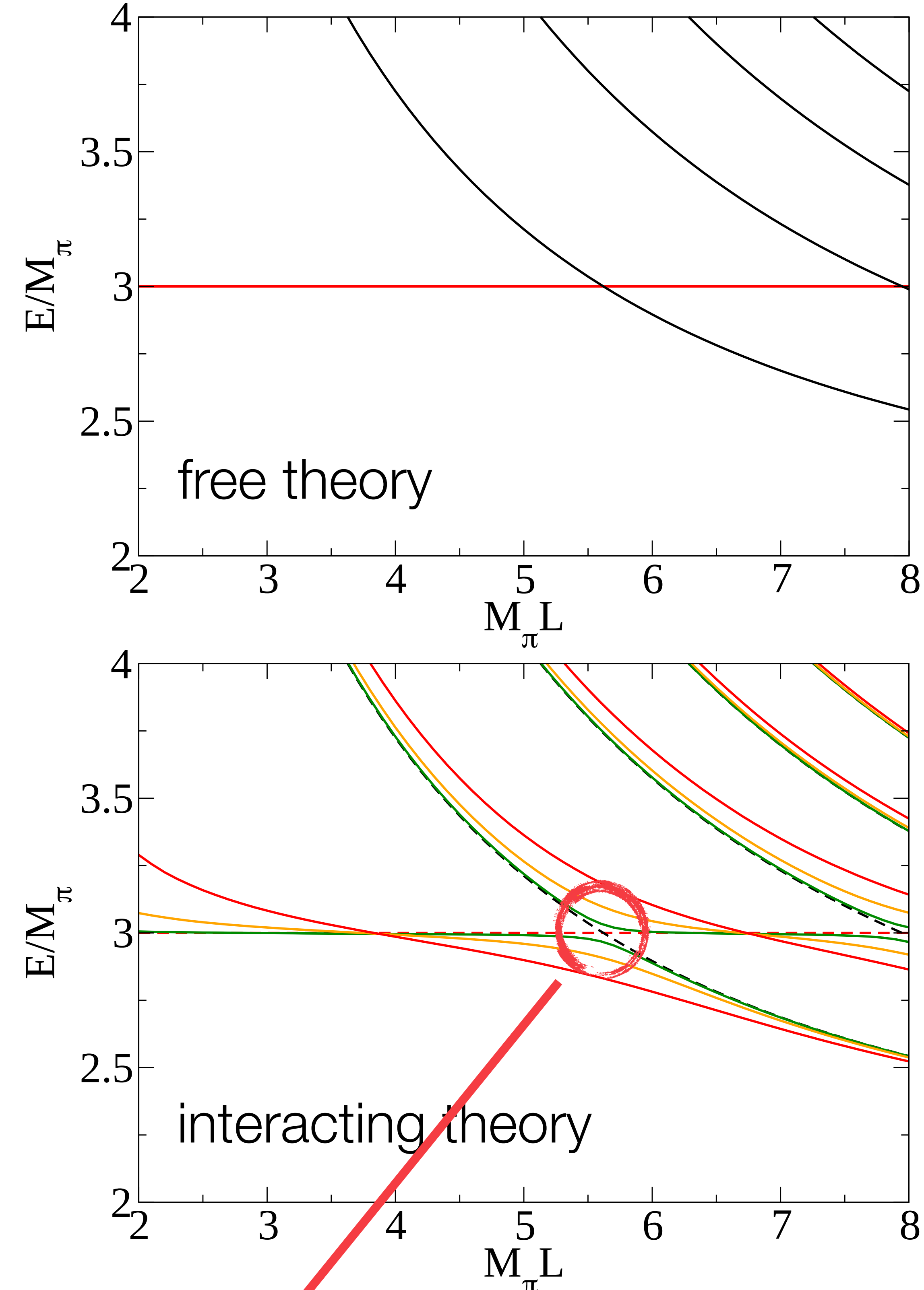
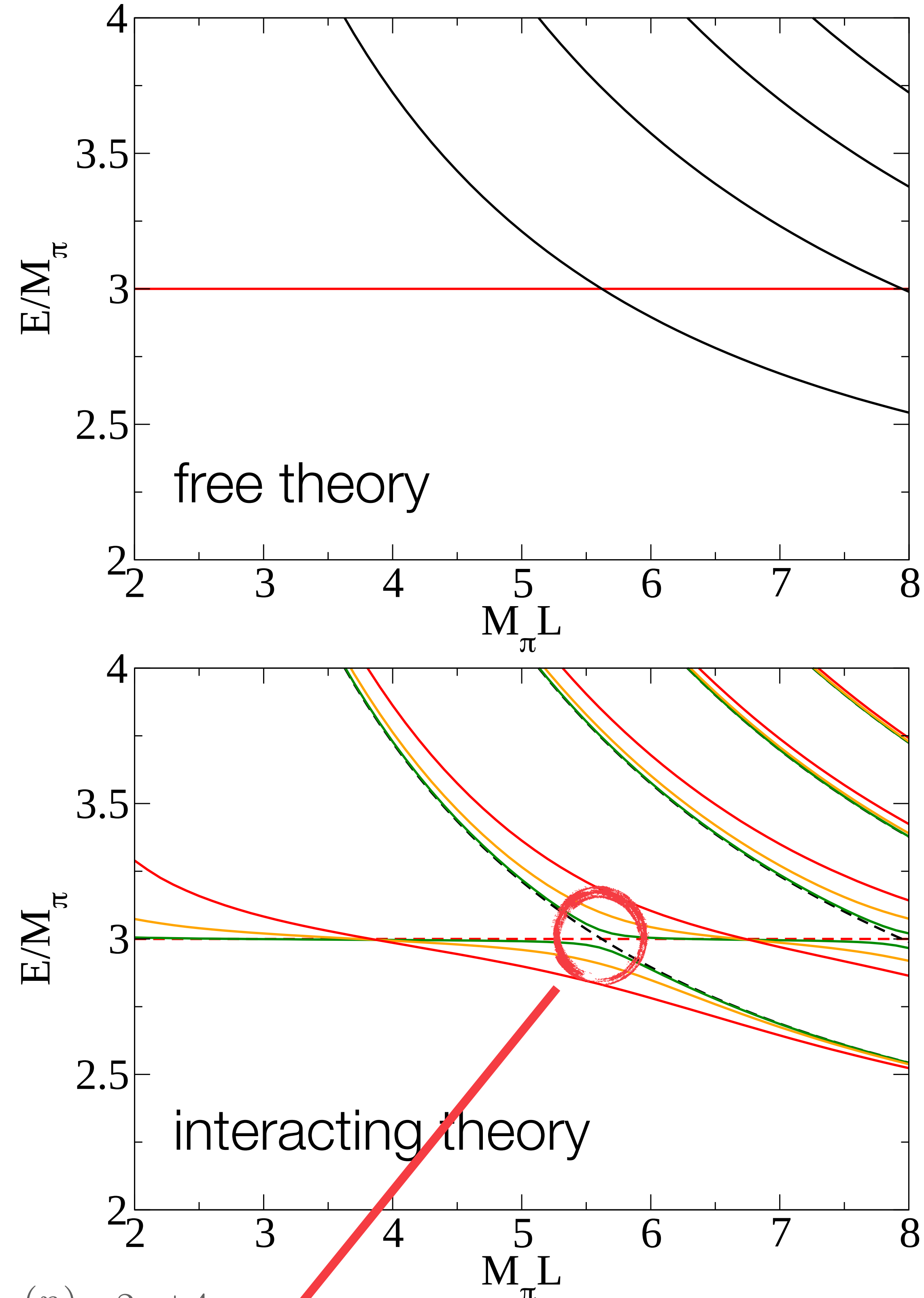


$$\Delta E \to k^2 \xrightarrow{\text{LFV}} \delta(k^2)$$

Nuclear Physics from Bottom Up

- compute multi-nucleon correlation functions
- measure energy difference between interacting and non-interacting system
- use Lüscher's finite volume formula to relate measured energies to phase shifts δ(k)
- compute low energy observables from effective range expansion

$$k^{2l+1}\cot\delta_l(k^2) = -\frac{1}{a_l} + \frac{1}{2}r_l\,k^2 + \sum_{n=0}^{\infty}(-)^{n+1}P_l^{(n)}\,k^{2n+4}$$



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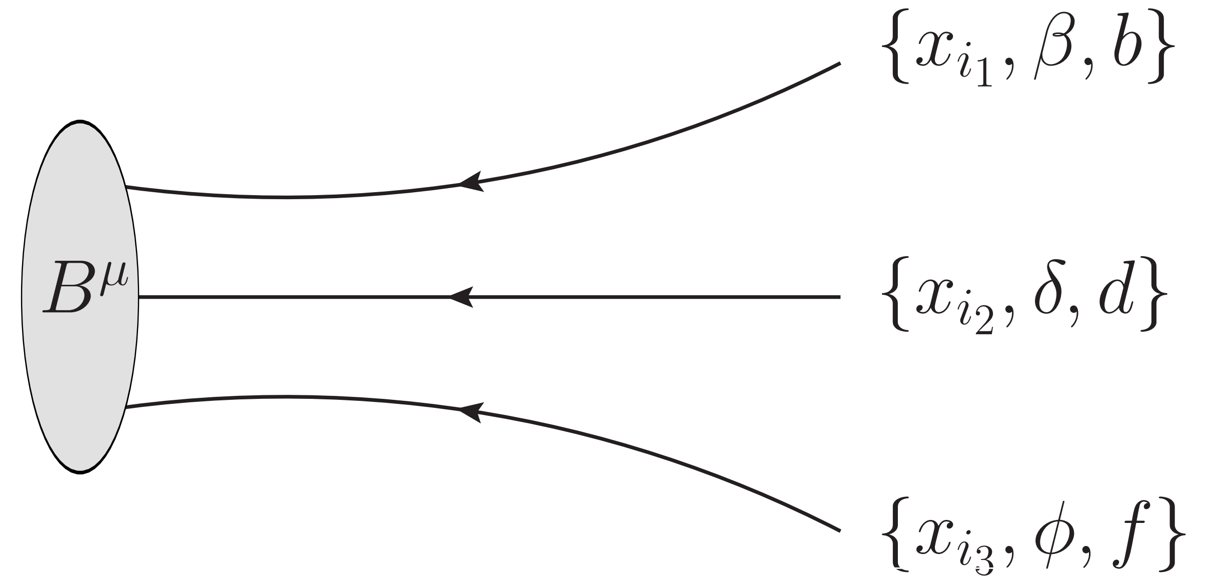

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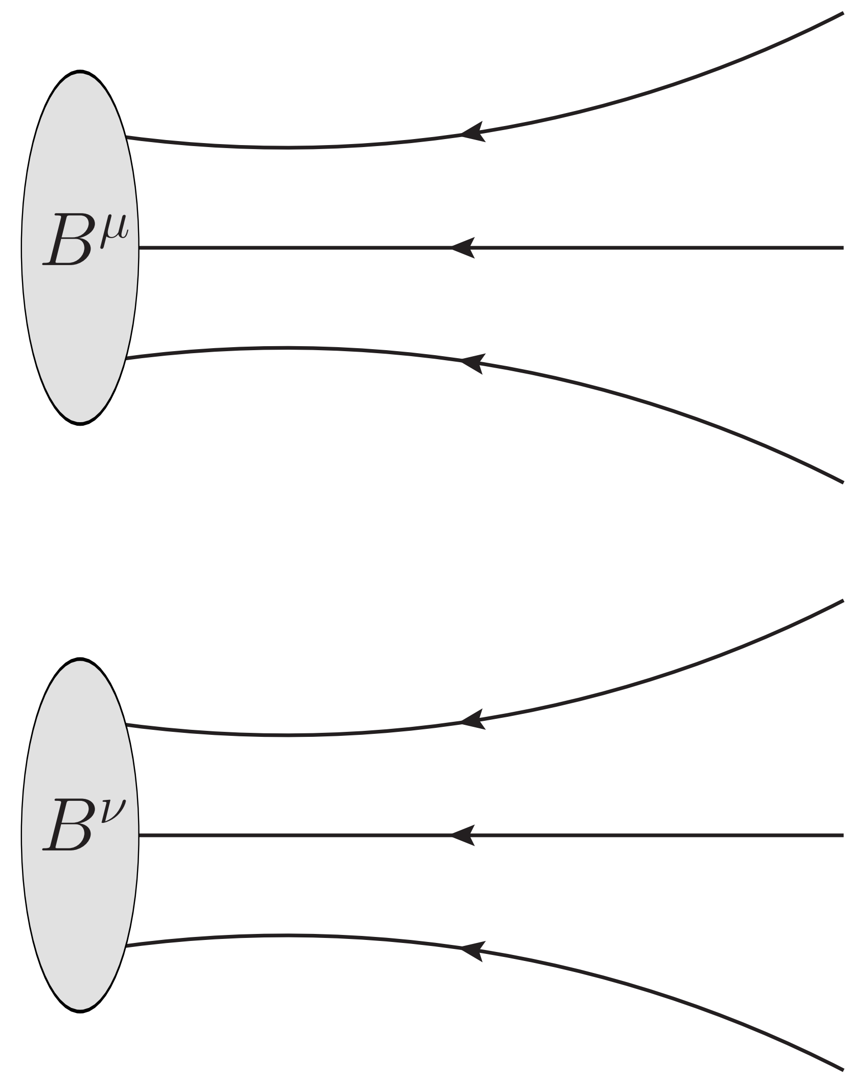

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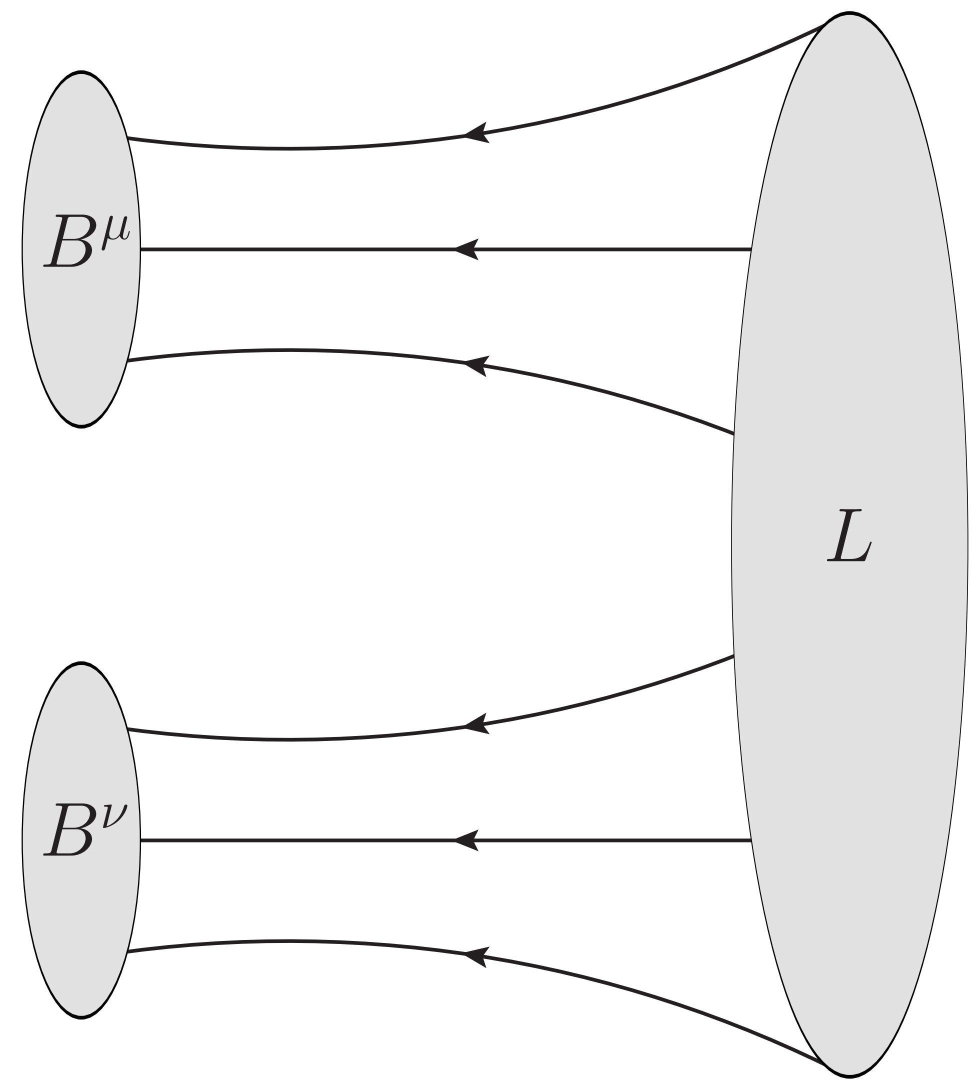

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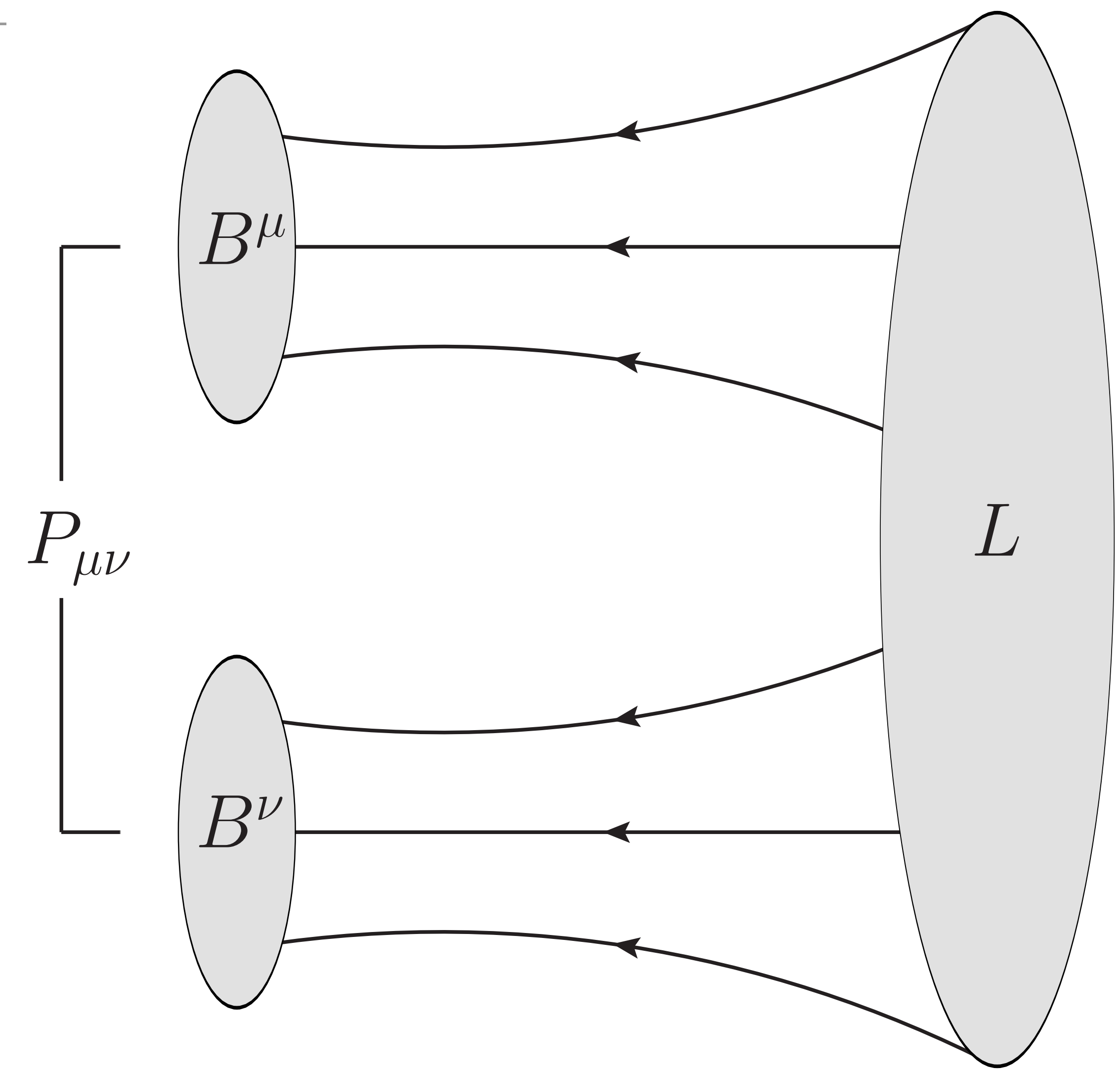

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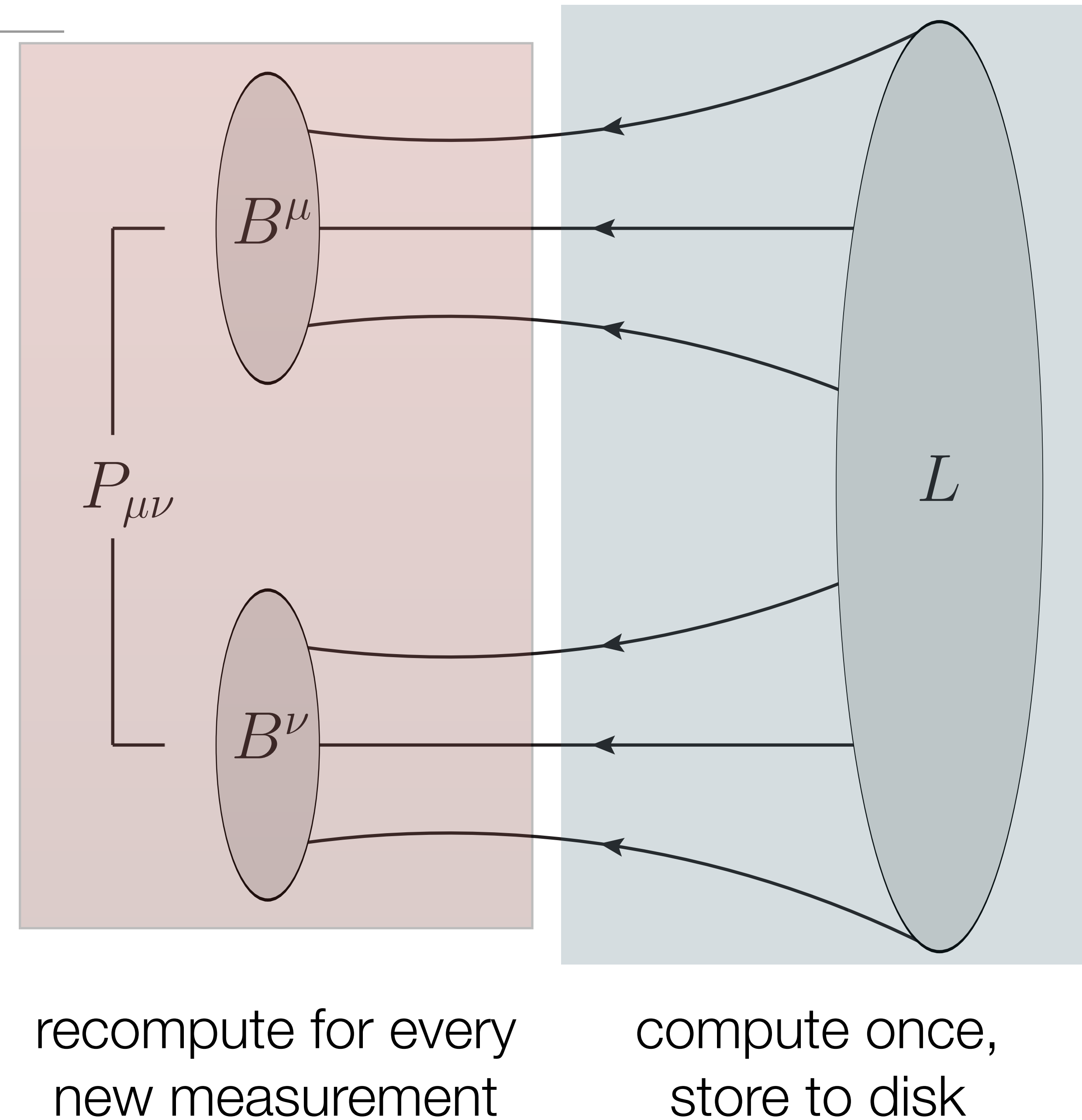

Challenges

- number of contractions/ diagrams grows combinatorially
  - Baryon blocks
  - use automatic code generation

```
pp = Proton[sink][xf, μ] ** bar[Proton[source][xi, ν]] ** SpinProjector[Same, Spin[ν, μ]];

contractions = Contract[pp];
Notation[contractions]
```

$$\mathrm{Same}_{\nu\mu}\, C\gamma_{5\,\nu''\,\rho''}\, C\gamma_{5\,\nu'\,\rho'}\, \mathrm{S}[\mathrm{down},\, \mathrm{xf}-\mathrm{xi}]^{b'b''}_{\nu'\nu''}\, \mathrm{S}[\mathrm{up},\, \mathrm{xf}-\mathrm{xi}]^{a'c''}_{\mu\rho''}\, \mathrm{S}[\mathrm{up},\, \mathrm{xf}-\mathrm{xi}]^{c'a''}_{\rho'\nu}\, \epsilon^{a''b''c''}\, \epsilon^{a'b'c'} - \mathrm{