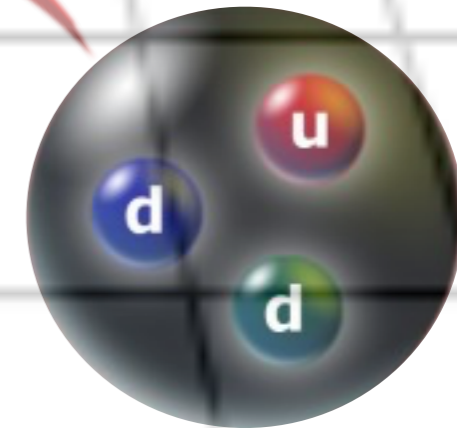




Advances in NN systems



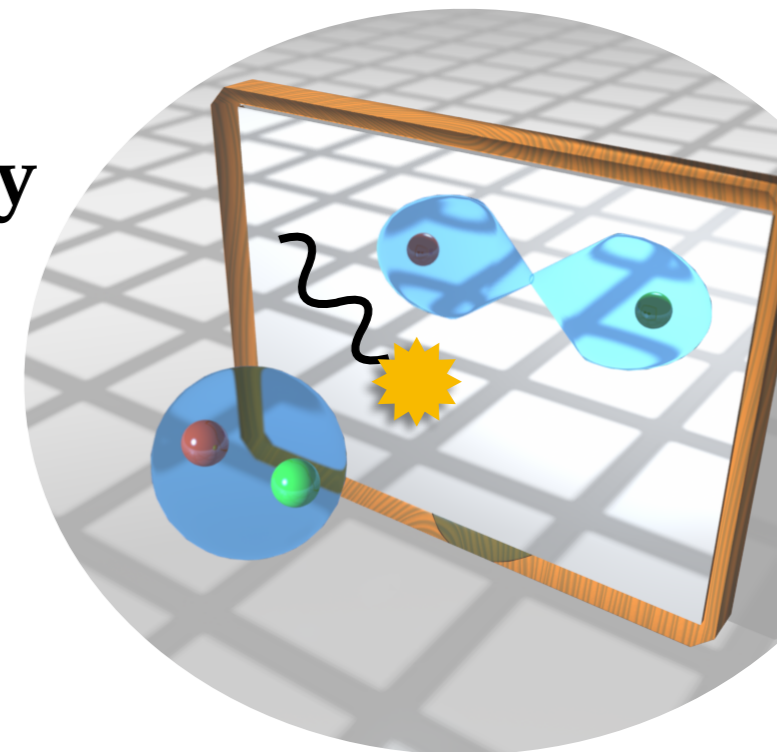
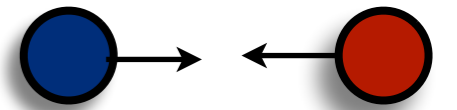
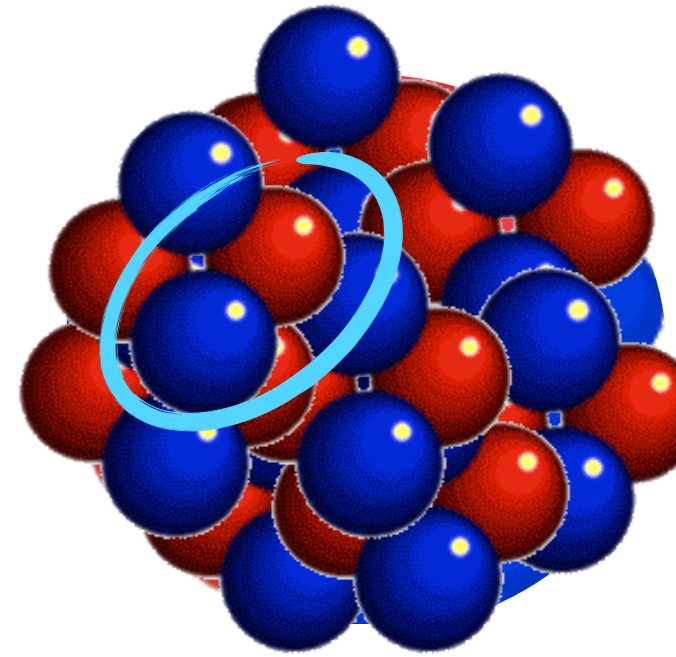
Amy Nicholson
UNC, Chapel Hill

Virtual DBD meeting, May 29, 2020

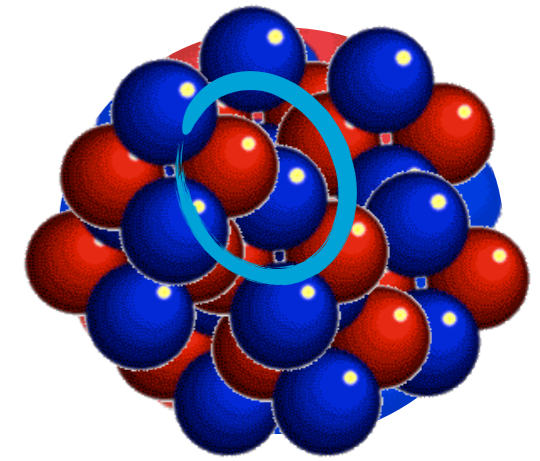


NN systems

- What do we need to get nuclear physics from LQCD?
 - Phase shifts required for infinite volume matching of MEs
 - Must have full control over 2-body systems
 - How do we project onto desired states?
 - How do we disentangle signals from closely spaced energy levels?
 - How do we beat the noise?



Methods for calculating few-body interactions from LQCD:



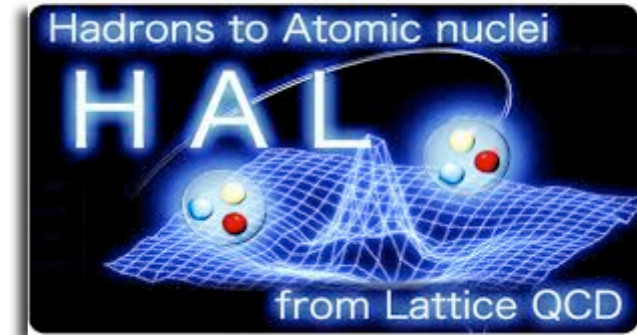
Spectroscopy + Lüscher Method



Yamazaki,
et. al.

Hanlon
et. al.

Potential Method

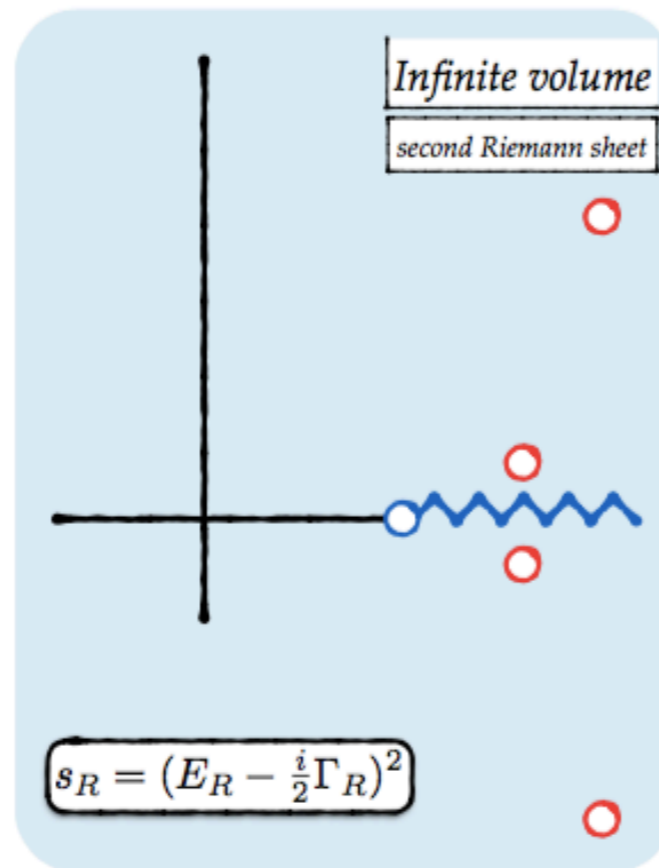
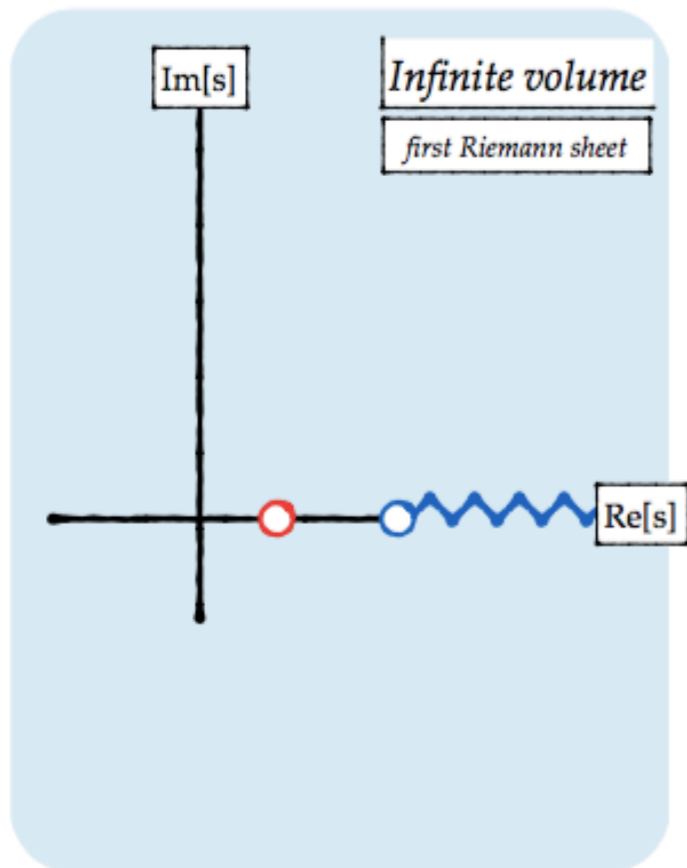


Spectroscopy + HOBET

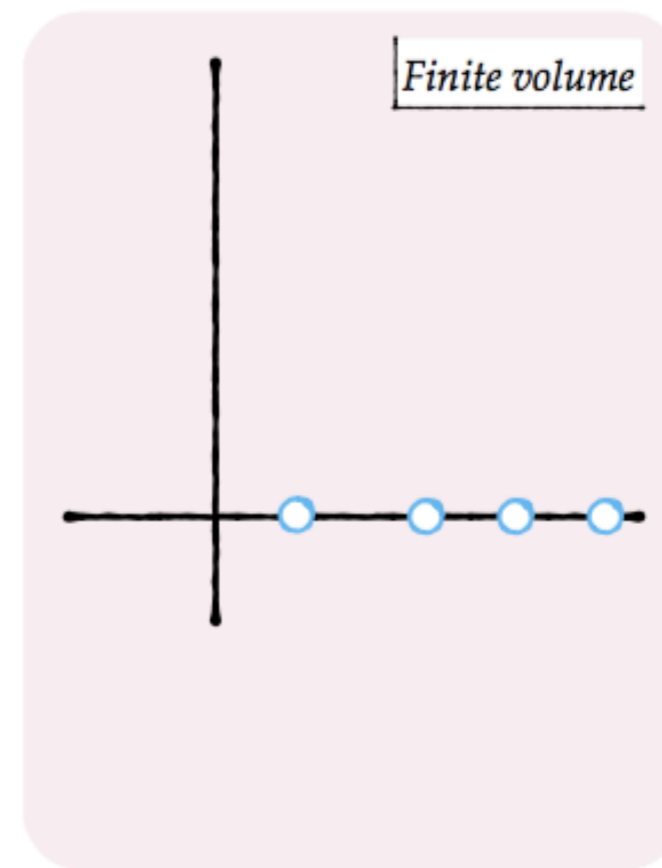
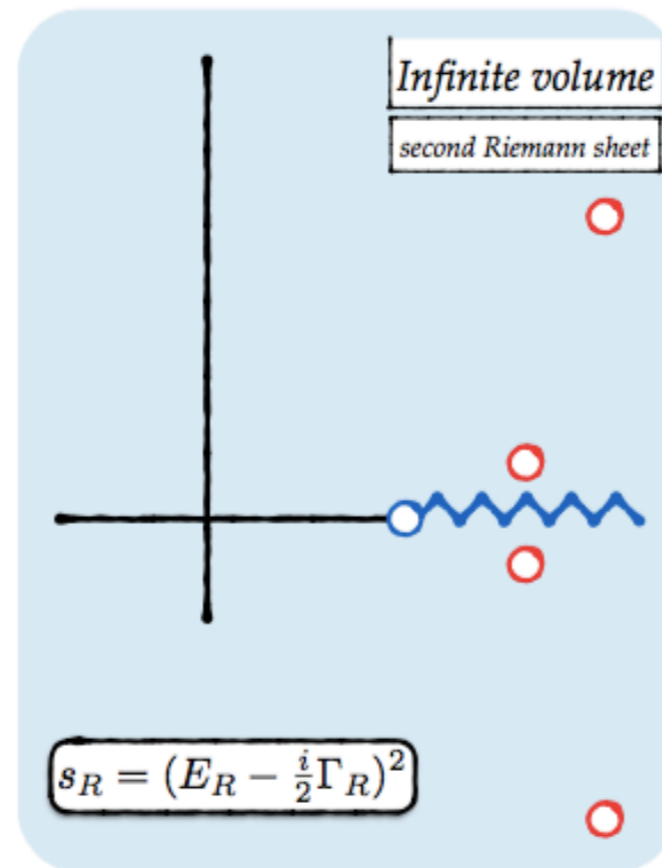
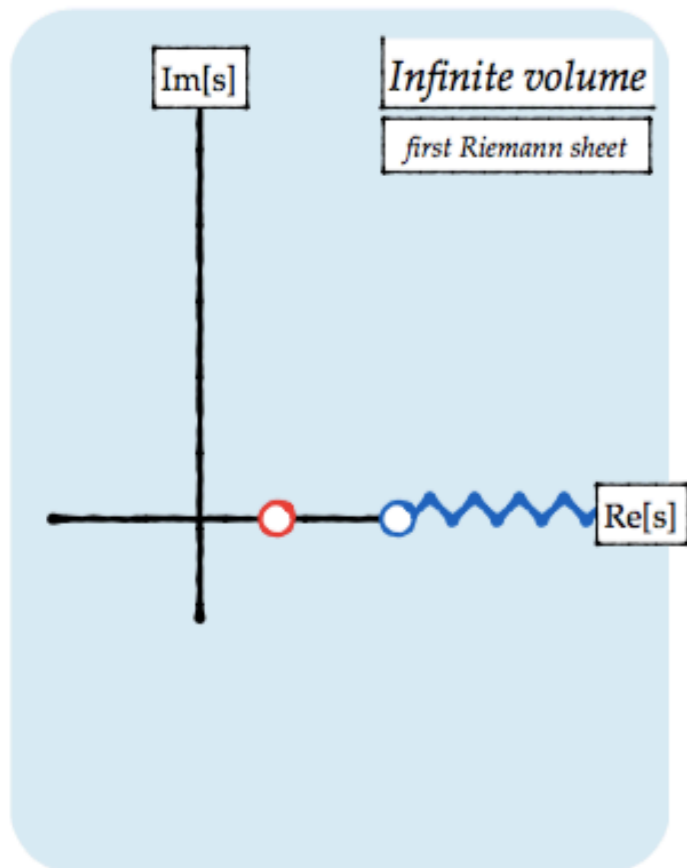


*not an official logo

Spectroscopy



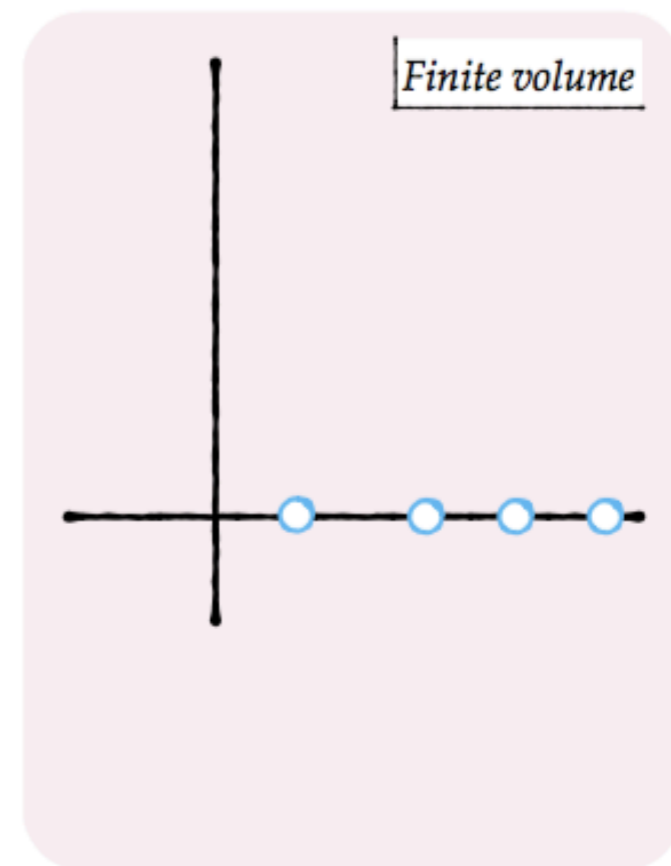
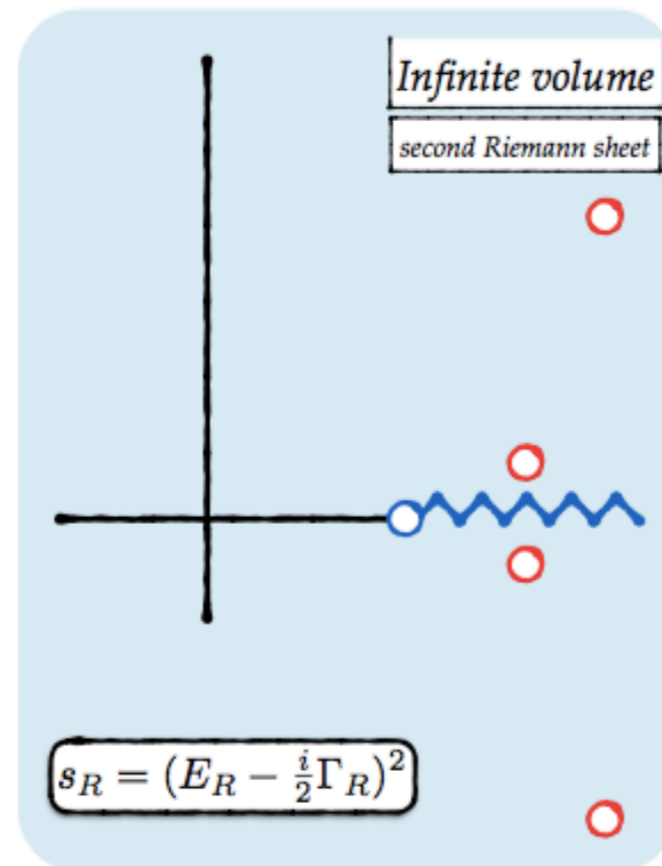
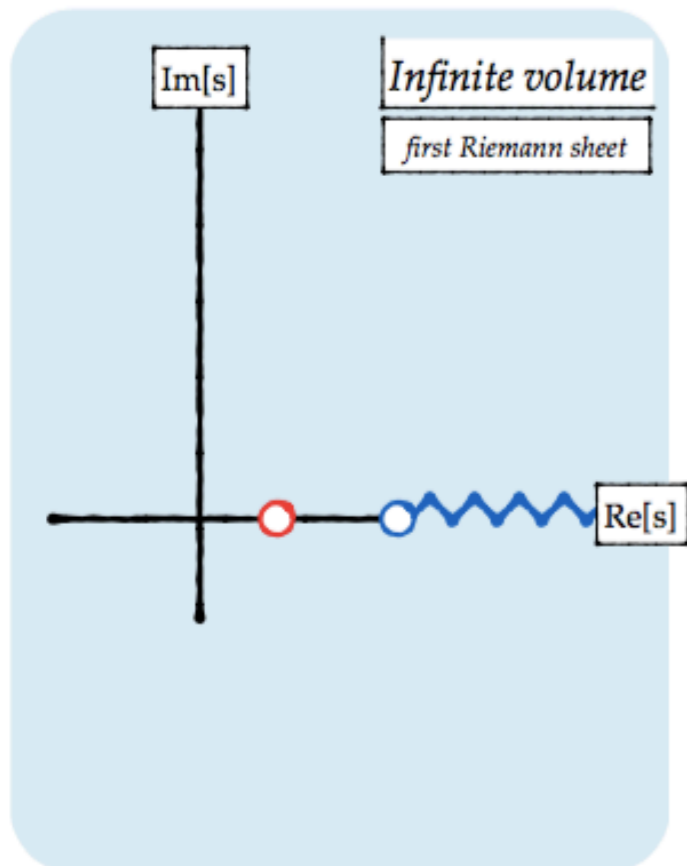
Spectroscopy



Spectroscopy

$$\langle \mathcal{O}(t) \mathcal{O}^\dagger(0) \rangle = \sum_n |\langle 0 | \mathcal{O} | n \rangle|^2 e^{-E_n t}$$

$$\xrightarrow[t \rightarrow \infty]{} \langle 0 | \mathcal{O} | E_0 \rangle \langle E_0 | \mathcal{O} | 0 \rangle e^{-E_0 t}$$



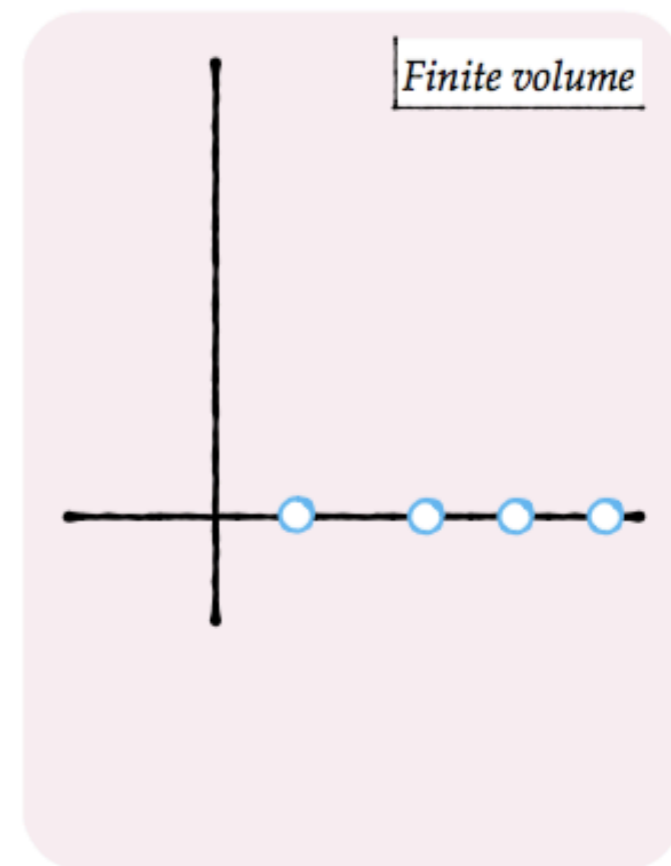
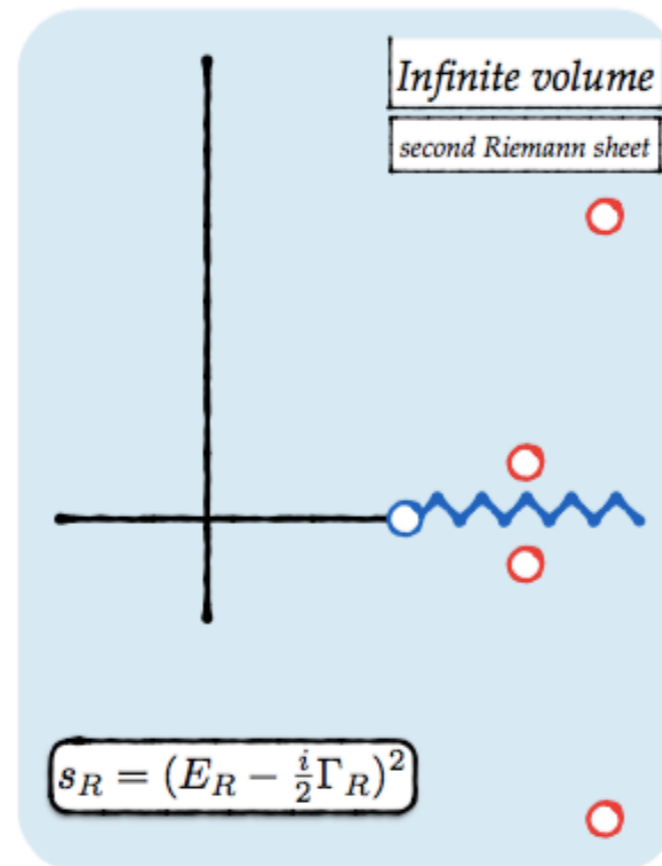
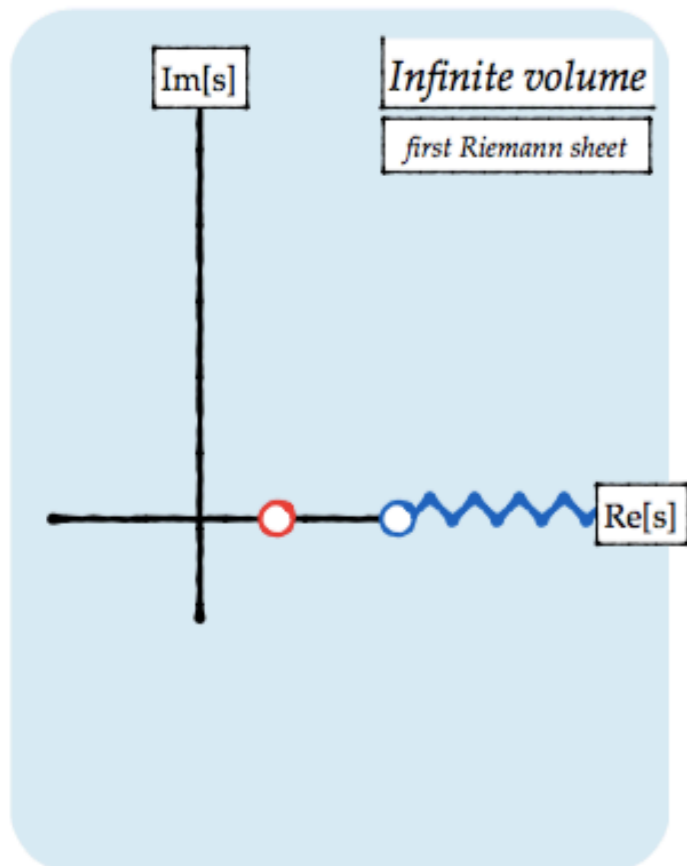
Figures courtesy
R. Briceno

Spectroscopy

- Finite volume energies simple to calculate from correlation functions at large Euclidean time:

$$\langle \mathcal{O}(t) \mathcal{O}^\dagger(0) \rangle = \sum_n |\langle 0 | \mathcal{O} | n \rangle|^2 e^{-E_n t}$$

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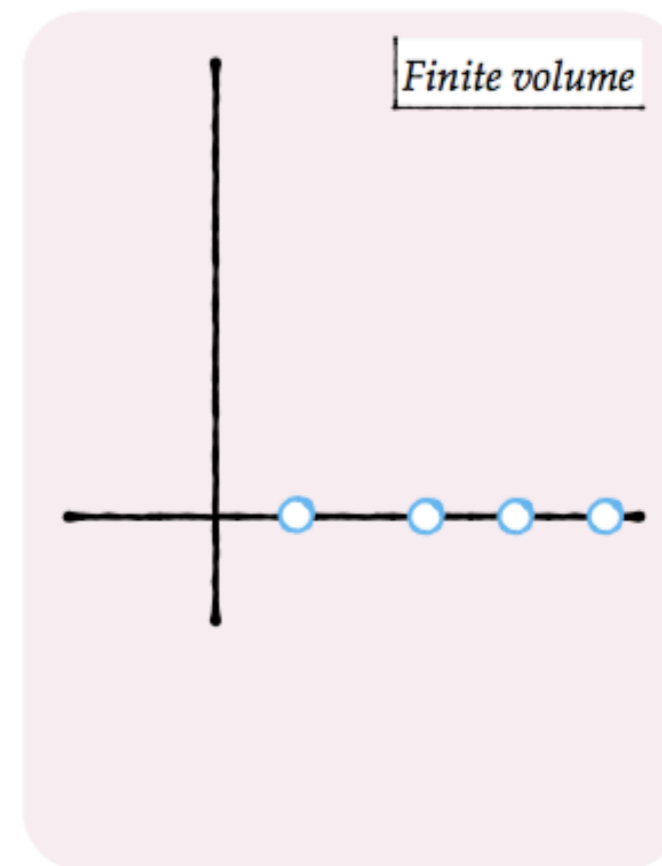
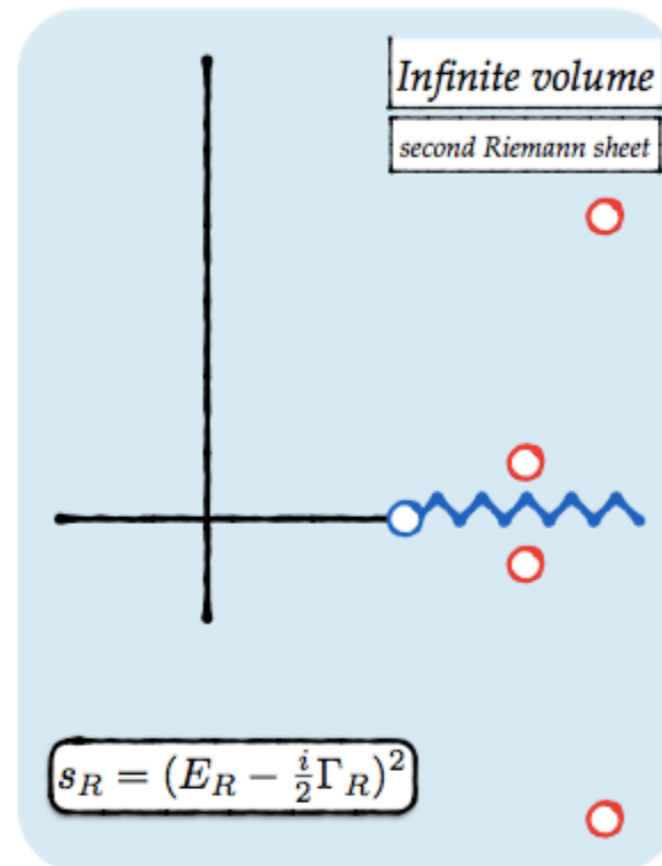
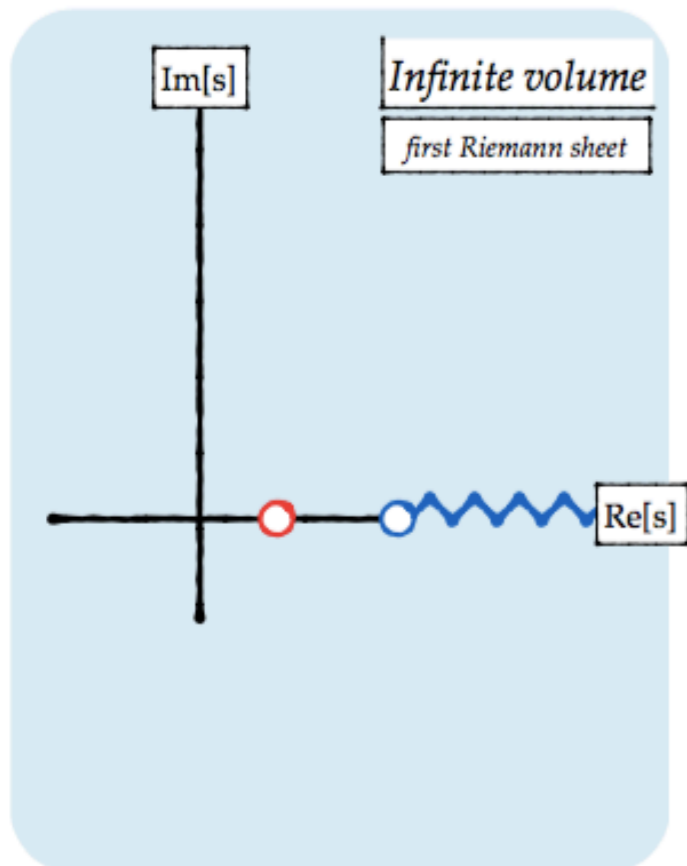
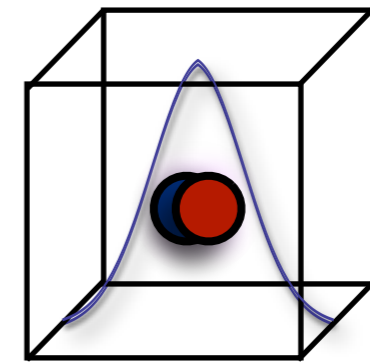
Figures courtesy R. Briceno

Spectroscopy

- Finite volume energies simple to calculate from correlation functions at large Euclidean time:
- Bound states: infinite volume extrapolation gives binding energies

$$\langle \mathcal{O}(t) \mathcal{O}^\dagger(0) \rangle = \sum_n |\langle 0 | \mathcal{O} | n \rangle|^2 e^{-E_n t}$$

$$\xrightarrow[t \rightarrow \infty]{} \langle 0 | \mathcal{O} | E_0 \rangle \langle E_0 | \mathcal{O} | 0 \rangle e^{-E_0 t}$$



