## Estimating excited-state contamination

## using experimental data

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$$
\text { July 29th, } 2016
$$

MTH and Harvey B. Meyer, to appear


The nucleon axial charge is a basic ingredient in describing neutron beta decay

$$
g_{A, \operatorname{expt}}=1.2723 \pm 0.0023
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Particle data group (2015 update)
In addition, $g_{A} \ldots$
parametrizes the nucleon-pion coupling in ChPT reveals how quark spin contributes to nucleon spin determines how nuclear properties vary with quark mass

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$$
\left\langle N, \mathbf{p}, \sigma^{\prime}\right| \overline{\mathcal{Q}} \tau^{a} \gamma^{\mu} \gamma_{5} \mathcal{Q}|N, \mathbf{p}, \sigma\rangle=g_{A} \bar{u}_{\sigma^{\prime}}(\mathbf{p}) \tau^{a} \gamma^{\mu} \gamma_{5} u_{\sigma}(\mathbf{p})
$$

Determining the QCD prediction for this benchmark quantity will improve our understanding of how nuclear structure emerges from the underlying theory

Nuclear charges are typically accessed from Lattice QCD (LQCD) by constructing ratios of correlators

$$
R(T, \tau) \equiv \frac{\langle\mathcal{O}(T) A(\tau) \overline{\mathcal{O}}(0)\rangle}{\langle\mathcal{O}(T) \overline{\mathcal{O}}(0)\rangle}=g_{A}+b_{1}\left(e^{-\Delta E_{1}(T-\tau)}+e^{-\Delta E_{1} \tau}\right)+\cdots
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At large separations excited state contamination is reduced but signal also degrades (Lepage, Parisi)

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Can excited state contamination explain why lattice values of $g_{A}$ tend to be below the experimental value?

At leading order in Chiral Perturbation Theory (ChPT) the value of excited state contamination is universal (interpolator-independent) and positive.

Brian Tiburzi, Phys. Rev. D91, 094510 (2015)
Oliver Bär, arXiv:1606.09385

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Using the LO ChPT prediction

| $T(\mathrm{fm})$ | $n_{\text {states }}(5 \%)$ | $n_{\text {states }}(3 \%)$ |
| :---: | :---: | :---: |
| 2 | 2 | 0 |
| 1.5 | 2 | 5 |
| 1 | 7 | 10 |

Note: Oliver Bär (arXiv:1606.09385) uses fewer states to stay in LO ChPT range of validity

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Ensemble N6 $\quad Q^{2}=0.0 \mathrm{GeV}^{2}$


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If higher finite-volume states are important, then the Roper could also play an important role.

To precisely define the excited state contamination we introduce

$$
R(T, \tau)=\frac{\langle\mathcal{O}(T) A(\tau) \overline{\mathcal{O}}(0)\rangle}{\langle\mathcal{O}(T) \overline{\mathcal{O}}(0)\rangle}=g_{A}+\mathcal{E}(T, \tau)\left\{\begin{array}{l}
A(\tau) \equiv 2 i \int d \mathbf{x} A_{z}^{3}(\tau, \mathbf{x}) \\
\mathcal{O}(\tau) \equiv \int d \mathbf{x} \frac{\bar{u}_{\uparrow}(0)}{\sqrt{m_{N}}} \cdot N(\tau, \mathbf{x})
\end{array}\right.
$$

$$
\mathcal{E}(T, \tau)=\sum_{n=1}^{\infty} b_{n}\left[e^{-\Delta E_{n}(T-\tau)}+e^{-\Delta E_{n} \tau}\right]+c_{n} e^{-\Delta E_{n} T}+\cdots
$$

$\Delta E_{n}=E_{n}(L)-m_{N}+\mathcal{O}\left(e^{-M_{\pi} L}\right)$
$b_{n}=\frac{\langle 0| \mathcal{O}(0)|n, L\rangle\langle n, L| A(0)|N, L\rangle}{\langle 0| \mathcal{O}(0)|N, L\rangle} \ll \quad \begin{gathered}\text { finite-volume } \\ \text { excited states }\end{gathered}$

We aim to estimate finite-volume energies and matrix elements using experimental scattering data

Finite-volume energies
$\Delta E_{n}=E_{n}(L)-m_{N}+\mathcal{O}\left(e^{-M_{\pi} L}\right)$

## Finite-volume energies


cubic, spatial volume (extent $L$ )
periodic boundary conditions

$$
\vec{p} \in(2 \pi / L) \mathbb{Z}^{3}
$$

$L$ large enough to drop $e^{-M_{\pi} L}$

## Finite-volume energies

$$
\begin{gathered}
\Delta E_{n}=E_{n}(L)-m_{N}+O\left(e^{-M_{\pi} L}\right) \\
L_{L}^{L} L_{L}^{L} \sum_{E_{2}(L)}^{E_{3}(L)} \\
\text { Isospin and parity are good quantum } \\
\text { numbers in finite-volume } \\
E_{1}(L)
\end{gathered} \quad I=1 / 2, \quad P=+
$$


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Can also project to a finite-volume irrep

$$
G_{1}^{+}=\left(J=\frac{1}{2}\right) \oplus\left(J=\frac{5}{2}\right) \oplus \cdots
$$

$$
\text { neglecting } \ell \geq 3 \rightarrow J \geq 5 / 2
$$ we find...