Same}_{\nu\mu}\, C\gamma_{5\,\nu''\,\rho''}\, C\gamma_{5\,\nu'\,\rho'}\, \mathrm{S}[\mathrm{down},\, \mathrm{xf}-\mathrm{xi}]^{b'b''}_{\nu'\nu''}\, \mathrm{S}[\mathrm{up},\, \mathrm{xf}-\mathrm{xi}]^{a'a''}_{\mu\nu}\, \mathrm{S}[\mathrm{up},\, \mathrm{xf}-\mathrm{xi}]^{c'c''}_{\rho'\rho''}\, \epsilon^{a''b''c''}\, \epsilon^{a'b'c'}$$

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```
Generate[BaryonBlocks][contractions] // Notation
```

$$-\mathrm{BaryonBlock}[\mathrm{Color}[b, d, f], \mathrm{Flavor}[\mathrm{down}, \mathrm{up}, \mathrm{up}], \mathrm{SpaceTime}[\mathrm{xf}, \{\mathrm{xi}, \mathrm{xi}, \mathrm{xi}\}], \mathrm{Spin}[\epsilon, \beta, \delta, \phi]]\left(\mathrm{Same}_{\phi\epsilon}\, C\gamma_{5\,\beta\,\delta} + \mathrm{Same}_{\delta\epsilon}\, C\gamma_{5\,\beta\,\phi}\right) \epsilon^{bdf}$$

Challenges

$$\sum_{\mu,\nu,A,B} P_{\mu\nu}\, B_A^{\mu}\, B_B^{\nu}\, L_{AB} = \mathbf{v}^T M \mathbf{v}$$

vector-Matrix-vector product

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- calculating the contractions is expensive: use GPUs

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vector-Matrix-vector product

```
p[tid] = v[I1[tid]] * M[tid] * v[I2[tid]];
```

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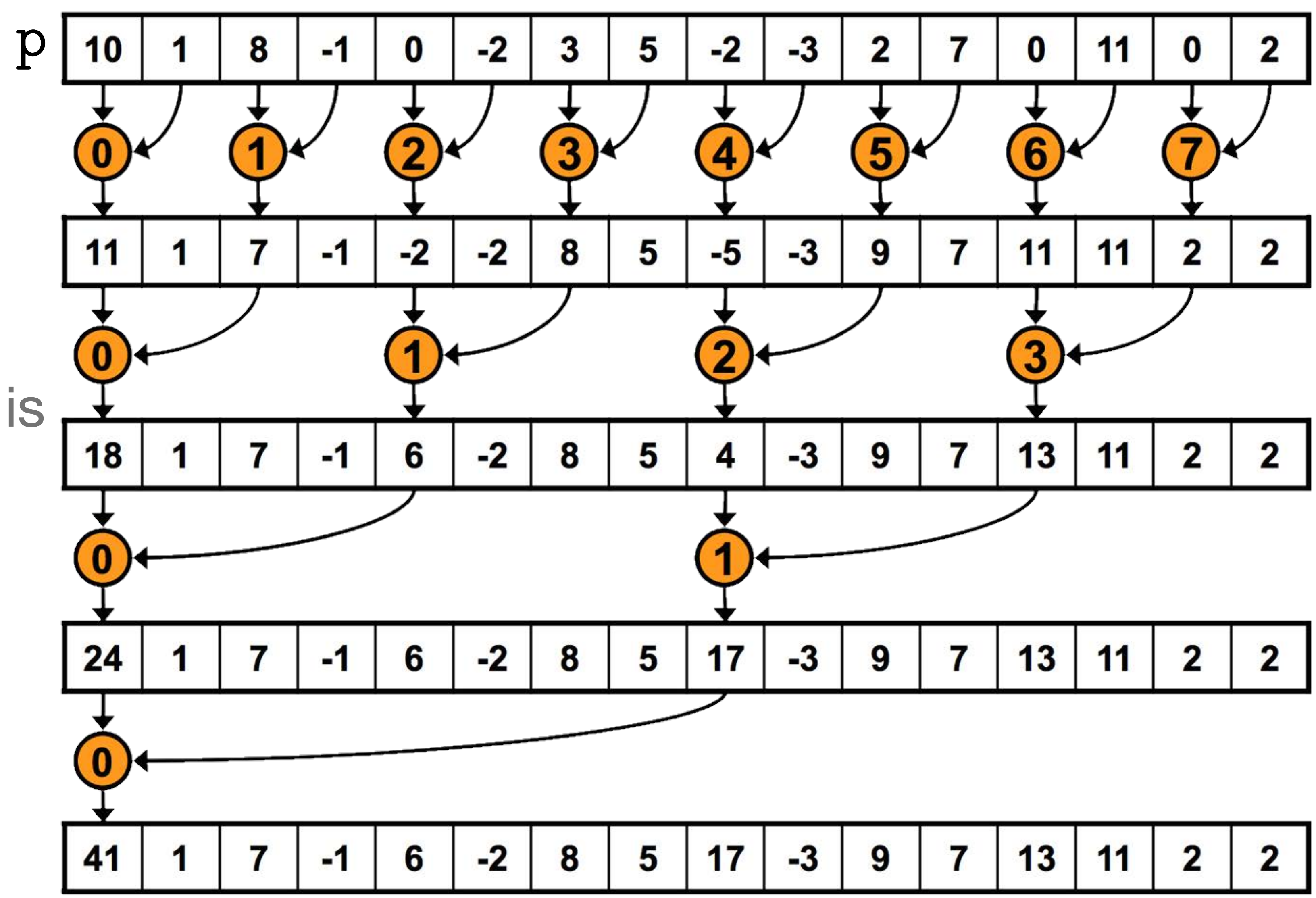

Challenges

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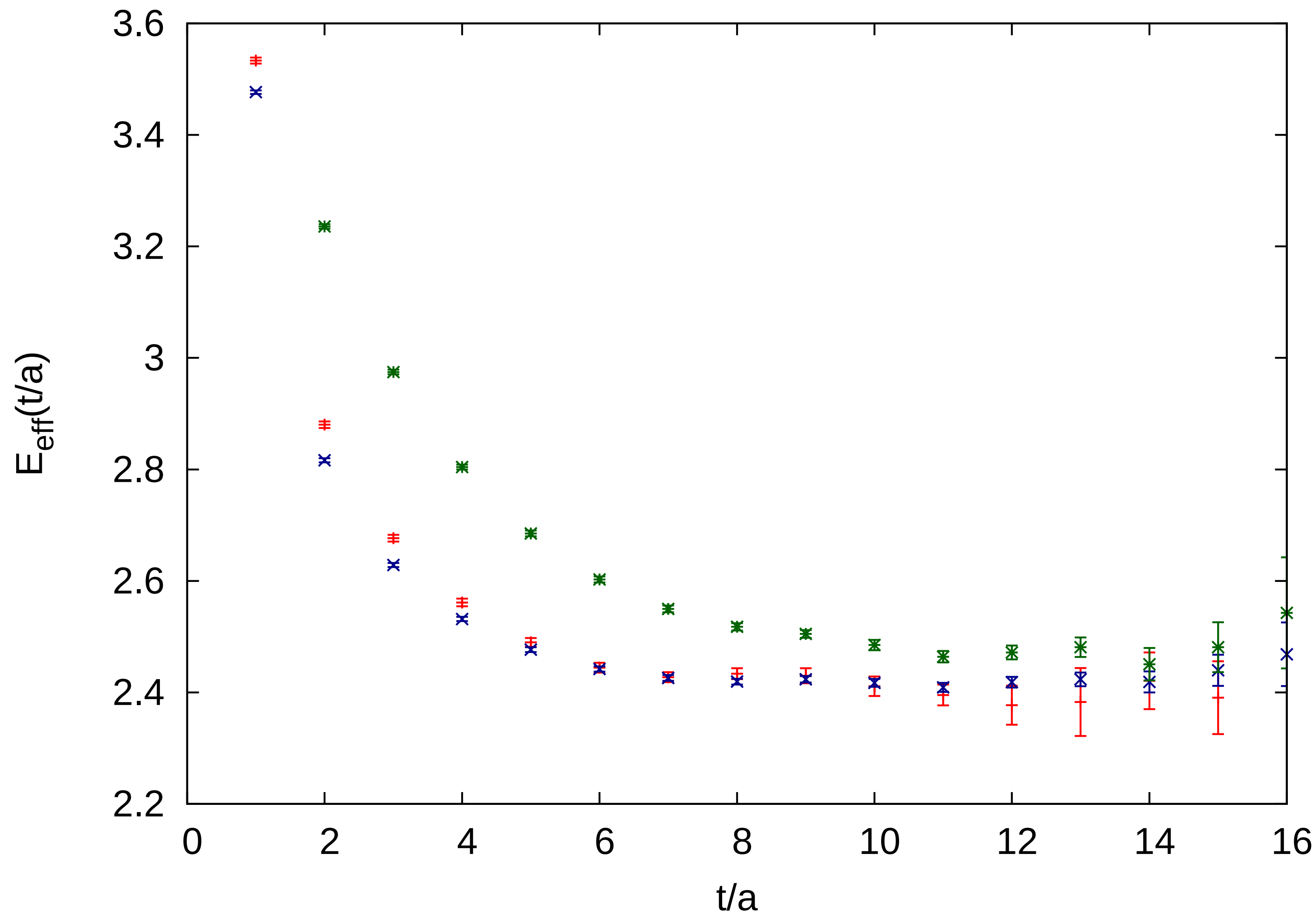
- excited states contributions: sink/source engineering

$$C(t,t_0) = \sum_{n=0}^{\infty} \tilde{Z}_n^* Z_n \, e^{-m_n(t-t_0)}$$



use sources/sinks with spatially displaced nuclei

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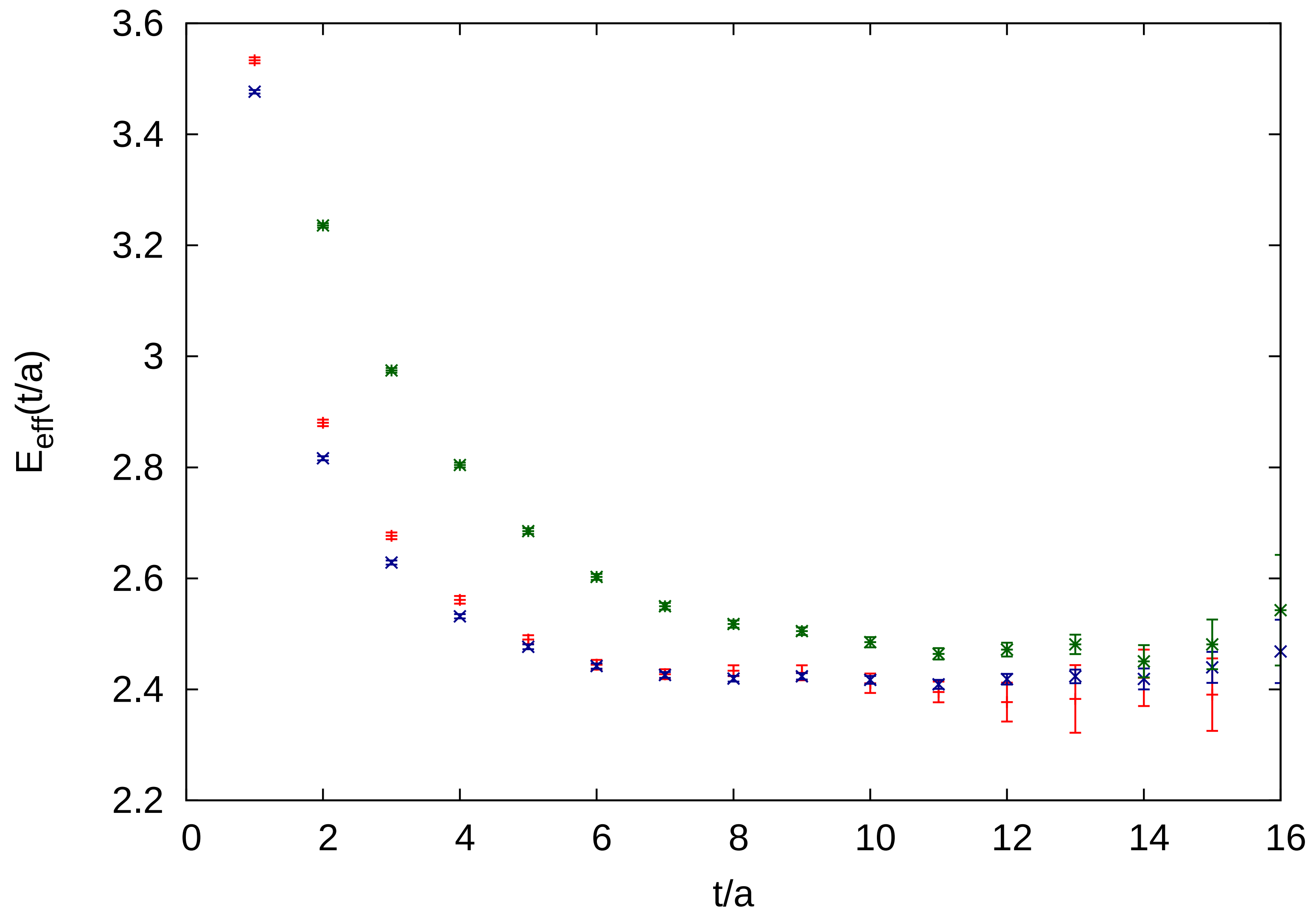