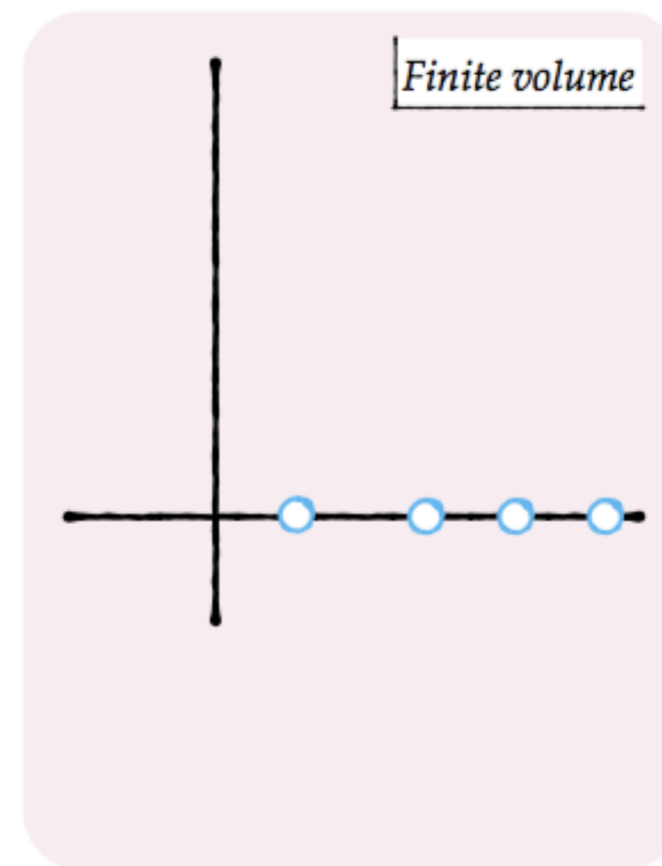
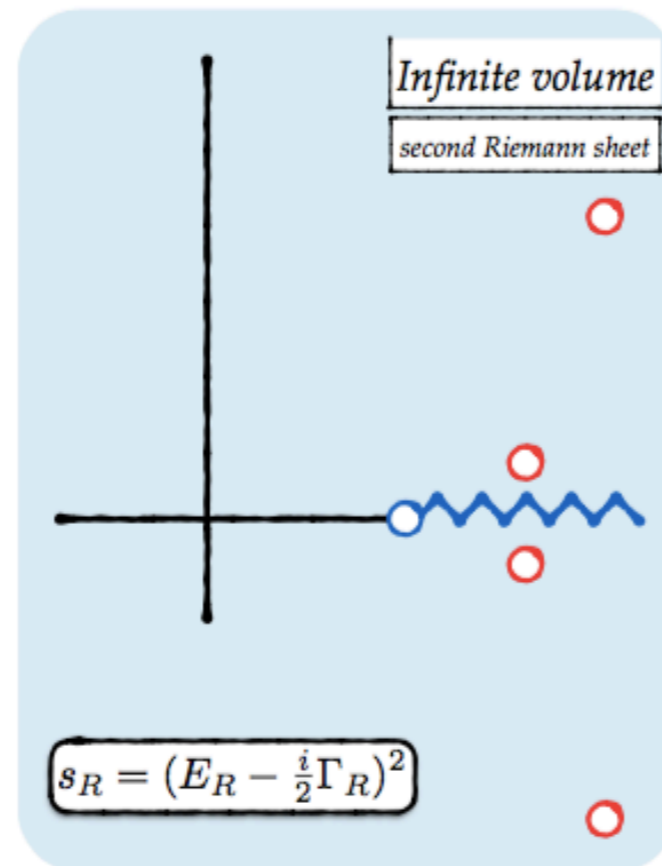
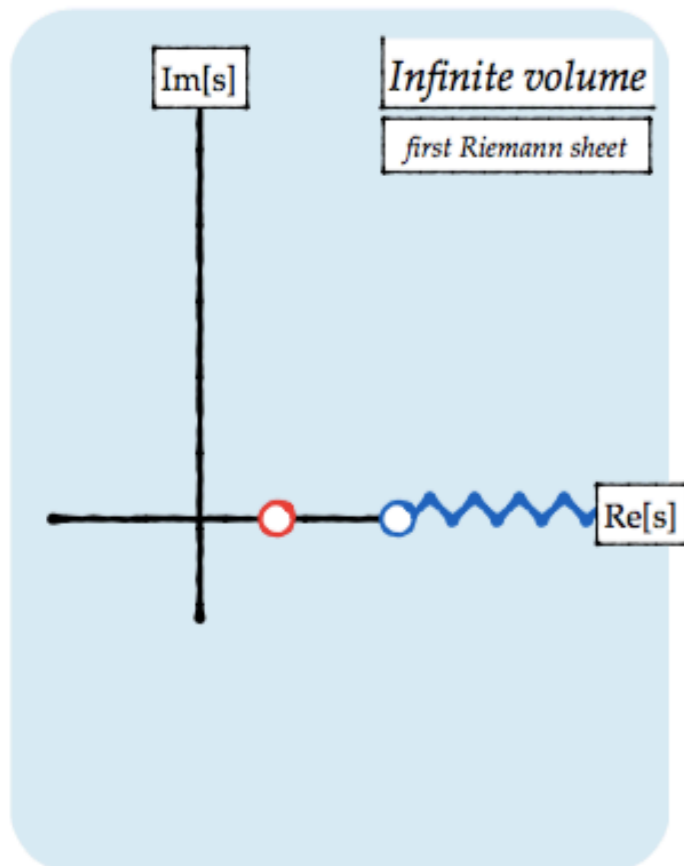
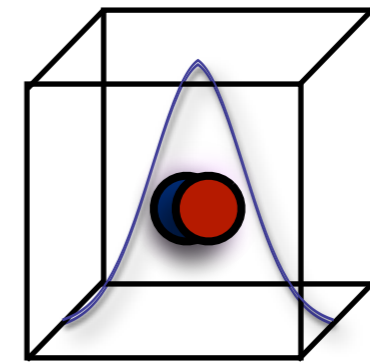
Figures courtesy R. Briceno

Spectroscopy

- Finite volume energies simple to calculate from correlation functions at large Euclidean time:
- Bound states: infinite volume extrapolation gives binding energies
- Can't directly resolve resonances or scattering states

$$\langle \mathcal{O}(t) \mathcal{O}^\dagger(0) \rangle = \sum_n |\langle 0 | \mathcal{O} | n \rangle|^2 e^{-E_n t}$$

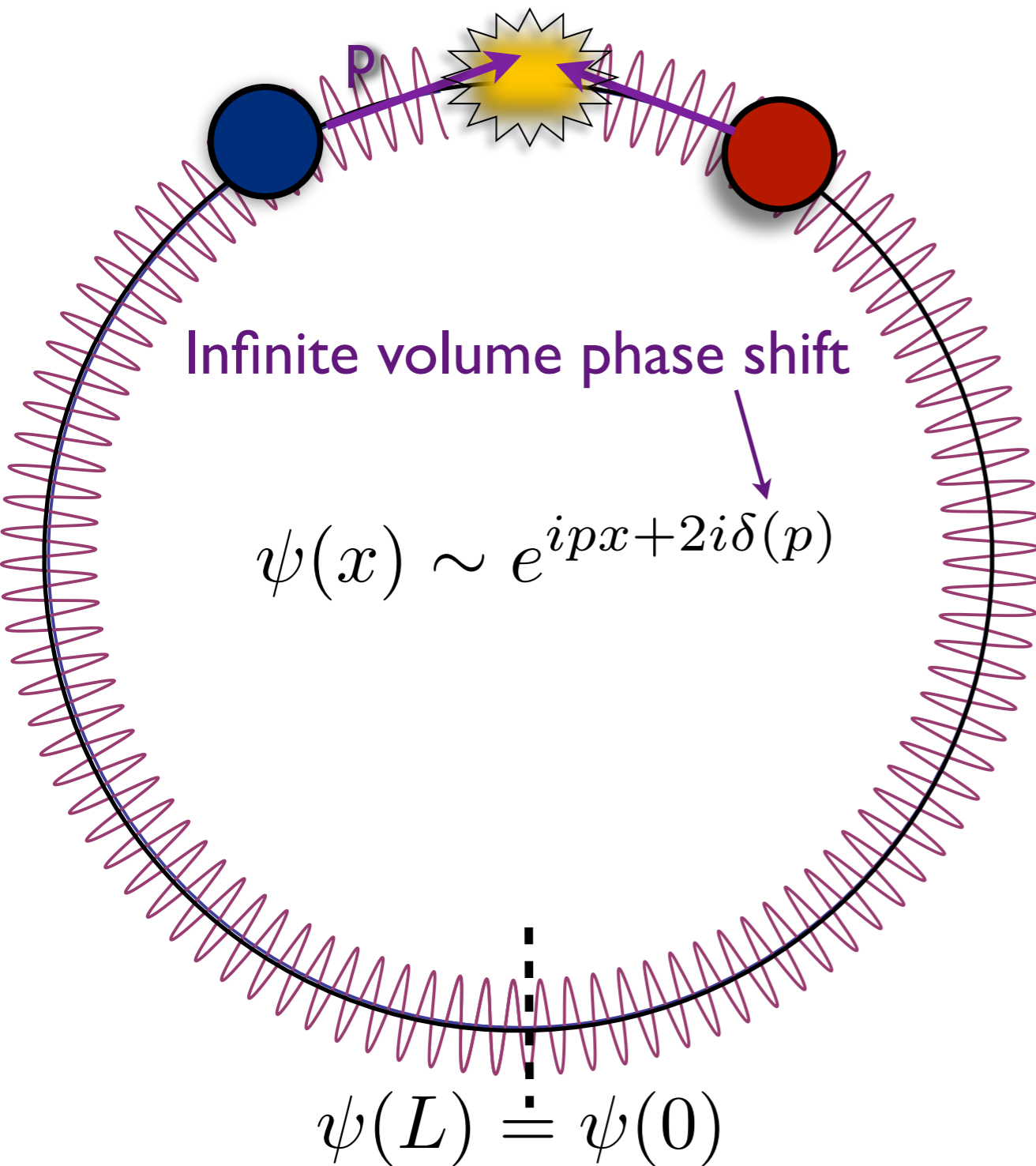
$$\xrightarrow[t \rightarrow \infty]{} \langle 0 | \mathcal{O} | E_0 \rangle \langle E_0 | \mathcal{O} | 0 \rangle e^{-E_0 t}$$



Figures courtesy R. Briceno

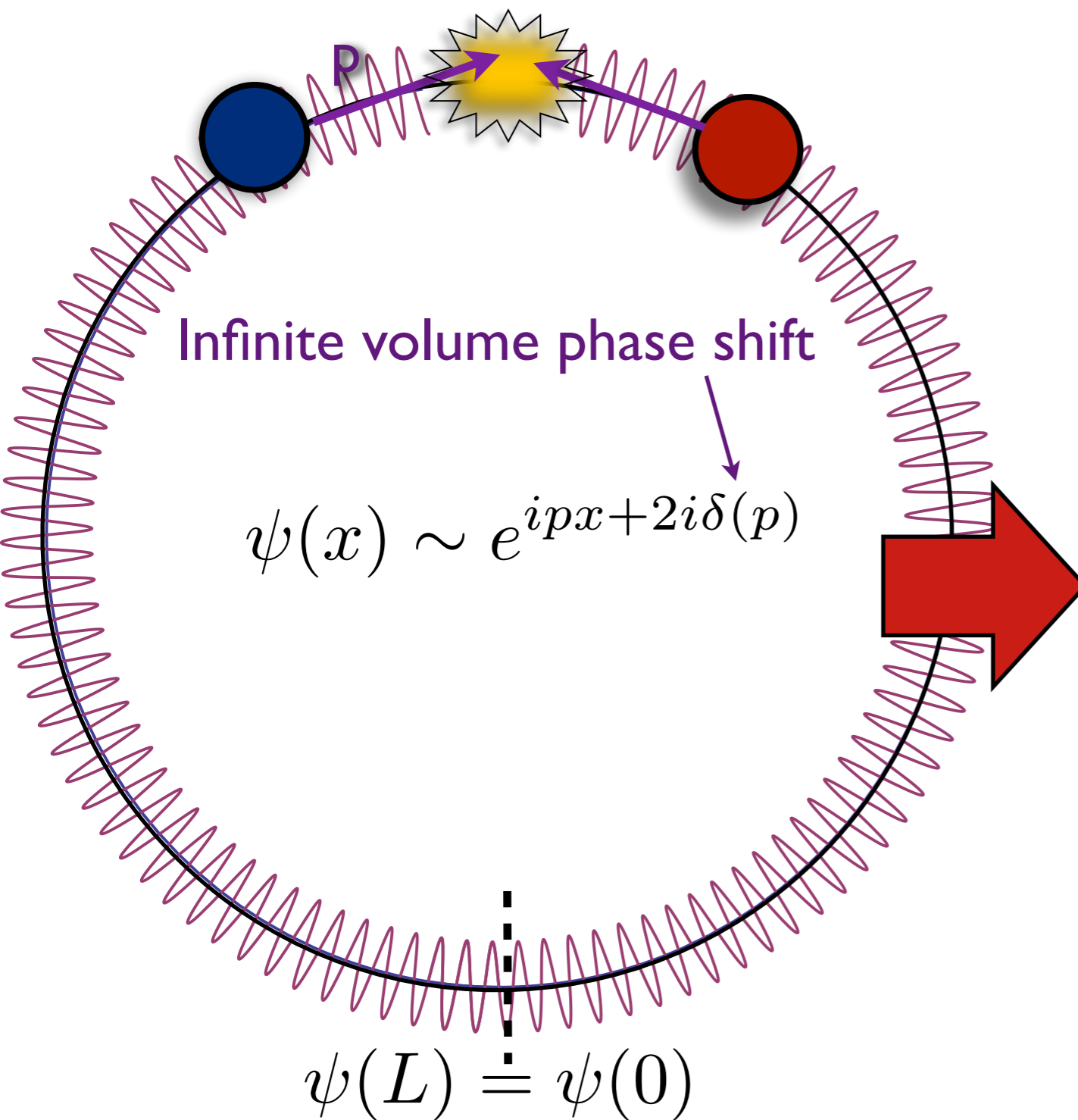
“Lüscher” in 1-d

Slide stolen unabashedly from R. Briceño



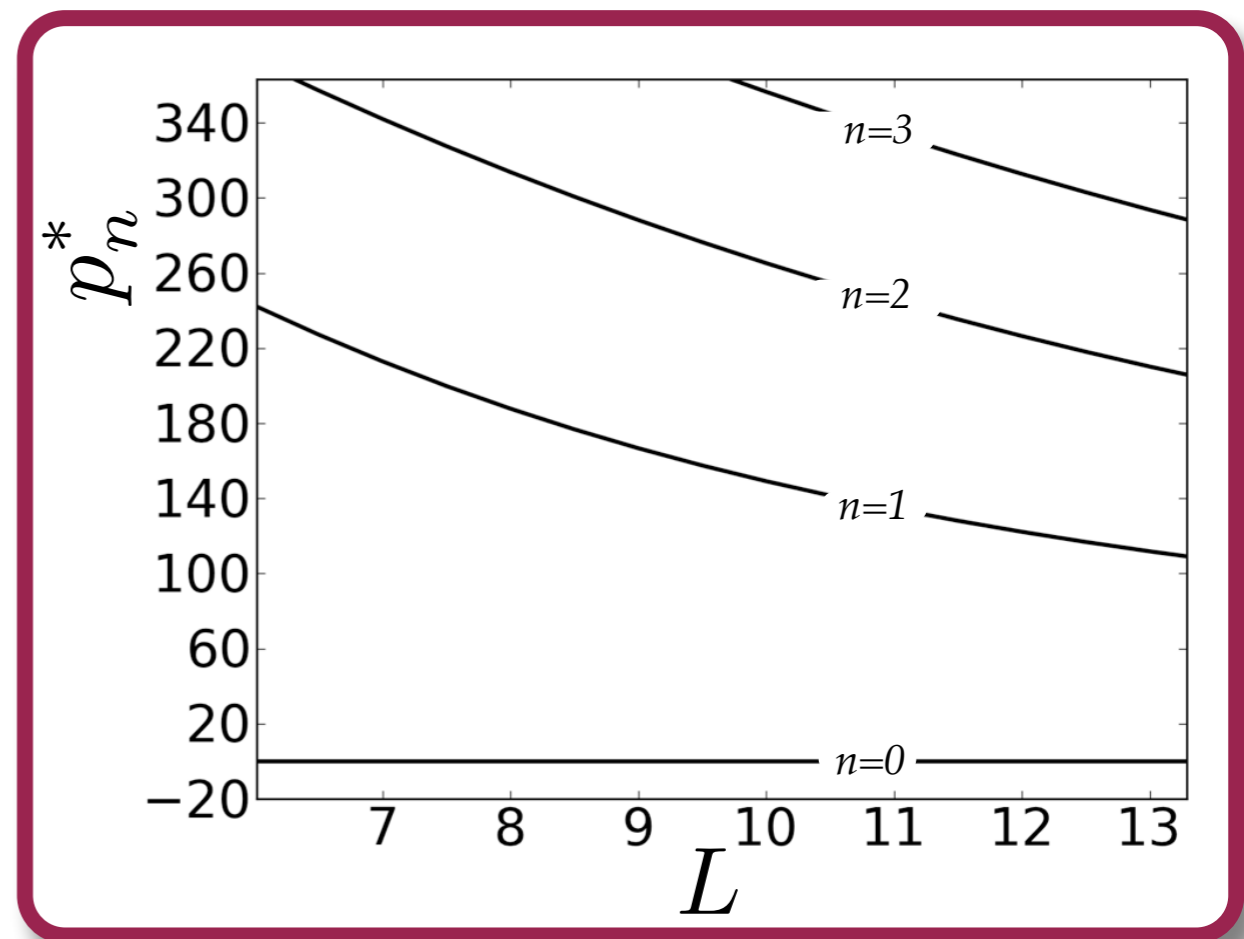
“Lüscher” in 1-d

Slide stolen unabashedly from R. Briceno



Quantization condition:

$$Lp_n^* + 2\delta(p_n^*) = 2\pi n$$



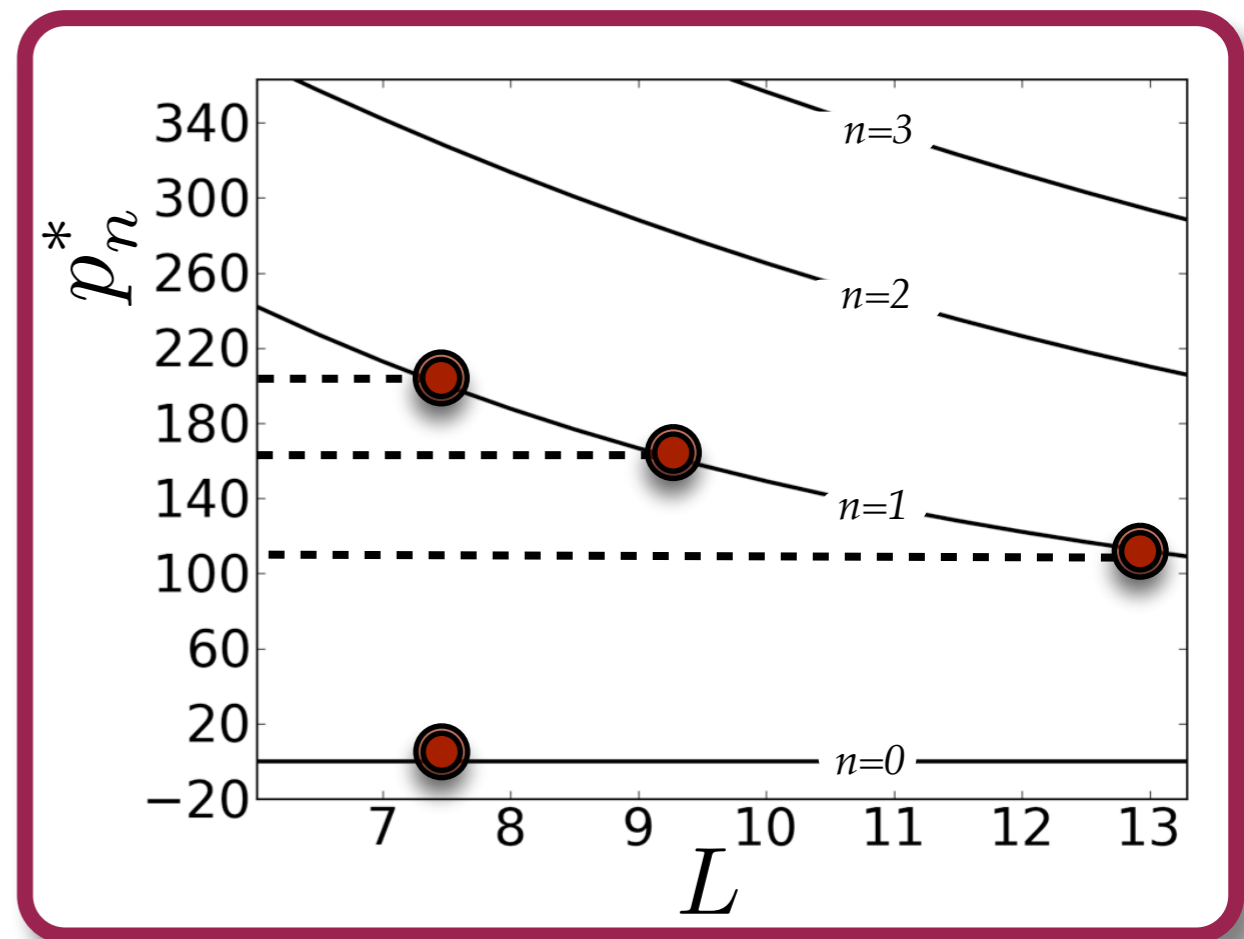
“Lüscher” in 1-d

Slide stolen unabashedly from R. Briceno

Quantization condition:

$$Lp_n^* + 2\delta(p_n^*) = 2\pi n$$

Lattice: measure energies at a given L

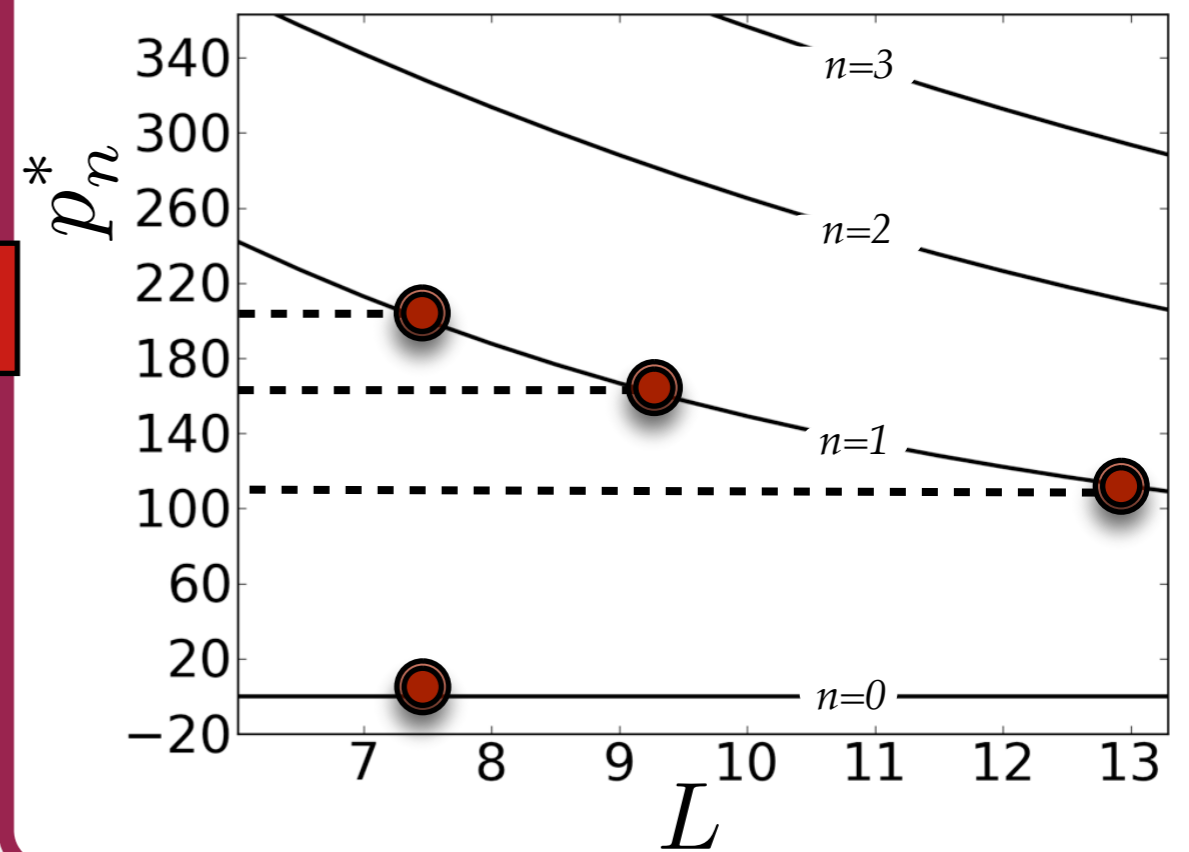
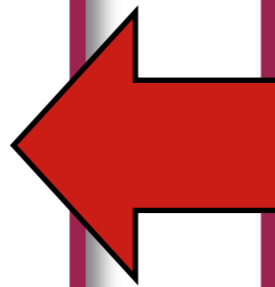
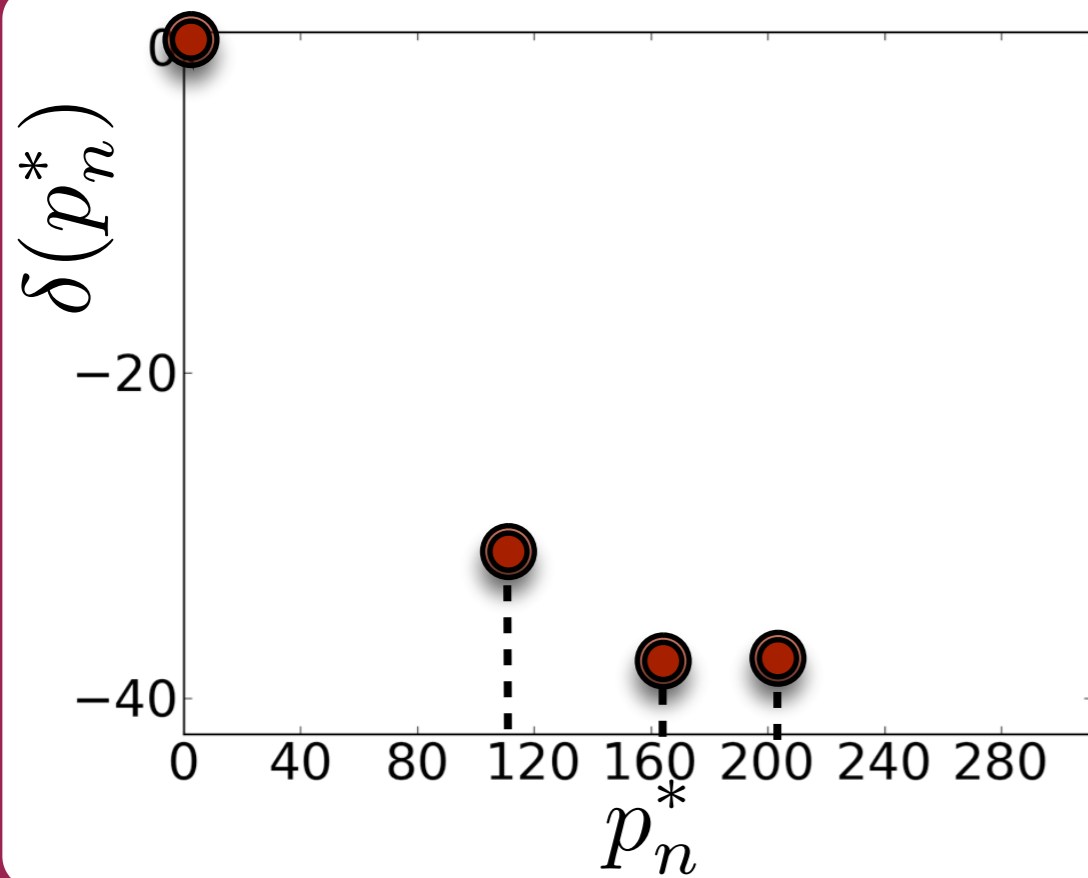


“Lüscher” in 1-d

Slide stolen unabashedly from R. Briceno

Quantization condition:

$$Lp_n^* + 2\delta(p_n^*) = 2\pi n$$

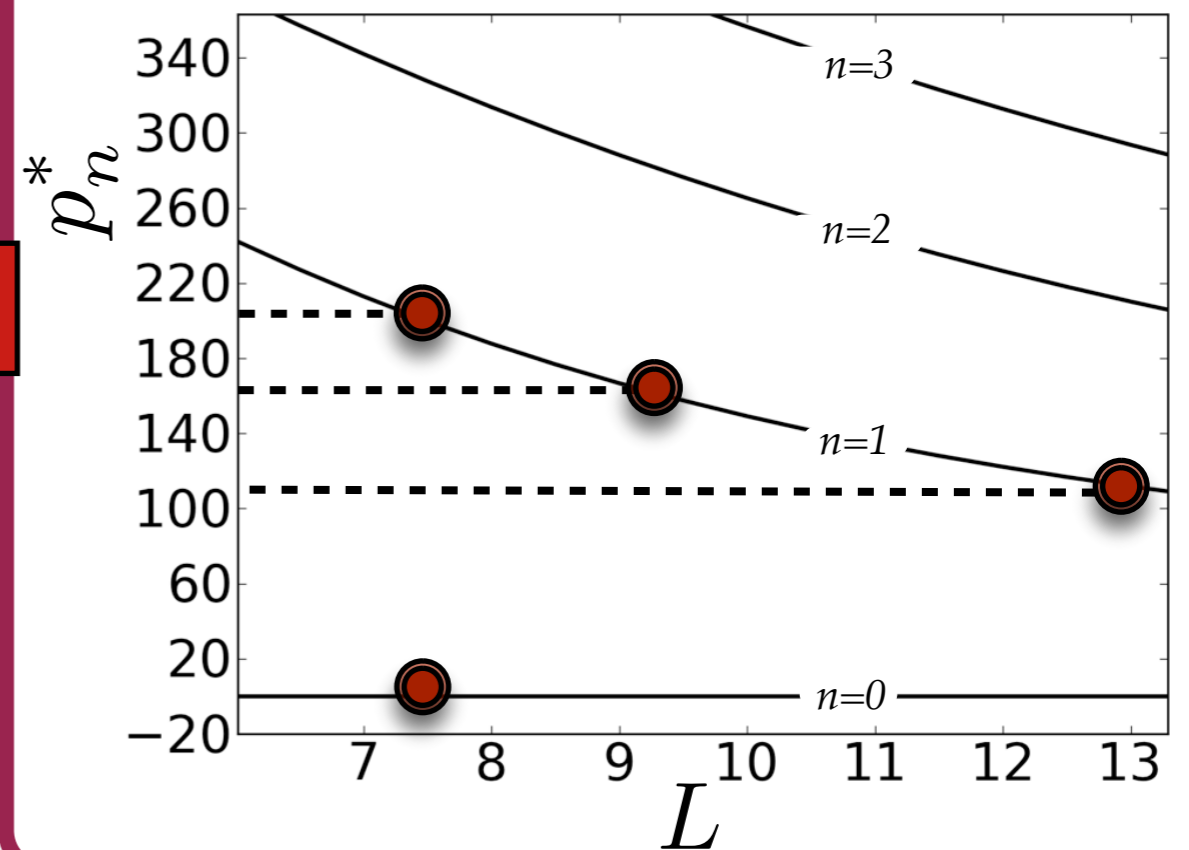
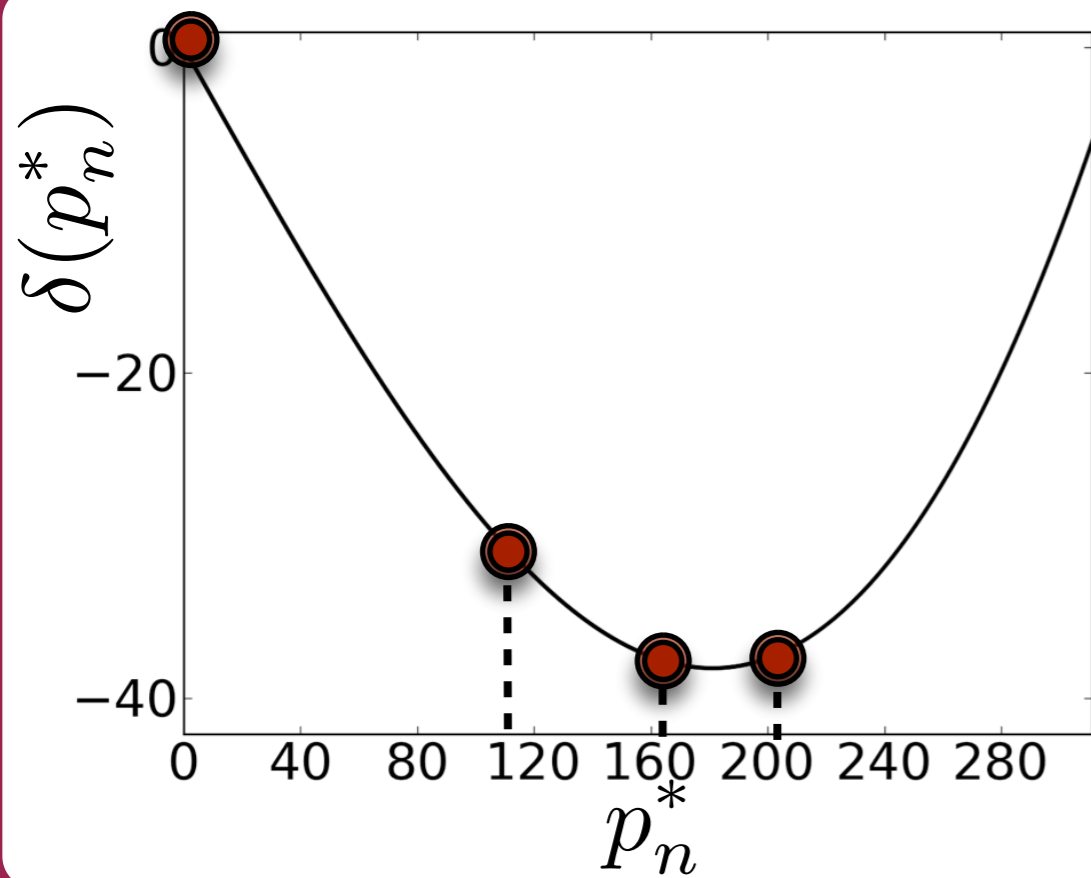


“Lüscher” in 1-d

Slide stolen unabashedly from R. Briceno

Quantization condition:

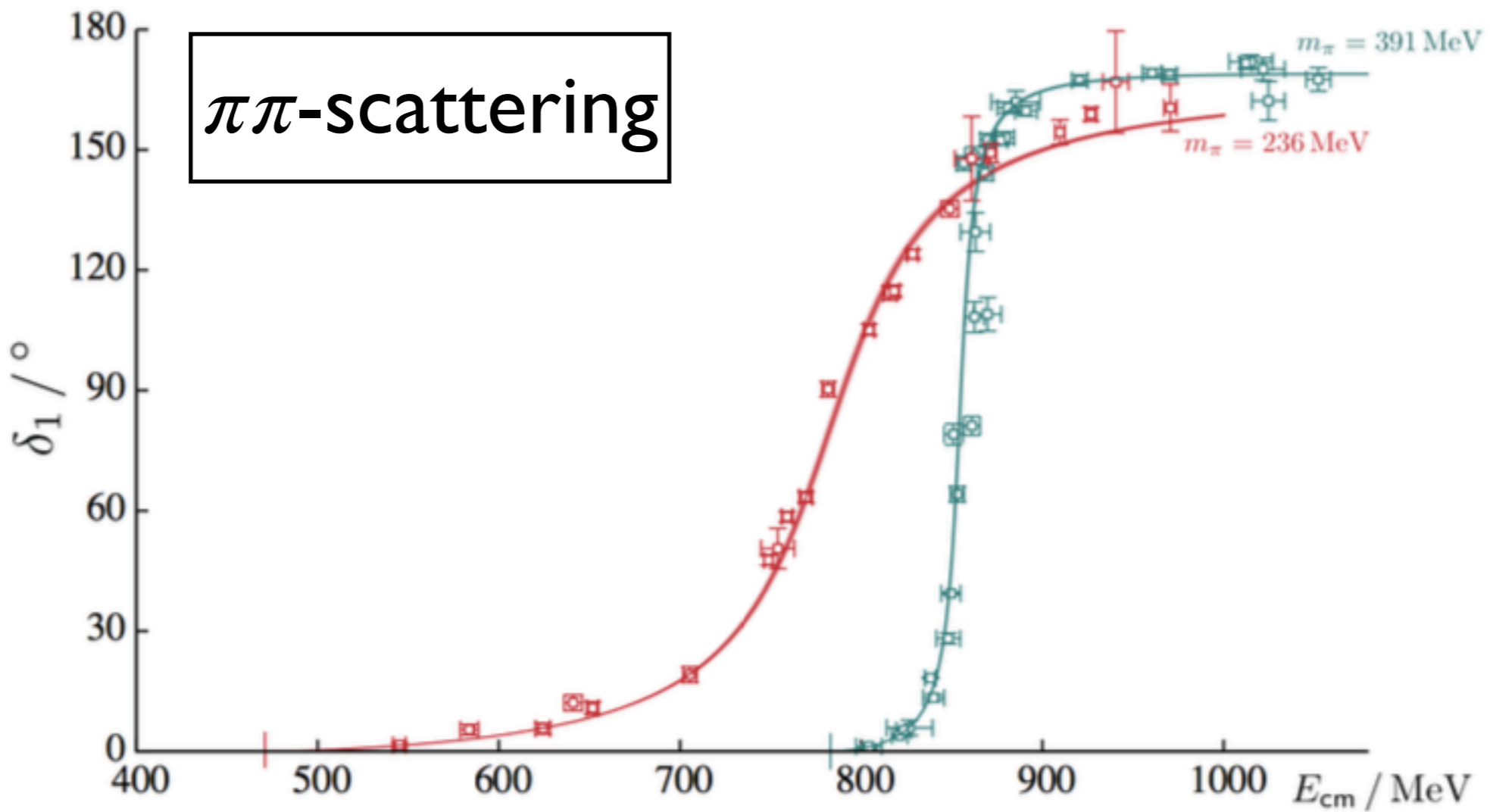
$$Lp_n^* + 2\delta(p_n^*) = 2\pi n$$



“Lüscher” in 1-d

D. J. Wilson, R. A. Briceno, J. J. Dudek, R. G. Edwards and C. E. Thomas, Phys. Rev. D 92, 094502 (2015)

Quantization condition:



$\delta(p_n^*)$

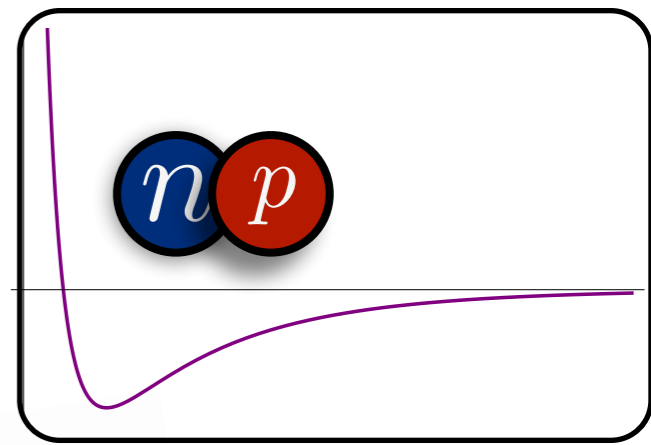
-20

-40

0

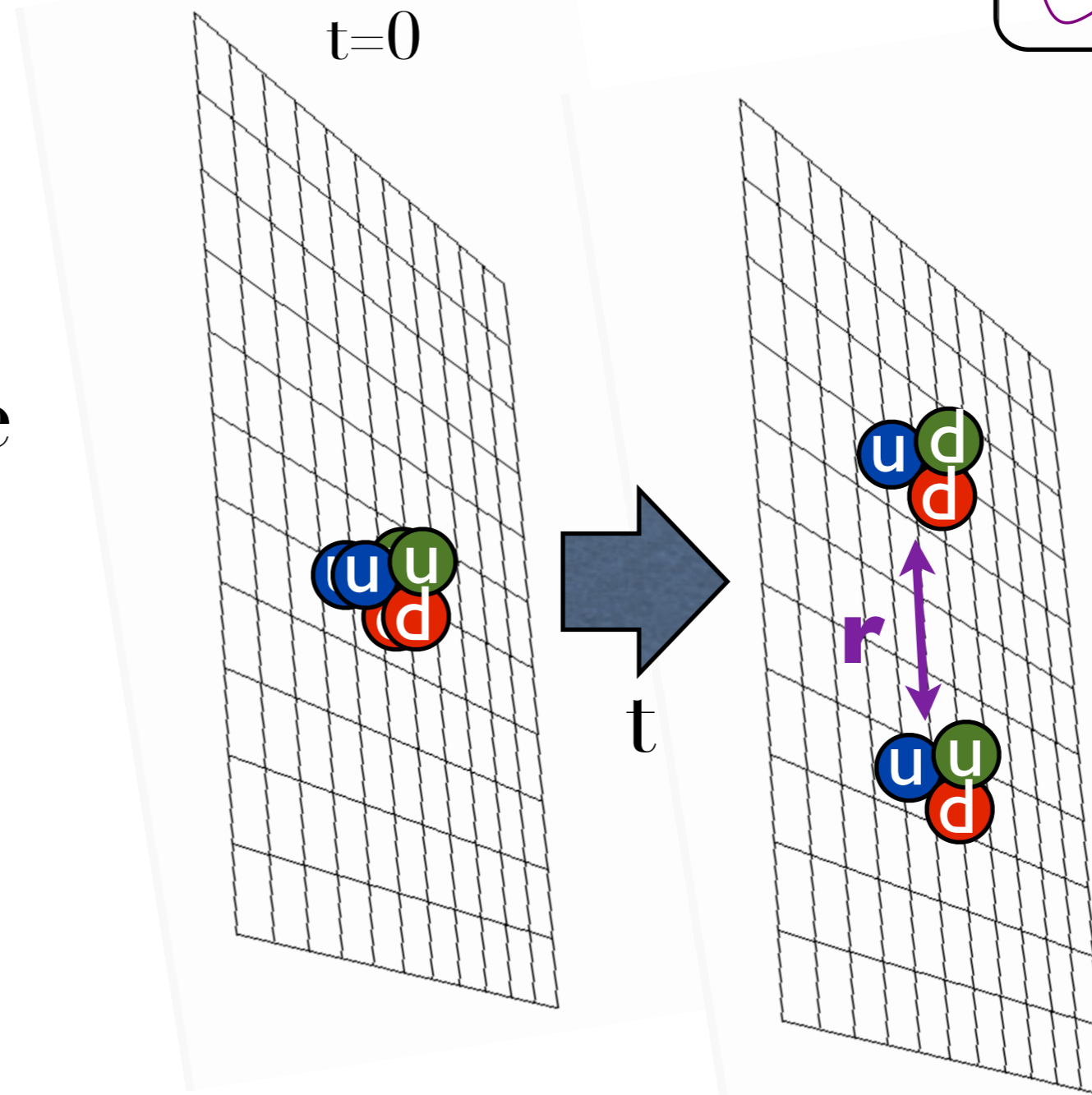
12 13

Potential method

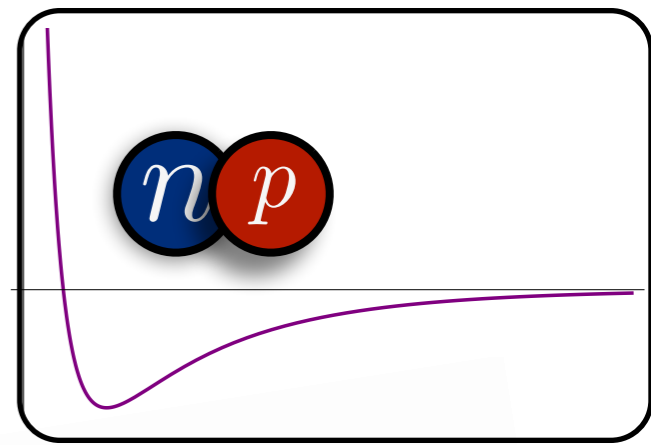


1. Create the following correlation function:

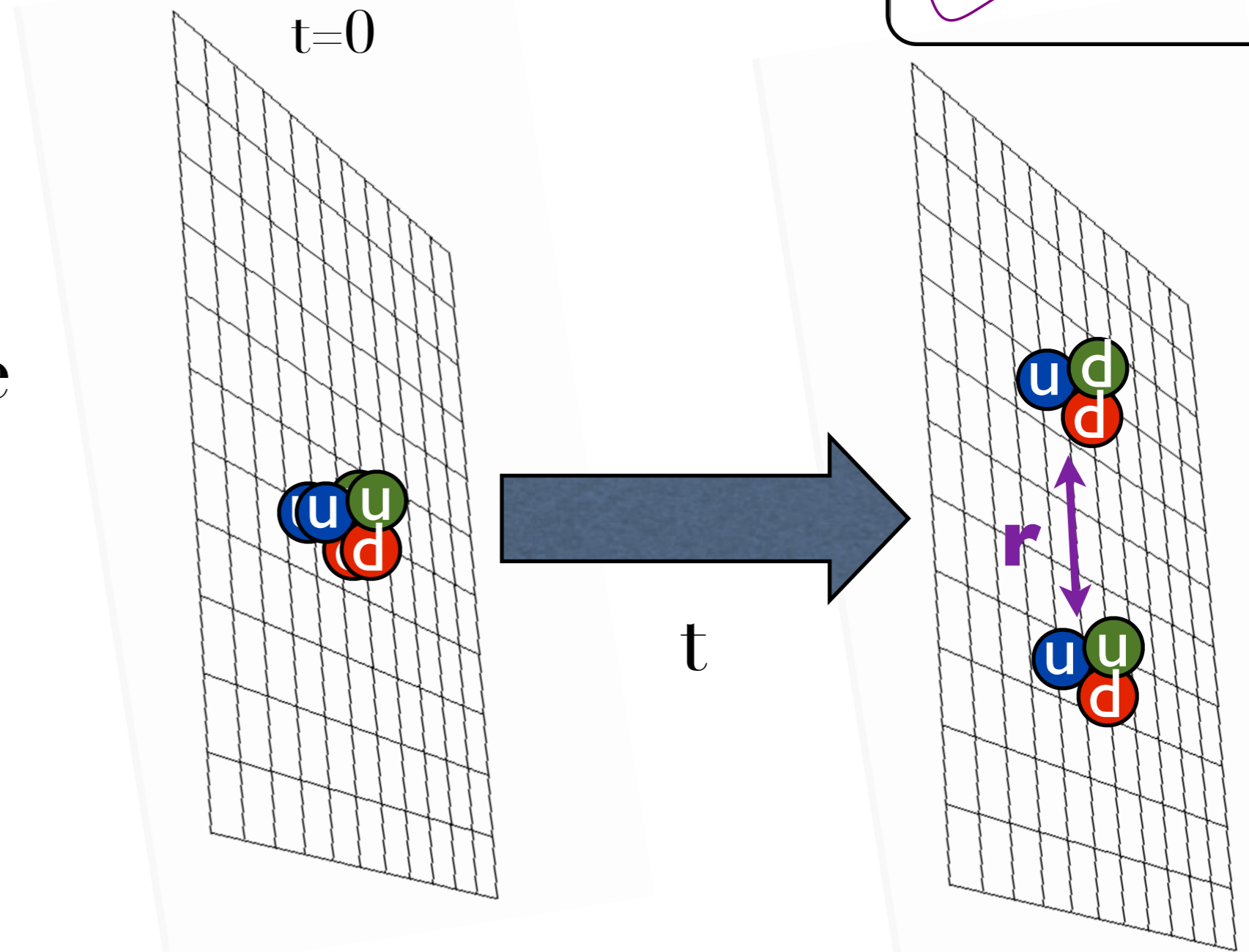
$$C_{NN}(\mathbf{r}, t)$$



Potential method

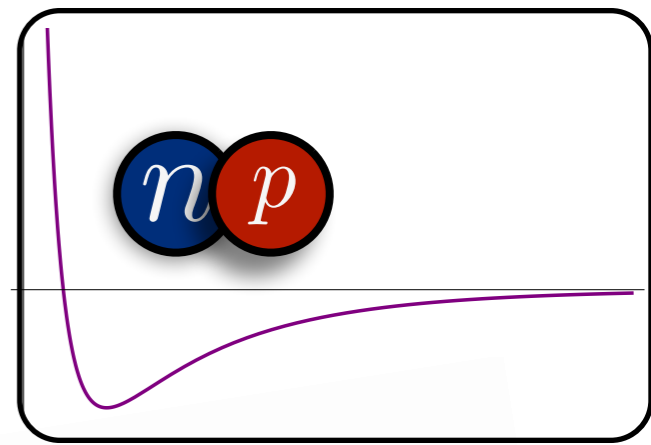


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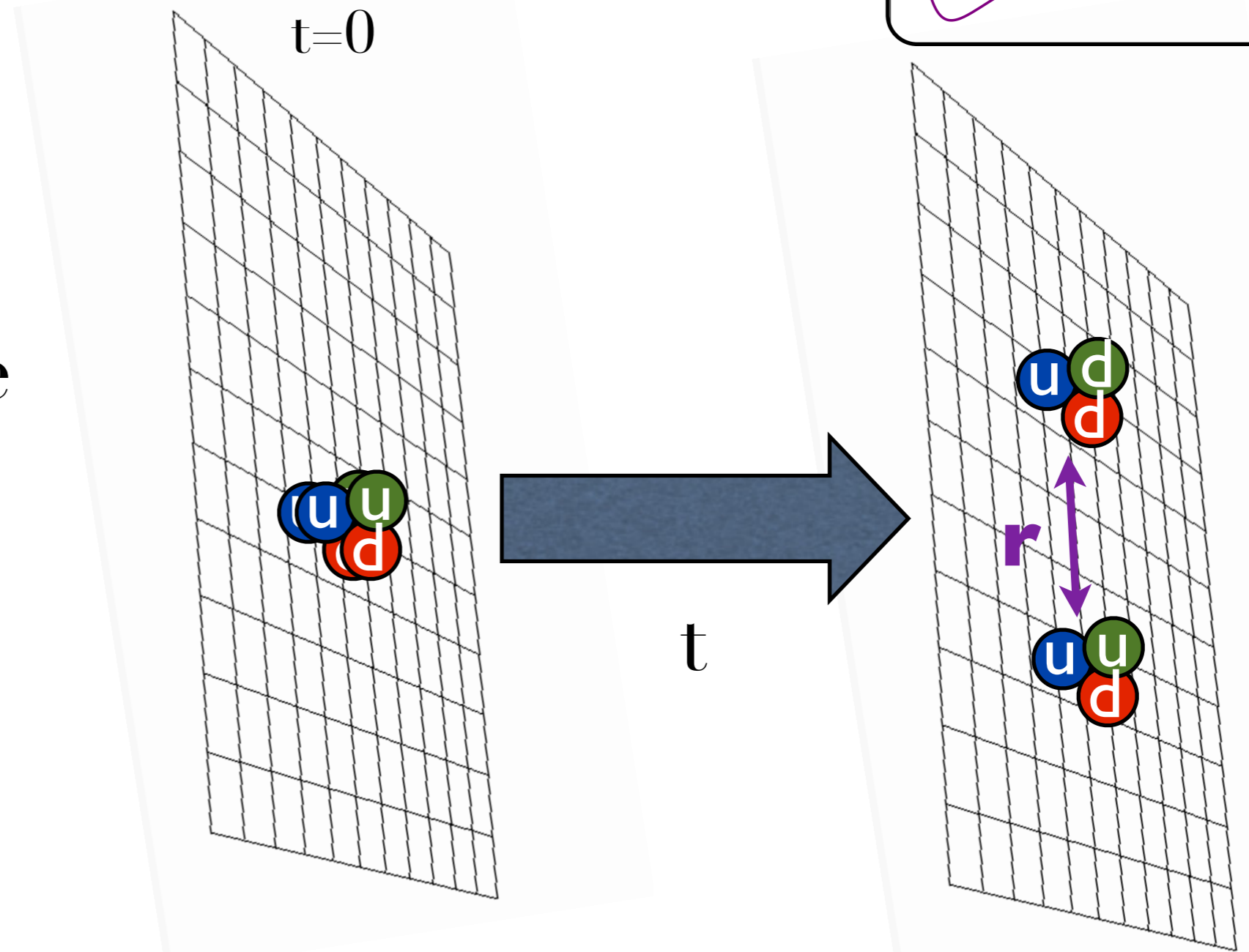


$$\lim_{t \rightarrow \infty} C_{NN}(\mathbf{r}, t) =$$

Potential method

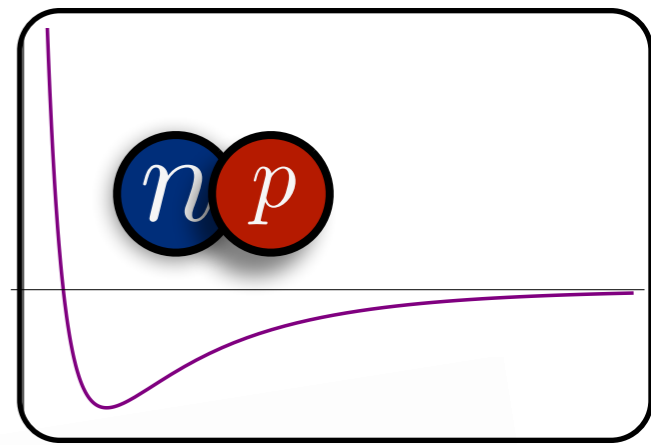


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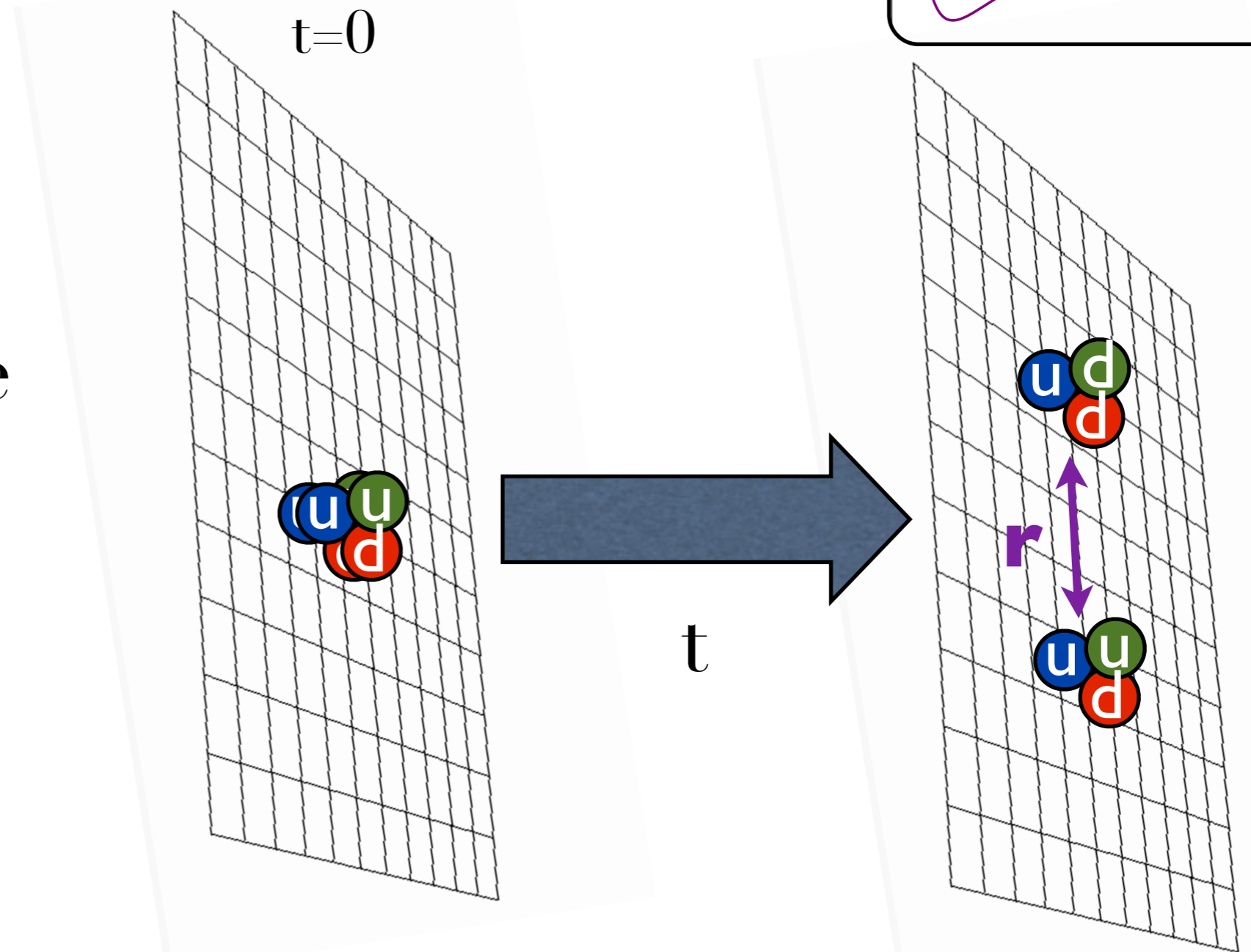


$$\lim_{t \rightarrow \infty} C_{NN}(\mathbf{r}, t) = \psi_0^\dagger$$

Potential method

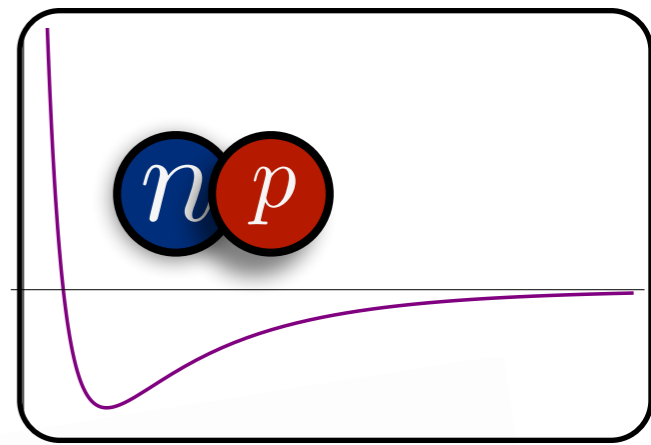


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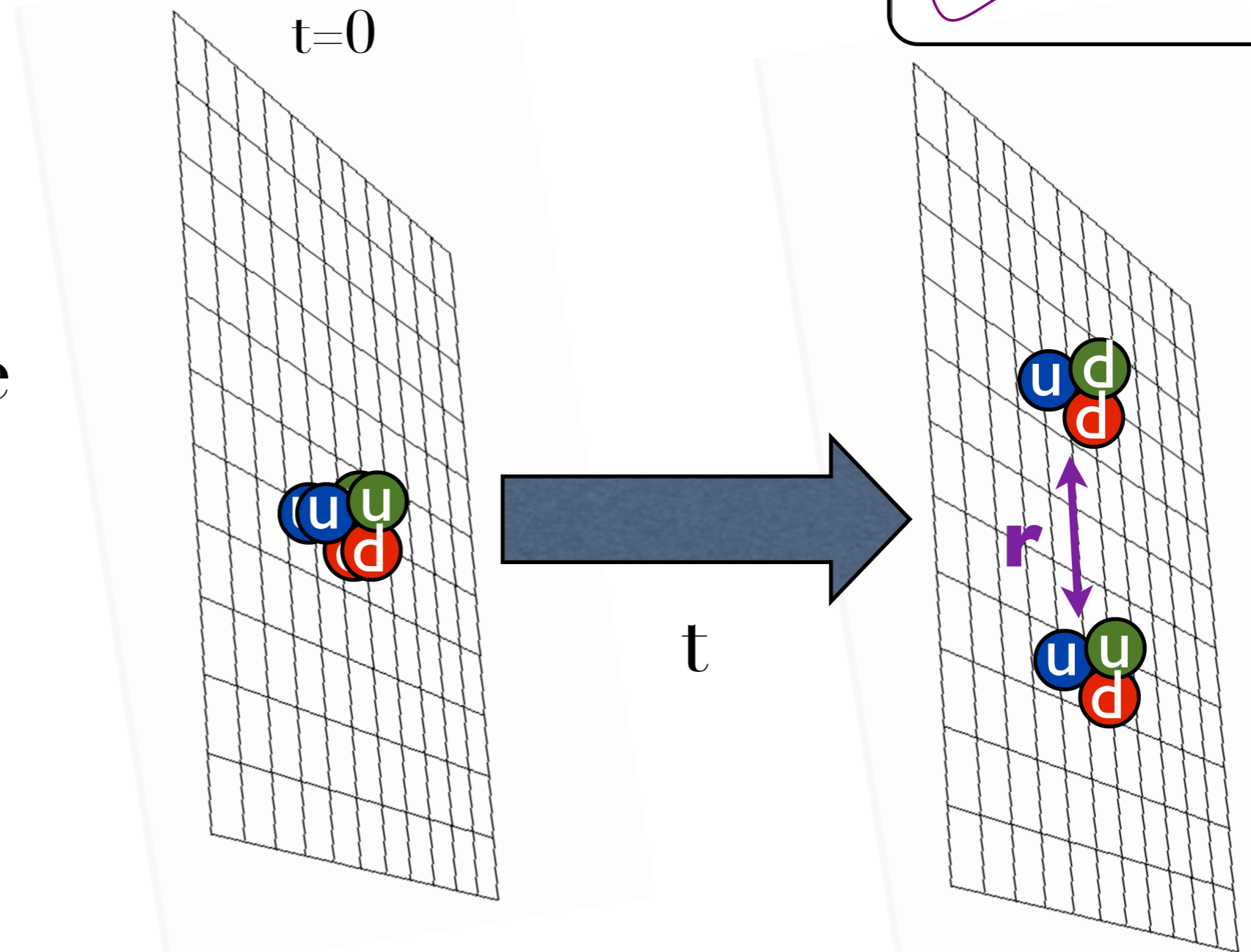


$$\lim_{t \rightarrow \infty} C_{NN}(\mathbf{r}, t) = \psi_0^\dagger \chi e^{-E_0 t}$$

Potential method

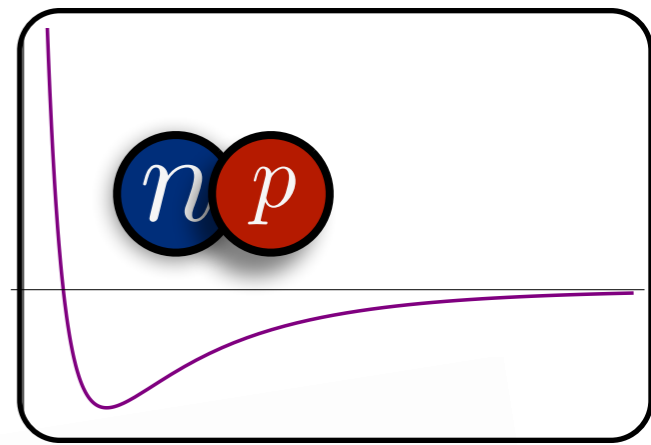


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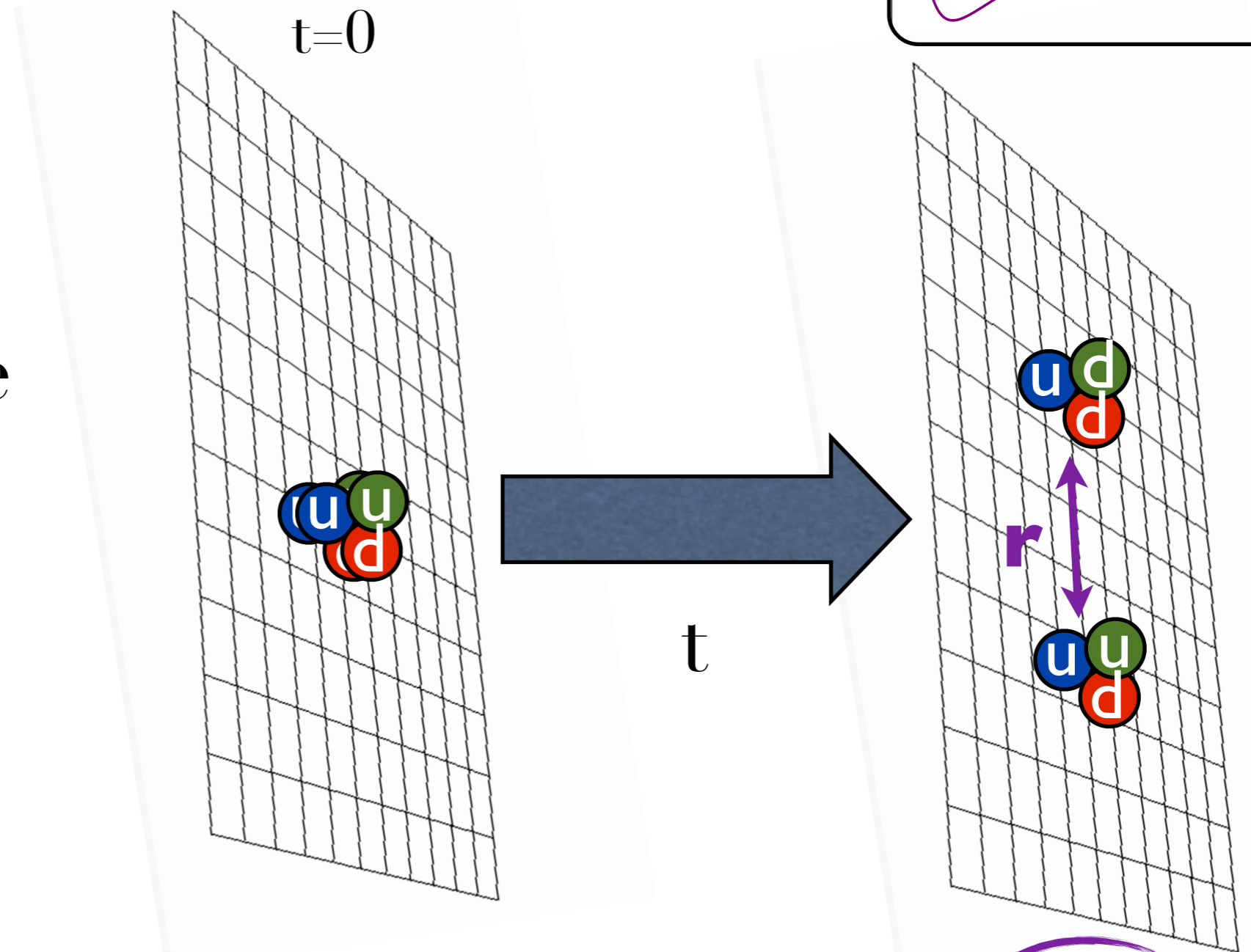


$$\lim_{t \rightarrow \infty} C_{NN}(\mathbf{r}, t) = \psi_0^\dagger \chi \cdot e^{-E_0 t} \chi \psi_0(\mathbf{r})$$

Potential method



1. Create the following correlation function:

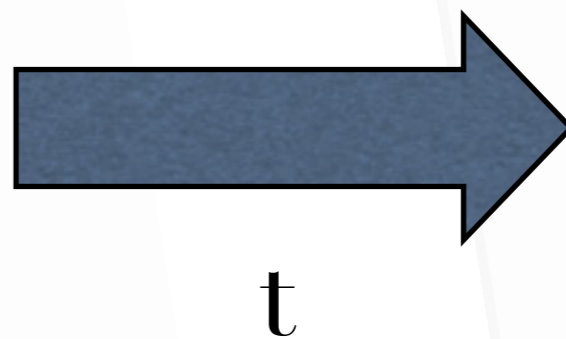
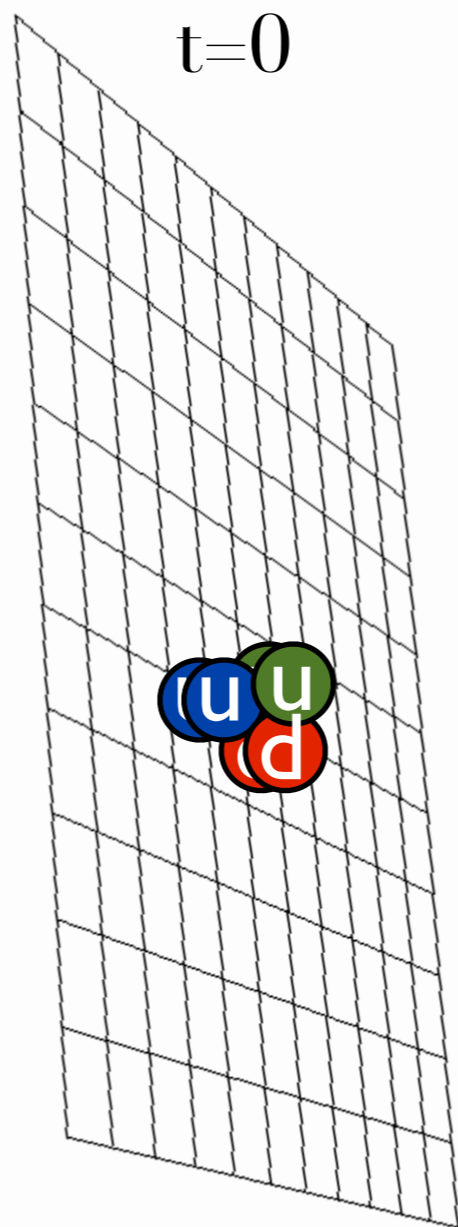


$$\lim_{t \rightarrow \infty} C_{NN}(\mathbf{r}, t) = \psi_0^\dagger \chi \cdot e^{-E_0 t} \chi \psi_0(\mathbf{r})$$

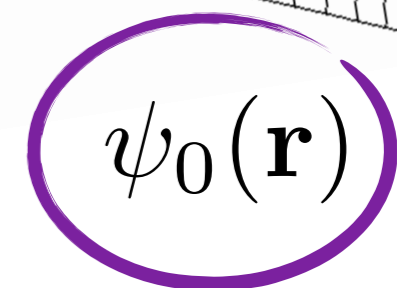
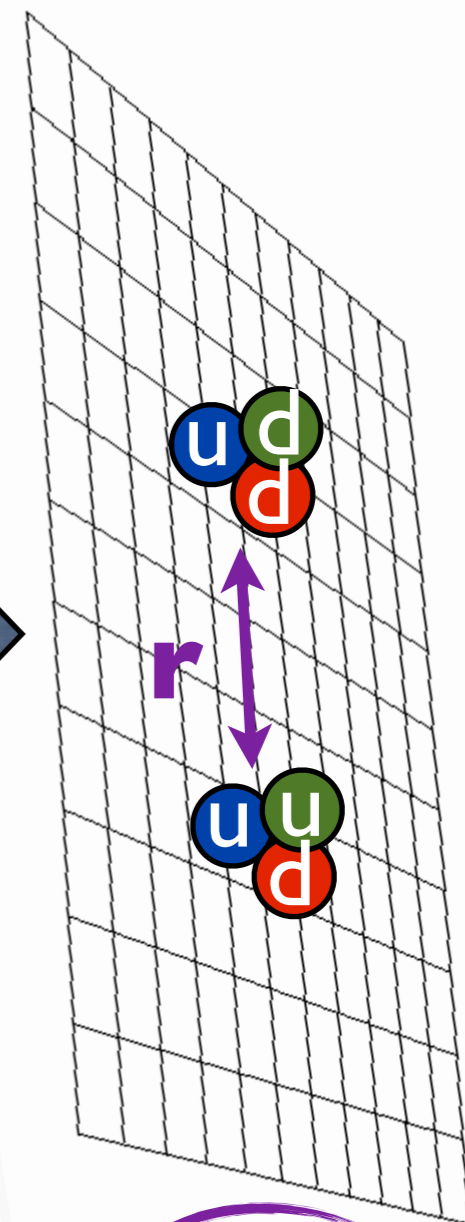
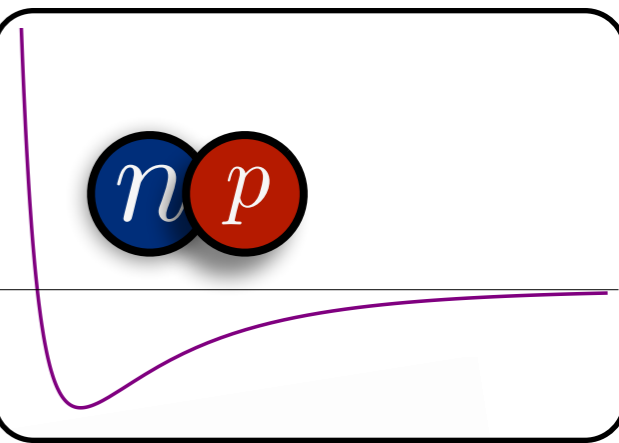
Potential method