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## Single channel quantization condition

$I\left(J^{P}\right)=1 / 2\left(1 / 2^{+}\right) \quad \delta\left(E_{n}\right)+\phi\left(E_{n}, L\right)=0 \quad$ known geometric scattering phase shift


Lüscher, M. Nucl. Phys B354, 531-578 (1991)
Beane et al., Nucl. Phys. A747, 55 (2005) Li and Liu, Phys. Rev. D87, 014502 (2013) Briceño, Phys. Rev. D 89, 074507 (2014) M. Göckeler et al., Phys. Rev. D86 094513 (2012)

## Single channel quantization condition

$\rightarrow \delta\left(E_{n}\right)+\phi\left(E_{n} L\right)=0$ known geometric $^{\text {k }}$
$\delta\left(E_{n}\right)+\phi\left(E_{n}, L\right)=0$ function
$I\left(J^{P}\right)=1 / 2\left(1 / 2^{+}\right)$


Phase shift data is determined using experimental data from CERN, JLab, LAMPF, TRIUMF, PSI
The data base is described in
Arndt et. al., Phys. Rev. C74, 045205 (2006)
The solution used here (WI08) is described in
Workman et. al., Phys. Rev. C86, 035202 (2012)
The fits were performed to eigenvalues of the S matrix



## $N \pi$ finite-volume states



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These are volume suppressed but may 100 become important near the resonance

|  |  |  |  |  |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 3.0 | 3.5 | 4.0 | 4.5 | 5.0 | 5.5 | 6.0 |
|  |  | $M_{\pi} L$ |  |  |  |  |

## $N \pi$ finite-volume states

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I\left(J^{P}\right)=1 / 2\left(1 / 2^{+}\right)
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Three-particle states can be included with generalized three-particle formalism MTH and Sharpe, 1408.5933, 1504.04248

Briceño, MTH, Sharpe, underway
Note: LO ChPT uses
non-interacting two-particle energies

$$
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$$

We now turn to the coefficients of excited state exponentials

$$
\begin{gathered}
b_{n}=\frac{\langle 0| \mathcal{O}|n, L\rangle\langle n, L| A|N, L\rangle}{\langle 0| \mathcal{O}|N, L\rangle} \\
c_{n}=-\frac{\langle 0| \mathcal{O}|n, L\rangle\langle n, L| \overline{\mathcal{O}}|0\rangle}{\langle 0| \mathcal{O}|N, L\rangle\langle N, L| \overline{\mathcal{O}}|0\rangle}+\frac{\langle 0| \mathcal{O}|n, L\rangle\langle n, L| A|n, L\rangle\langle n, L| \overline{\mathcal{O}}|0\rangle}{\langle 0| \mathcal{O}|N, L\rangle\langle N, L| \overline{\mathcal{O}}|0\rangle}
\end{gathered}
$$

## Finite-volume matrix elements

One can rewrite $b_{n}$ using extensions of the Lellouch-Lüscher formalism

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b_{n}=\frac{\langle 0| \widetilde{\mathcal{O}}|n, L\rangle\langle n, L| \widetilde{A}|N, L\rangle}{\langle 0| \widetilde{\mathcal{O}}|N, L\rangle}
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& =\frac{i}{2 \omega_{\pi} \omega_{N} L^{3}} \mathcal{C}\left(E_{n}, L\right) \frac{\langle 0| \mathcal{O} \mid N \pi, \text { in }\rangle\langle N \pi, \text { out }| A_{z}^{3}|N\rangle}{\langle 0| \mathcal{O}|N\rangle}
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infinite-volume matrix elements

## Lellouch-Lüscher factor

$$
\mathcal{C}\left(E_{n}, L\right)=4 \pi^{2} q^{3} e^{-2 i \delta}\left(q \frac{\partial \phi}{\partial q}+p^{*} \frac{\partial \delta}{\partial p^{*}}\right)^{-1} \quad\left(q \equiv \frac{p^{*} L}{2 \pi}\right)
$$

(Neglects higher angular momenta and three-particle states)

Agadjanov et al., (2014), Nucl.Phys. B886, 1199 (2014).
Briceño and MTH, Phys. Rev. D92, 074509 (2015)

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infinite-volume matrix elements