use sources/sinks with spatially displaced nuclei

Lepage Argument

- signal-to-noise ratio of correlation functions

$$\mathrm{SNR} \sim \frac{\langle N\bar{N}\rangle}{\sqrt{\langle (N\bar{N})(N\bar{N})^\dagger\rangle - \langle N\bar{N}\rangle^2}}$$

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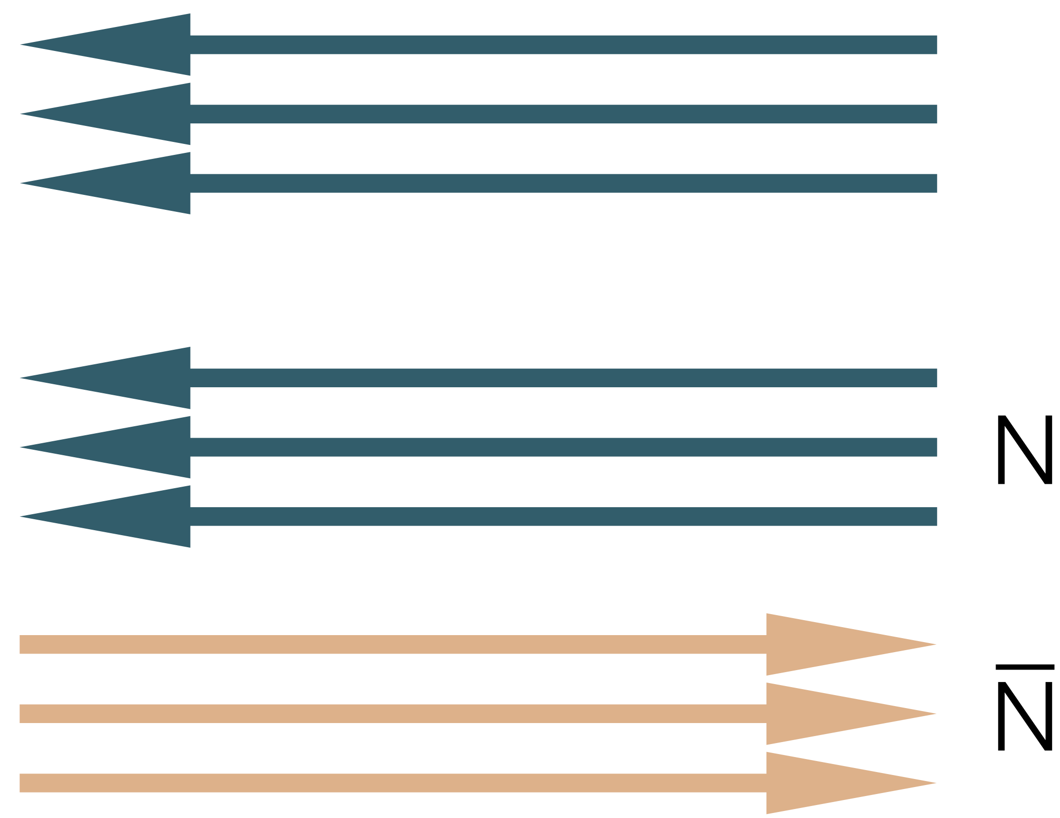
- numerator $\sim \exp(-m_N t)$
- denominator



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- numerator
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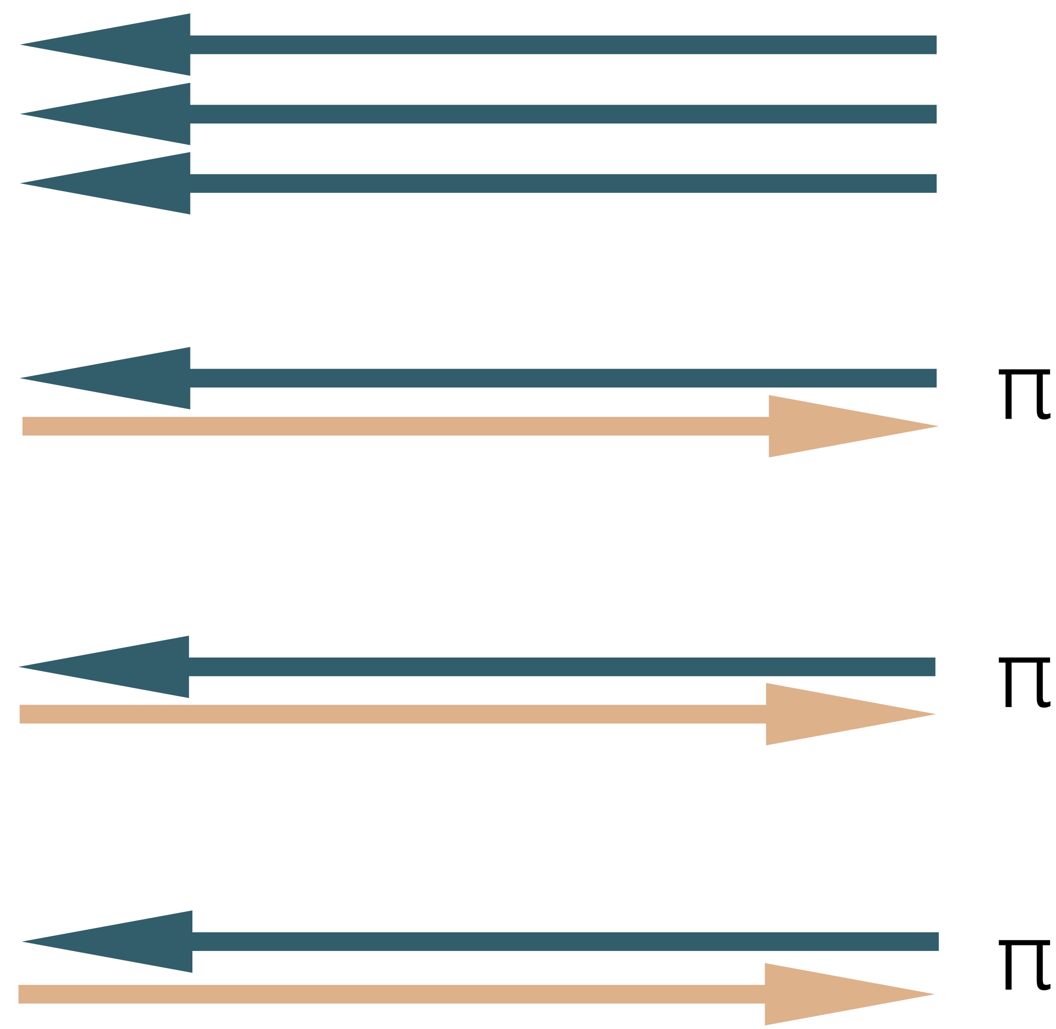
- denominator
  $\sim \exp\left(-\frac{3}{2}m_\pi t\right)$



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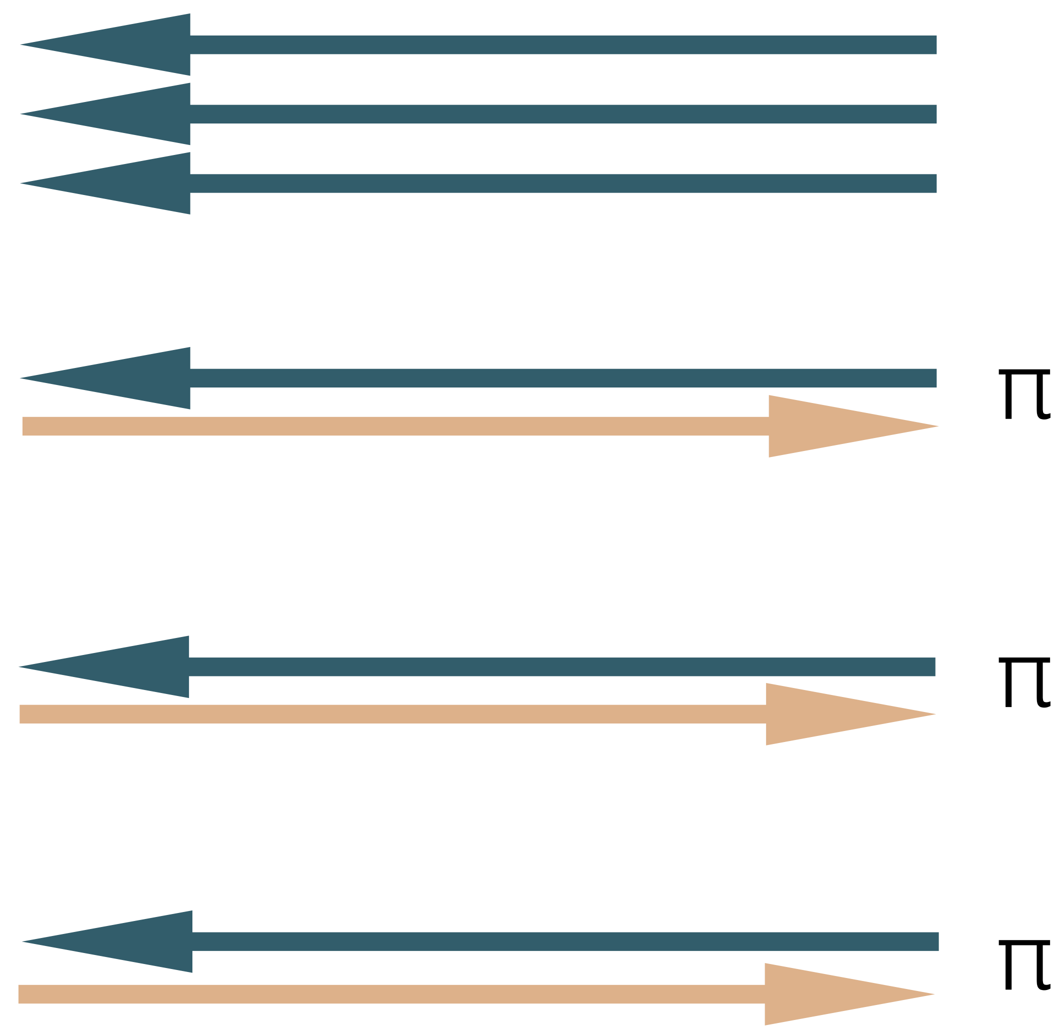
- signal-to-noise ratio of correlation functions
- numerator
  $\sim \exp(-m_N t)$
- denominator
  $\sim \exp\left(-\frac{3}{2}m_\pi t\right)$
- time-dependence of SNR
  $\sim \sqrt{N}\exp\left[-A\left(m_N - \frac{3}{2}m_\pi\right)t\right]$



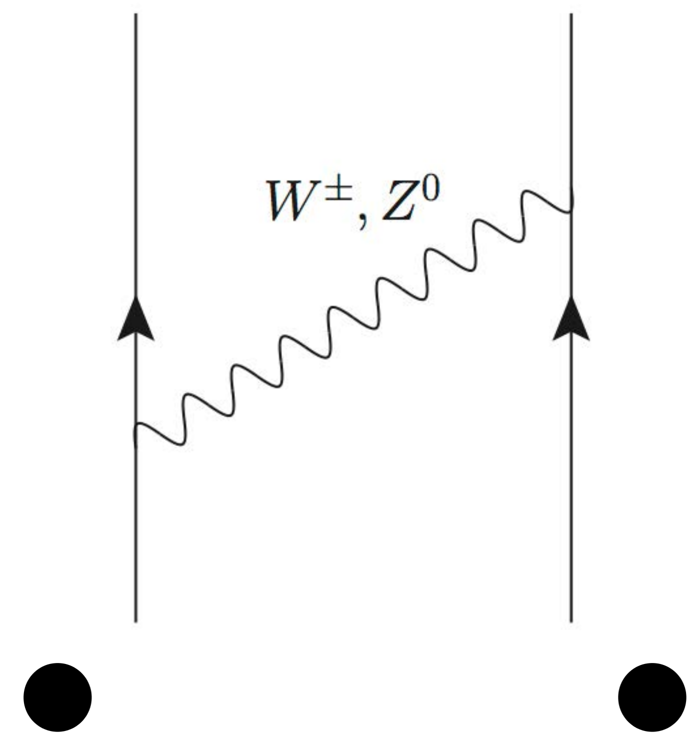
huge statistics needed (MG)
huge amount of storage needed (HDF5)
large pion mass

Parity Violation - Contractions $\Delta I = 2$

- 2 Baryon s-wave source

Parity Violation - Contractions ΔI=2

- 2 Baryon s-wave source
- EW vertices ⇒ 4-quark operator insertion



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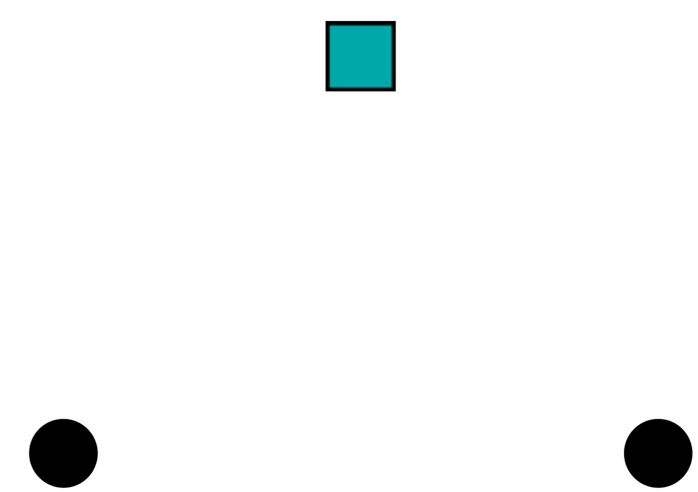

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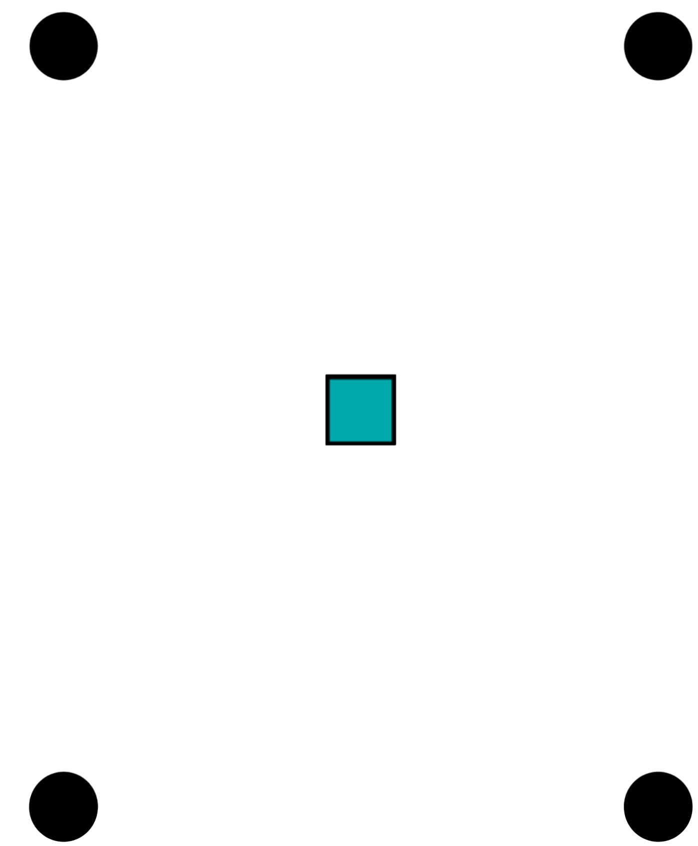

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- 2 Baryon s-wave source
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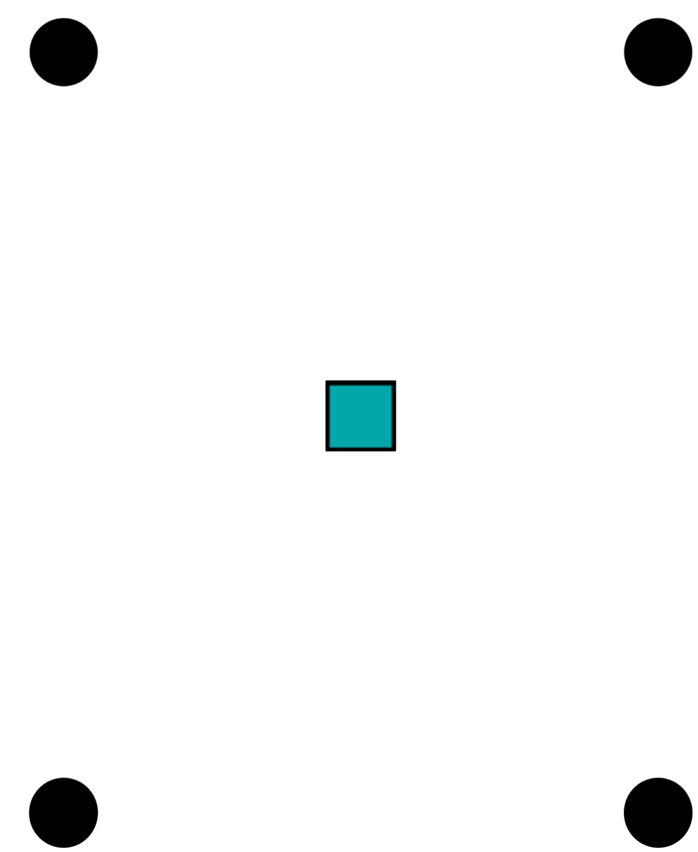
- In total there are 4896 contractions.