2. Plug NBS wave-function into Schrödinger Eq. to determine the potential:

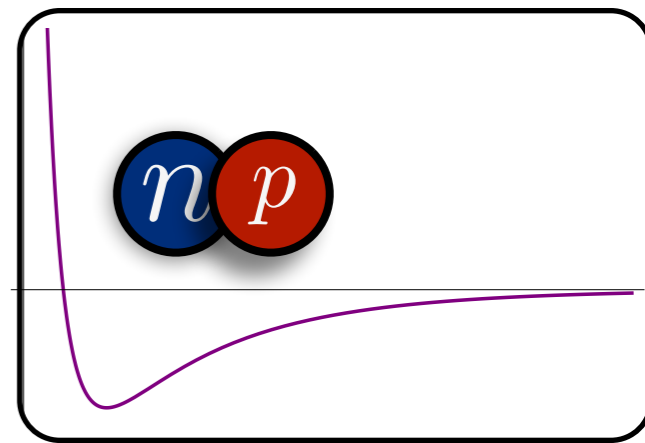
$$\left[\frac{\mathbf{p}^2}{2\mu} - H_0 \right] \psi_{\mathbf{p}}(\mathbf{r}) = \int d^3 r' U(\mathbf{r}, \mathbf{r}') \psi_{\mathbf{p}}(\mathbf{r}') \leftarrow \psi_0(\mathbf{r})$$



t



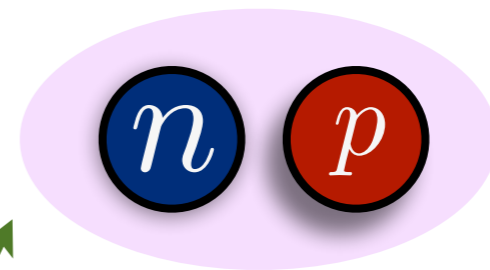
Potential method



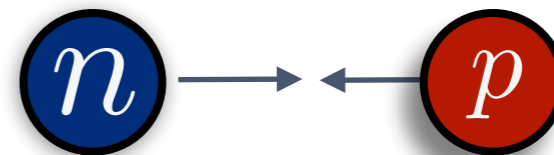
2. Plug NBS
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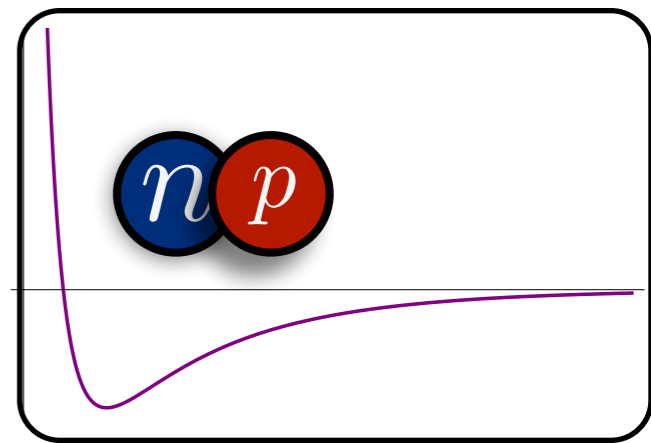
Binding energies



Phase shifts



Potential method



3. Use derivative expansion to determine the leading order potential:

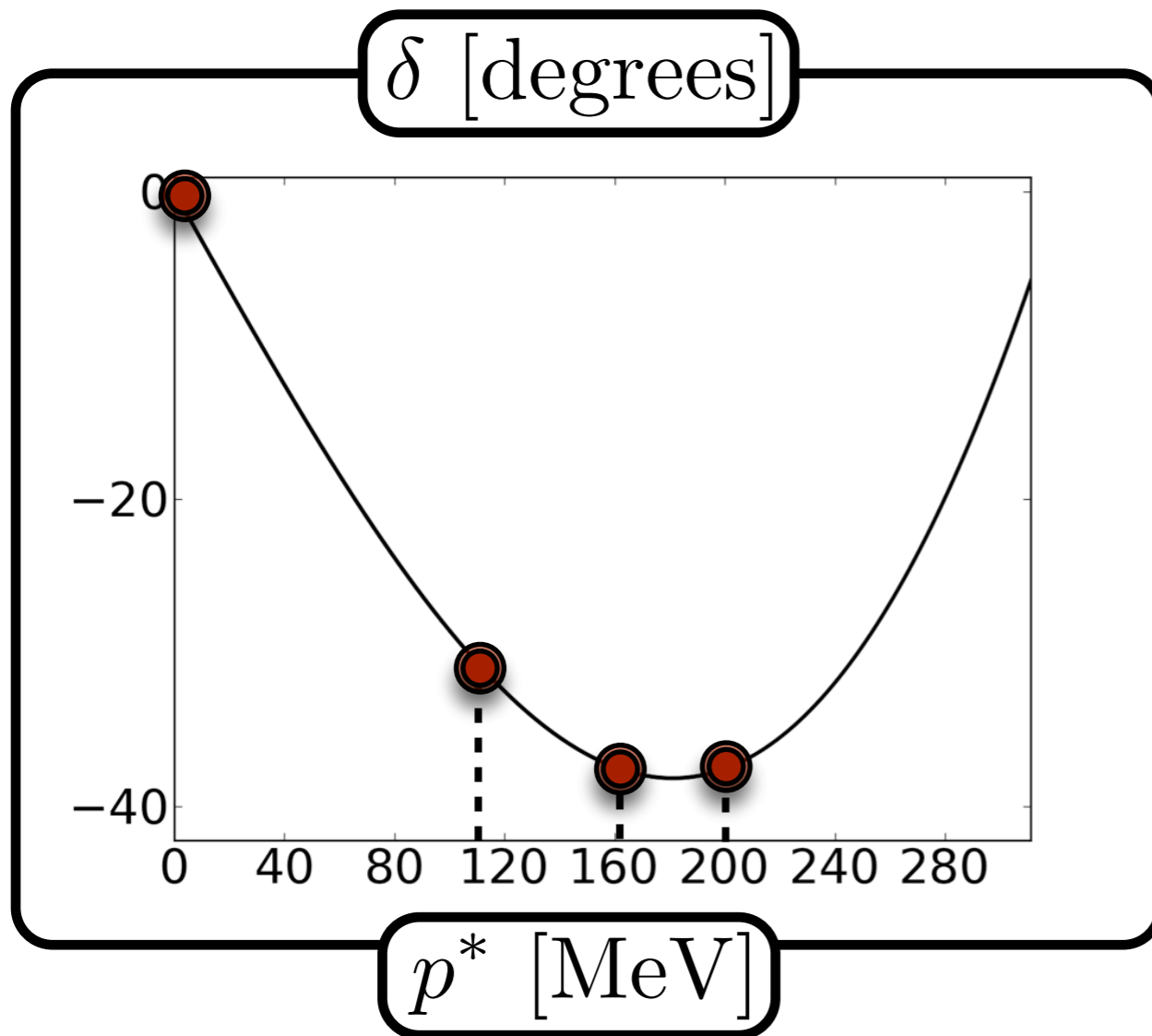
$$U(\mathbf{r}, \mathbf{r}') = V_C(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}') + \mathcal{O}(\nabla_{\mathbf{r}}^2/\Lambda^2)$$

$$V_C(\mathbf{r}) \simeq \frac{\mathbf{p}^2}{2\mu} + \lim_{t \rightarrow \infty} \frac{1}{2\mu} \frac{\nabla_{\mathbf{r}}^2 C_{NN}(\mathbf{r}, t)}{C_{NN}(\mathbf{r}, t)}$$

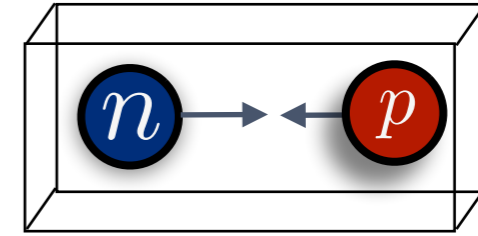
$$\left[\frac{\mathbf{p}^2}{2\mu} - H_0 \right] \psi_{\mathbf{p}}(\mathbf{r}) = \int d^3 r' U(\mathbf{r}, \mathbf{r}') \psi_{\mathbf{p}}(\mathbf{r}') \leftarrow \psi_0(\mathbf{r})$$

Some comparisons

see Drischler, et al, 1910.07961

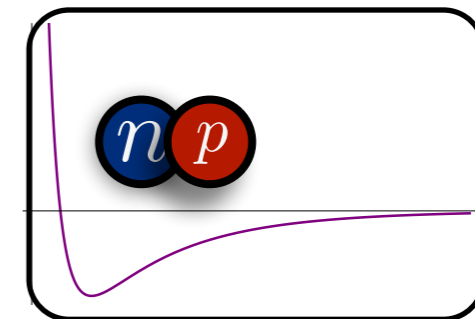


$$U(\mathbf{r}, \mathbf{r}') = V_C(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}') + \mathcal{O}(\nabla_{\mathbf{r}}^2/\Lambda^2)$$



Lüscher

- discrete phase shifts
- need ground state saturation
- no volume extrapolation
- no uncontrolled approximations

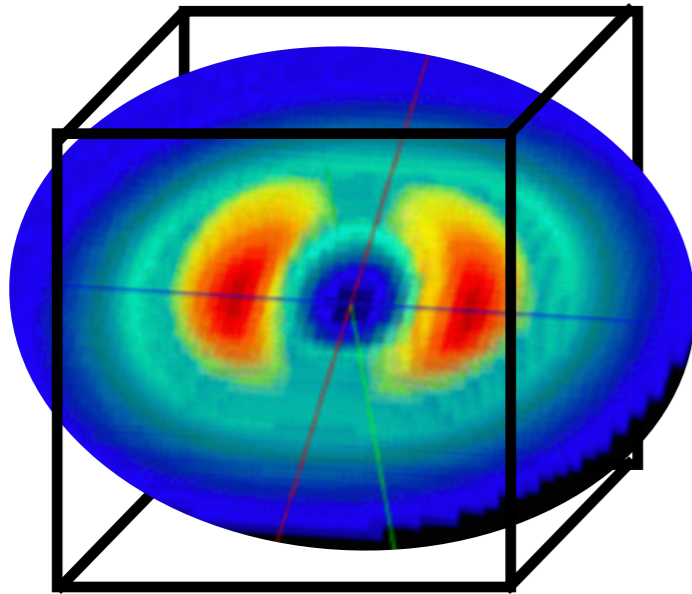


Potential

- nearly continuous phase shifts
- only need elastic state saturation
- need volume extrapolation
- cutoff in gradient expansion

LQCD connection to HOBET

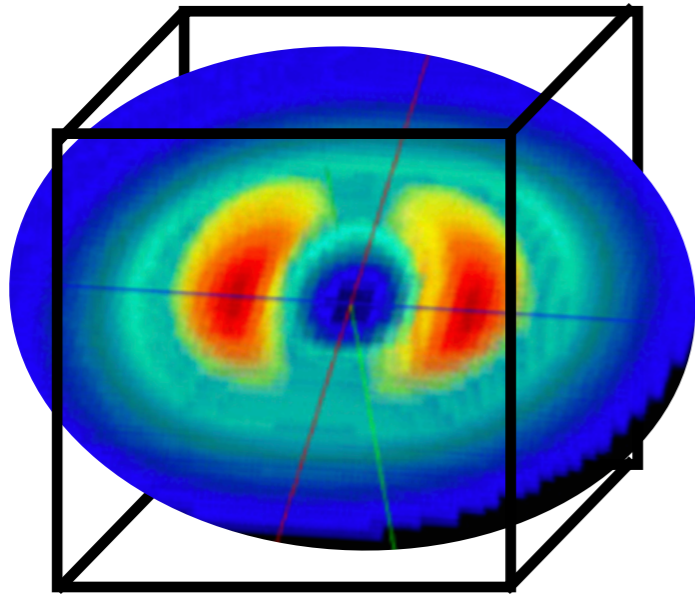
(K. McElvain and W. Haxton)



Formulate HOBET with the same (IR) BC as LQCD, fix (UV) couplings to reproduce LQCD energy levels, then remove the BC and make predictions

LQCD connection to HOBET

(K. McElvain and W. Haxton)

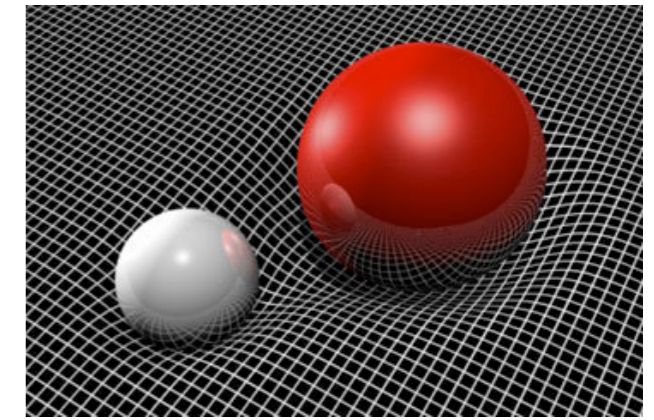


Formulate HOBET with the same (IR) BC as LQCD, fix (UV) couplings to reproduce LQCD energy levels, then remove the BC and make predictions

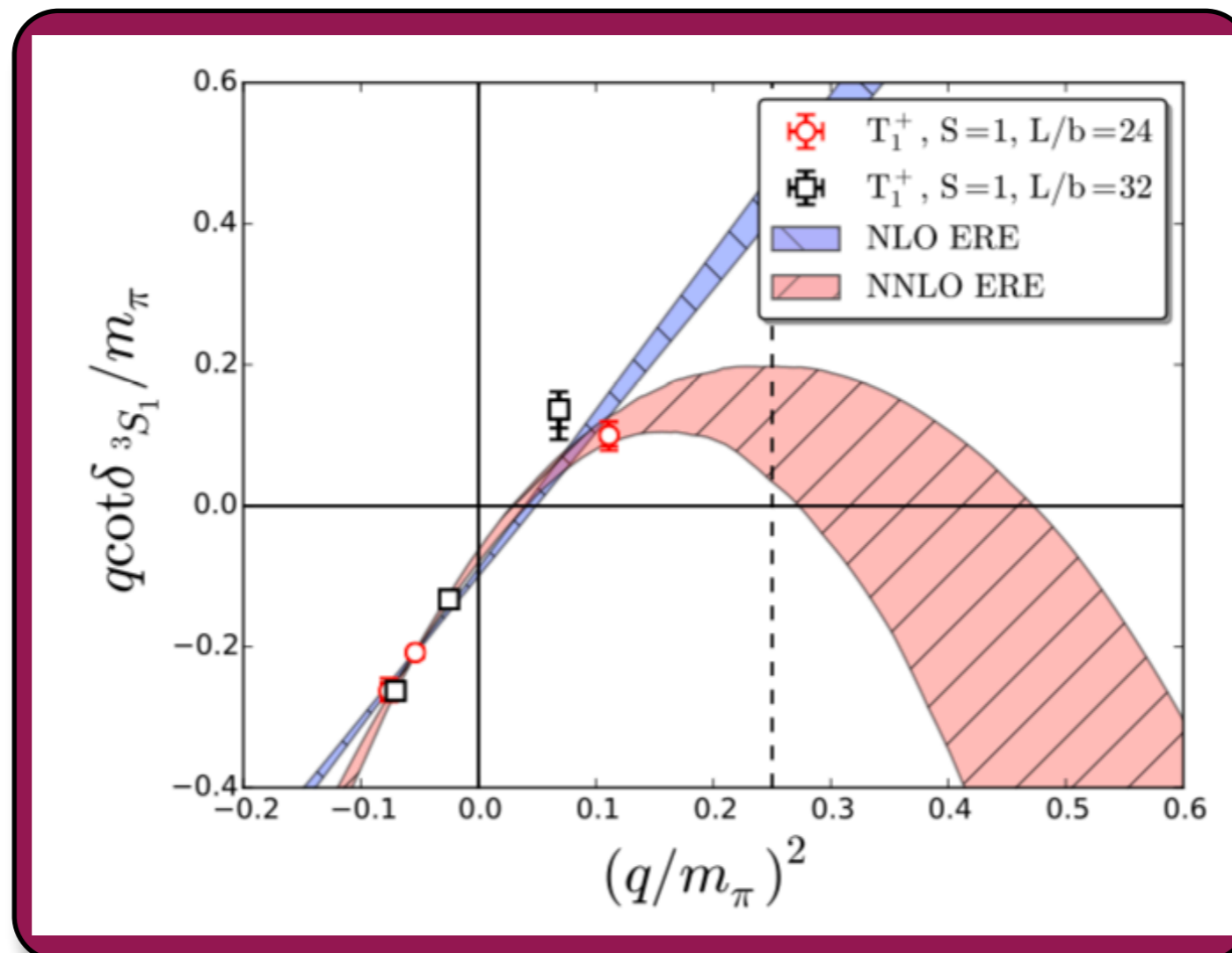
- No need to truncate partial wave expansion
- Can deal with volumes smaller than Compton wavelength of the pion
- Luscher formalism for $N > 2$ is messy
- Alternate method for determining binding energies

Composite states at $m_\pi \sim 800 \text{ MeV}$

- L=32
- L=24

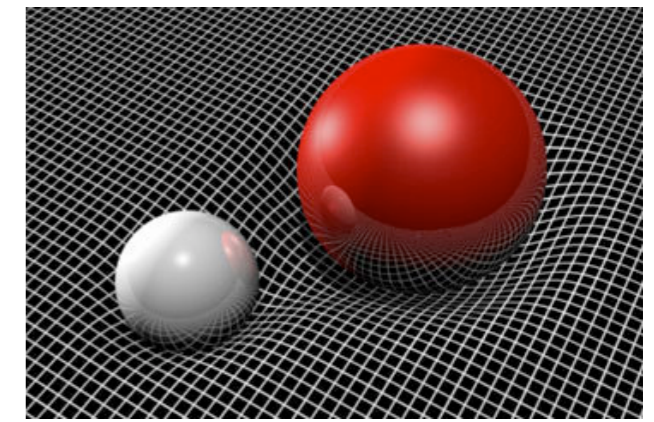


$$p \cot \delta = ip$$

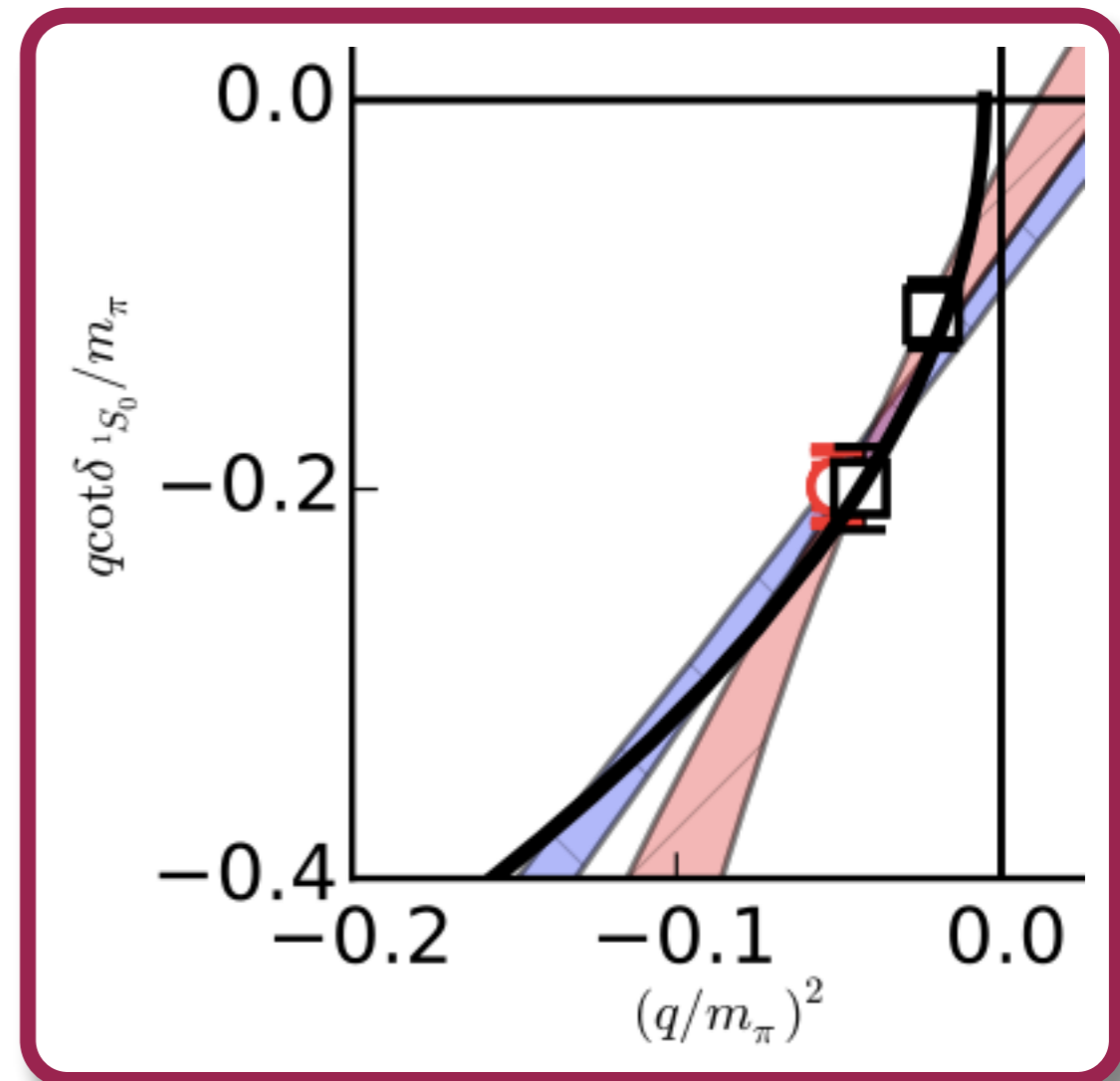
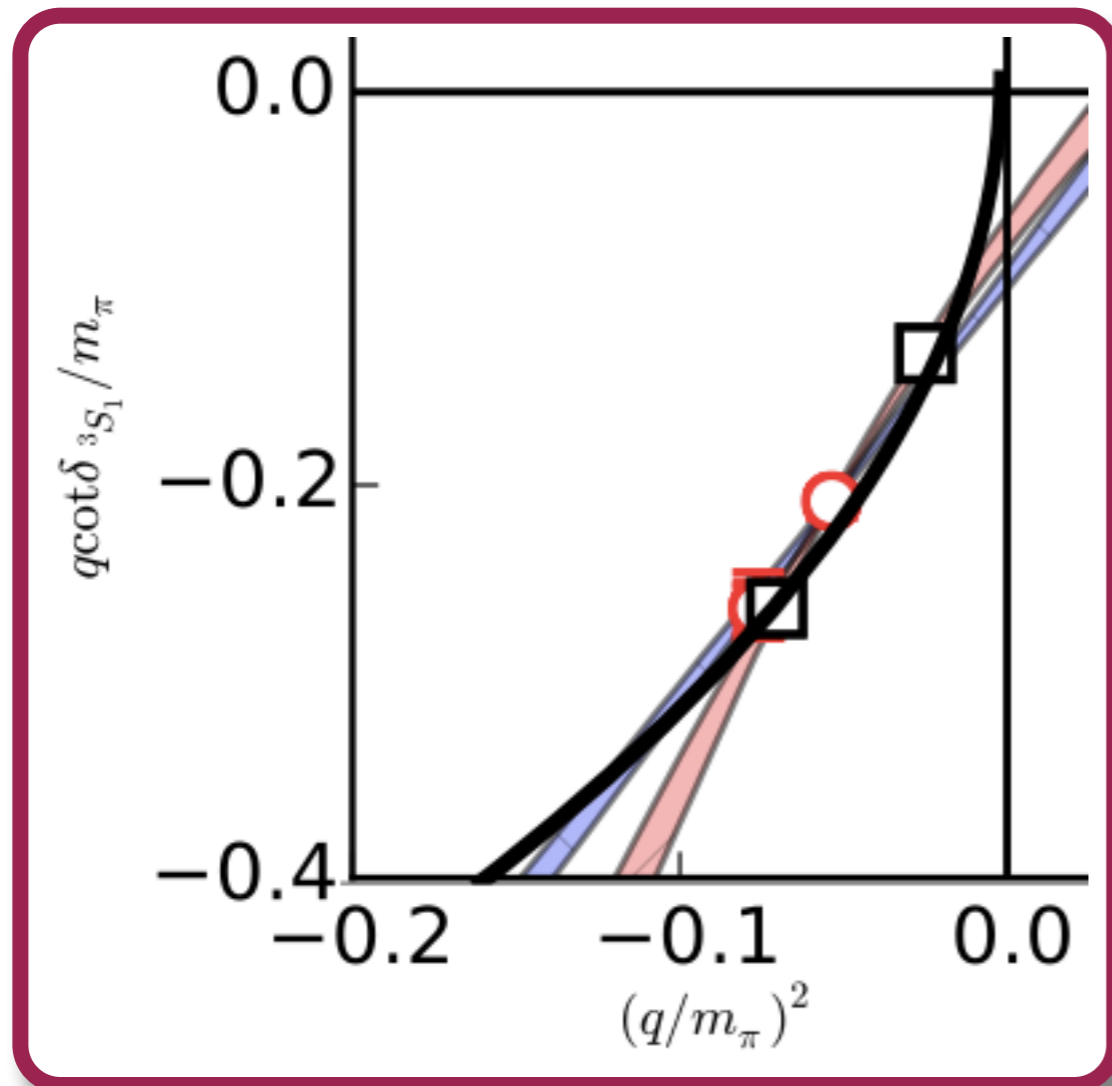


Composite states at $m_\pi \sim 800$ MeV

- L=32
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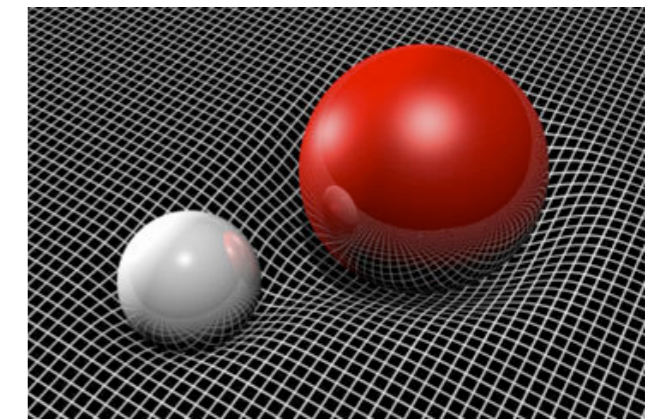


$$p \cot \delta = ip$$



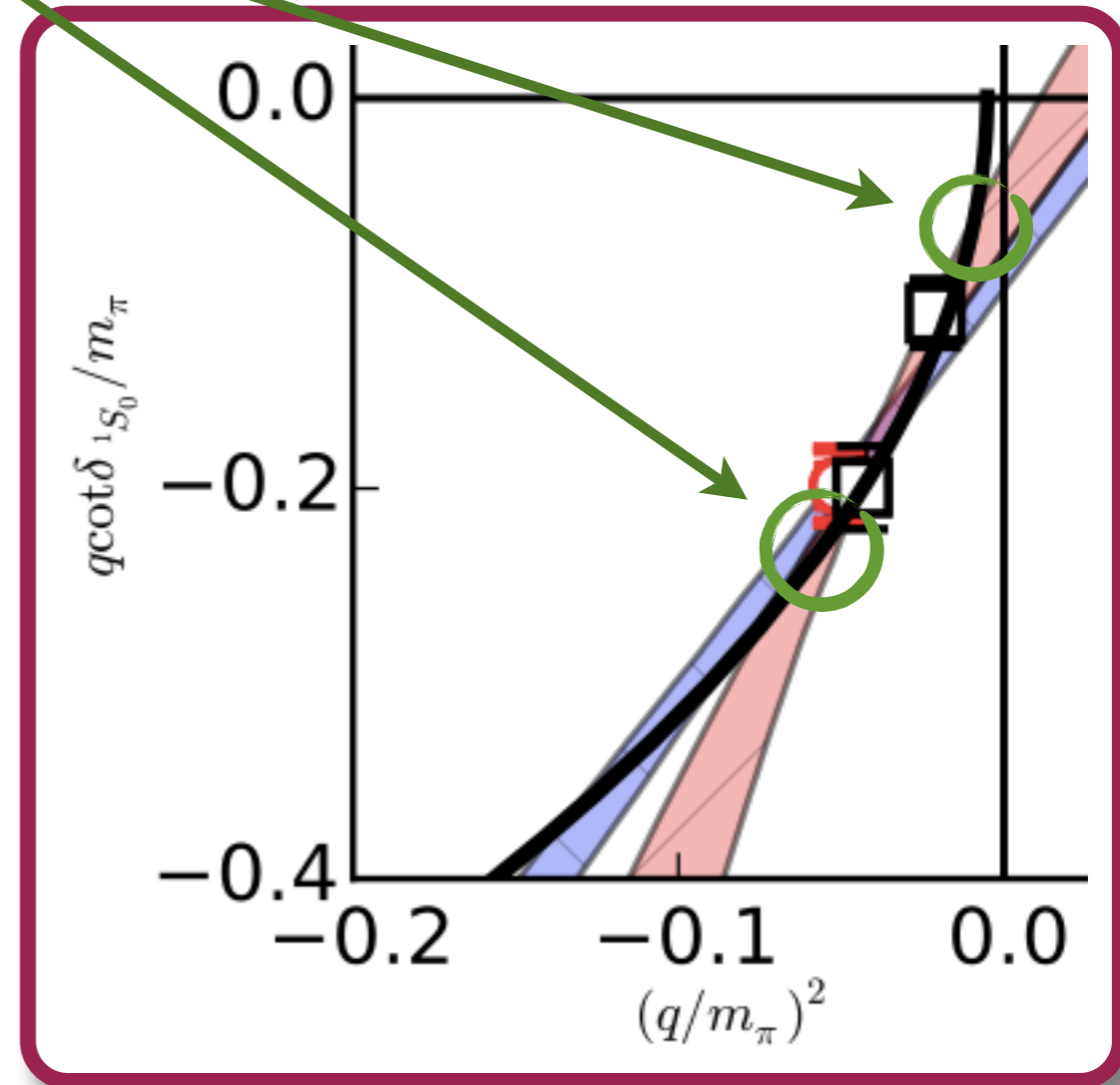
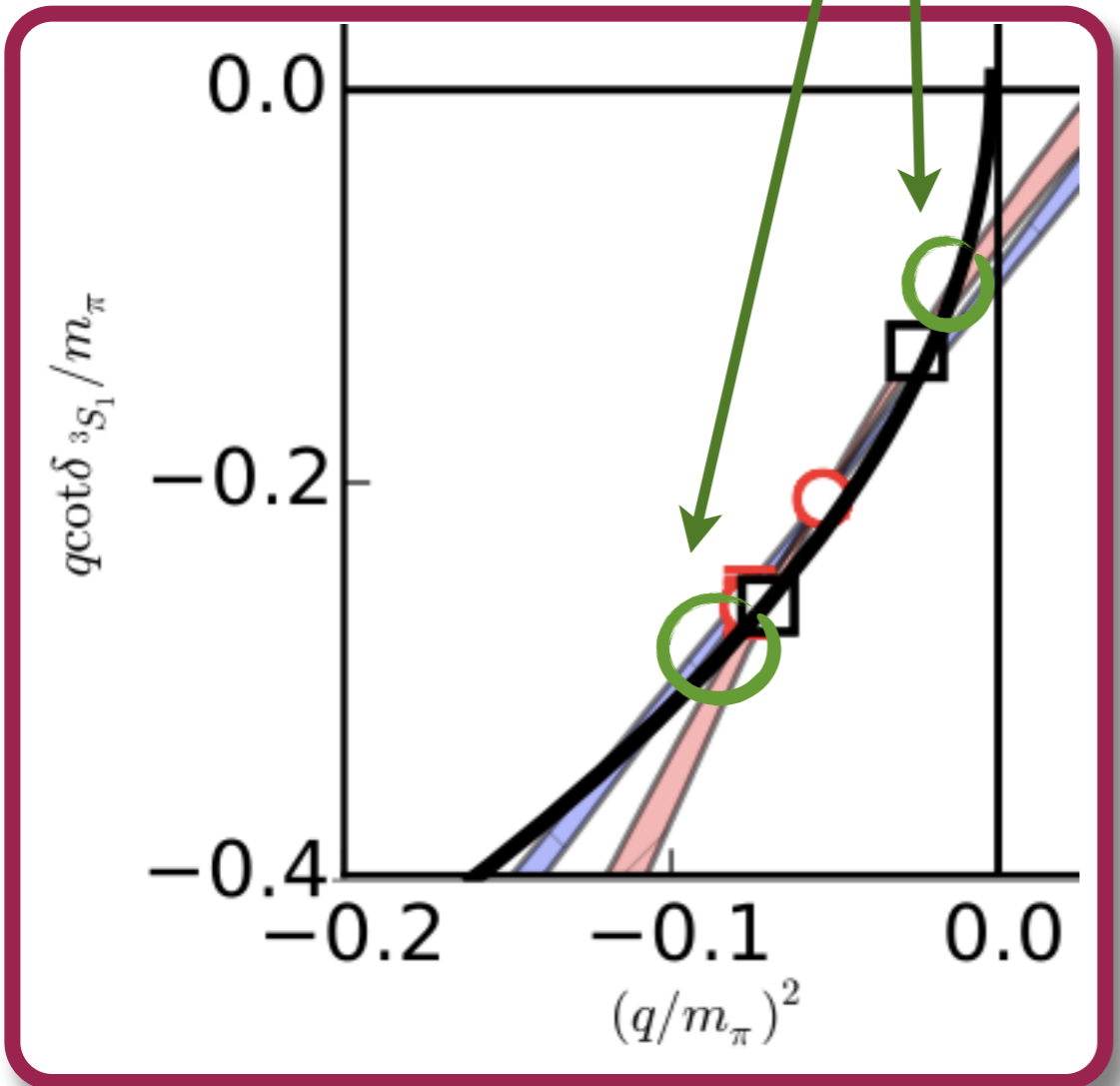
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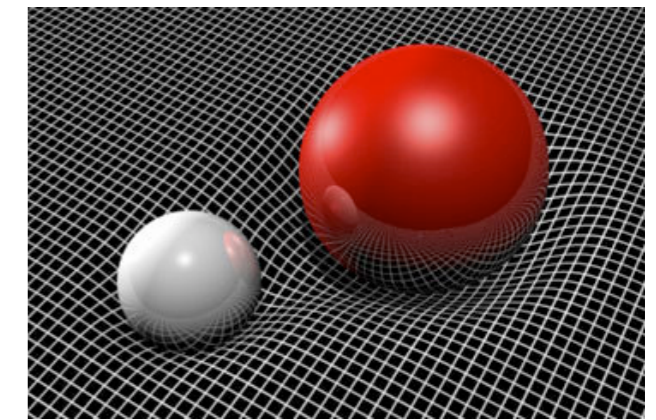
$$p \cot \delta = ip$$