## Lellouch-Lüscher factor

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\left.\mathcal{C}\left(E_{n}, L\right)=4 \pi^{2} q^{3} e^{-2 i \delta}\left(q \frac{\partial \phi}{\partial q}+p^{*} \frac{\partial \delta}{\partial p^{*}}\right)^{-1} \xrightarrow[\Delta \rightarrow 0]{ } \nu_{n}\right)
$$

In the free theory this counts the degeneracy of finite-volume states
(Neglects higher angular momenta and three-particle states)

Agadjanov et al., (2014), Nucl.Phys. B886, 1199 (2014).
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Can use this result to evaluate $b_{n}$ in ChPT

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\mathcal{C}\left(E_{n}, L\right)=\nu_{n}+\cdots
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Result agrees with Oliver Bär, arXiv:1606.09385

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$\langle N \pi$, out $| A_{z}^{3}|N\rangle=$


Result agrees with Oliver Bär, arXiv:1606.09385
Can one use experimental scattering data to go beyond the ChPT prediction?

## $\mathcal{C}\left(E_{n}, L\right)$ beyond LO ChPT

non-interacting result

$$
4 \pi^{2} q^{2}\left(\frac{\partial \phi}{\partial q}\right)^{-1}
$$

interacting result

$$
4 \pi^{2} q^{3}\left(q \frac{\partial \phi}{\partial q}+p^{*} \frac{\partial \delta}{\partial p^{*}}\right)^{-1}
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Two distinct effects:
Lellouch-Lüscher curve is lowered Places on the curve with physical meaning change

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## $\langle N \pi$, out $| A_{z}^{3}|N\rangle$ beyond LO ChPT

In principle this can be extracted from experiment but present data is insufficient

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N \nu \rightarrow N \pi
$$

Here we consider a (primitive) model of the matrix element

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We approximate the amplitude and kernel to be on-shell and use experimental value

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We approximate the amplitude and kernel to be on-shell and use experimental value

This model produces the correct phase (Watson's theorem)

The loop must be regulated, here we choose a cutoff at

$$
p=800 \mathrm{MeV}
$$

Not a rigorous determination... But a plausible value that gives insight into the problem of excited state contamination

$$
R(T, \tau)=\frac{\langle\mathcal{O}(T) A(\tau) \overline{\mathcal{O}}(0)\rangle}{\langle\mathcal{O}(T) \overline{\mathcal{O}}(0)\rangle}=g_{A}+\mathcal{E}(T, \tau)
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Effect of modifying $\Delta E_{n}, \mathcal{C}\left(E_{n}, L\right)$, and $\langle N \pi$, out $| A_{z}^{3}|N\rangle$


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## ChPT, 2 states ChPT, 5 states

Oliver Bär, arXiv:1606.09385

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## Summary

The Lüscher and Lellouch-Lüscher formalisms allow one to use experimental inputs to estimate excited state contamination

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The Lellouch-Lüscher relation gives a great deal of insight about the coefficients including some surprises:

Amputated tree-level diagrams can be used to extract the same LO ChPT predictions given by standard one-loop diagrams

Interactions can shift the Lellouch-Lüscher factors dramatically due to the highly oscillatory function


A sign flip in the axial matrix element could lead to the observed sign of the excited state contamination


## Conclusions

Many finite-volume states can be important in excited state contamination

It may be that the positive ChPT result is flipped by higher states
This emphasizes the importance of well-known techniques to reduce excited state contamination: e.g. variational method

## Future work

Better estimate the infinite-volume matrix element
Include the effects of heavier than physical pions
Include the effects of three-particle states

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Effect of modifying $\Delta E_{n}, \mathcal{C}\left(E_{n}, L\right)$, and $\langle N \pi$, out $| A_{z}^{3}|N\rangle$


$$
R(T, \tau)=\frac{\langle\mathcal{O}(T) A(\tau) \overline{\mathcal{O}}(0)\rangle}{\langle\mathcal{O}(T) \overline{\mathcal{O}}(0)\rangle}=g_{A}+\mathcal{E}(T, \tau)
$$

$$
\mathcal{E}(T, \tau)=\sum_{n=1}^{\infty} b_{n}\left[e^{-\Delta E_{n}(T-\tau)}+e^{-\Delta E_{n} \tau}\right]+c_{n} e^{-\Delta E_{n} T}+\cdots
$$

Effect of modifying $\Delta E_{n}, \mathcal{C}\left(E_{n}, L\right)$, and $\langle N \pi$, out $| A_{z}^{3}|N\rangle$


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$$

Effect of modifying $\Delta E_{n}, \mathcal{C}\left(E_{n}, L\right)$, and $\langle N \pi$, out $| A_{z}^{3}|N\rangle$


## $\frac{R(T=1.5 \mathrm{fm}, \tau)}{g_{A}}$ <br> ChPT, 20 states

Oliver Bär, arXiv:1606.09385
this work, 8 states