- Degenerate light quarks reduce this to 2208.
- Requires 15 tensors.



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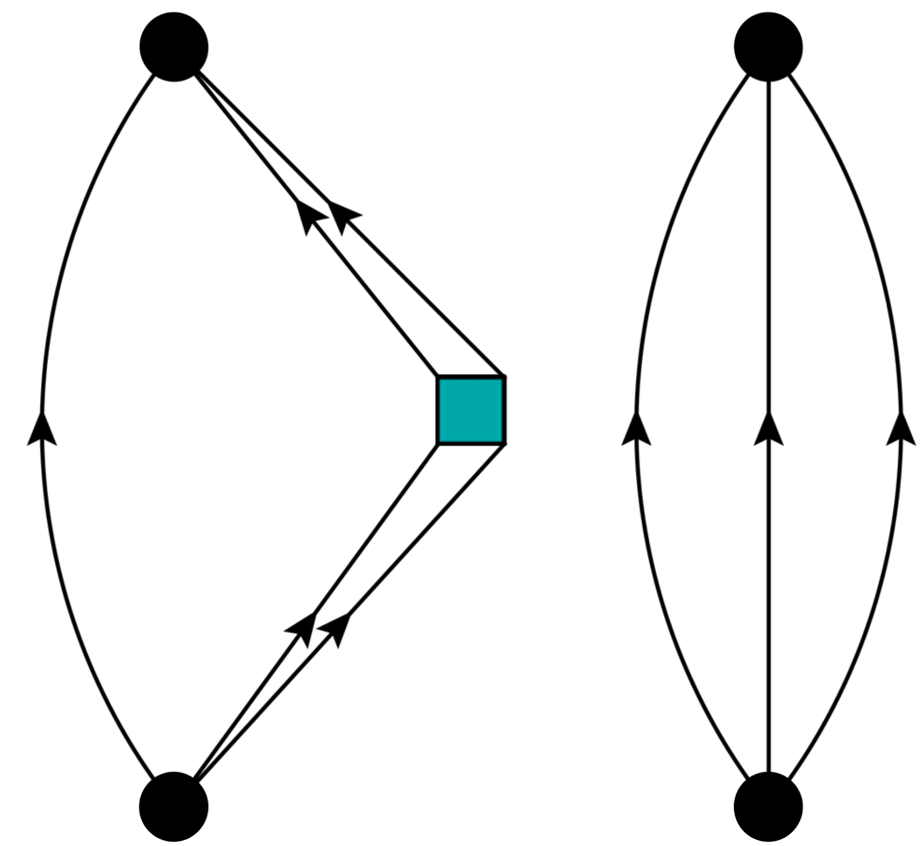

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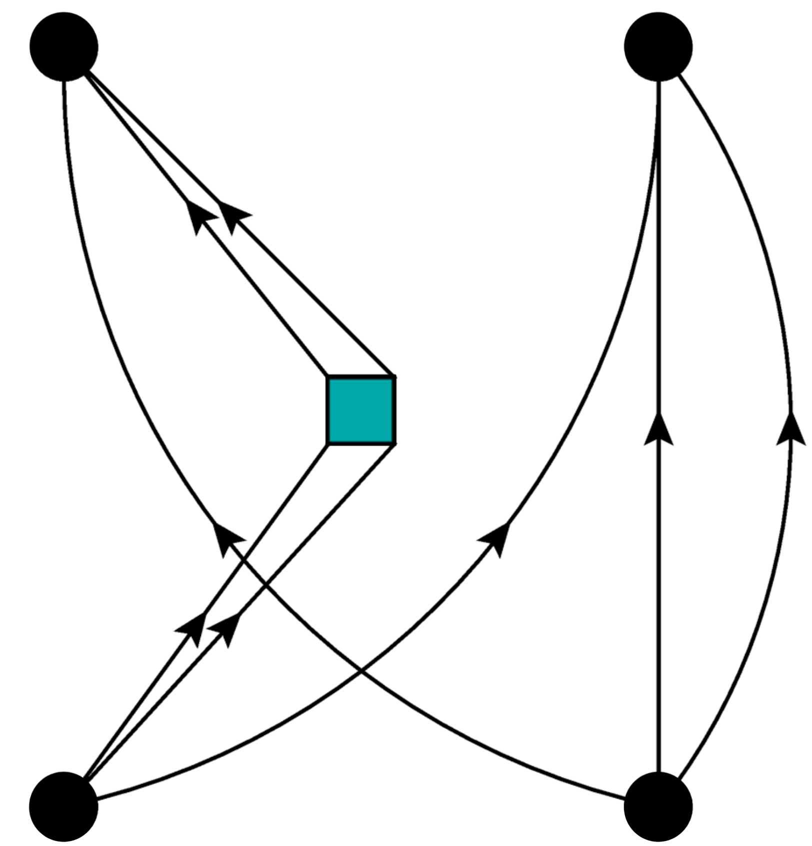

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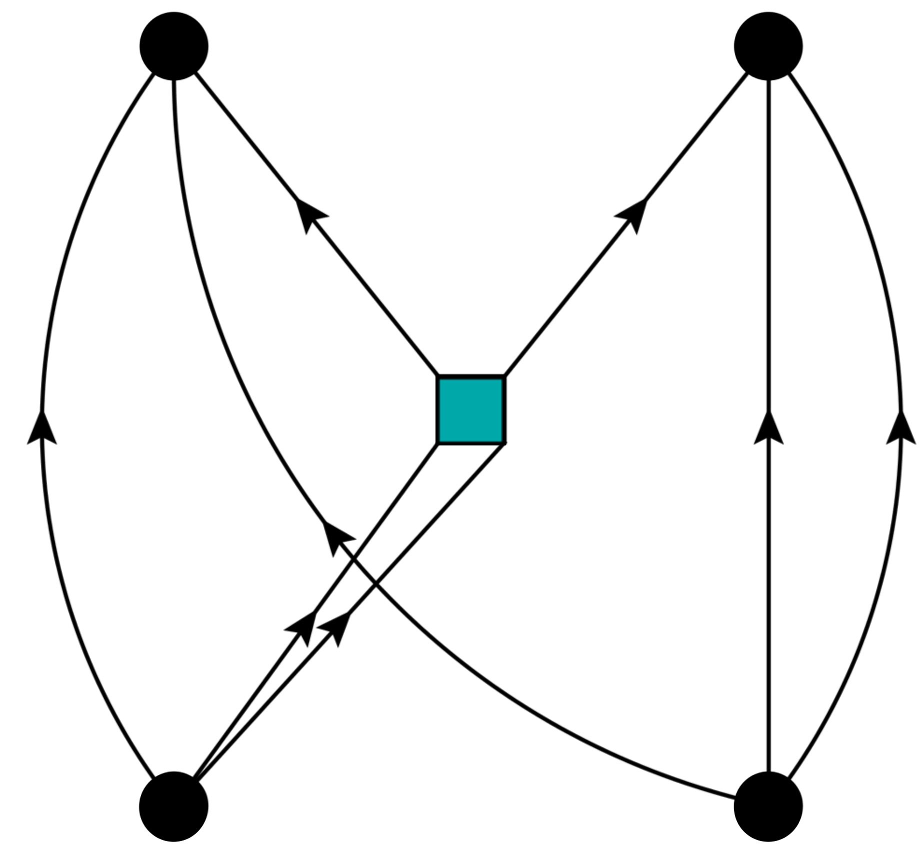

Parity Violation - Contractions ΔI=2

- 2 Baryon s-wave source
- EW vertices ⇒ 4-quark operator insertion
- 2 Baryon p-wave sink
- In total there are 4896 contractions.
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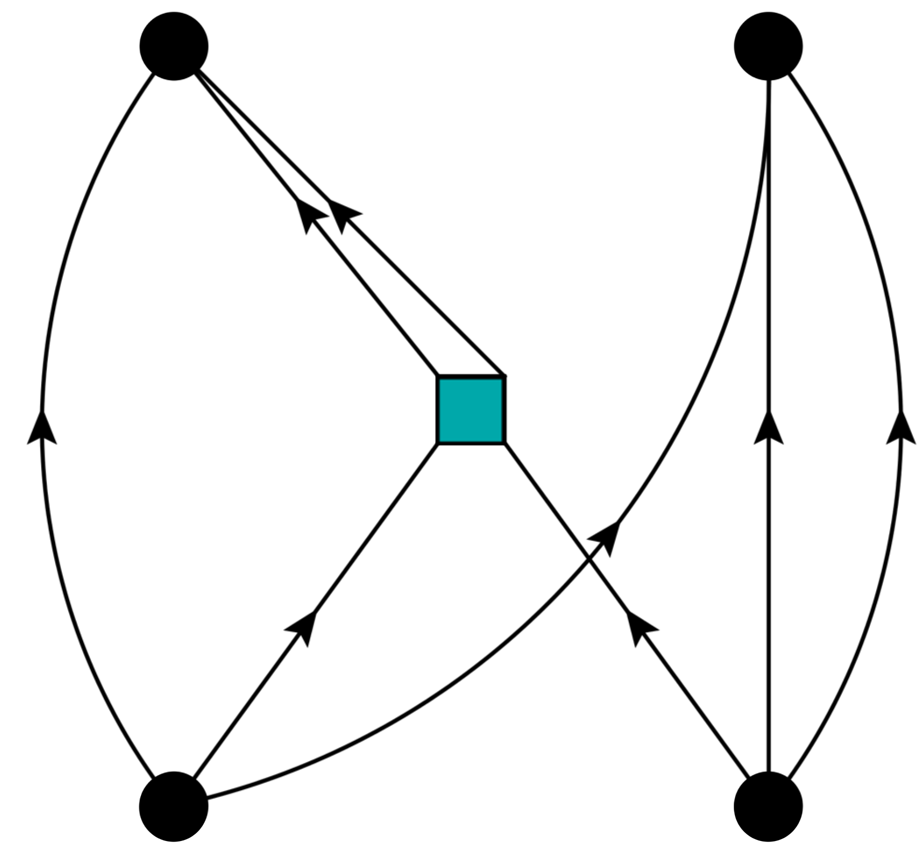

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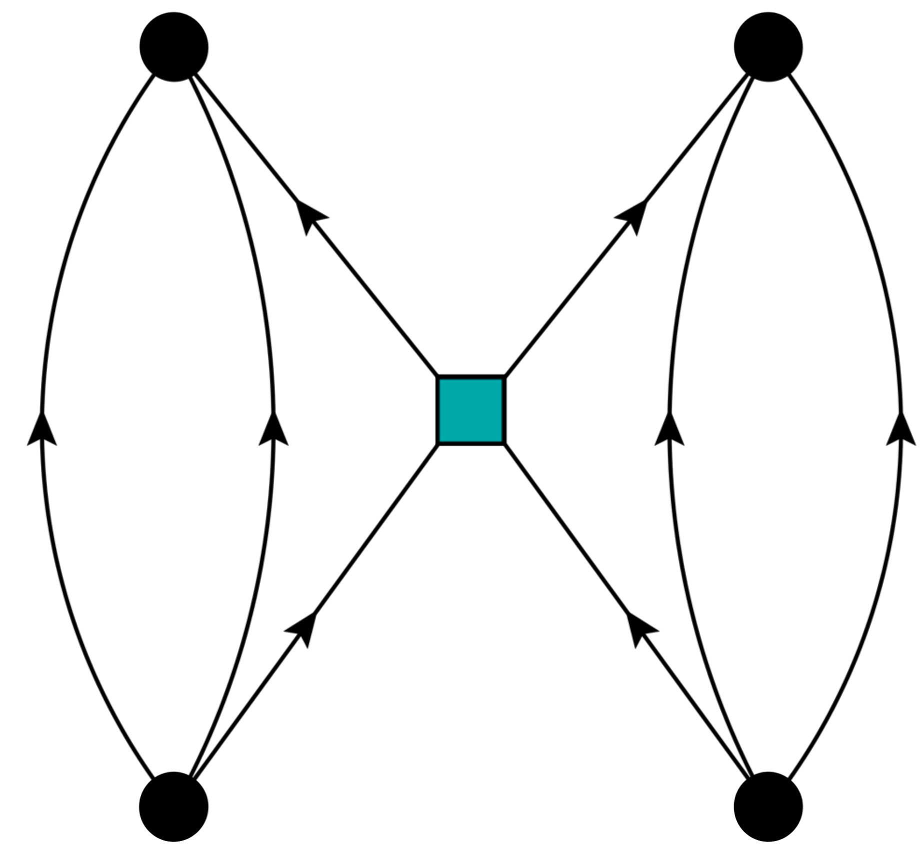

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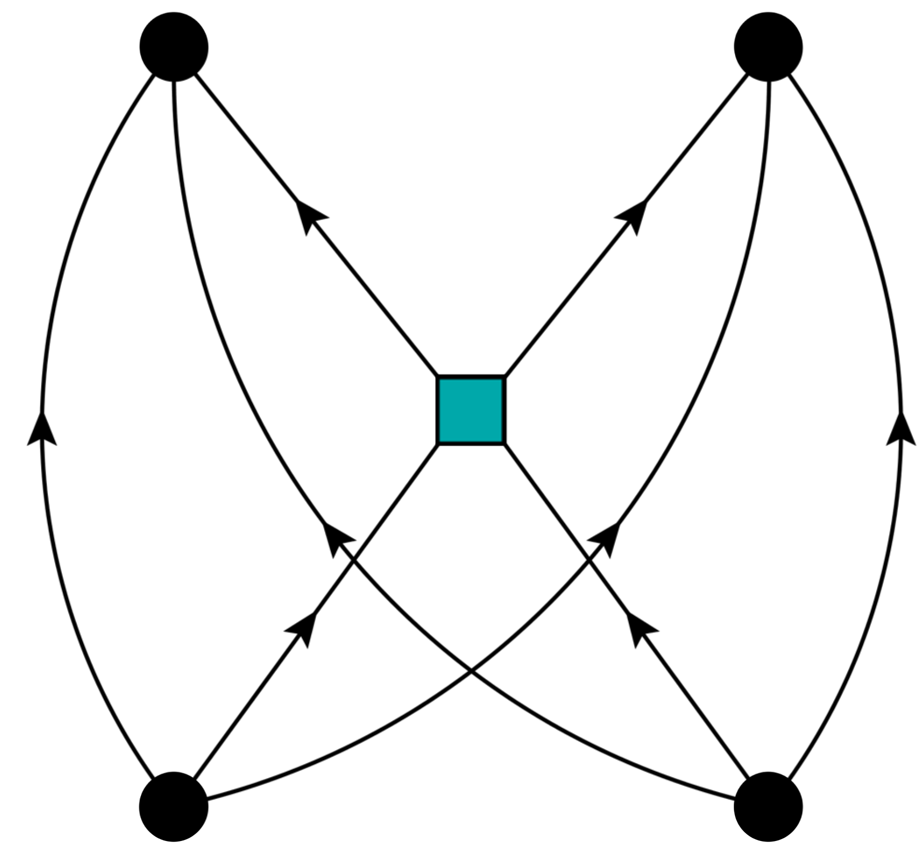

Parity Violation - Contractions $\Delta I = 2$

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- 2 Baryon p-wave sink
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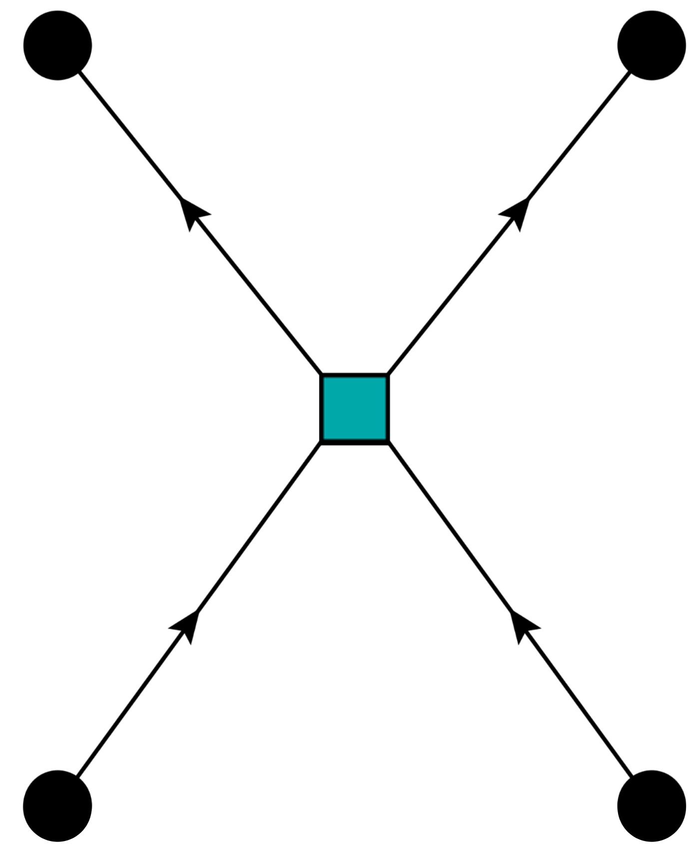
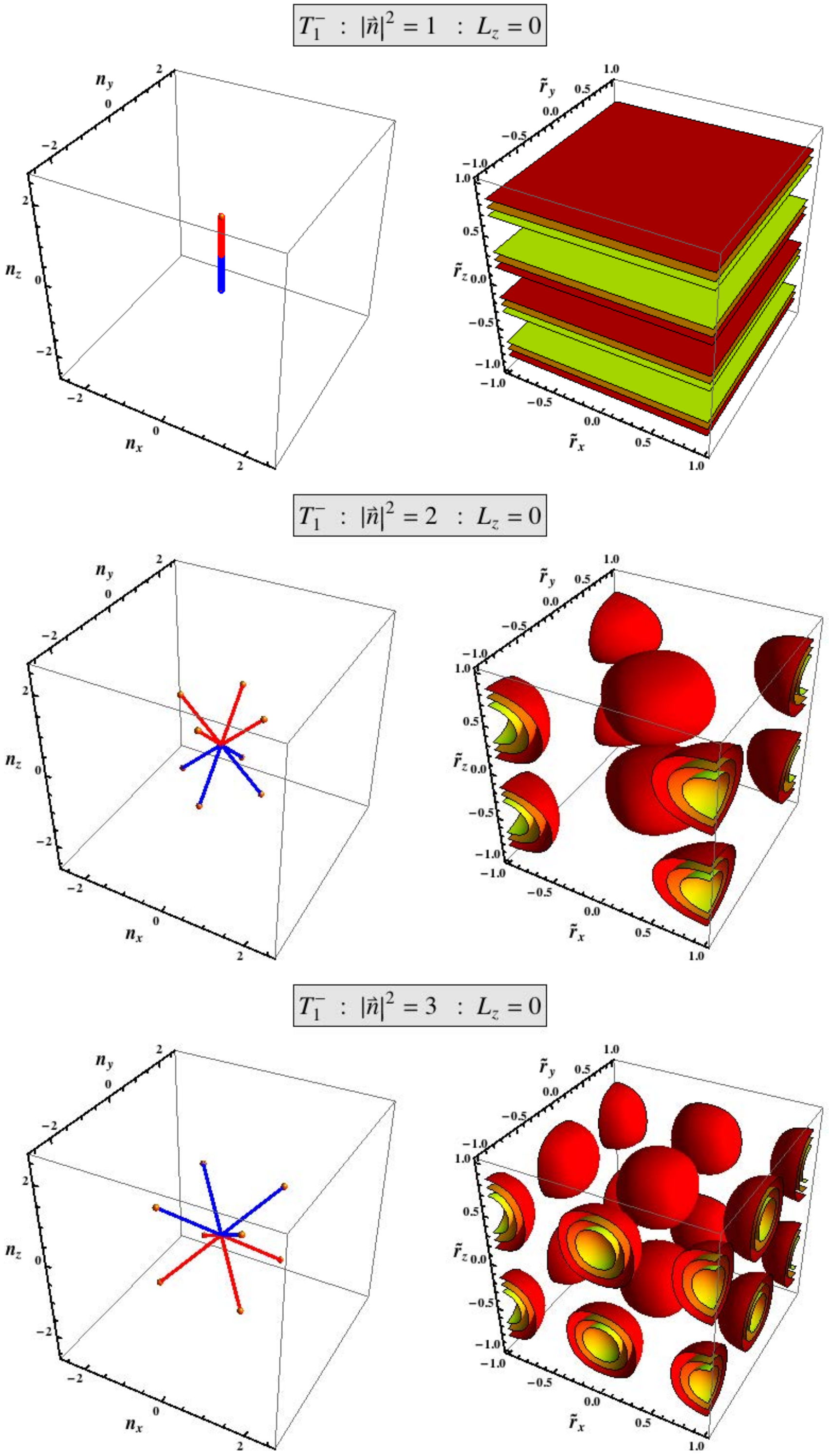
- Degenerate light quarks reduce this to 2208.
- Requires 15 tensors.
- 2 baryon blocks & 1 four-quark object



Source and Sink Construction

- use of momentum sources and sinks (non-local in coordinate space) would be optimal



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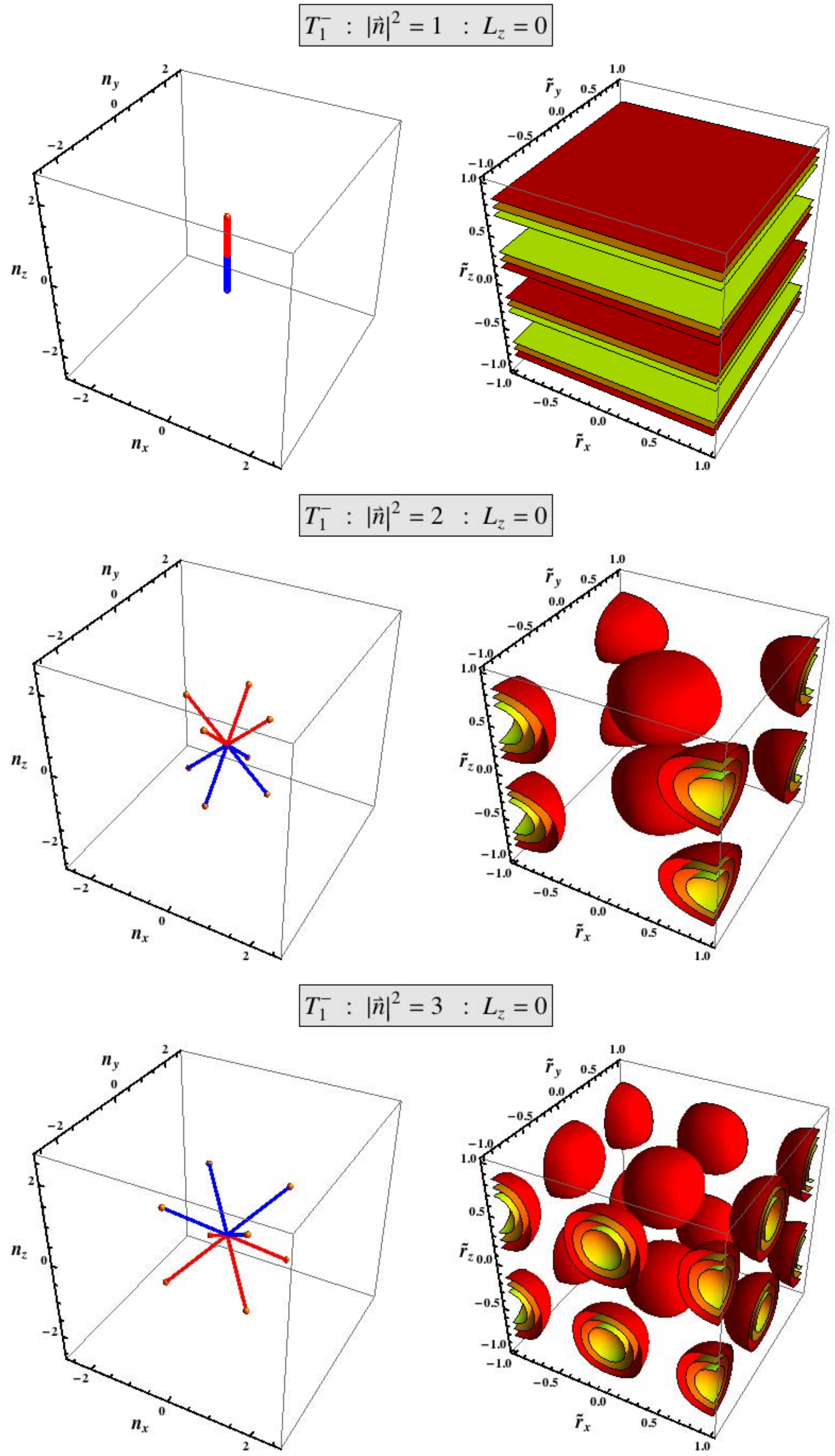


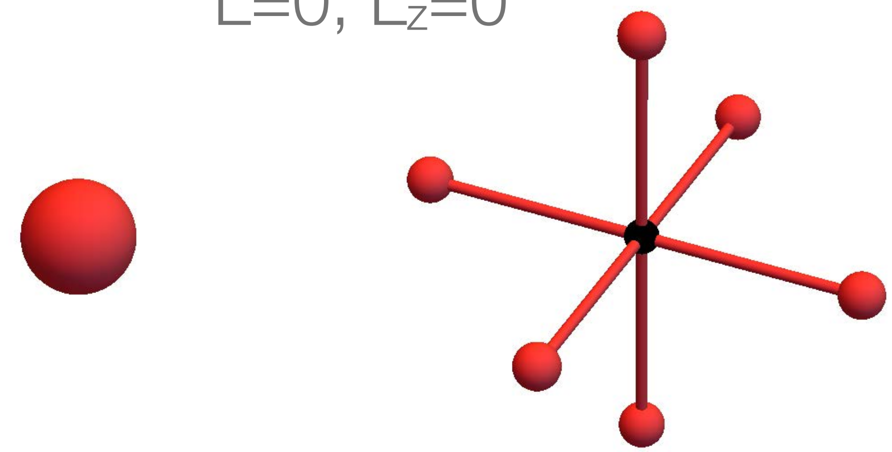
we wish to use: $\bar{N}(p) = \sum_x e^{ipx} \bar{q}_1(x)\, \bar{q}_2(x)\, \bar{q}_3(x)$