NNLO crossings



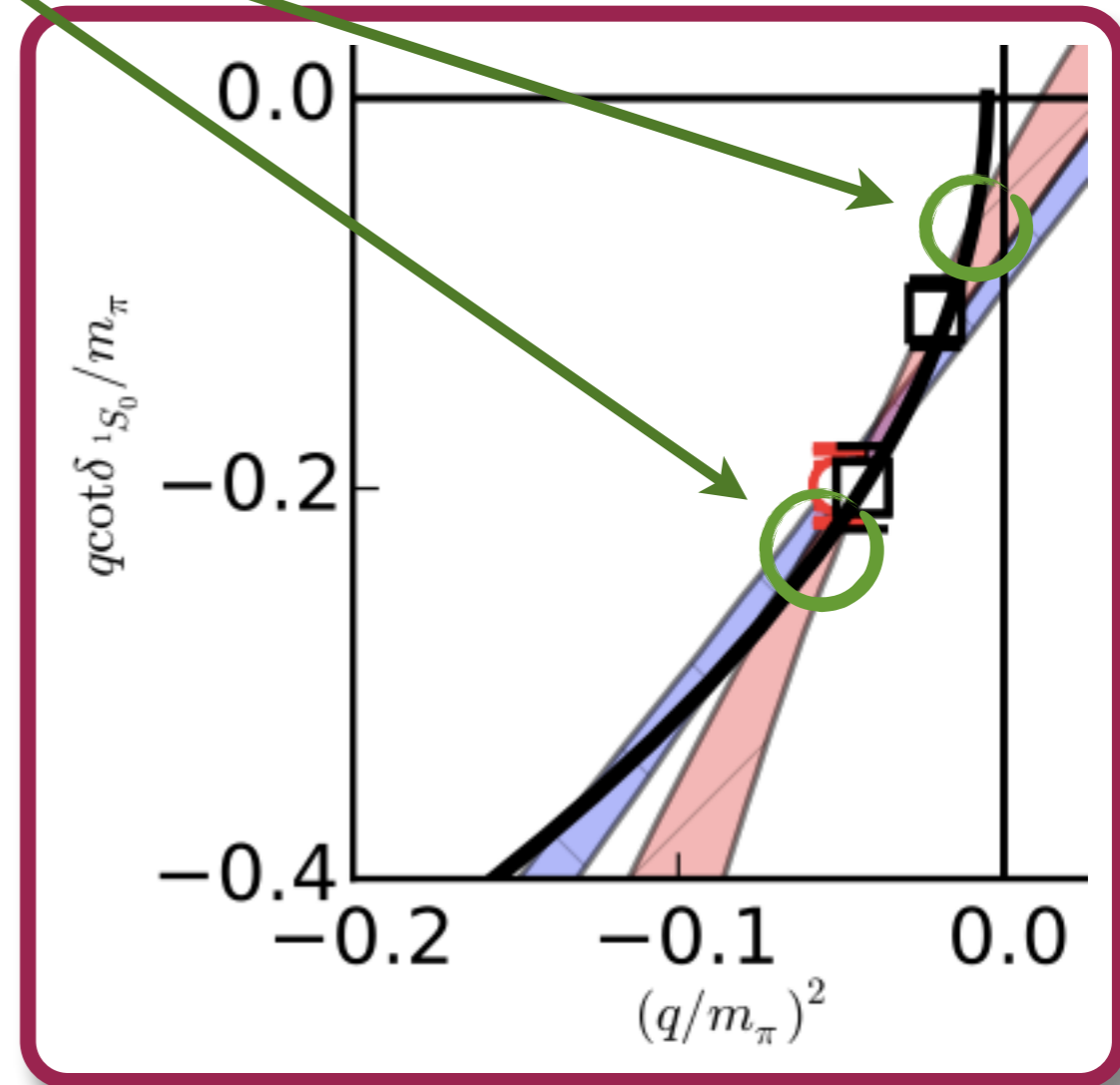
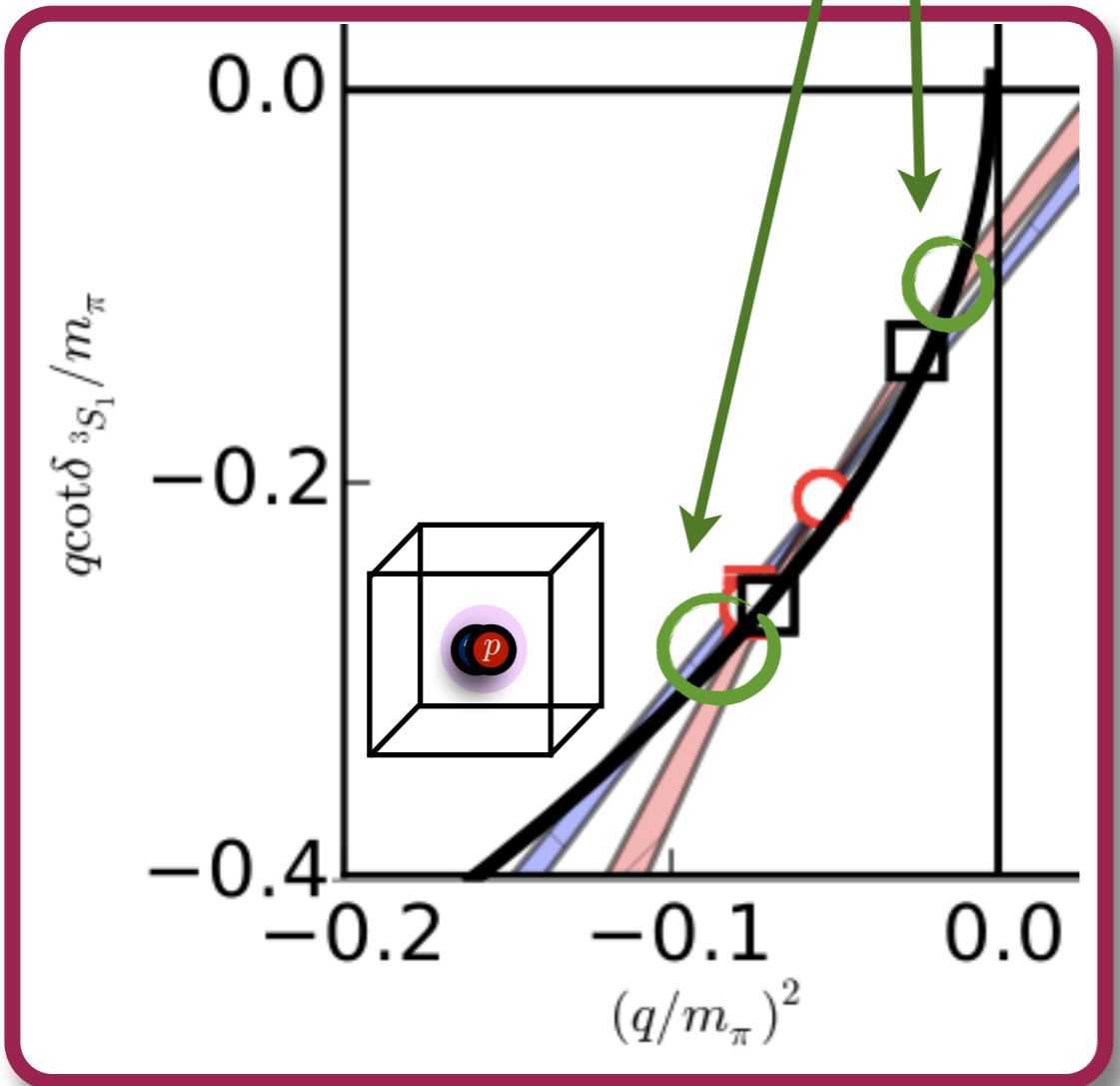
Composite states at $m_\pi \sim 800$ MeV

- L=32
- L=24



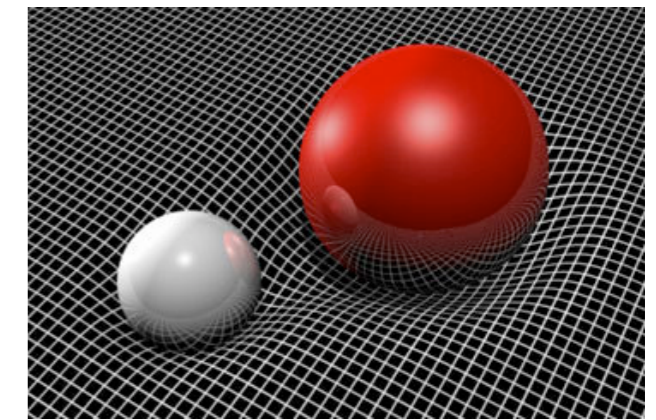
$$p \cot \delta = ip$$

NNLO crossings



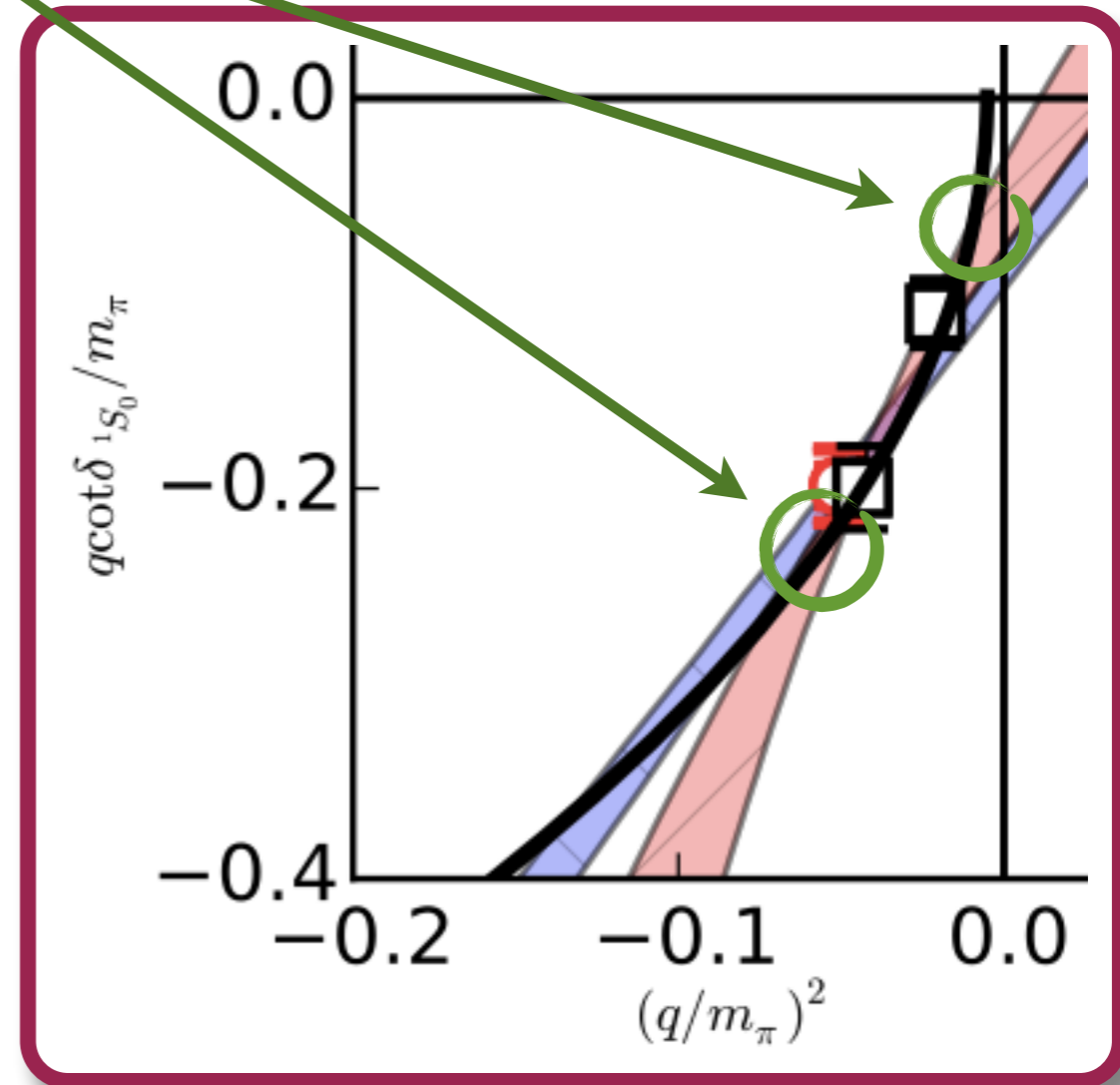
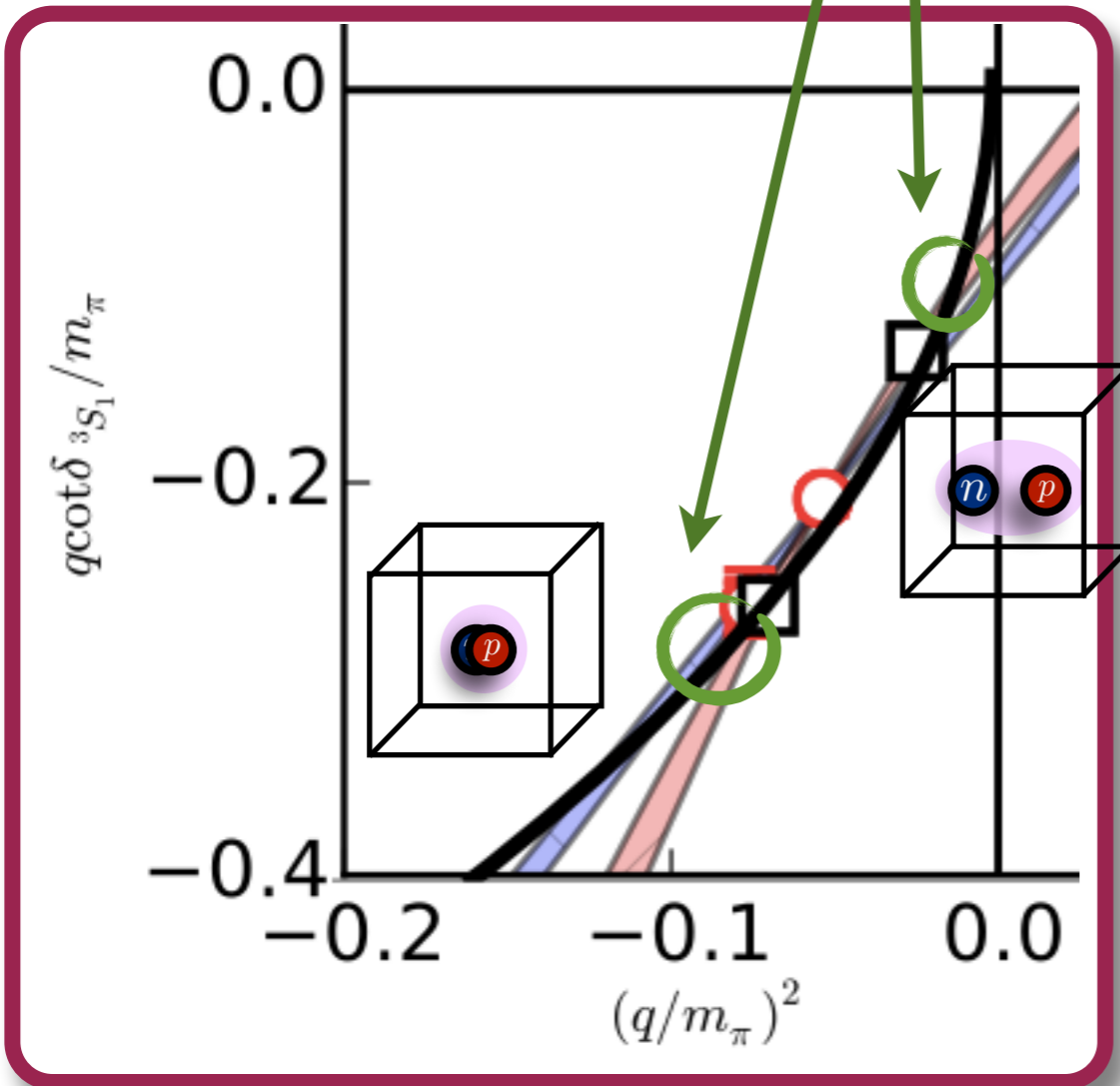
Composite states at $m_\pi \sim 800$ MeV

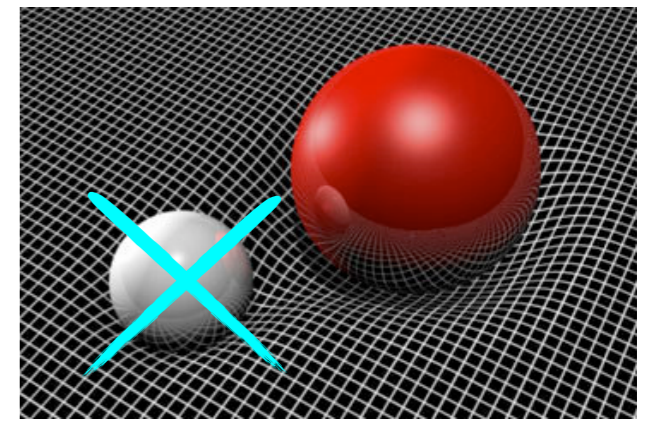
- L=32
- L=24



$$p \cot \delta = ip$$

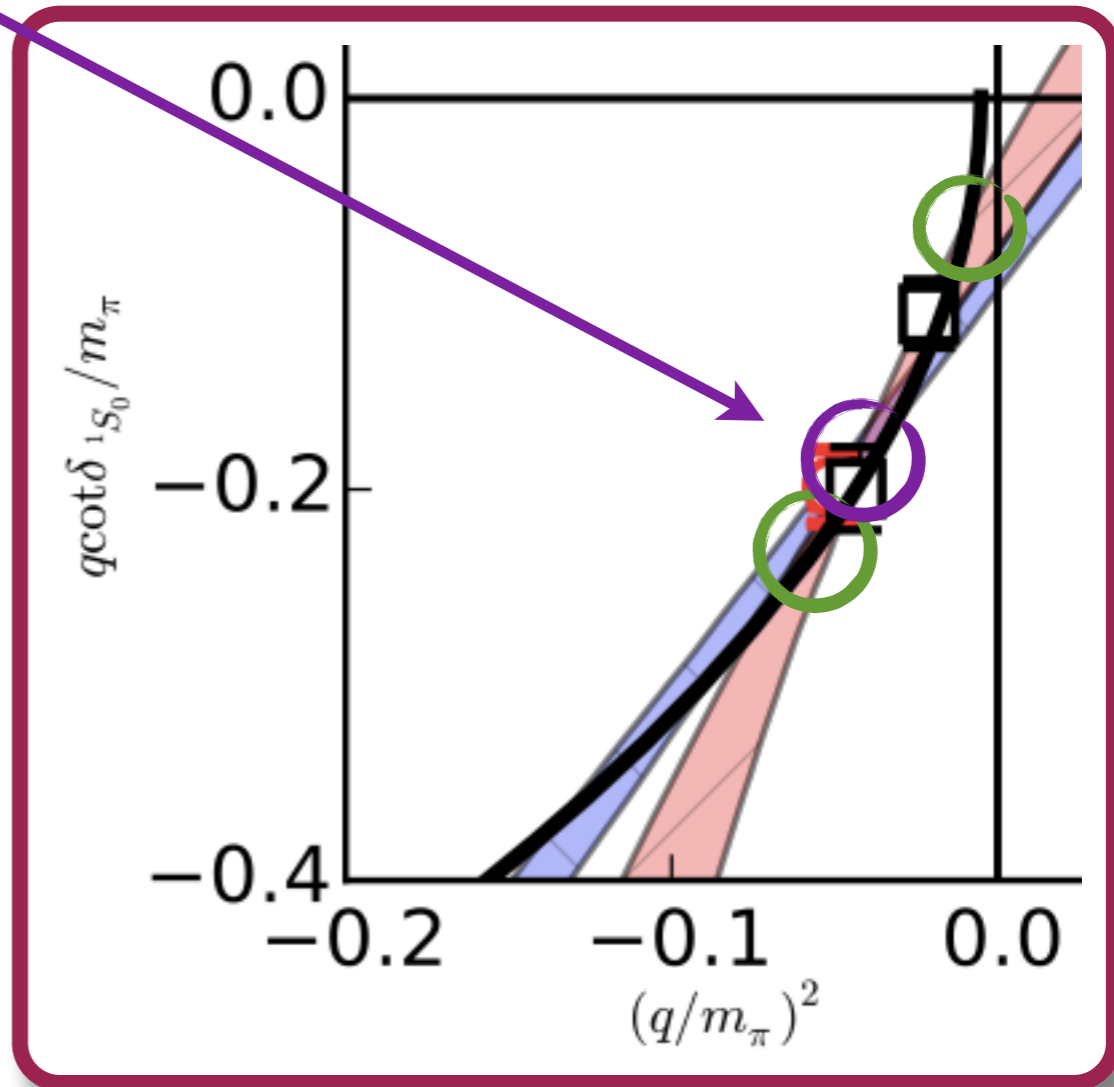
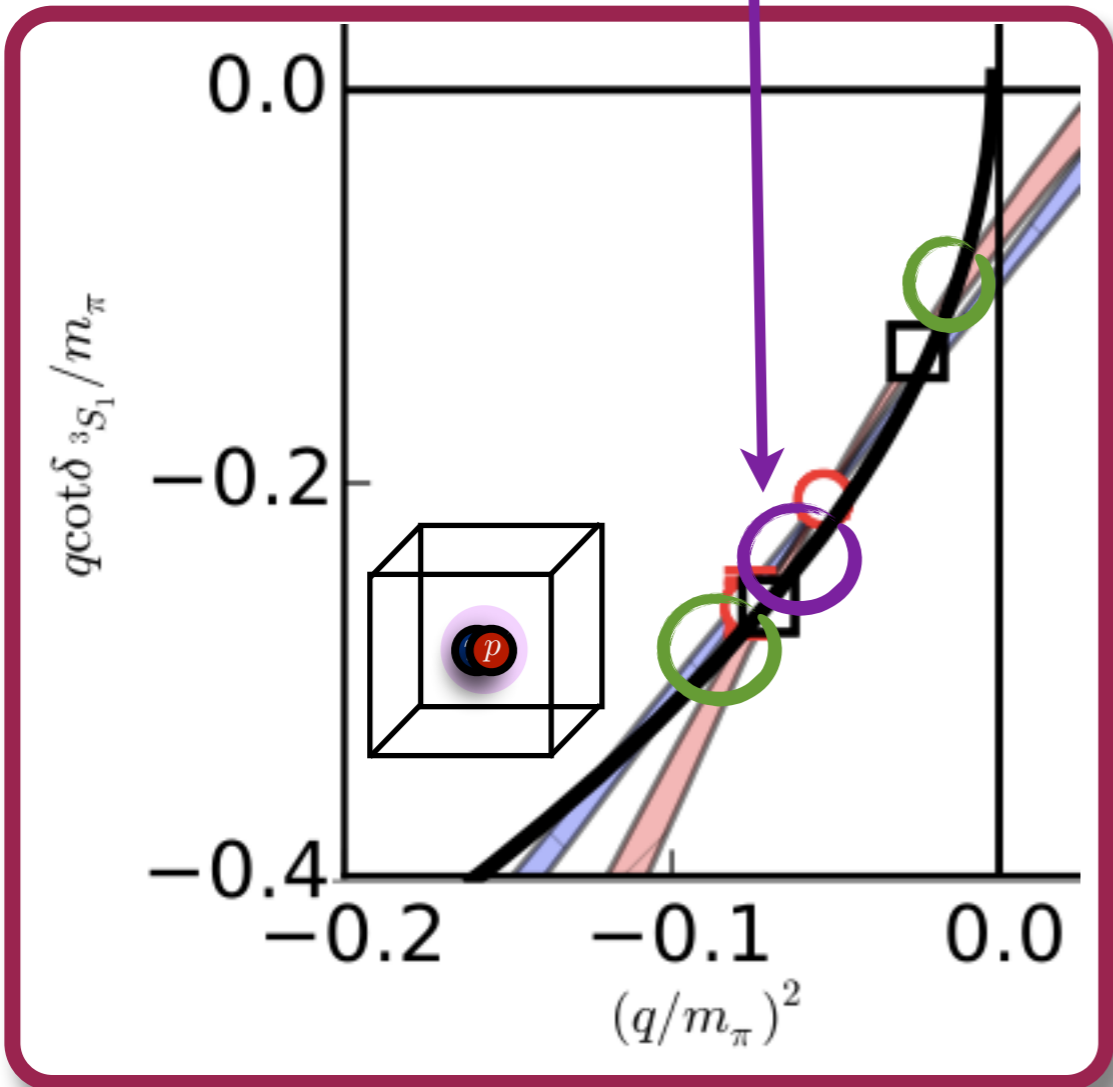
NNLO crossings

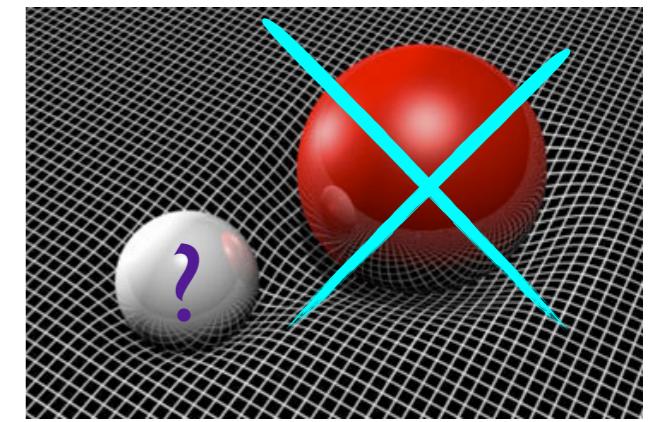
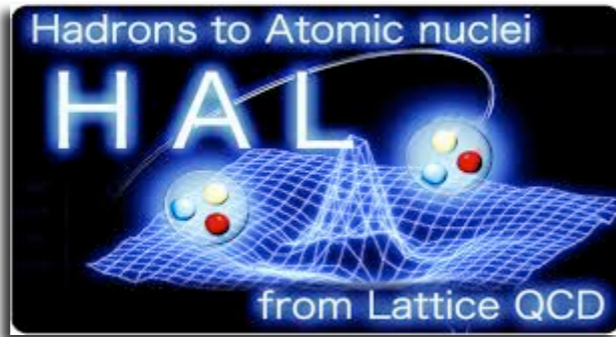




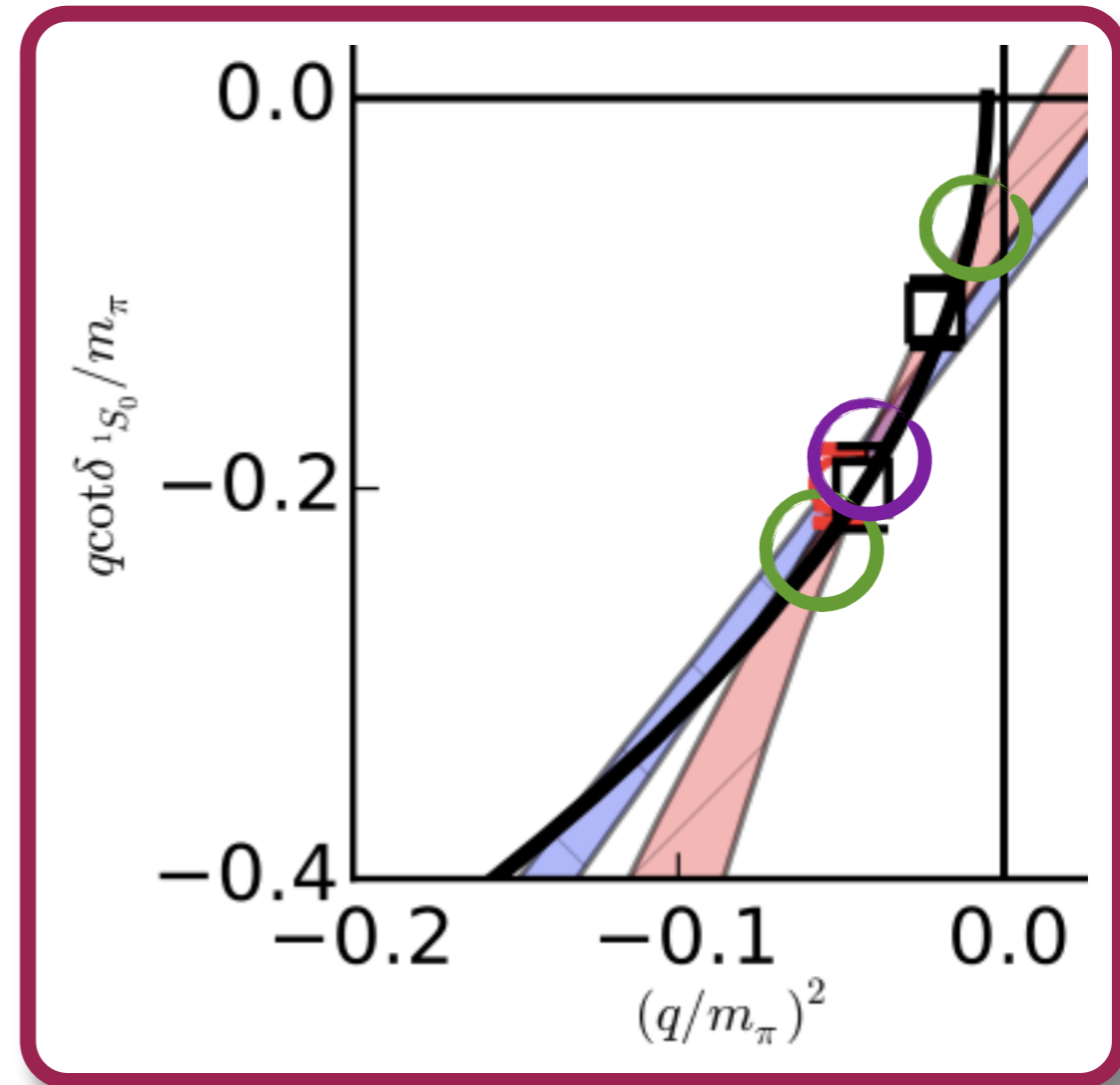
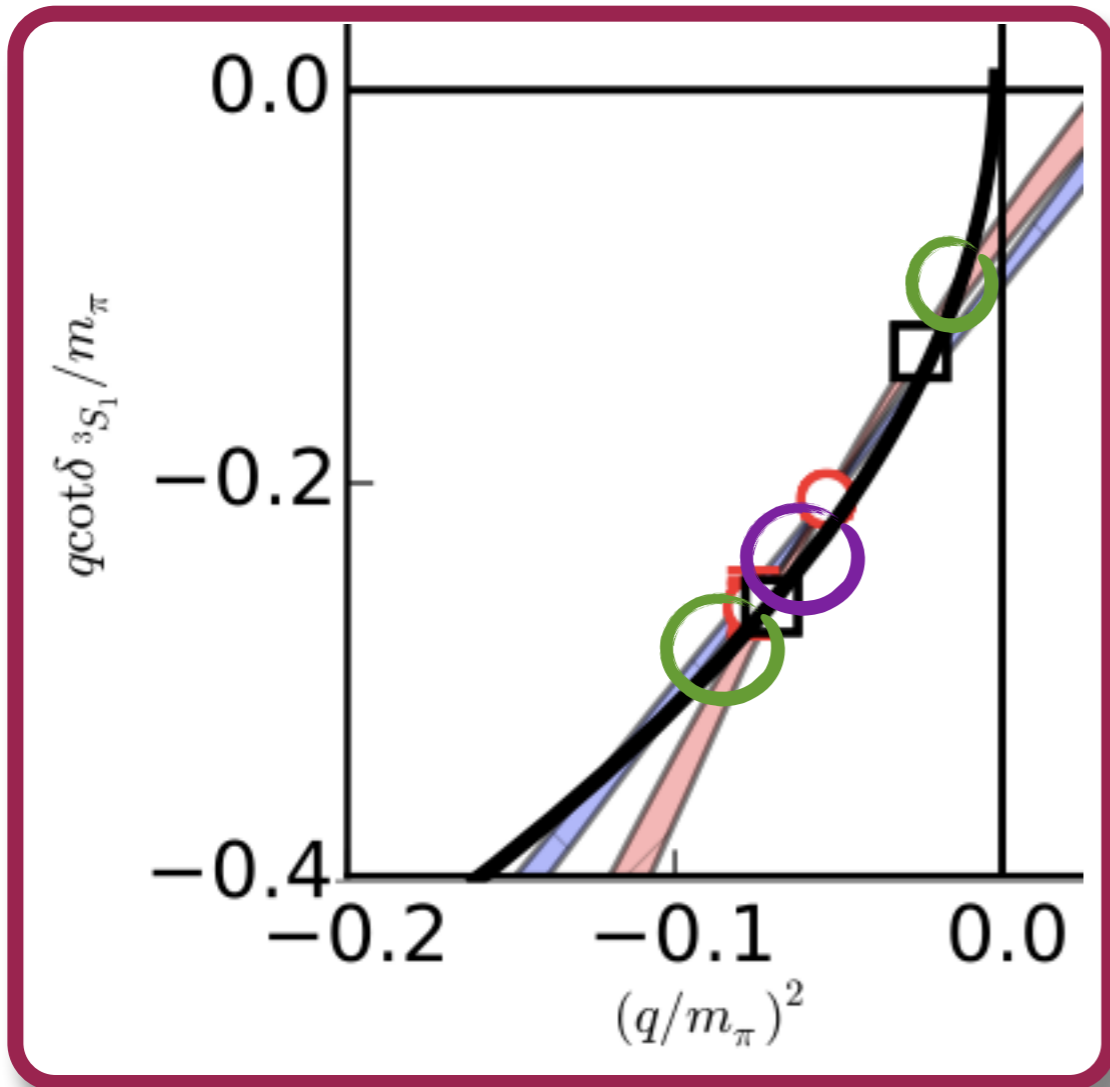
Yamazaki, et. al.