we are limited to: $\bar{N}'(p; p_1, p_2) = \sum_{x_1, x_2, x_3} e^{ip_1 x_1} \bar{q}_1(x_1)\, e^{ip_2 x_2} \bar{q}_2(x_2)\, e^{i(p - p_1 - p_2) x_3} \bar{q}_3(x_3)$

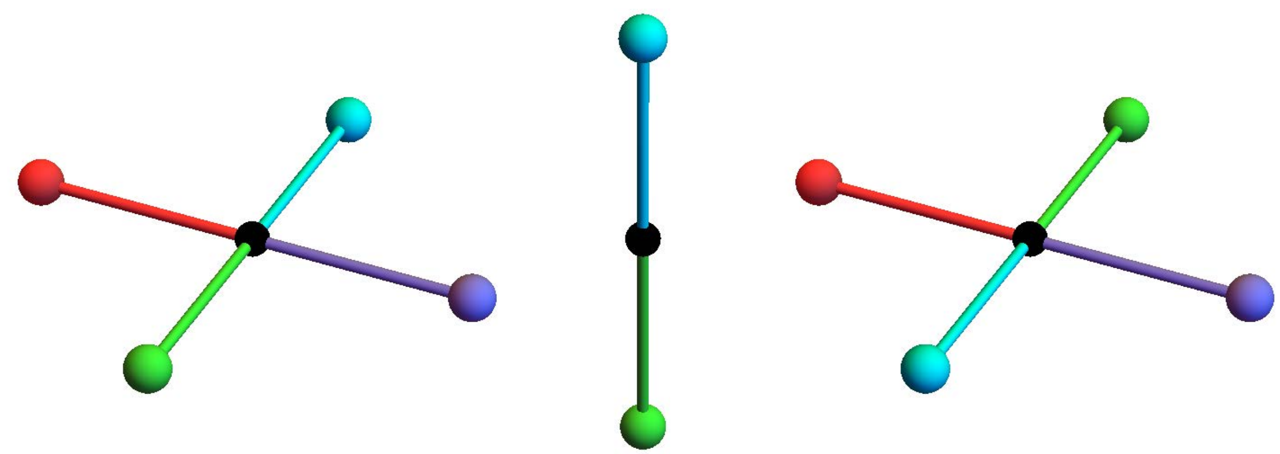
Source and Sink Construction

- use of momentum sources and sinks (non-local in coordinate space) would be optimal
- we use coordinate-space sources (and sinks) instead

$L=0,\ L_Z=0$



$L=1,\ L_Z=+1,0,-1$



Source and Sink Construction

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- mix different lattice irreducible representations ⇒ excited states

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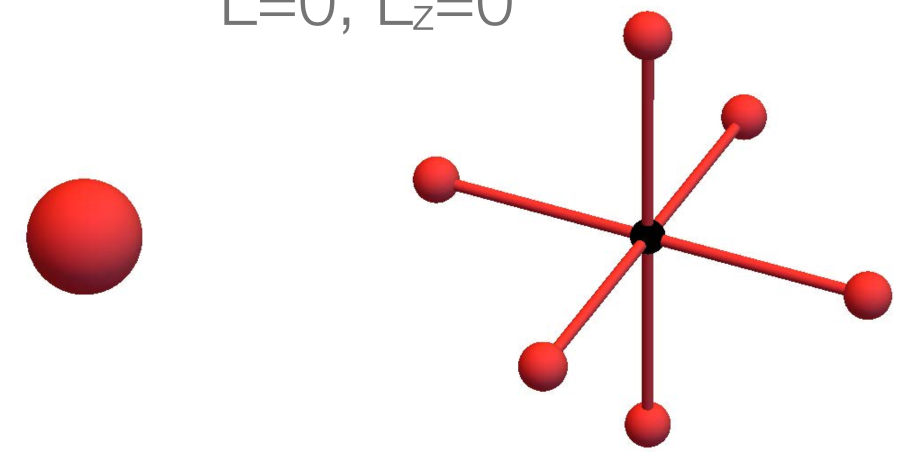

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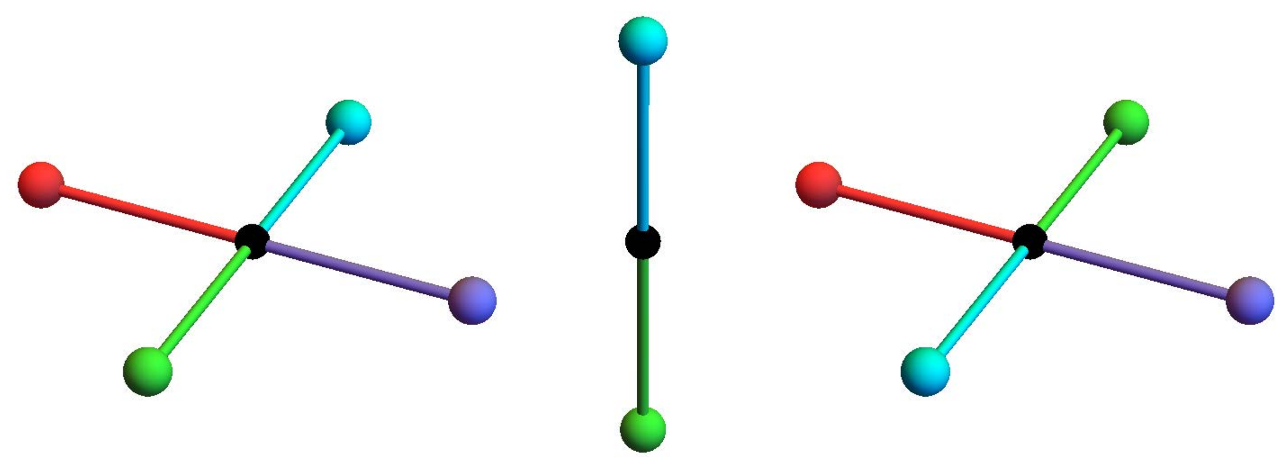
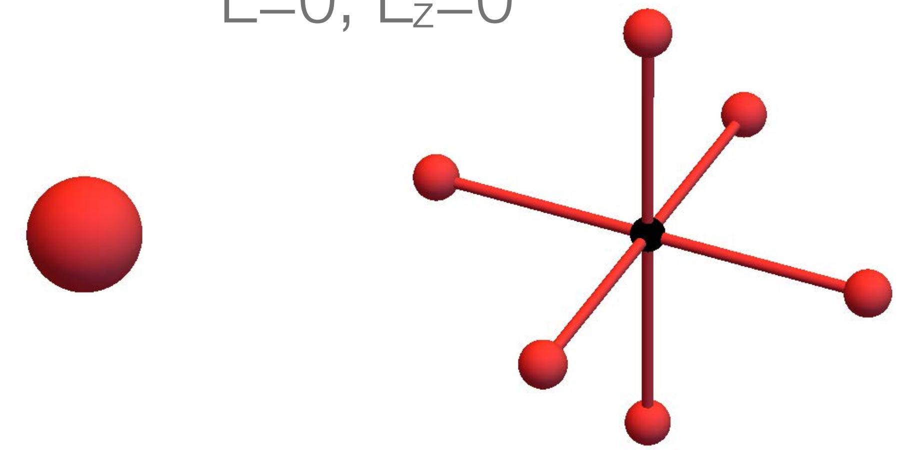


Source and Sink Construction

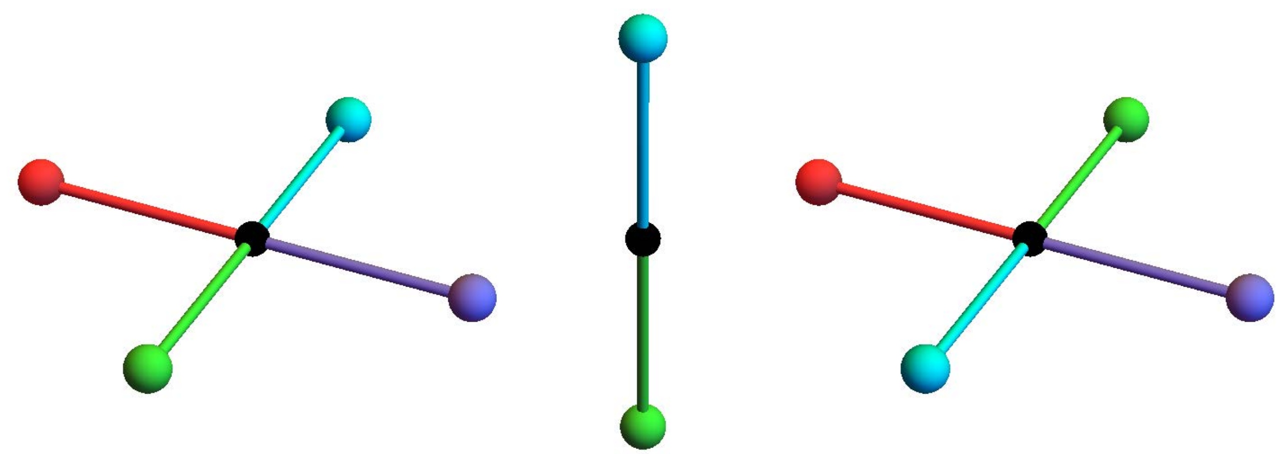
- use of momentum sources and sinks (non-local in coordinate space) would be optimal
- we use coordinate-space sources (and sinks) instead
- mix different lattice irreducible representations ⇒ excited states
- rotational symmetry breaking: mixing of different continuum multiplets

$L=0$, $L_z=0$



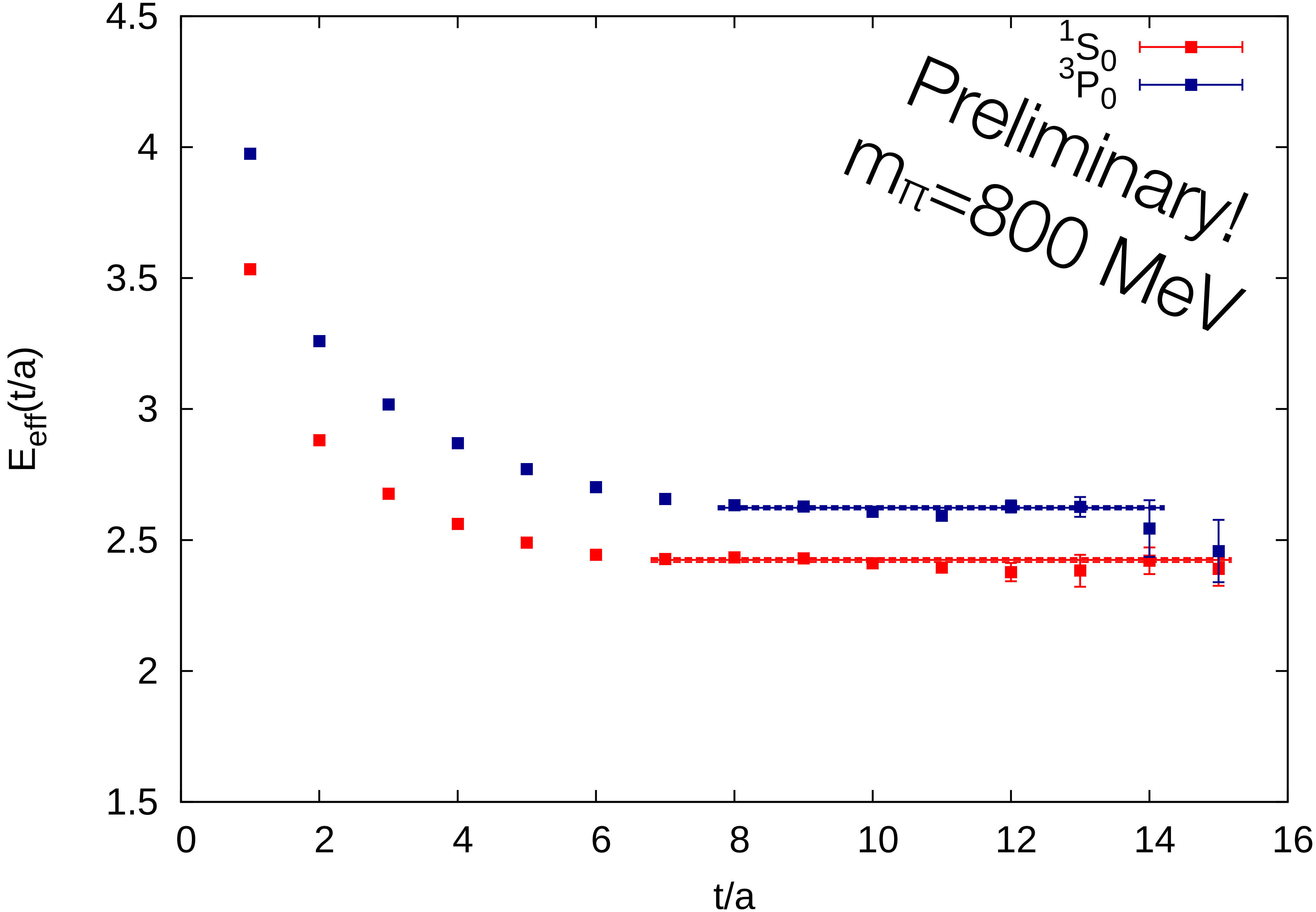
$L=4,6, \ldots$

$L=1$, $L_z=+1,0,-1$

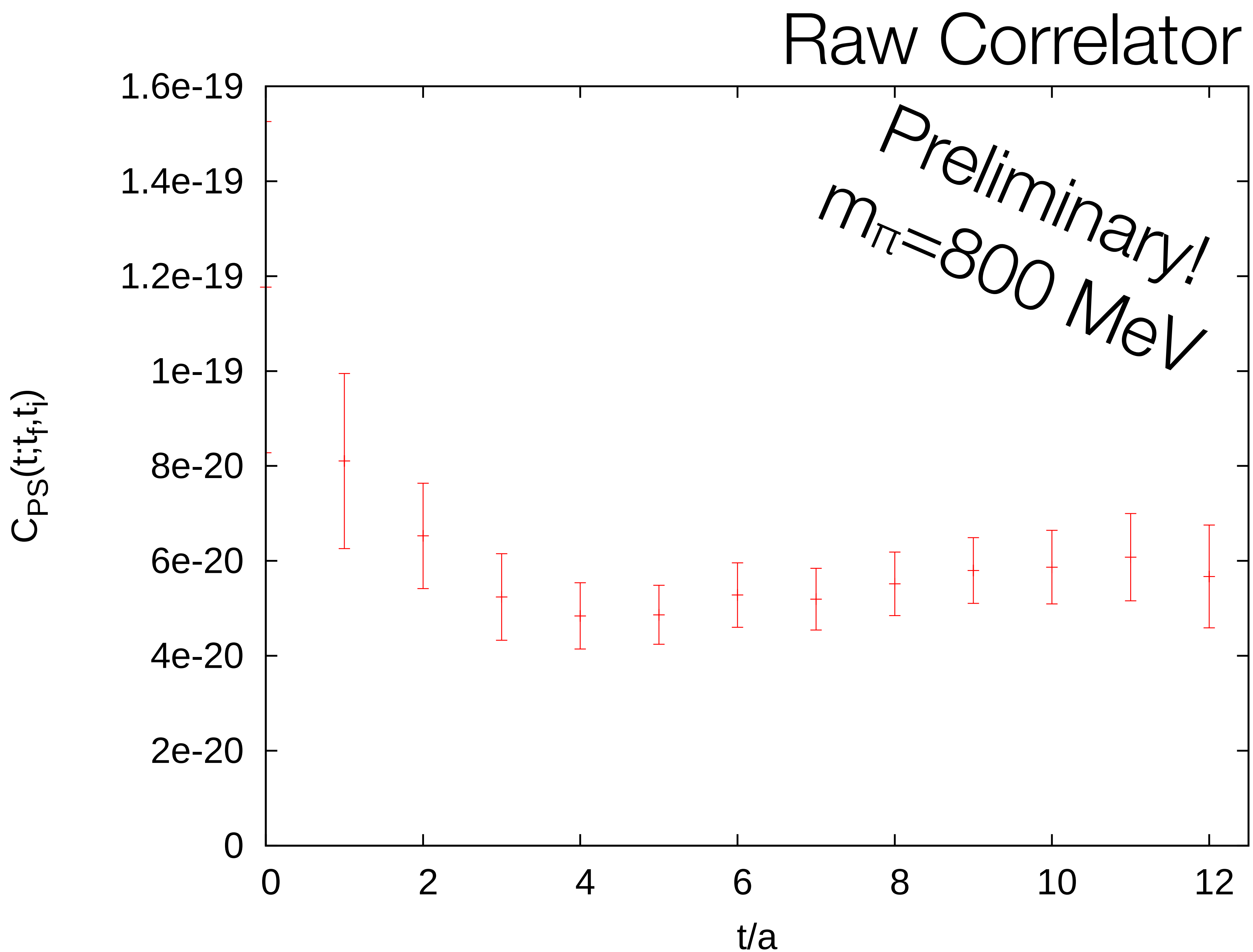


$L=3,5, \ldots$

Preliminary Results:
Partial Wave Scattering at m_π=800 MeV



Preliminary Results: Parity Violation Matrix Element at m_π=800 MeV



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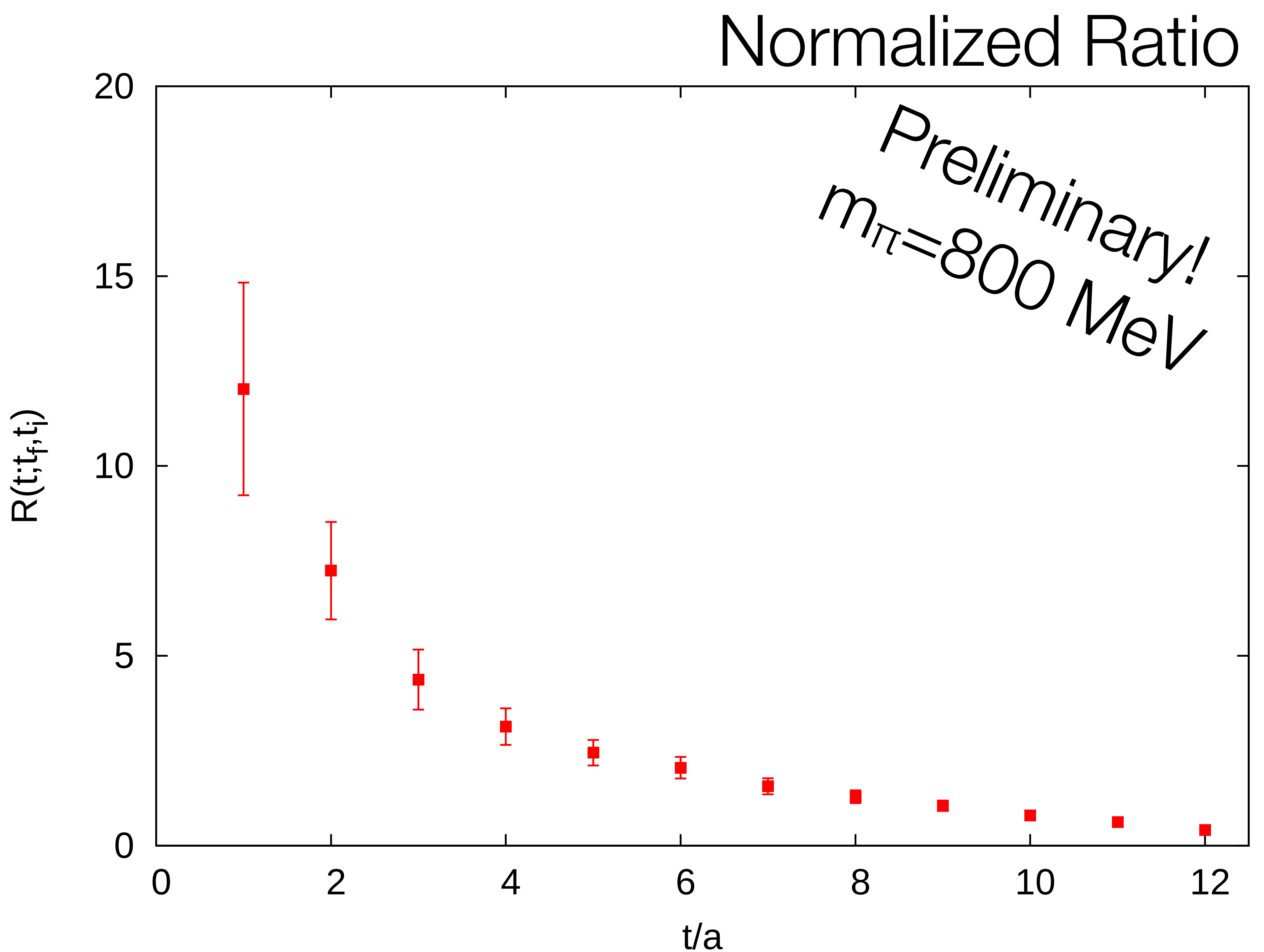
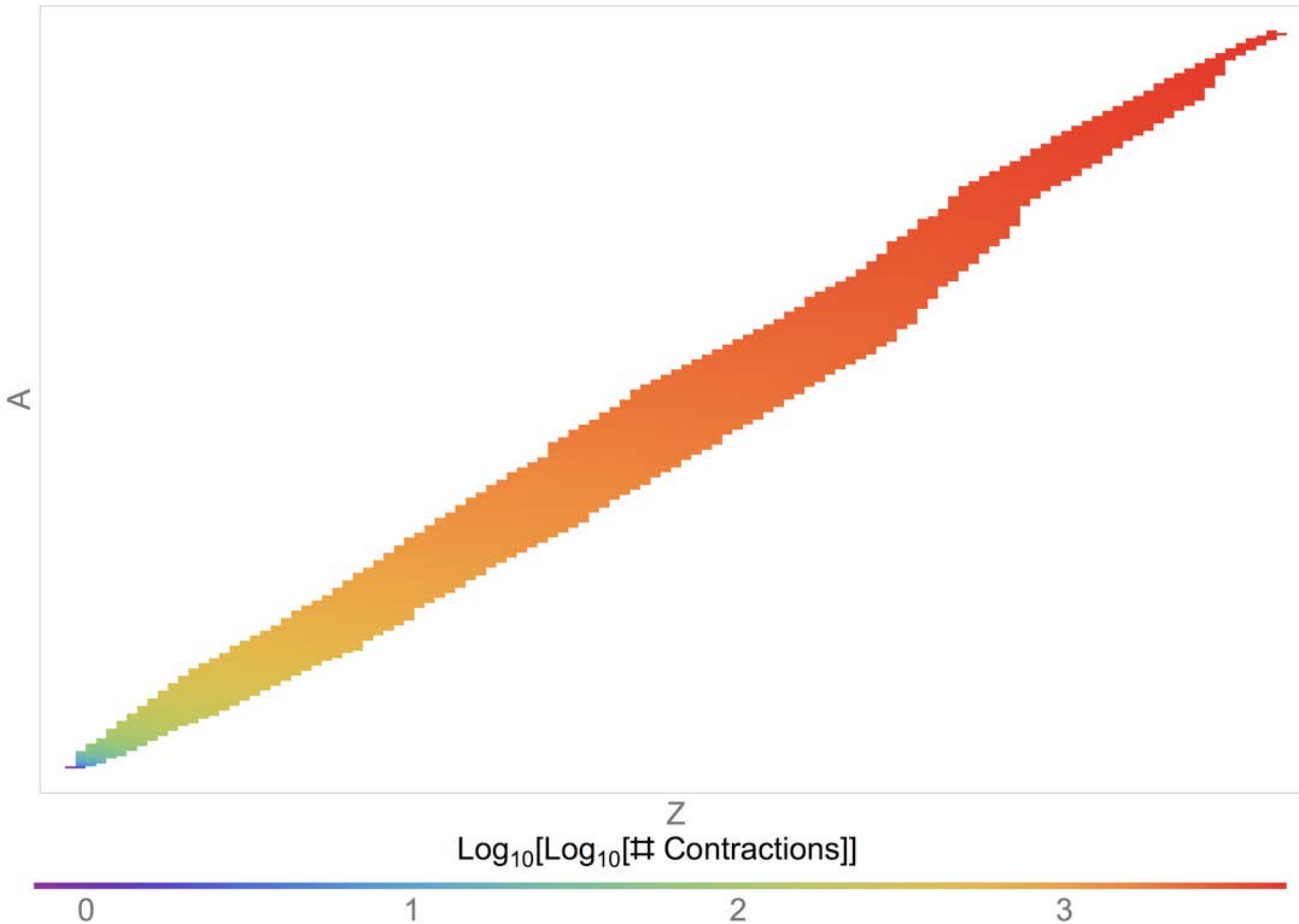


Reach



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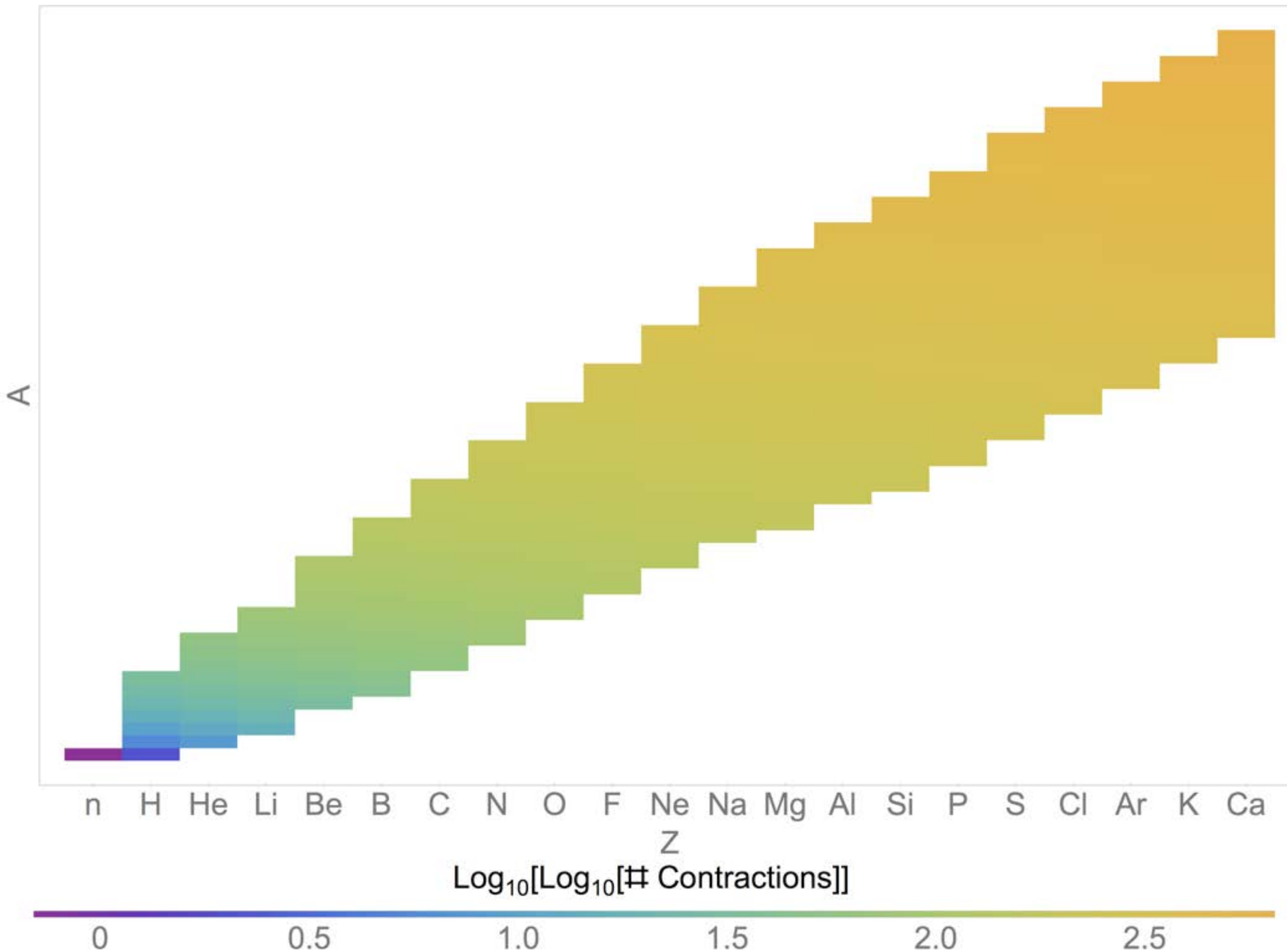
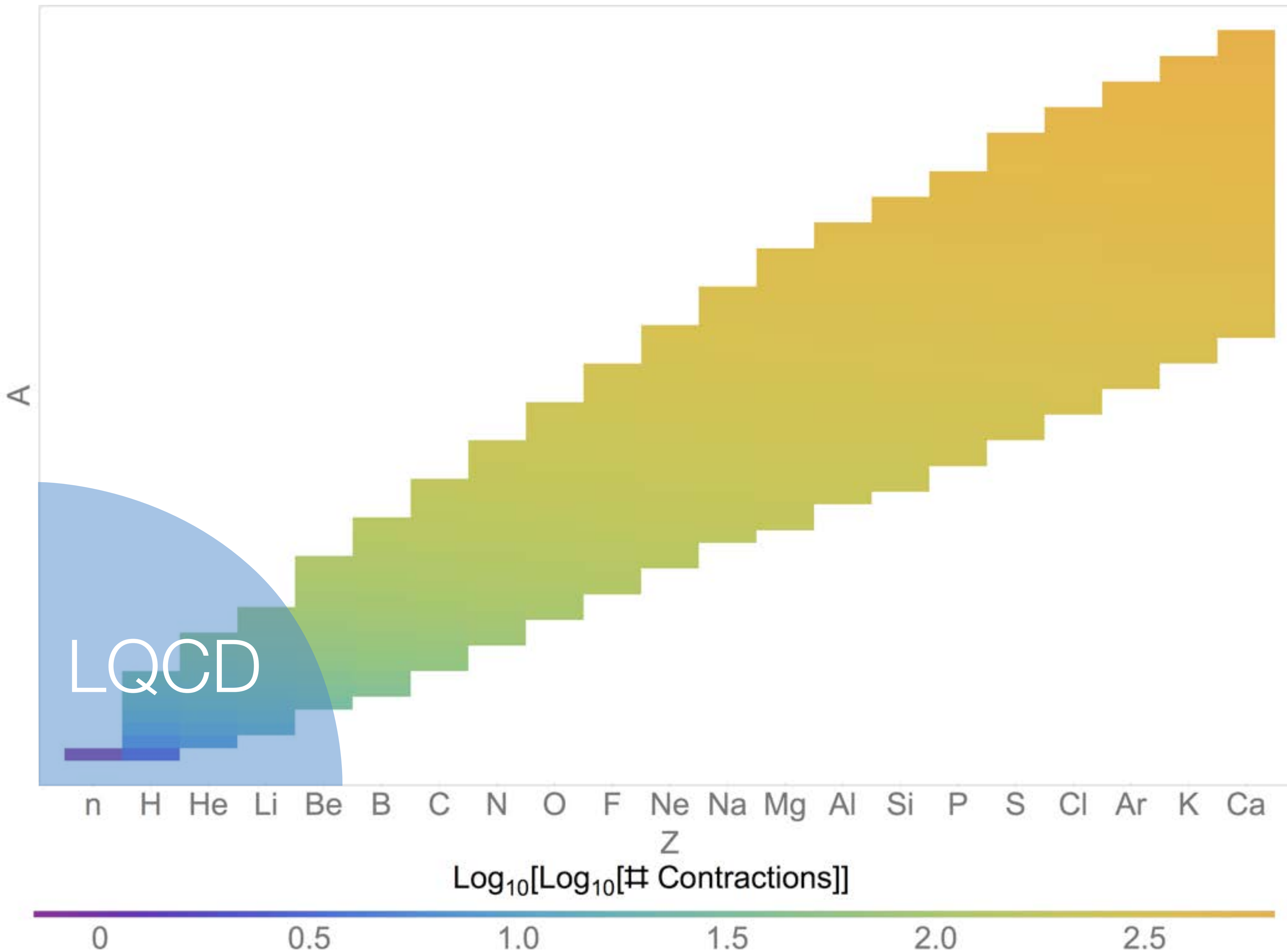


A
n
H
He
Li
Be
B
C
N
O
F
Ne
Na
Mg
Al
Si
P
S
Cl
Ar
K
Ca
Z
Log10[Log10[# Contractions]]
0
0.5
1.0
1.5
2.0
2.5

Reach



A
LQCD
n
H
He
Li
Be
B
C
N
O
F
Ne
Na
Mg
Al
Si
P
S
Cl
Ar
K
Ca
Z
Log10[Log10[# Contractions]]
0
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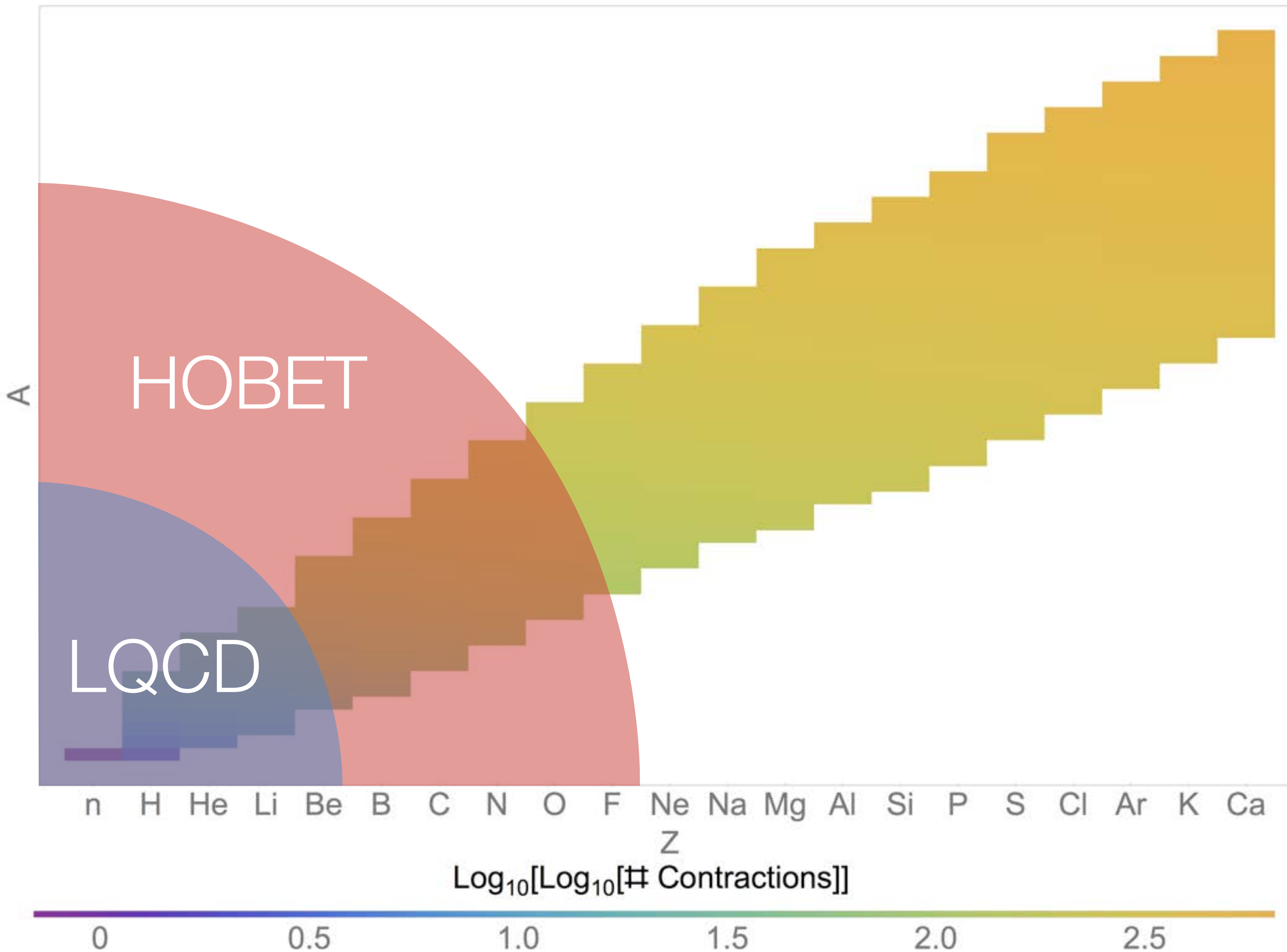
Reach



HOBET
LQCD
A
n H He Li Be B C N O F Ne Na Mg Al Si P S Cl Ar K Ca
Z
Log10[Log10[# Contractions]]
0 0.5 1.0 1.5 2.0 2.5

HOBET: Connecting a non-relativistic effective theory to the lattice

- Idea: Build an effective theory that can utilize lattice input to fix parameters that are unknown, while taking other parameters from experiment

- This includes utilizing either experiment or lattice input on the NN interaction to predict properties of light nuclei

- HOBET is a true ET: the effective interaction is constructed directly in the soft — or "included" — P-space

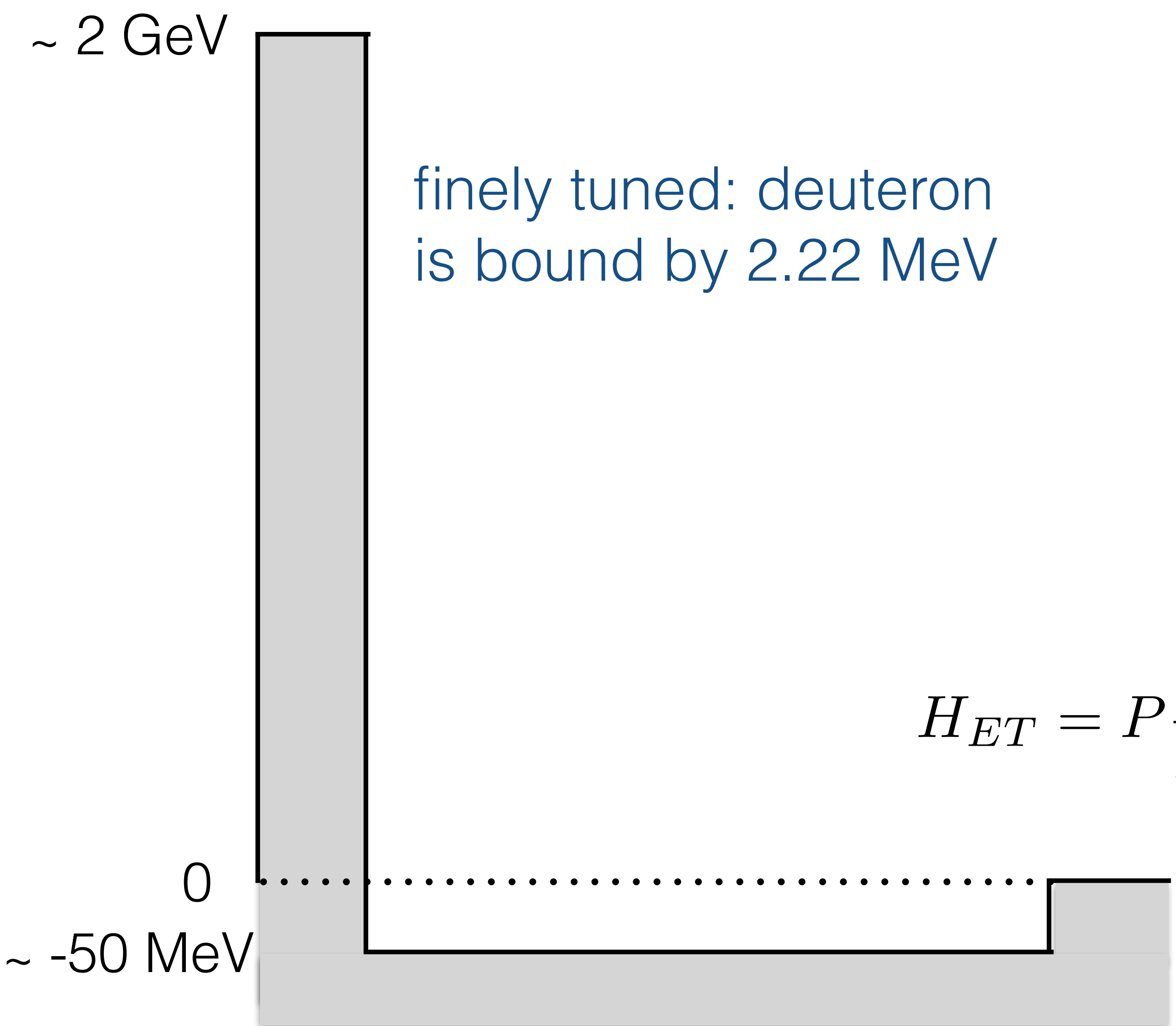
- Usual nuclear physics approach:
  QCD → singular NN potential → P-space effective interaction

- HOBET: QCD → P-space effective interaction

- The difficult effective interactions problem is avoided

- How is this done? HOBET's unique infra-red/ultraviolet separation allows us to utilize NN phase shifts to fix ET parameters

Simplified analytic example: hard-core s-wave interaction, chosen to reproduce deuteron binding energy



finely tuned: deuteron is bound by 2.22 MeV