$$p \cot \delta = ip$$



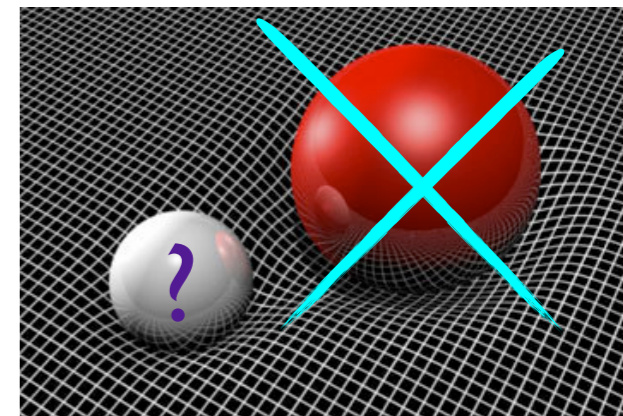


$$p \cot \delta = ip$$

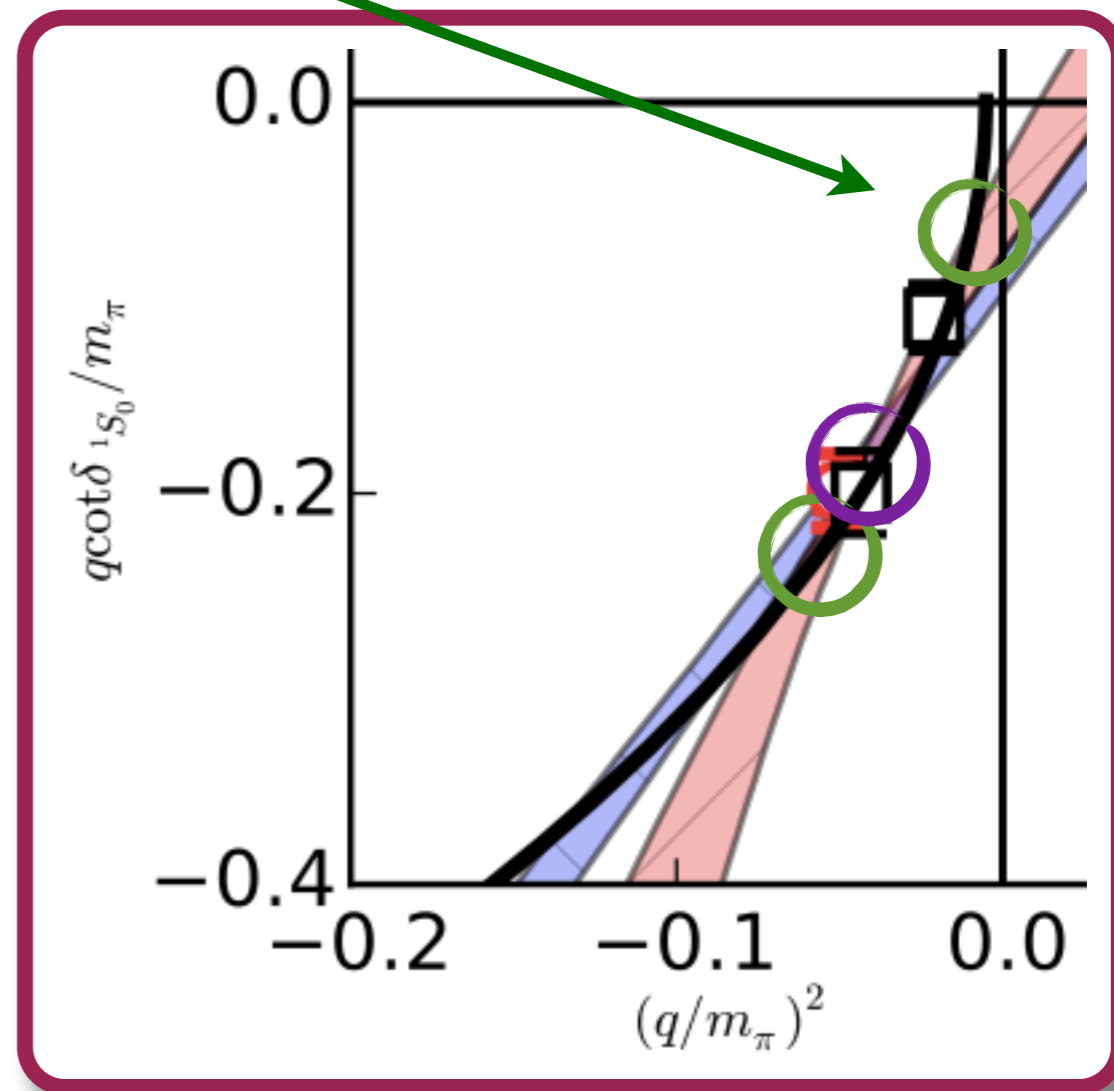
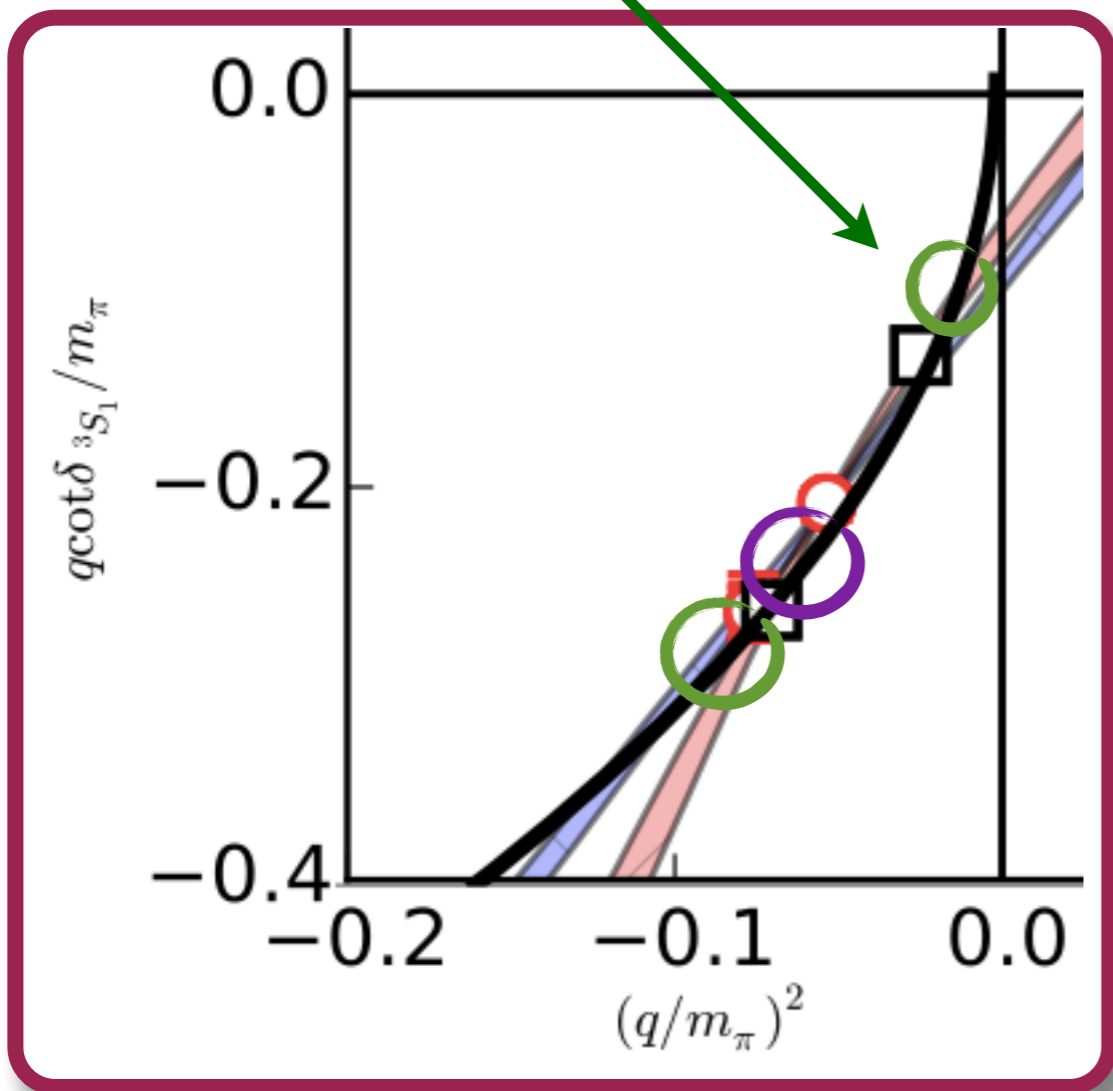


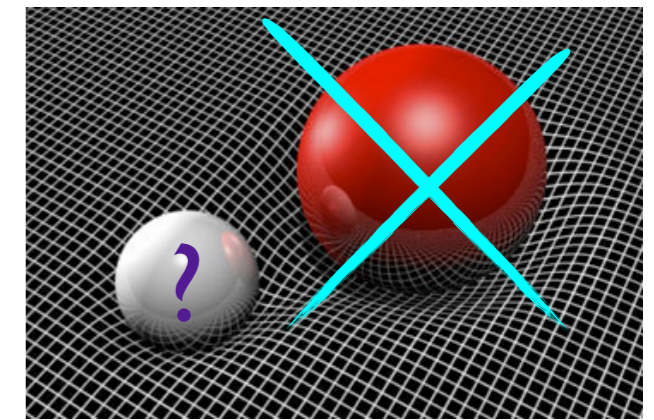


?



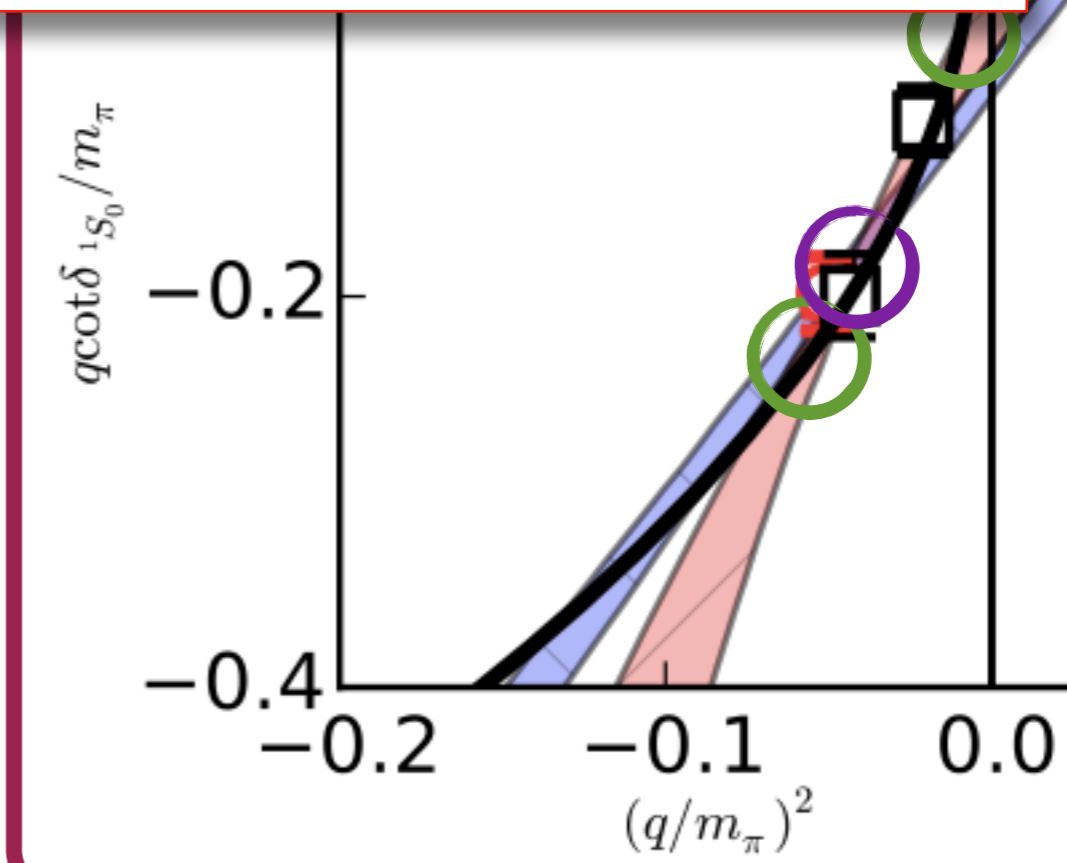
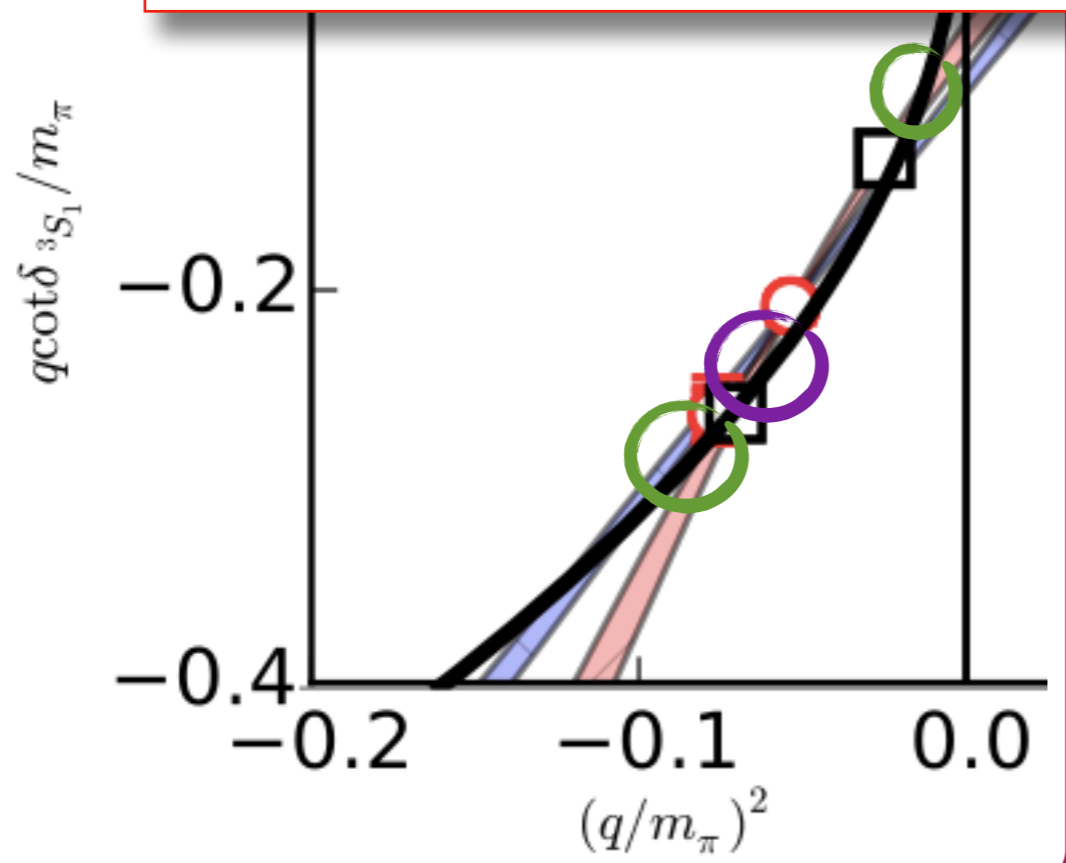
$$p \cot \delta = ip$$



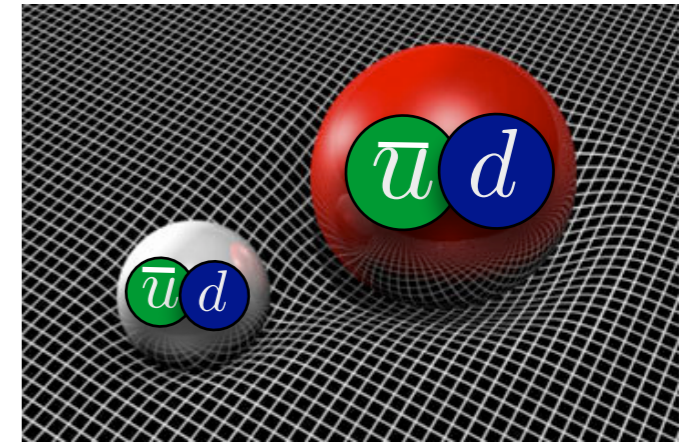


$$p \cot \delta = ip$$

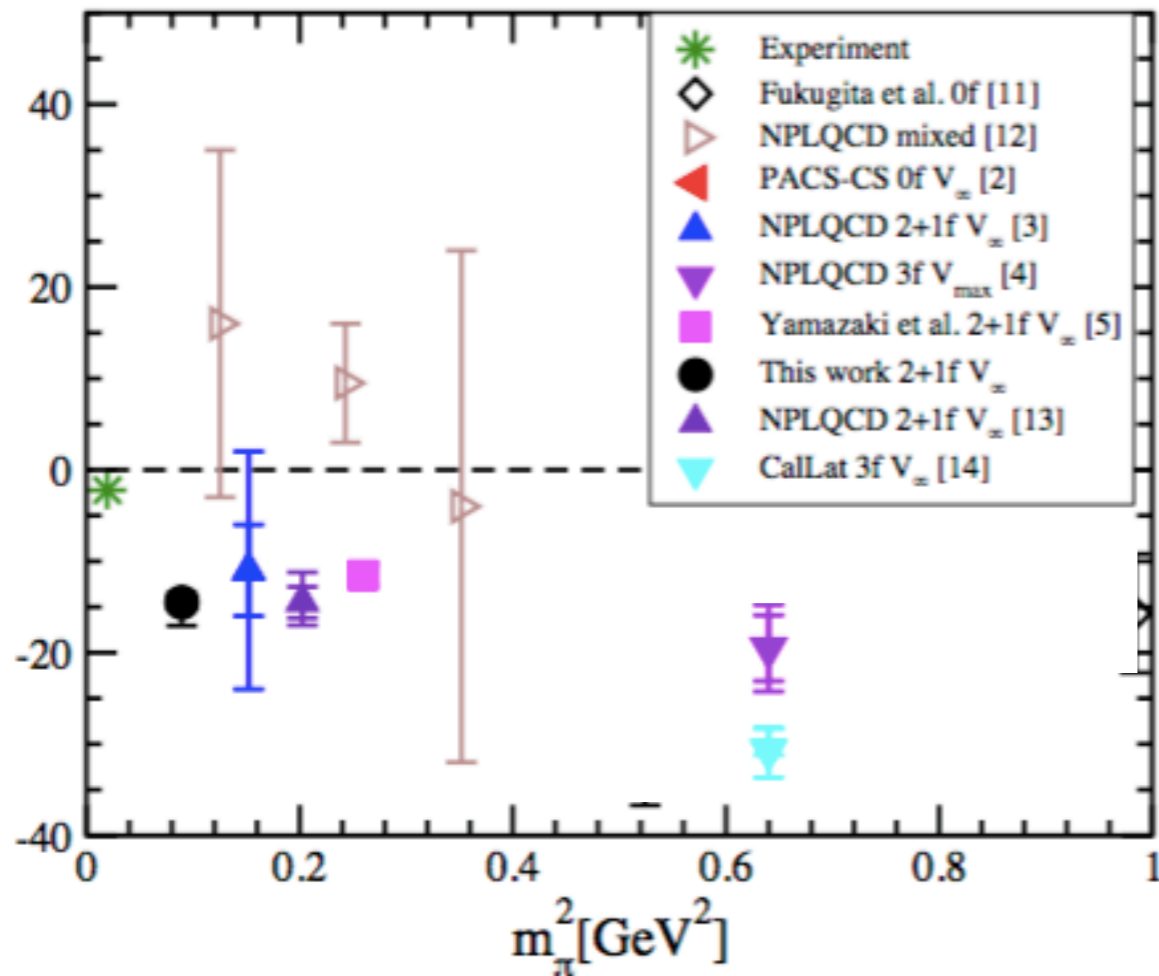
HAL has pointed to issues with an ERE interpretation of some of these results



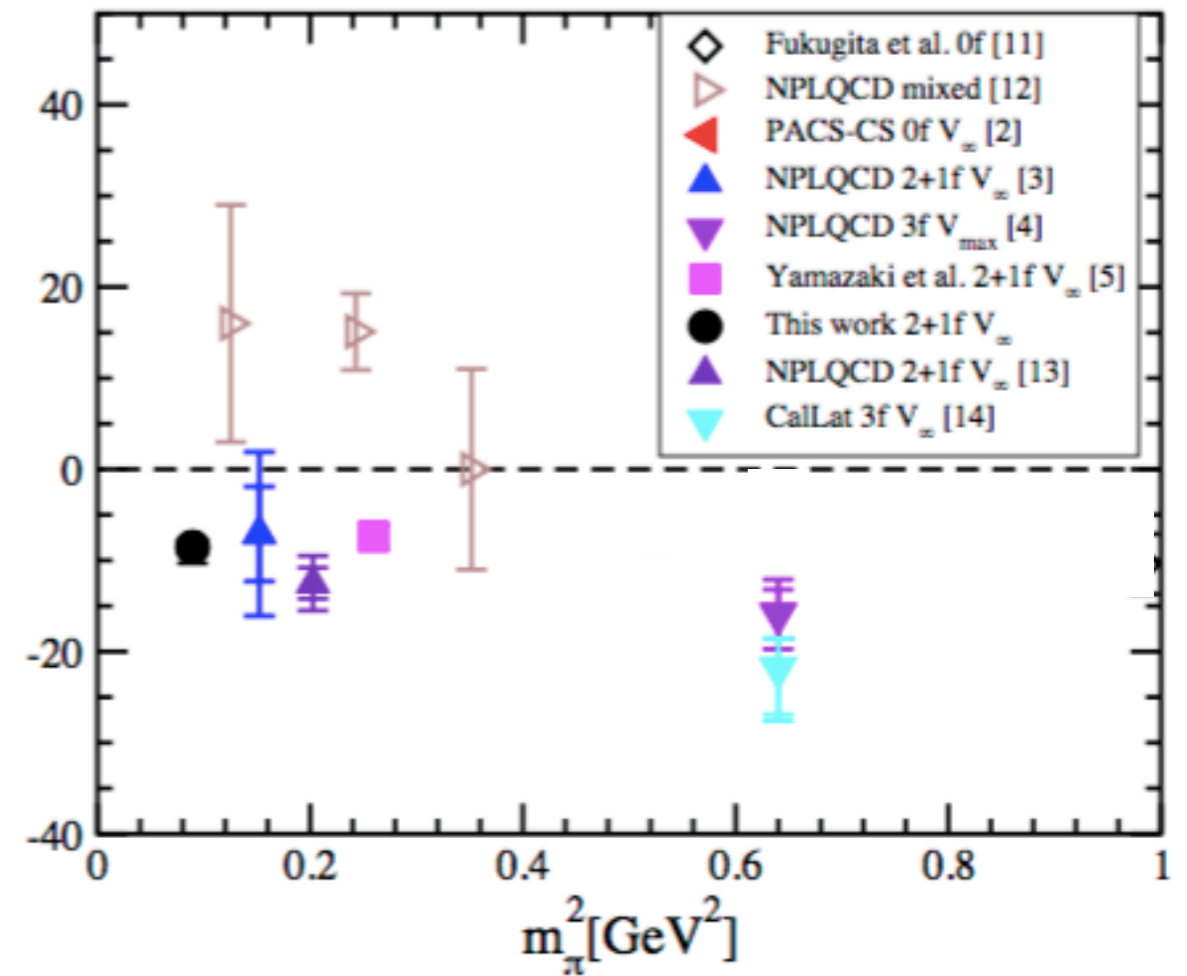
NN Binding energies



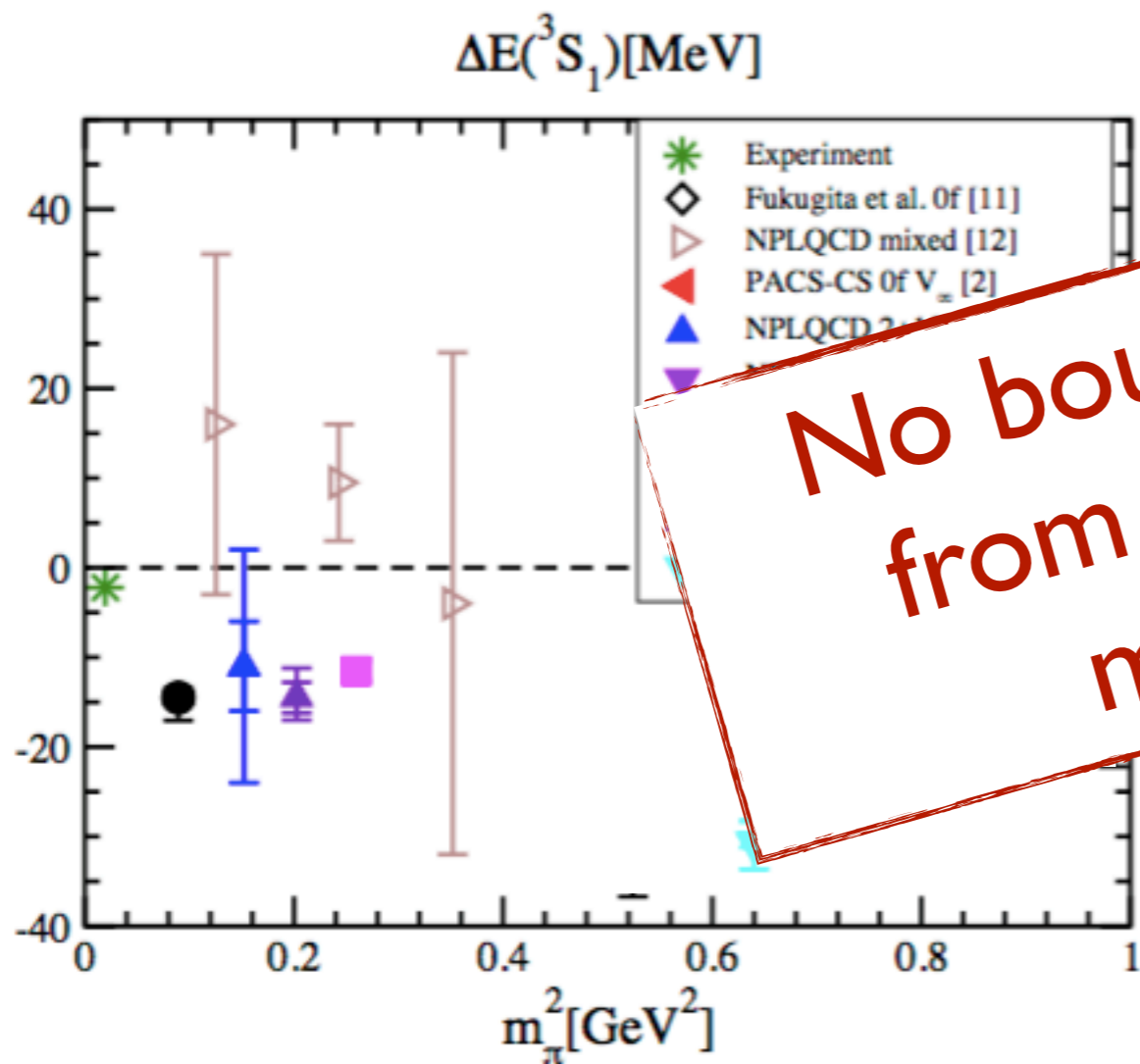
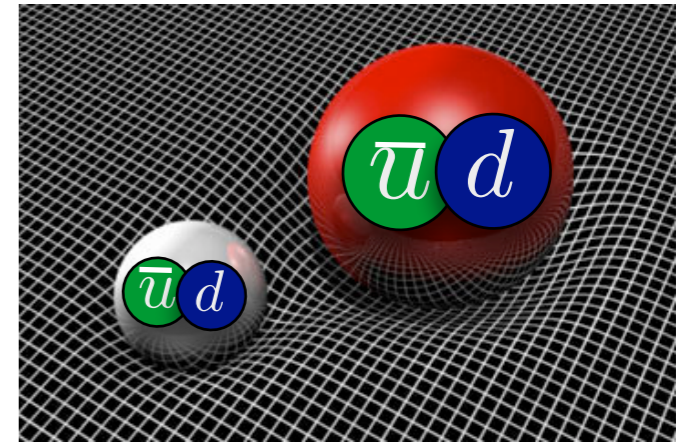
$\Delta E(^3S_1)$ [MeV]



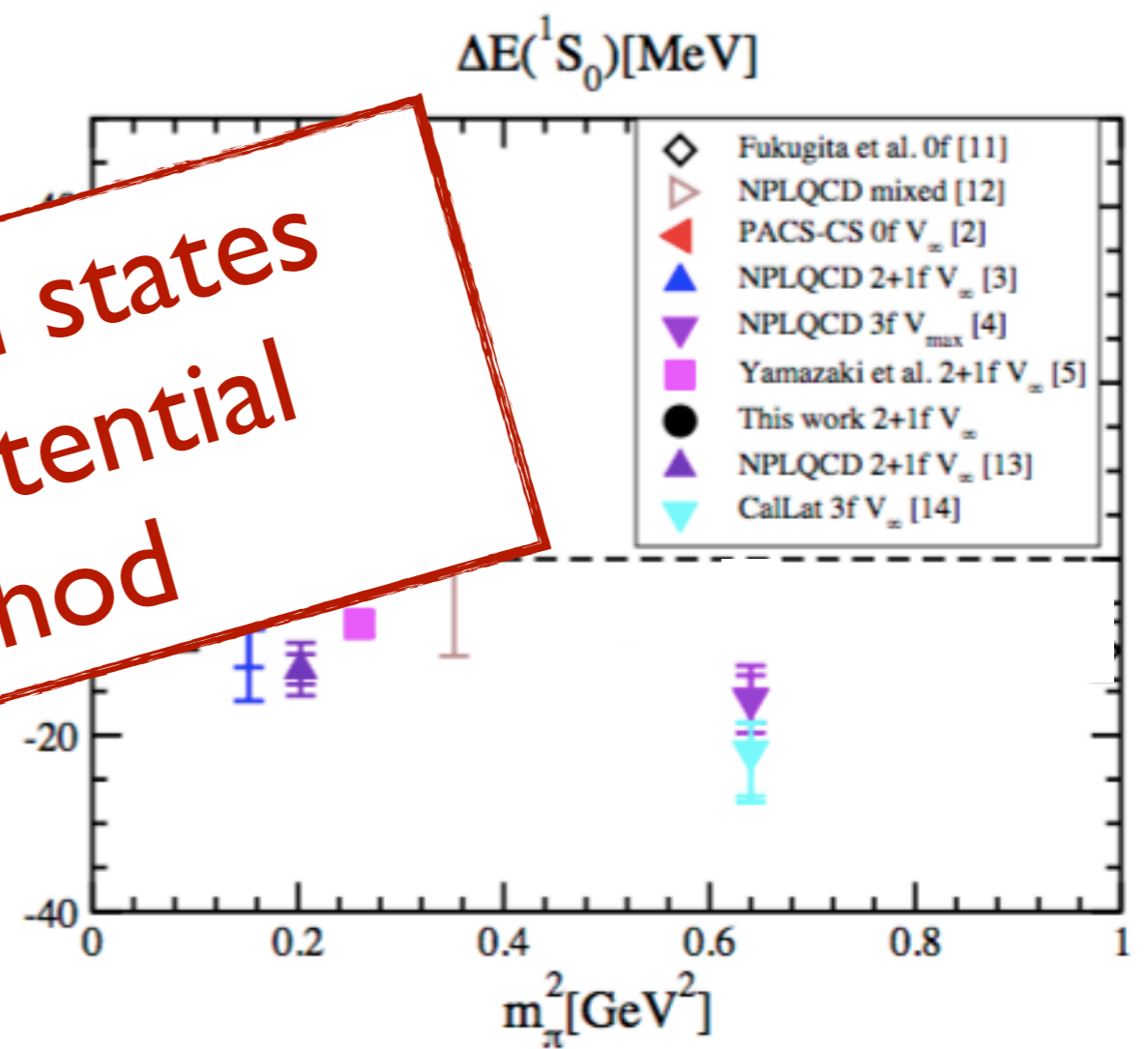
$\Delta E(^1S_0)$ [MeV]



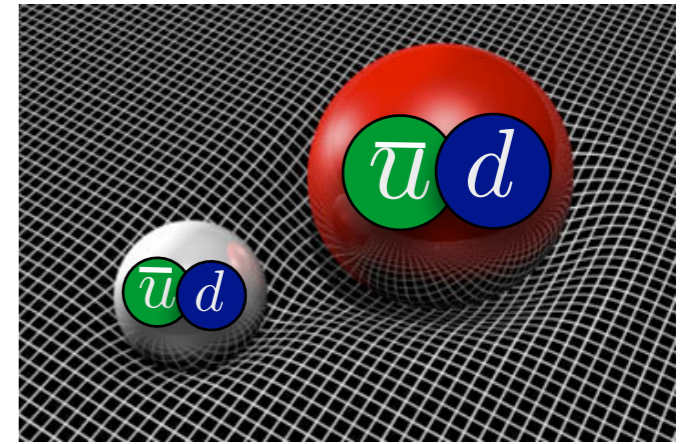
NN Binding energies



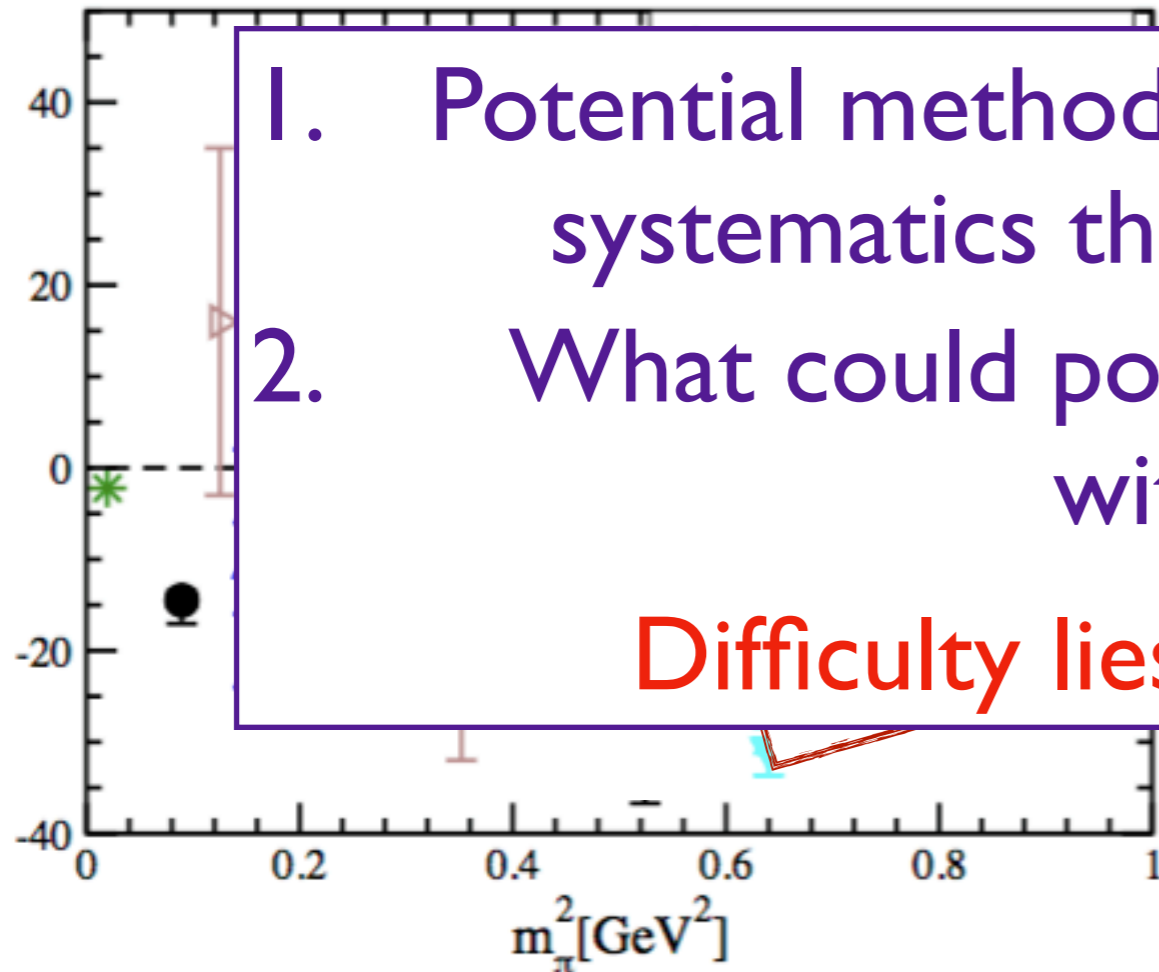
No bound states
from potential
method



NN Binding energies



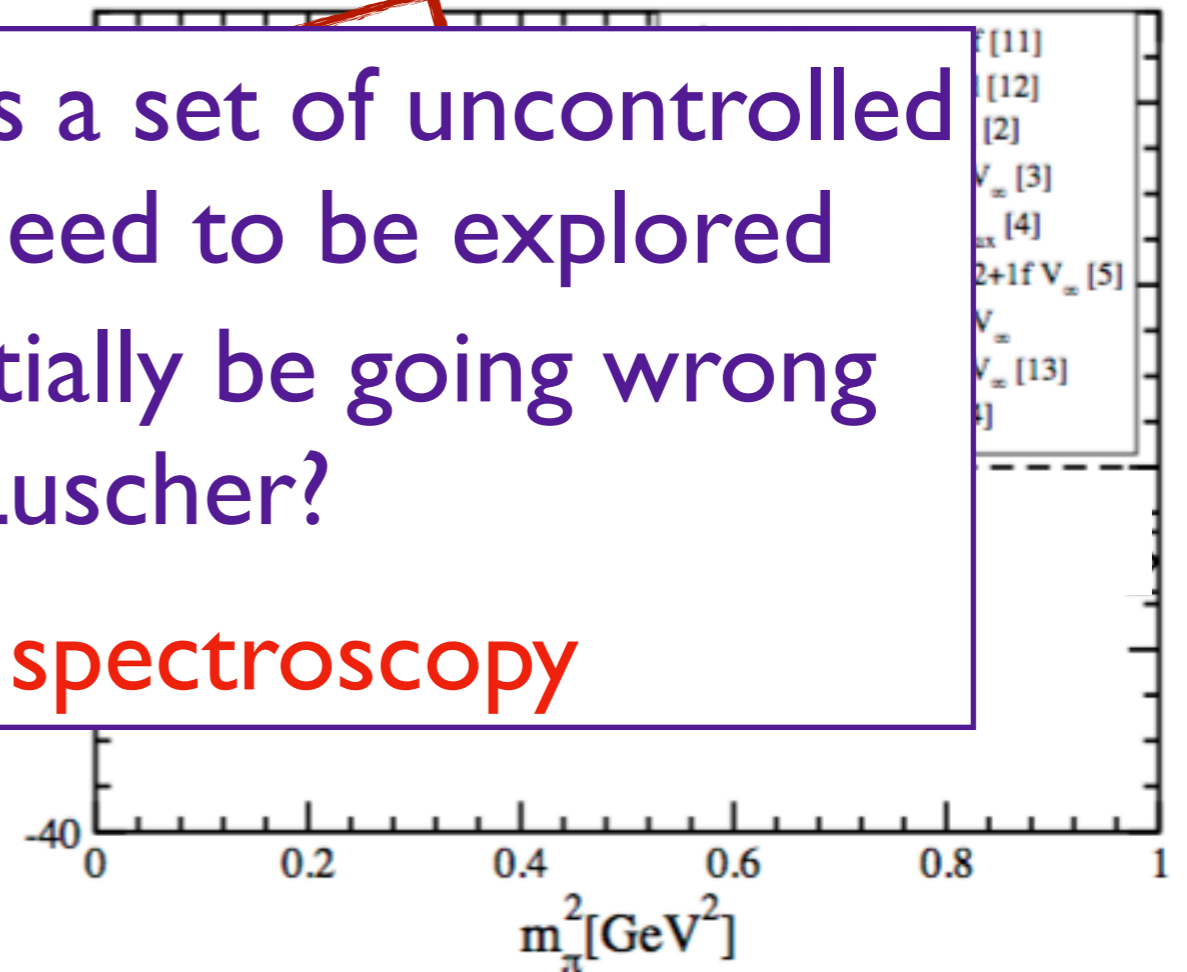
$\Delta E(^3S_1)[\text{MeV}]$



1. Potential method has a set of uncontrolled systematics that need to be explored
2. What could potentially be going wrong with Luscher?