P is the soft ET space
Q=1-P
H = T+V

use the Haxton/Luu factorization of the Bloch-Horowitz equation

$$H_{ET} = P \frac{E}{E-TQ} \left[T - T\frac{Q}{E}T + V + V_\delta \right] \frac{E}{E-QT} P$$

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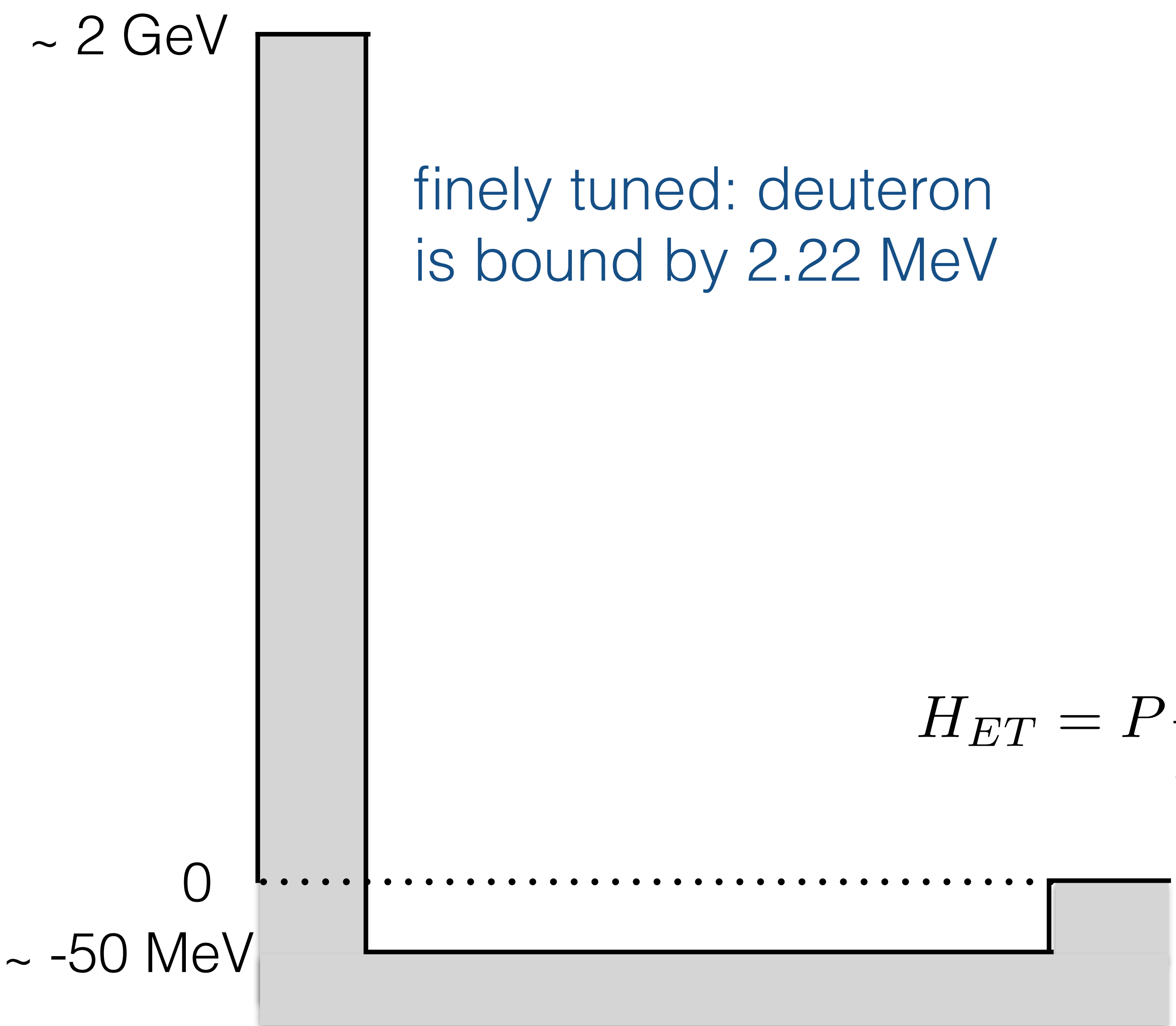

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sums kinetic energy T to all orders

outgoing solution for a specific E depends on the phase shift δ(E)

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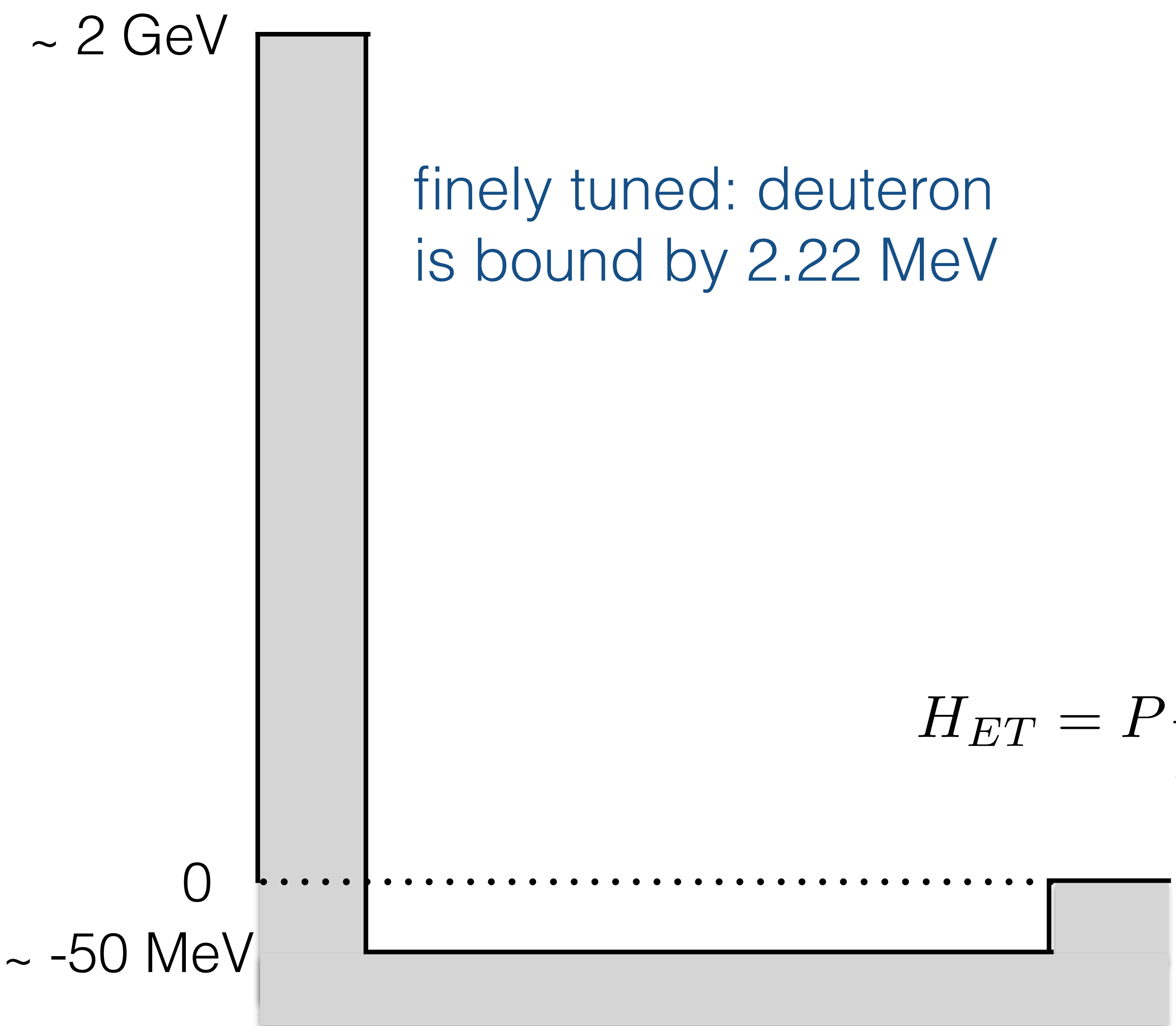

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short-range operator that corrects for the effects of V acting outside P: can be efficiently expanded in terms of contact operators

The BH equation must be solved self-consistently: $H_{ET} = H_{ET}(E)$

So one picks an E, supplies δ(E), calculates $H_{ET}(E)$, diagonalizes in P

A solution must exist at every E>0

But the diagonalization does not give an eigenvalue at E

Thus we "dial" V_δ - this can be done order-by-order to reproduce δ(E) over a range of E

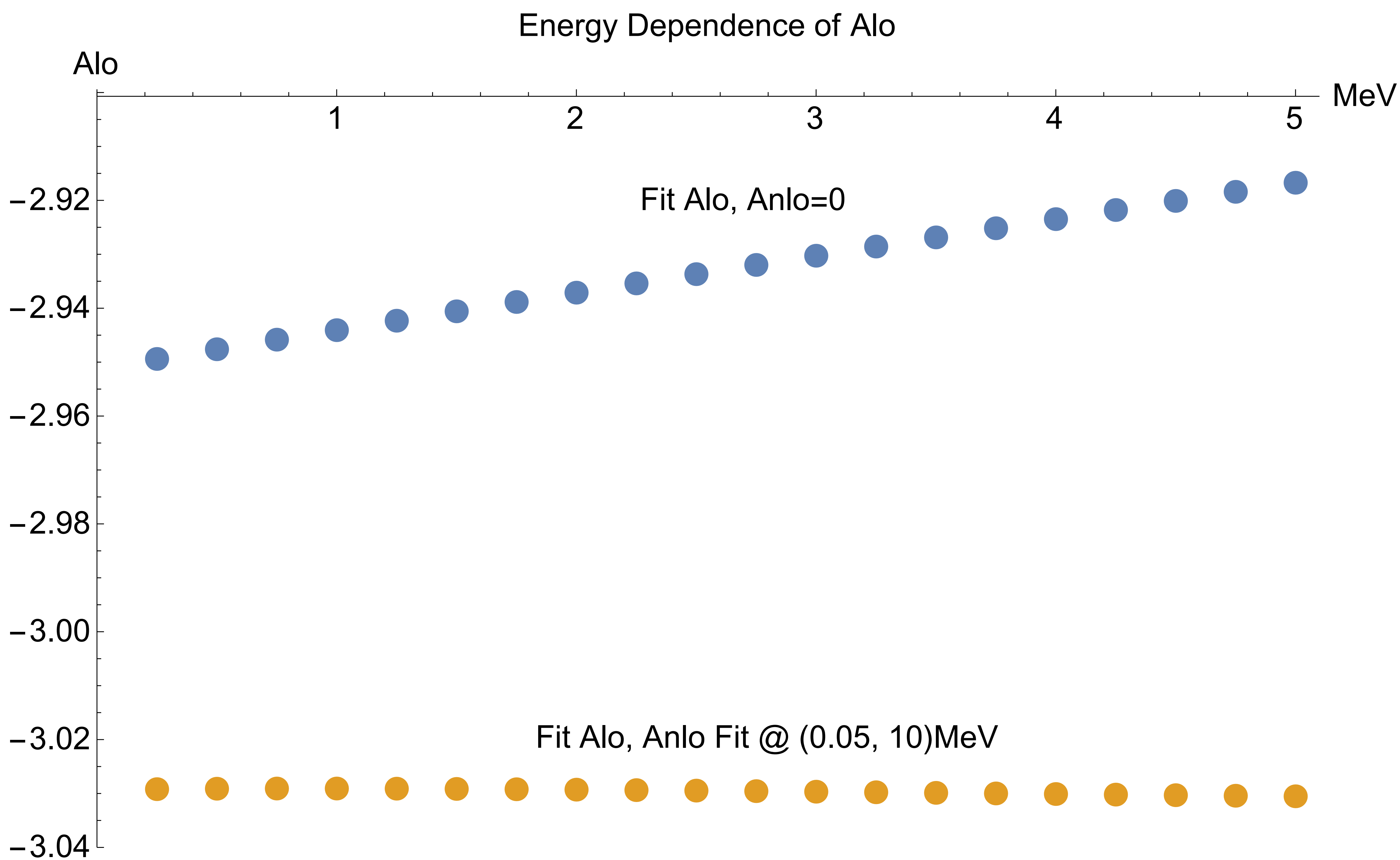
Through NNLO:

$$V_\delta = a_{LO}\delta(\vec{r}) + a_{NLO}\left(\overleftarrow{\nabla}^2\,\delta(\vec{r}) + \delta(\vec{r})\,\overrightarrow{\nabla}^2\right) + a^1_{NNLO}\,\overleftarrow{\nabla}^2\,\delta(\vec{r})\,\overrightarrow{\nabla}^2 + a^2_{NNLO}\left(\overleftarrow{\nabla}^4\,\delta(\vec{r}) + \delta(\vec{r})\,\overrightarrow{\nabla}^4\right)$$

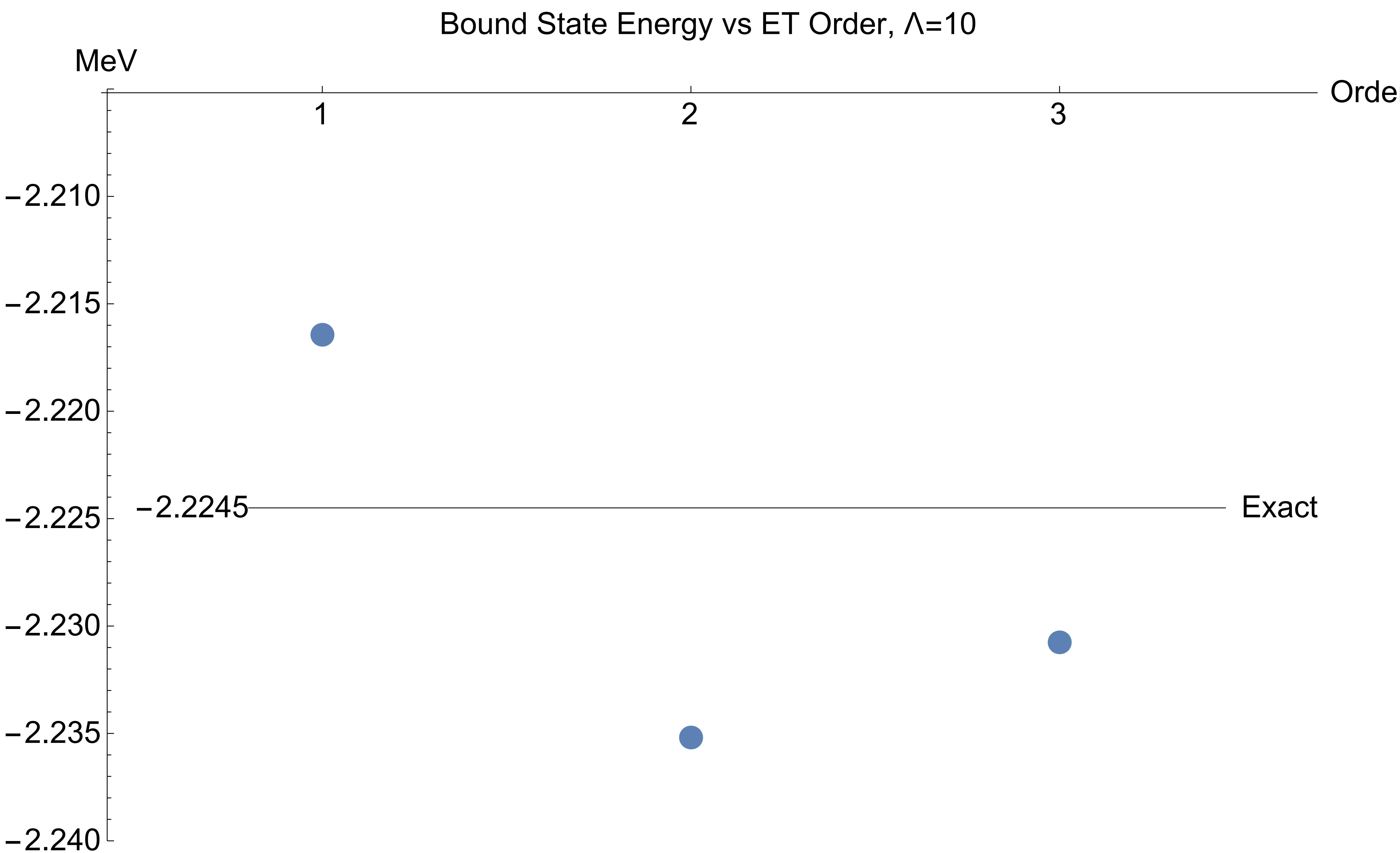
The larger the range in E over which δ(E) is fit, the more terms needed

Phase shifts yield the deuteron binding energy, in a calculation limited to P

Low-energy constants become constant, as higher orders are included



For $V_\delta = 0$ the predicted binding energy is -0.68 MeV



CalLat is applying these techniques to the parity-violating asymmetry in

$$n + p \to D + \gamma$$

Ongoing SNS experiment to measure the neutral current in the hadronic weak interaction (see poster)

We will use HOBET + lattice to fully determine this system, and to relate this observable to other parity-violating observables

Experimental strong phase shifts: fix all strong interaction low-energy constants

Lattice: provides the experimentally unknown parameter — the parity-violating weak phase shift

Conclusions

- Nuclear physics can be done on the Lattice
  - Baryon blocks and tensors tame Wick Contractions
    ⇒ automatic code generation, parallelization (GPUs)
  - sophisticated, expensive non-local sources/sinks for higher partial waves ⇒ treating excited states effects
  - exponential decrease of SNR ⇒ large m_π, huge statistics (MG), huge amount of data to store (HDF5)
  - preliminary higher partial wave and PV results look promising, but might need to disentangle angular momentum multiplets

Conclusions

- Expected computational costs:
  - $m_\pi\downarrow$: inversions$\Uparrow$, SNR$\Downarrow$
  - $L\uparrow$: inversions$\uparrow$, FFT$\Uparrow$, contractions$\uparrow$, SNR$\uparrow$
- feed lattice results into HOBET ⇒ solve complex nuclear systems

Thank You