Difficulty lies in spectroscopy

$\Delta E(^1S_0)[\text{MeV}]$



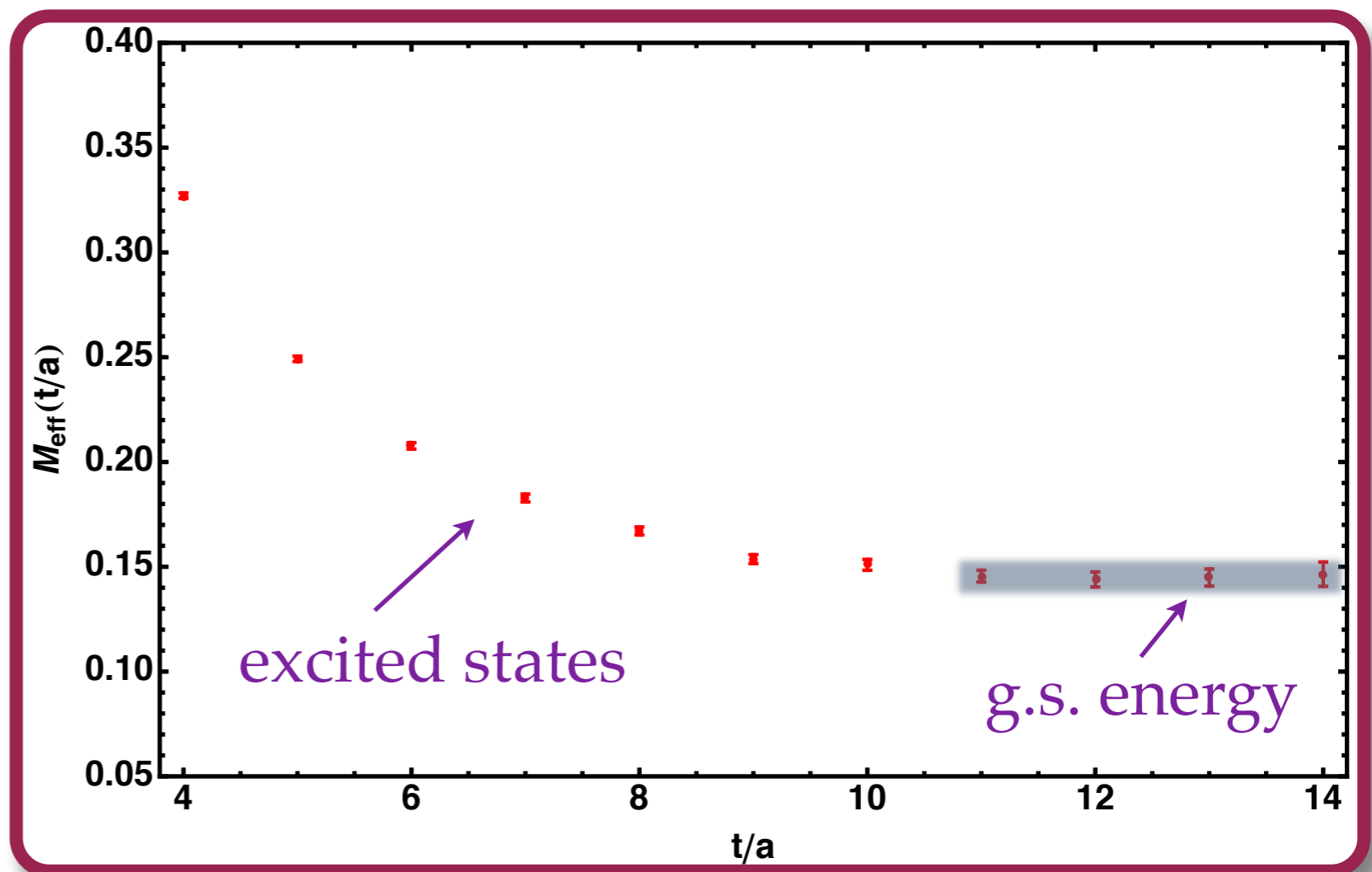
Calculating the energies

Imaginary time
projection:

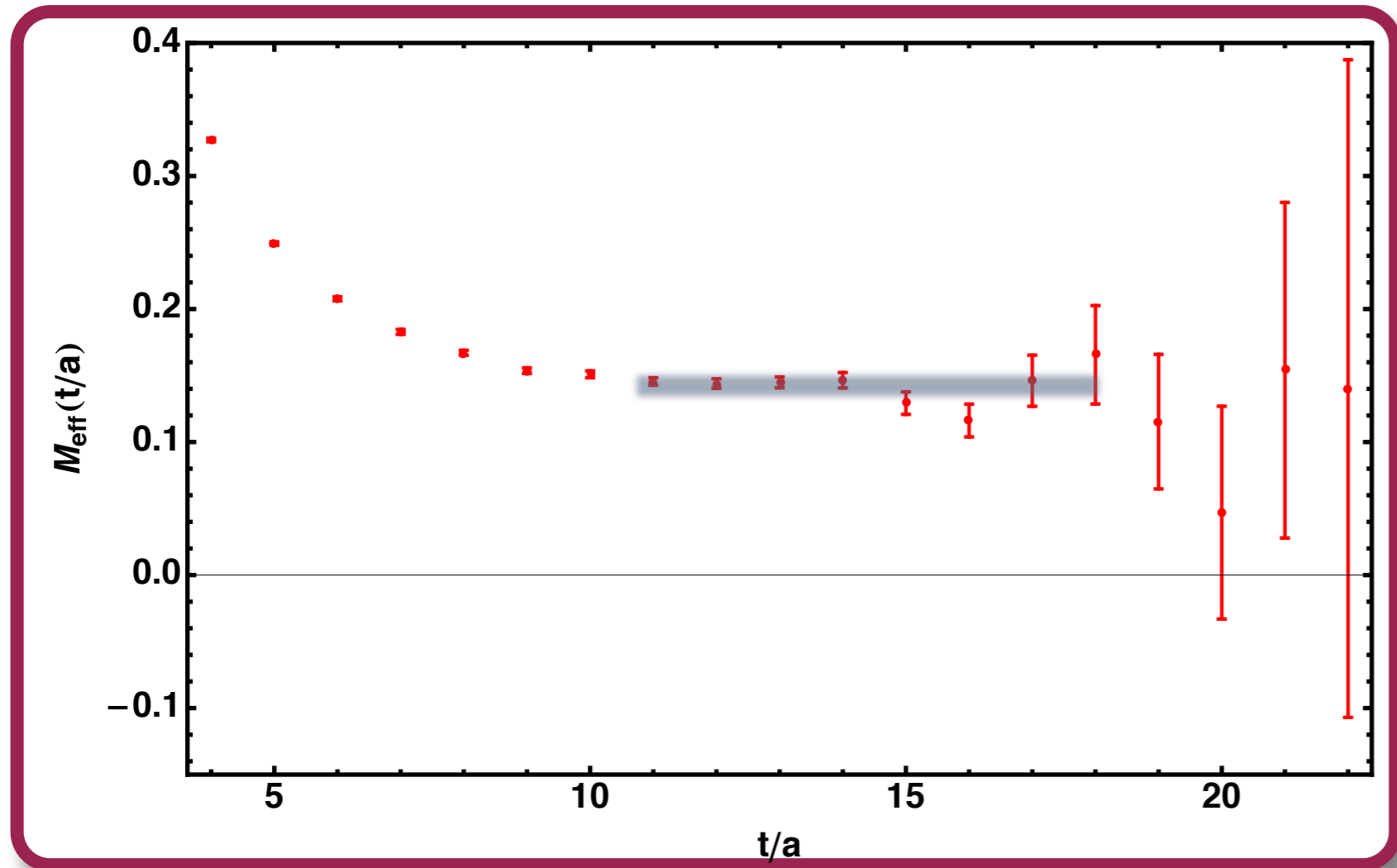
$$C(t) = \langle \mathcal{O}(t) \mathcal{O}^\dagger(0) \rangle = \sum_n |\langle 0 | \mathcal{O} | n \rangle|^2 e^{-E_n t}$$
$$\xrightarrow{t \rightarrow \infty} Z_0 e^{-E_0 t}$$

Effective mass plot:

$$M_{\text{eff}} \equiv \ln \frac{C(t)}{C(t+1)}$$
$$\xrightarrow{t \rightarrow \infty} E_0$$

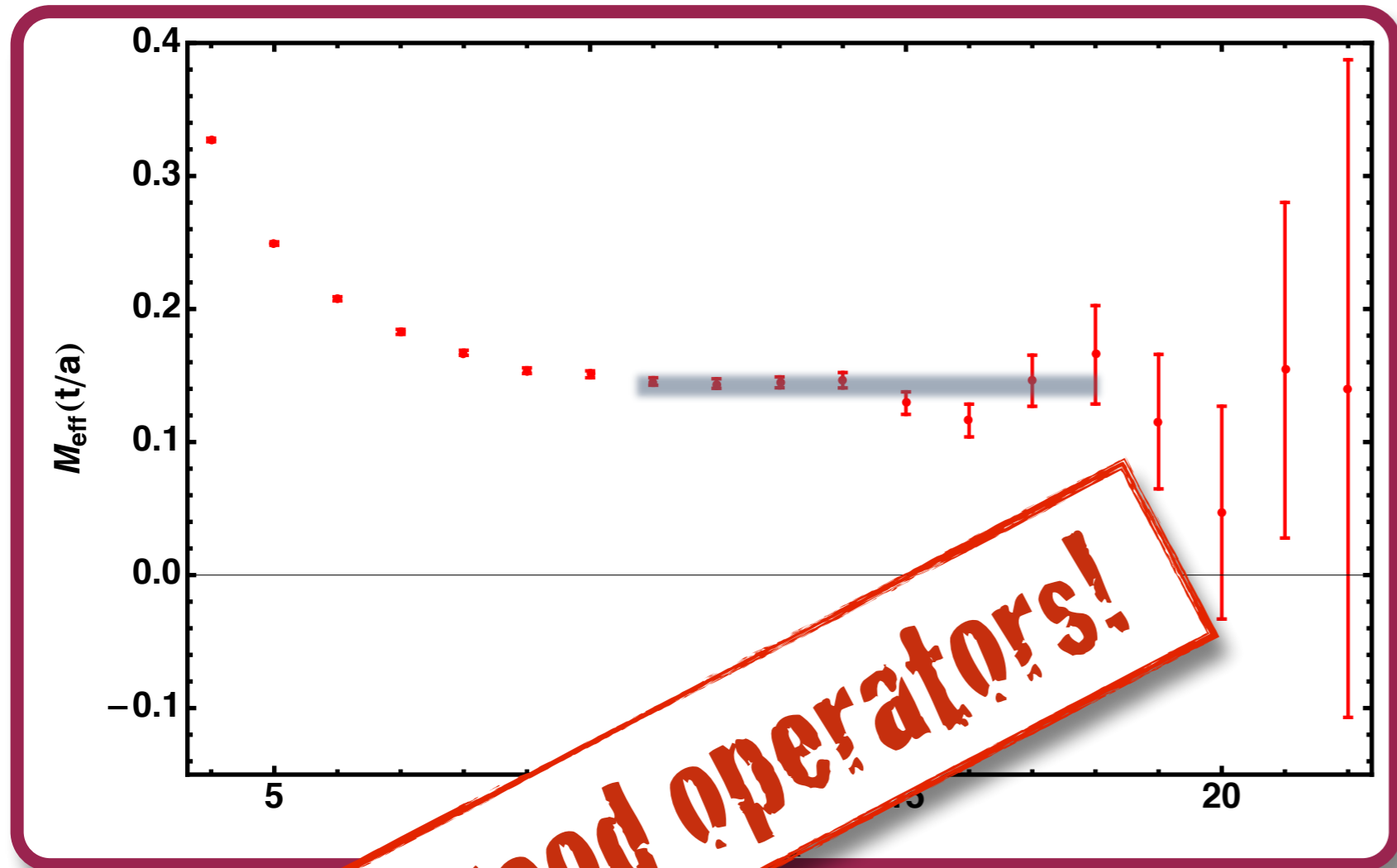


Nucleons: Signal-to-noise



$$\left. \vphantom{e^{A(M_n - 3/2m_\pi)t}} \right\} \sim e^{A(M_n - 3/2m_\pi)t}$$

Nucleons: Signal-to-noise

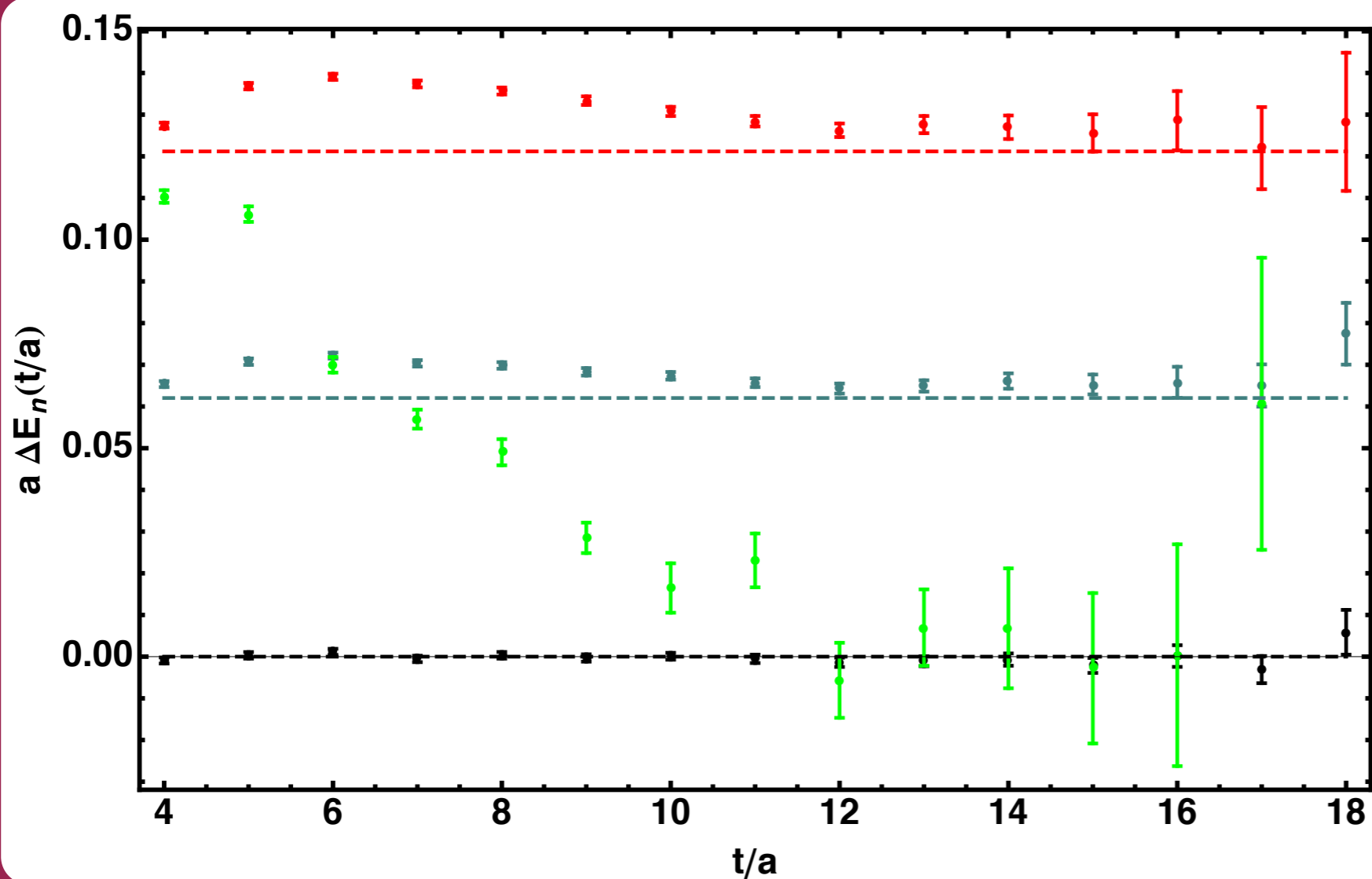


$$\left. \vphantom{e^{A(M_n - 3/2m_\pi)t}} \right\} \sim e^{A(M_n - 3/2m_\pi)t}$$

Need good operators!

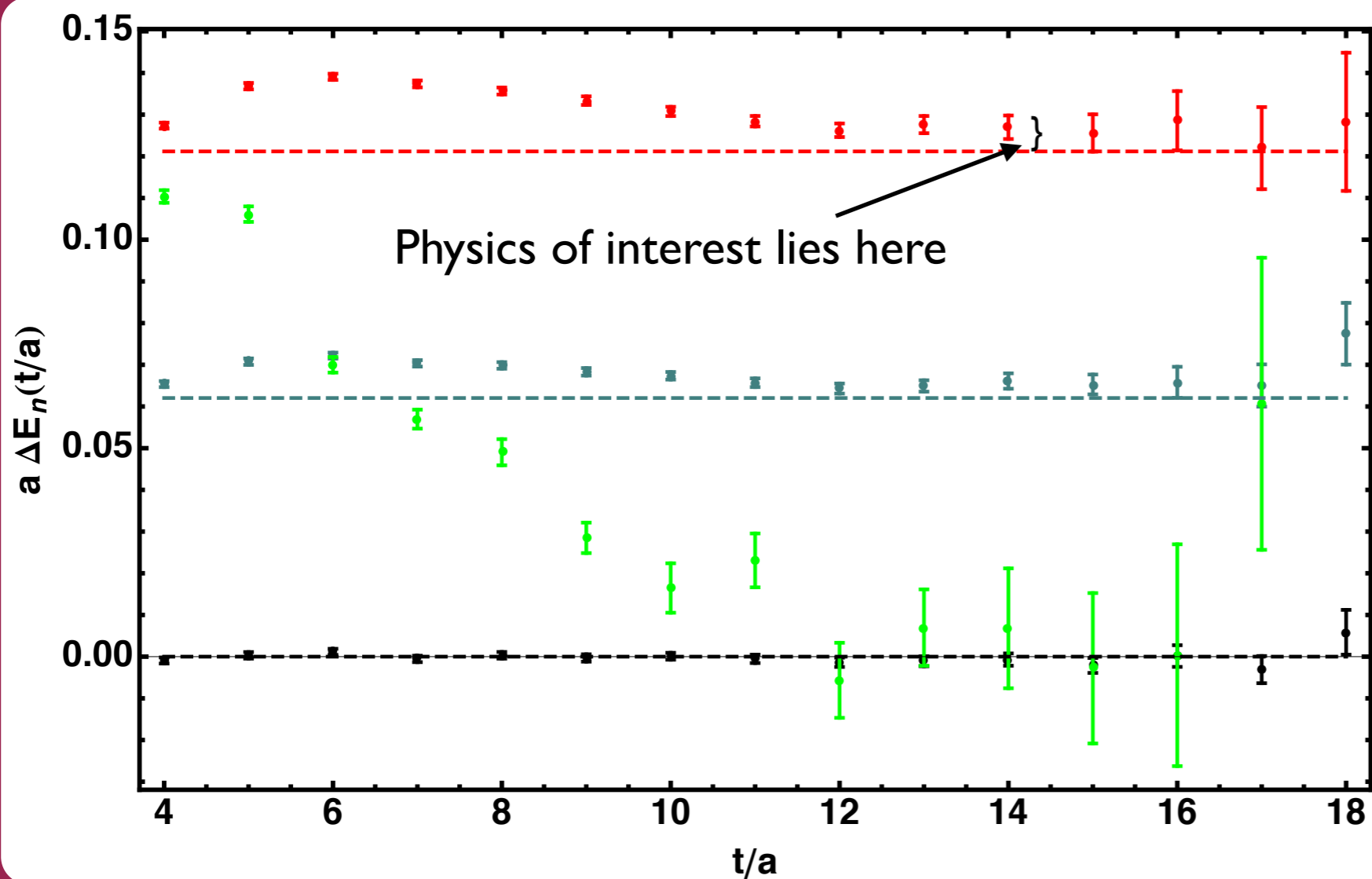
Trying to pull off tiny correction
compared to large nucleon mass:

$$\Delta E = E_{NN} - 2E_N$$

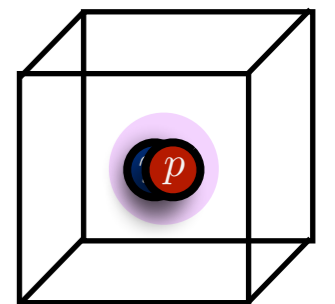
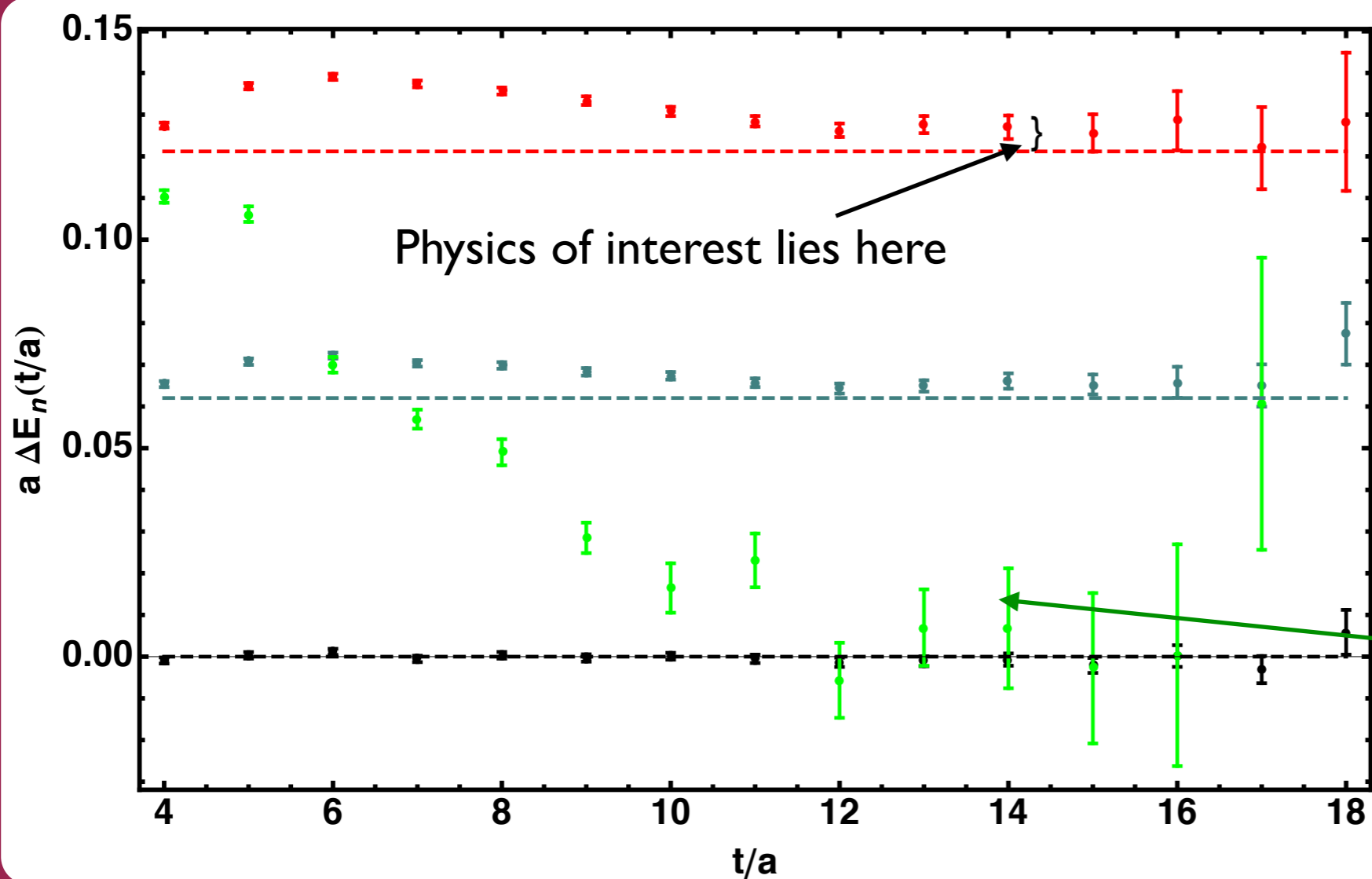


Trying to pull off tiny correction
compared to large nucleon mass:

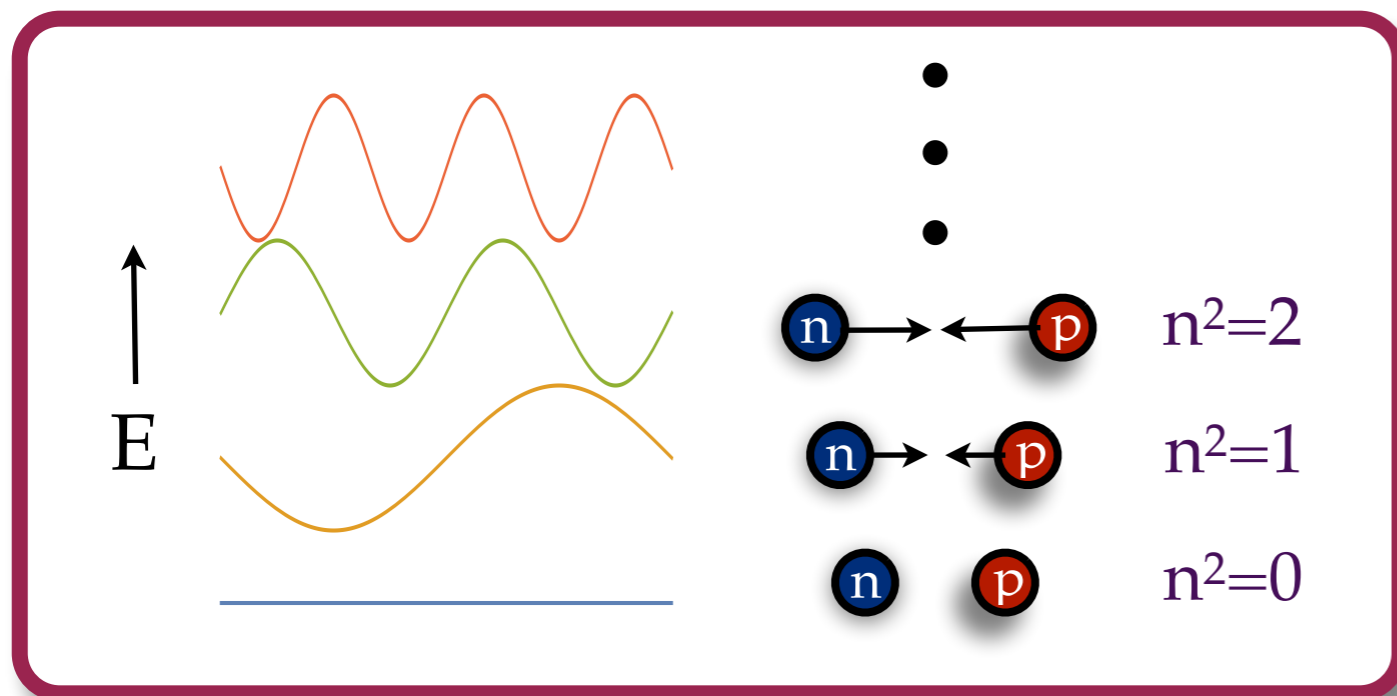
$$\Delta E = E_{NN} - 2E_N$$



Trying to pull off tiny correction
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 $\Delta E = E_{NN} - 2E_N$

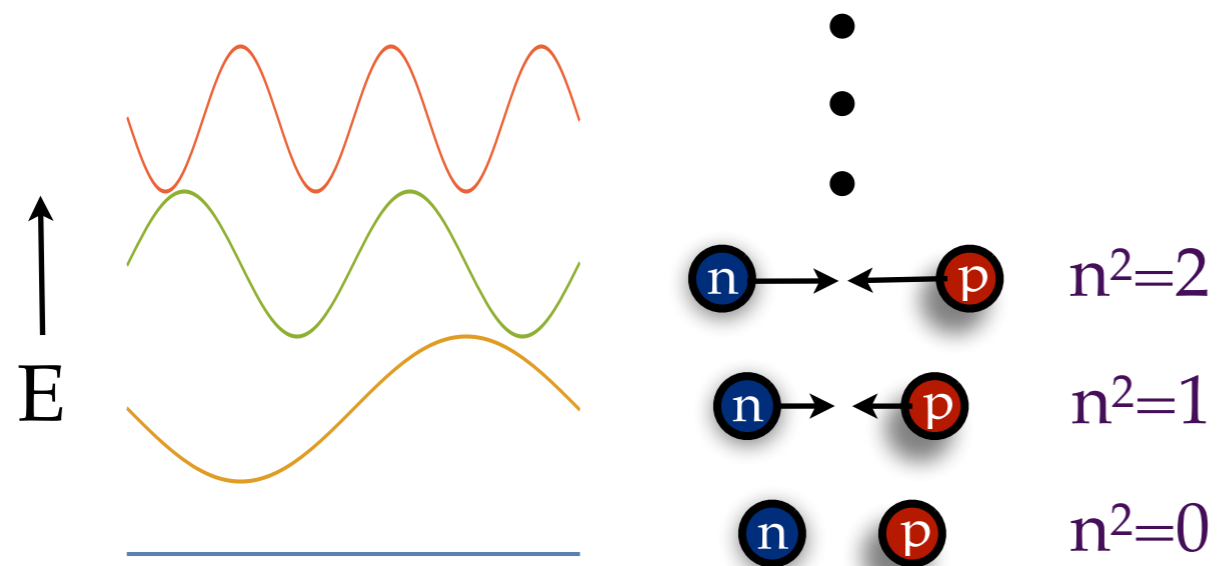


Excited state contamination

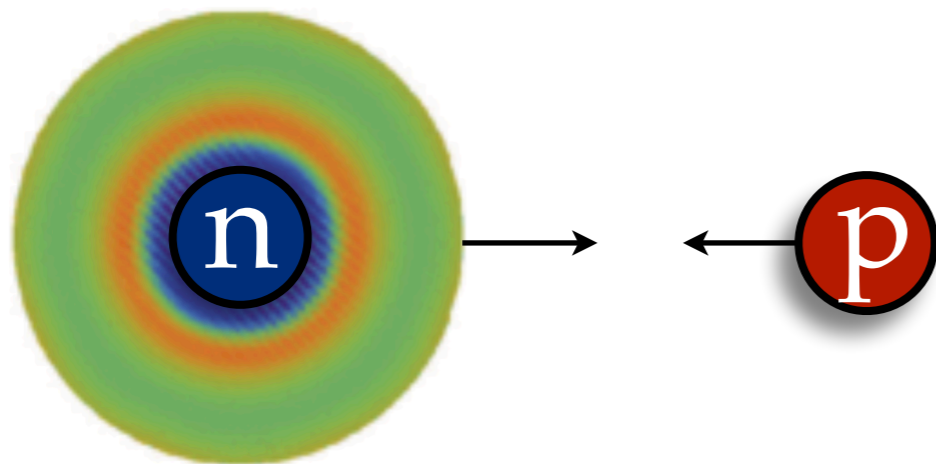


Elastic scattering
(2-body)
 $\Delta E \sim 50 \text{ MeV}$
(Lüscher)

Excited state contamination



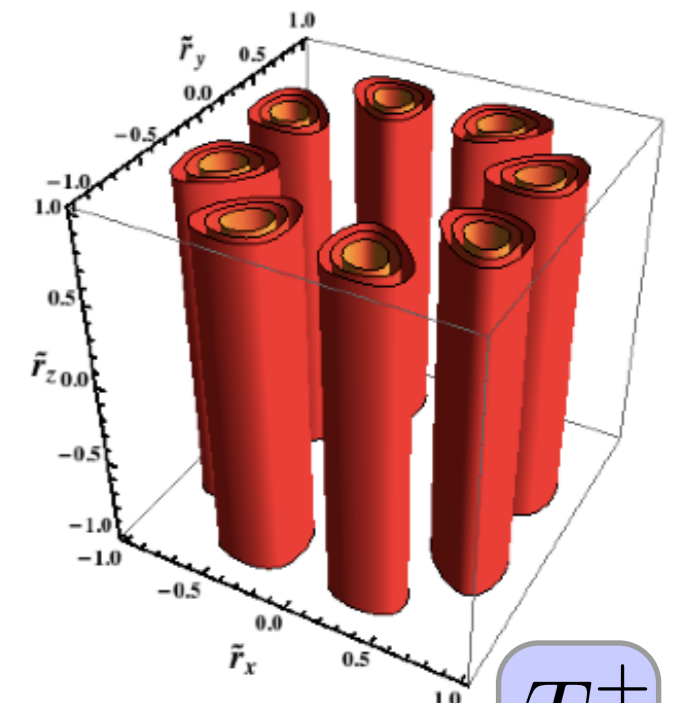
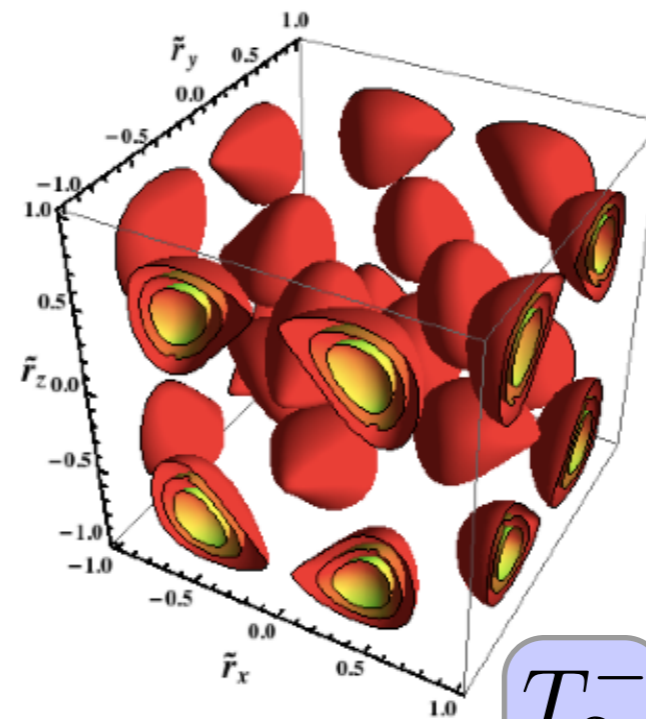
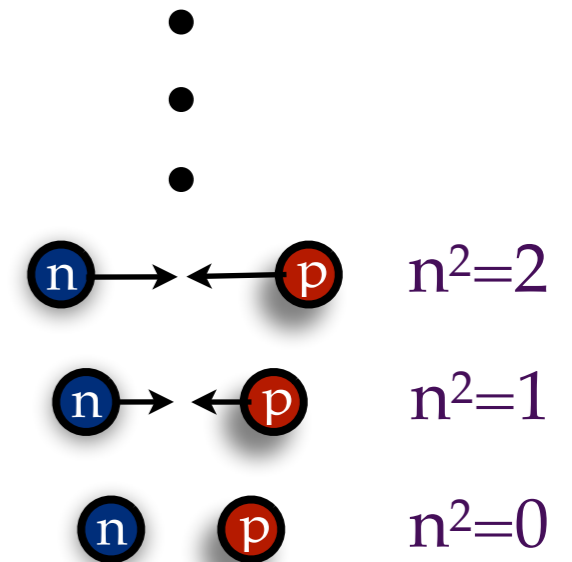
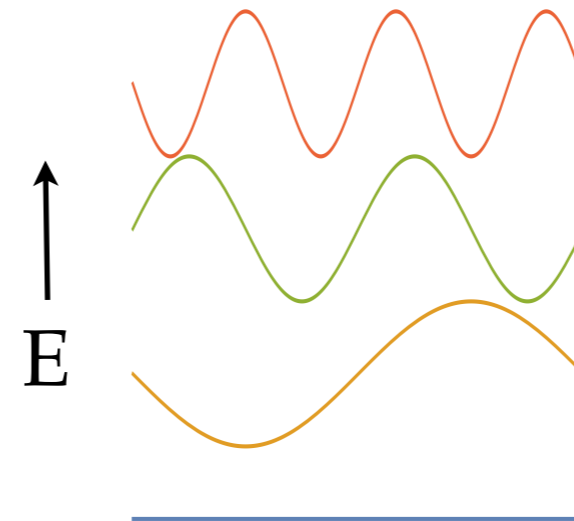
Elastic scattering
(2-body)
 $\Delta E \sim 50 \text{ MeV}$
(Luscher)



Inelastic single body
 $\Delta E \sim m_\pi$
(HAL, Luscher)

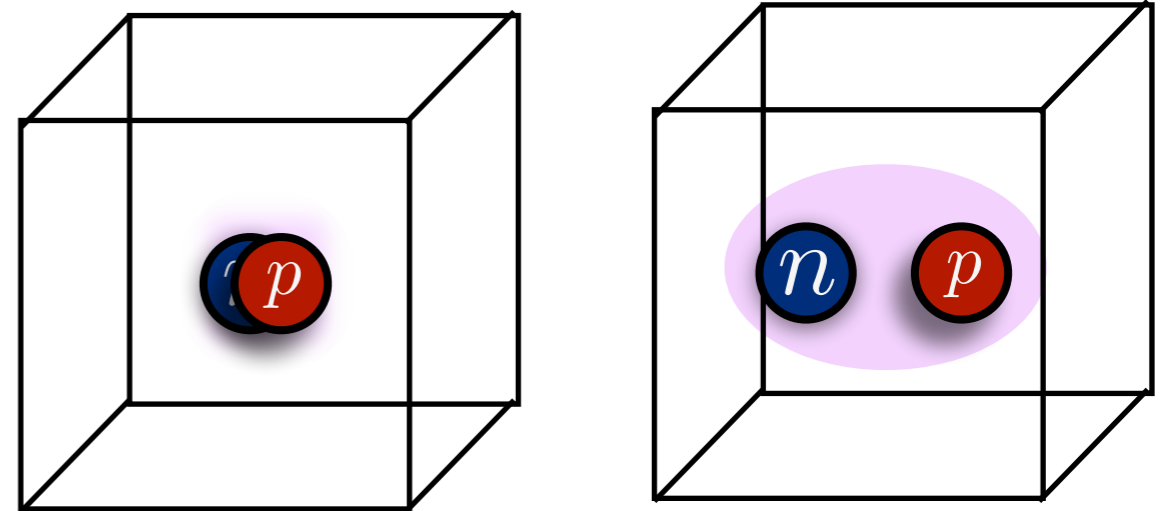
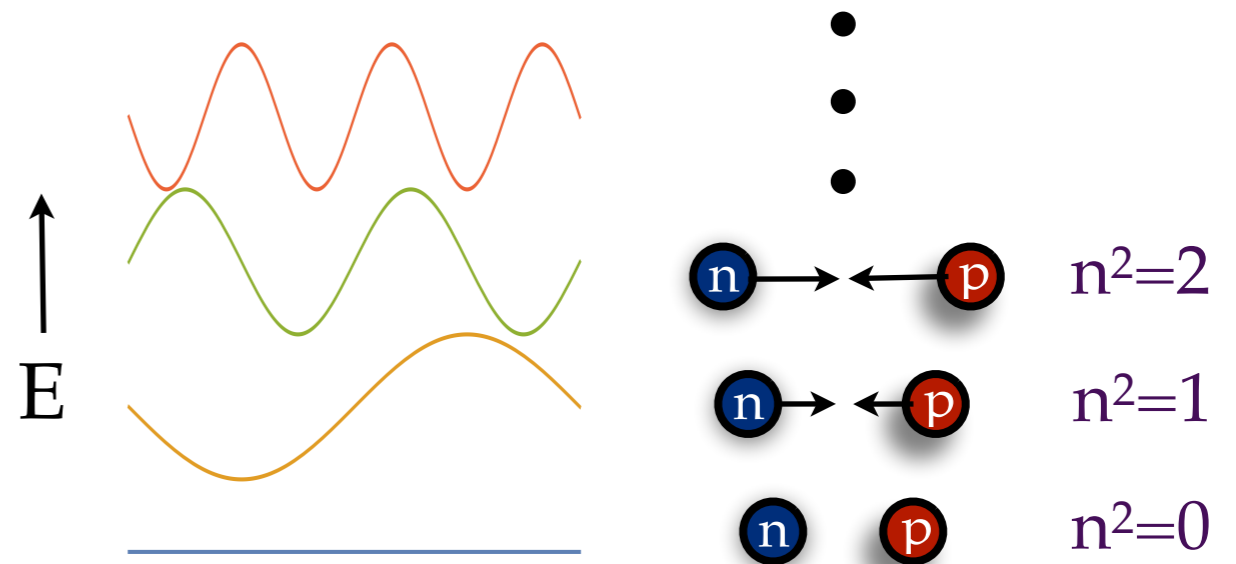
Reducing elastic 2-body excited states

- Project onto non-interacting eigenstates of the box
- Very costly to perform exact momentum/angular momentum projection at both source & sink ($\sim V$)
- Perform exact projection only at the sink

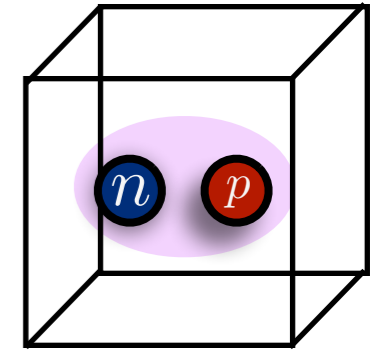
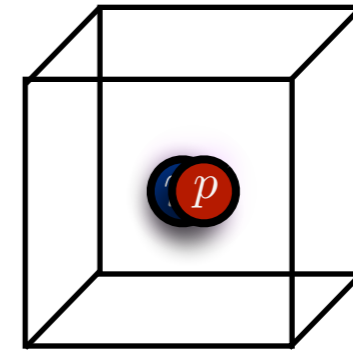


Reducing elastic 2-body excited states

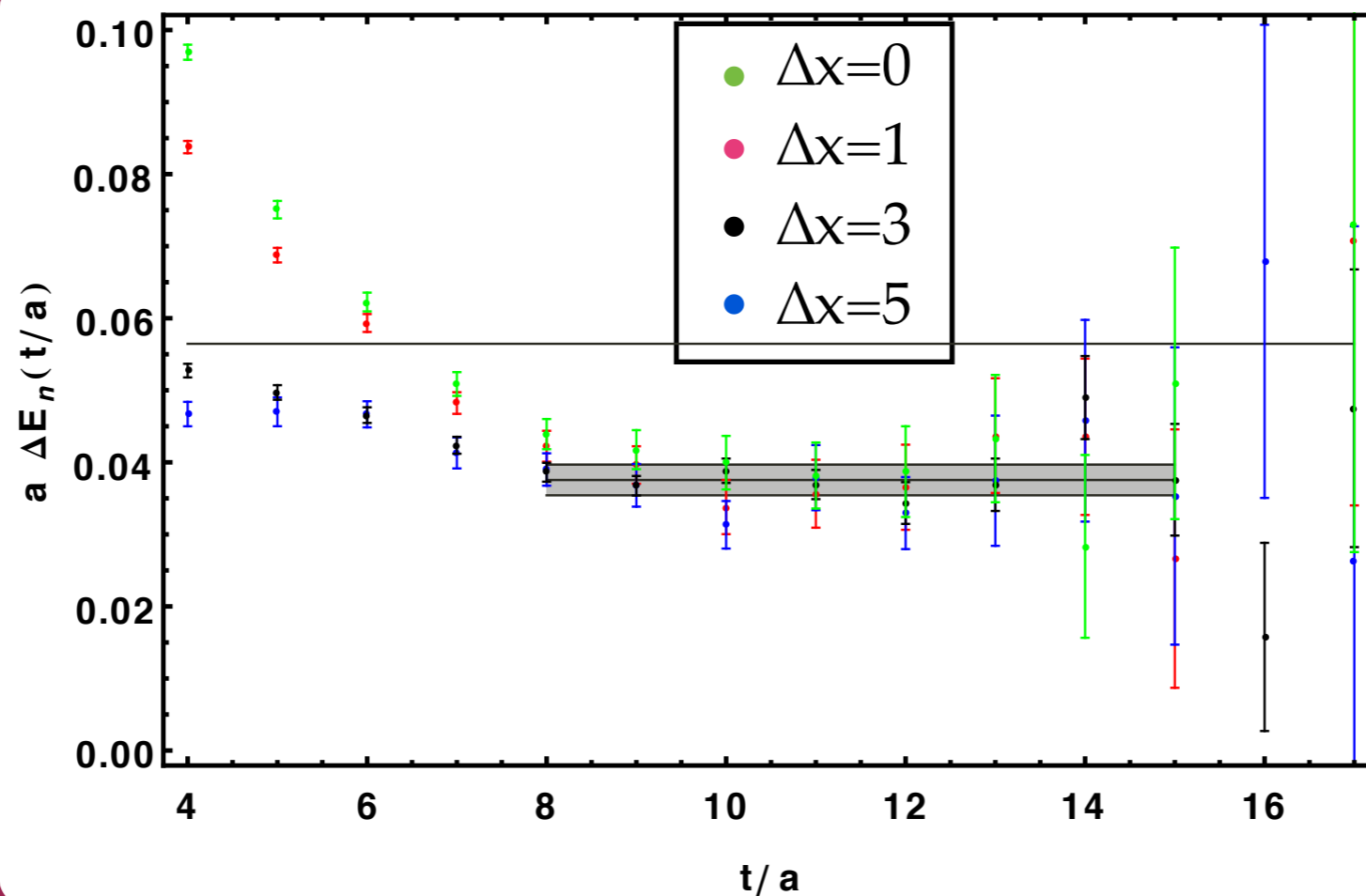
- Project onto non-interacting eigenstates of the box
- Very costly to perform exact momentum/angular momentum projection at both source & sink ($\sim V$)
- Source: need spatially displaced source operators to have overlap with $\ell > 0$
- Even for s-wave, displaced sources are cleaner



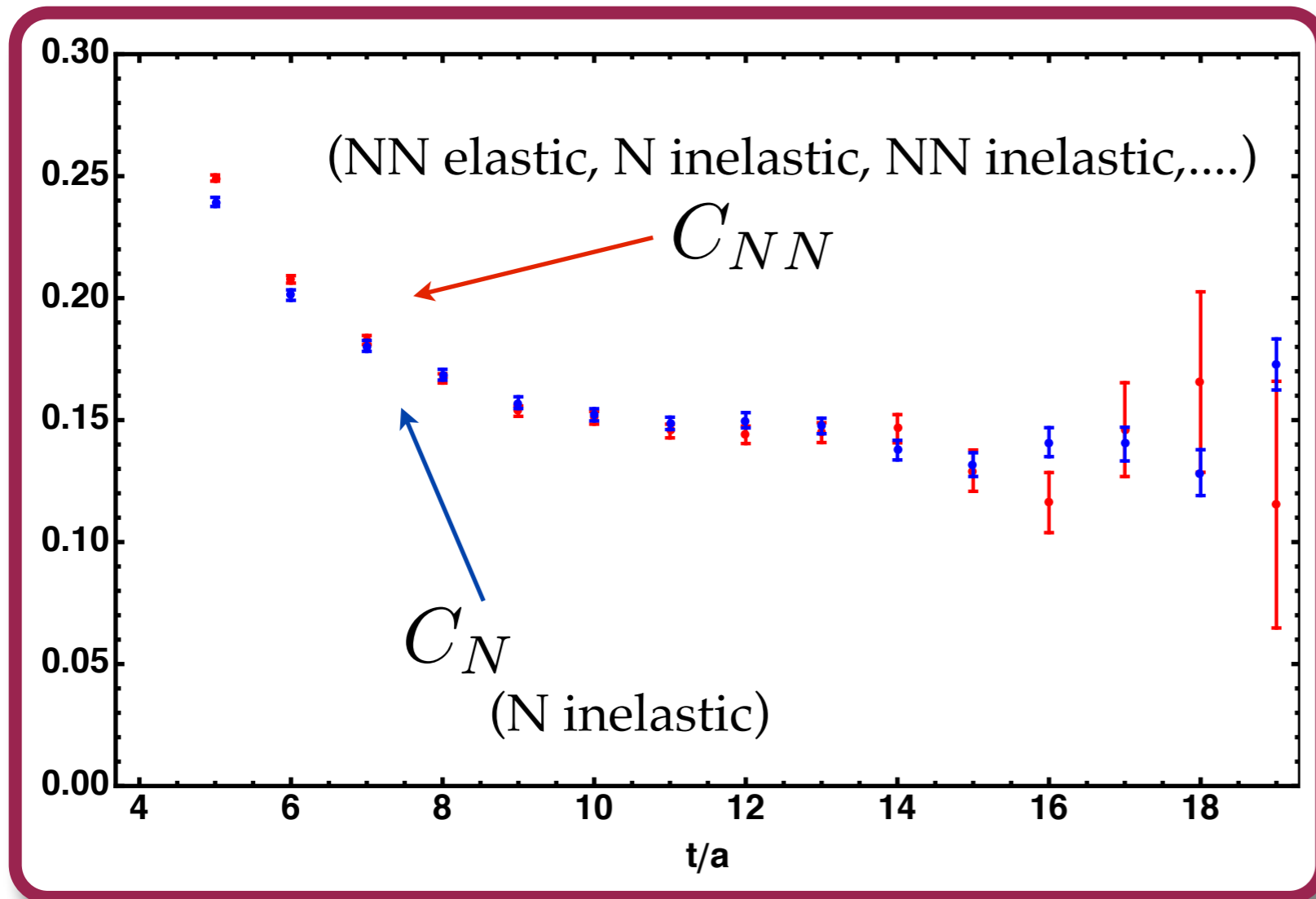
Source: position space



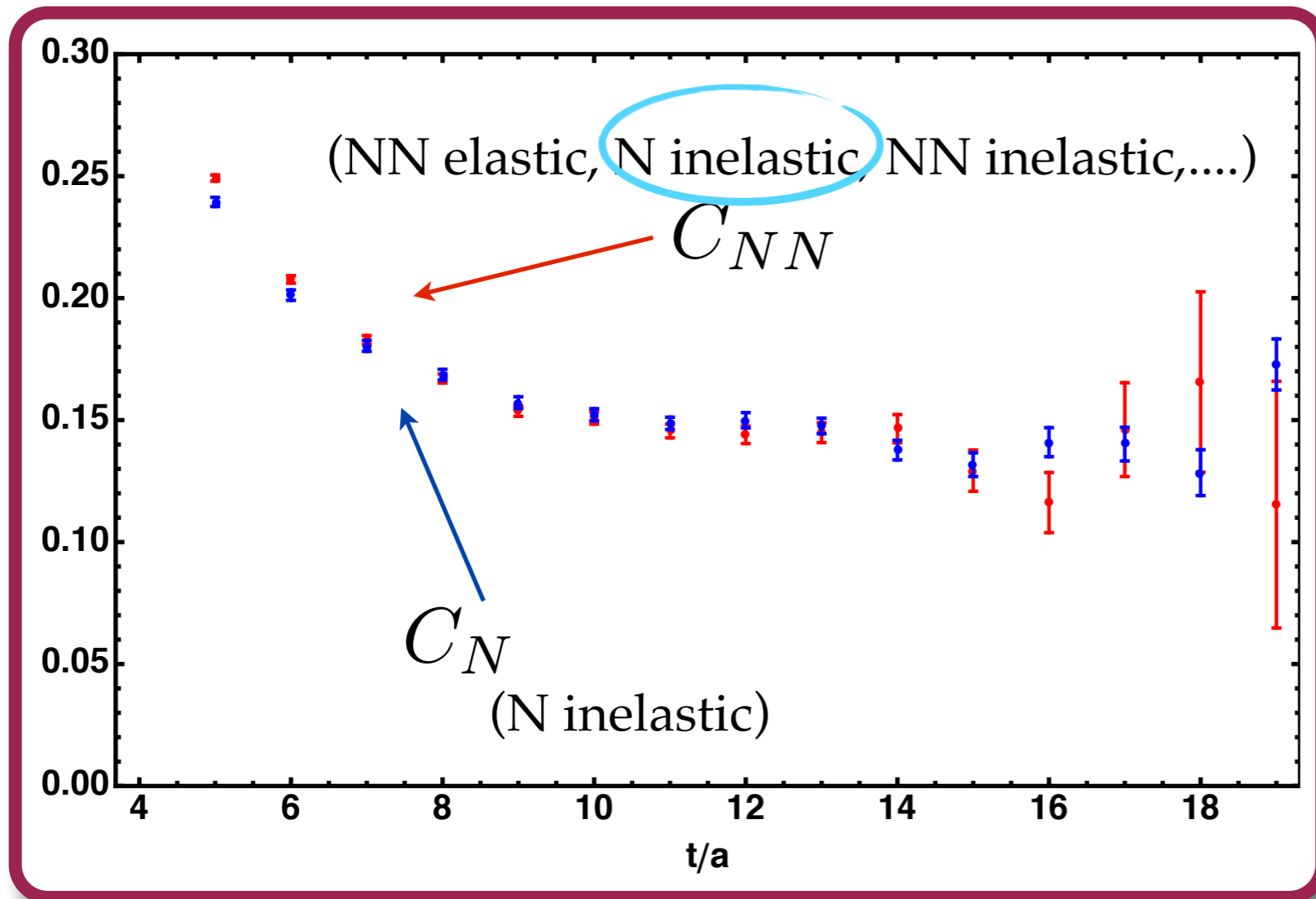
Large displacements are necessary for maximal overlap with low-energy states



Excited state contributions to NN

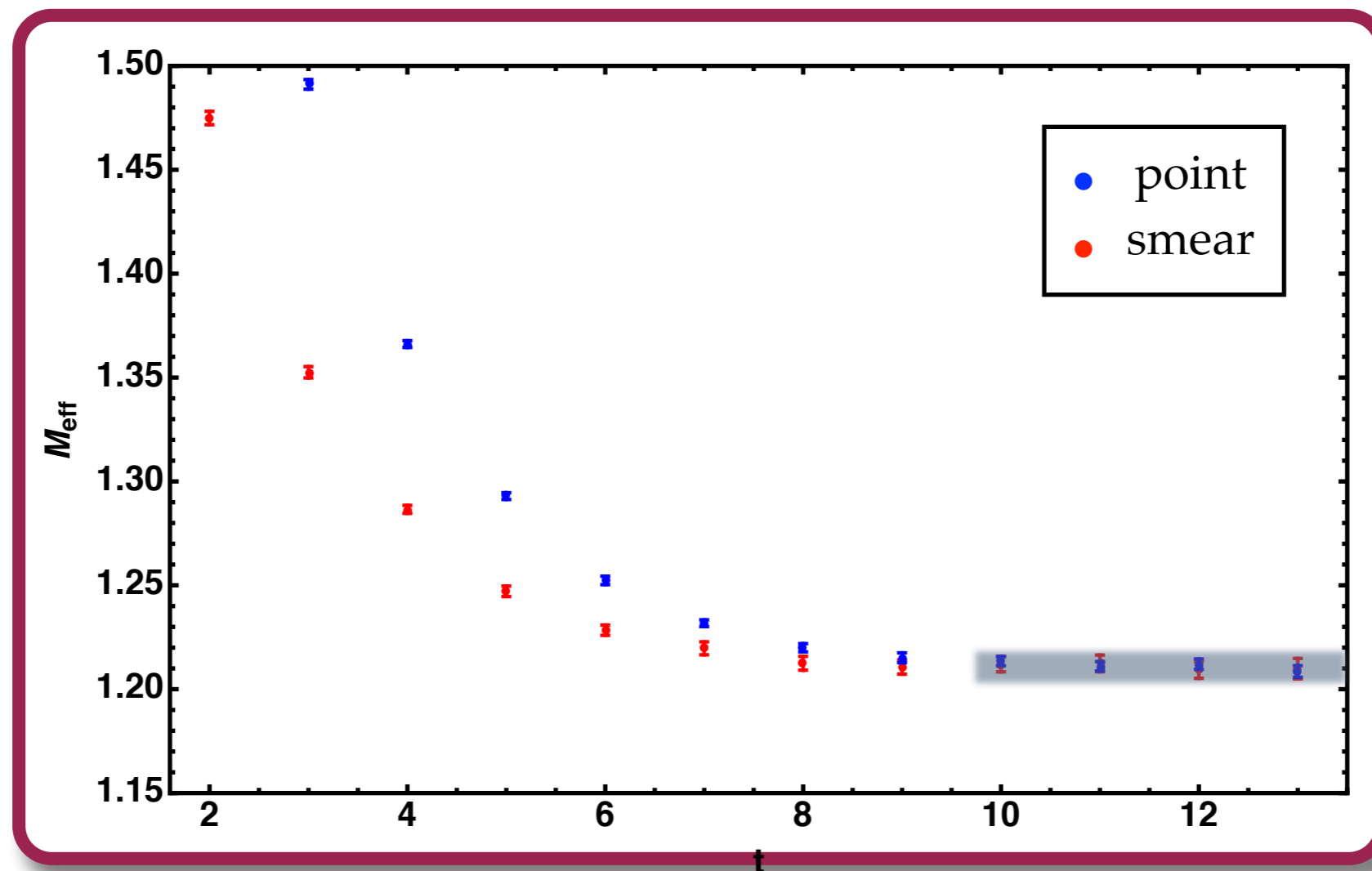
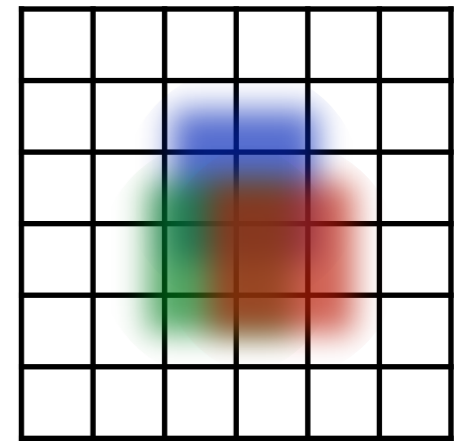
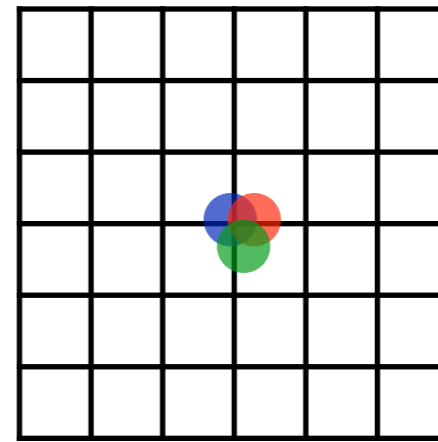


Excited state contributions to NN



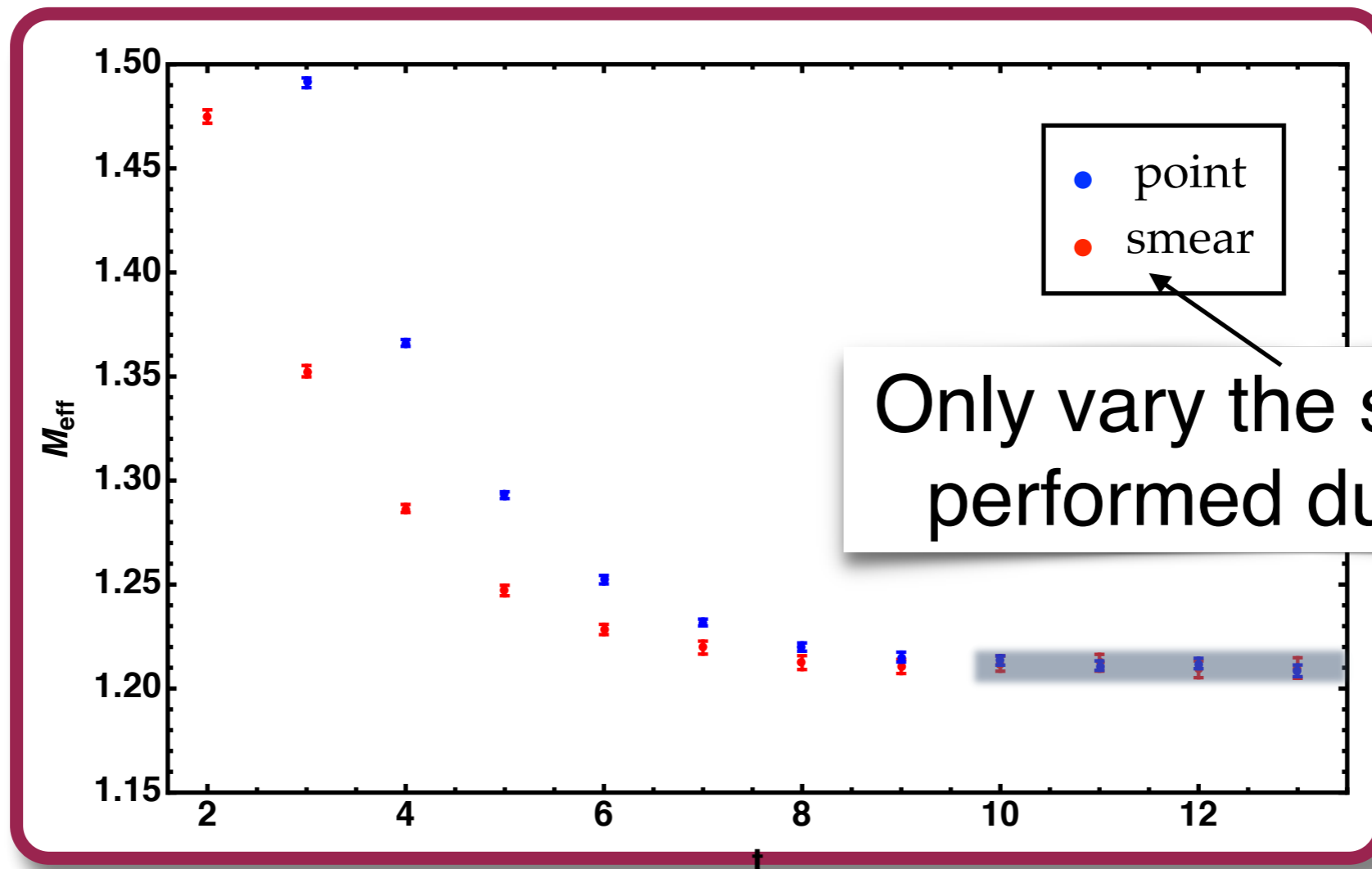
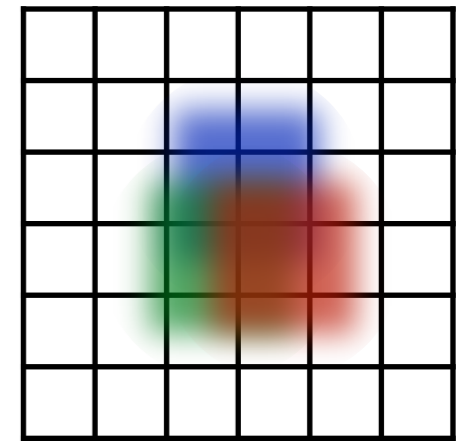
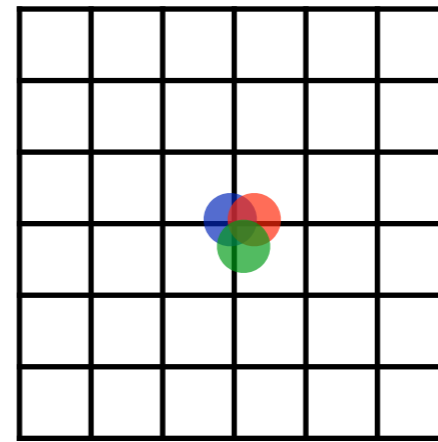
Long time behavior
of NN correlator
dominated by
inelastic single
nucleon excited state
(problem for HAL
method!)

Reducing single nucleon inelastic states: Matrix Prony (poor man's GEVP)



Single nucleon correlator

Reducing single nucleon inelastic states: Matrix Prony (poor man's GEVP)



Only vary the sink: easily performed during FFT

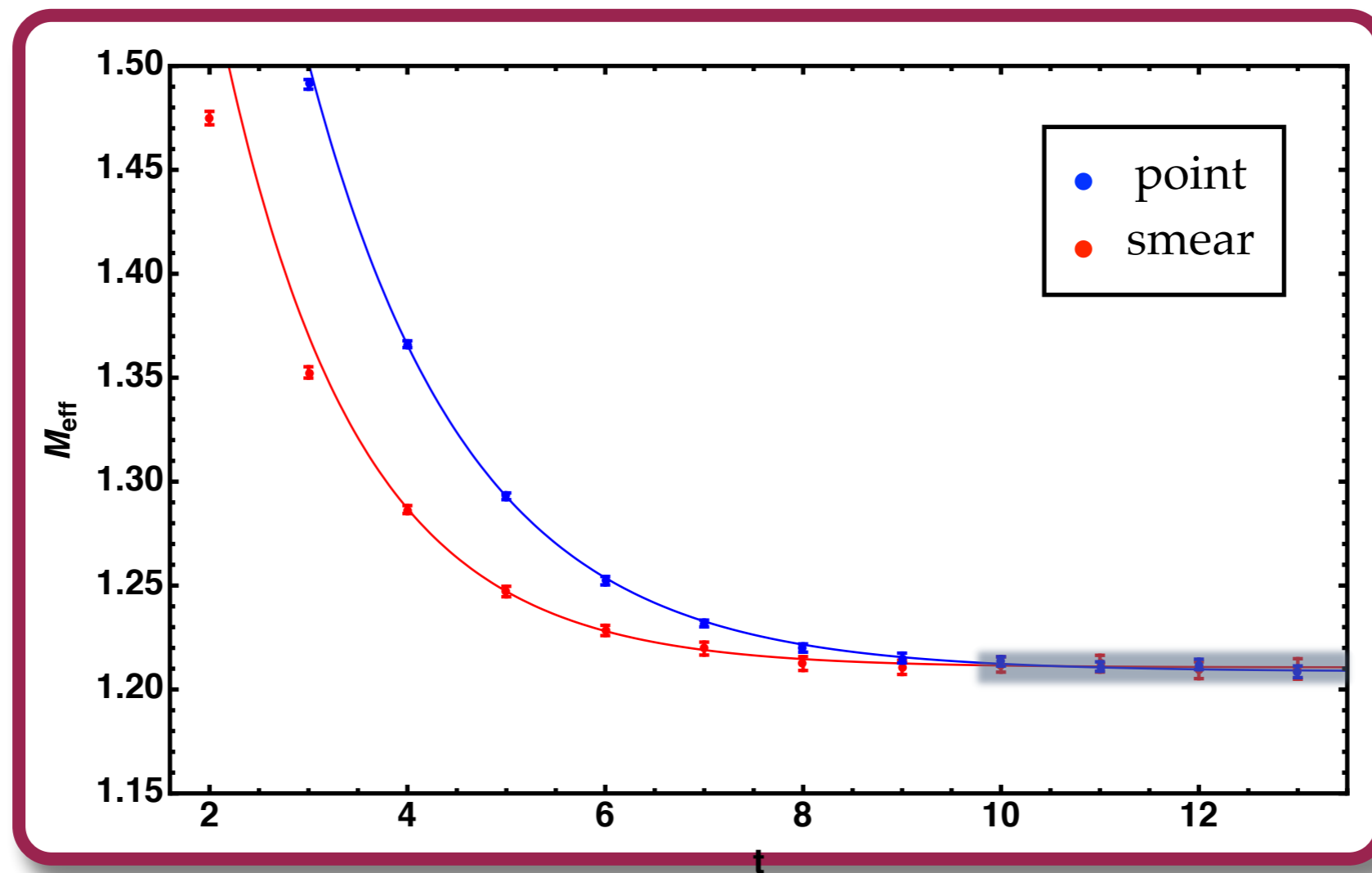
Single nucleon correlator

Reducing single nucleon inelastic states: Matrix Prony (poor man's GEVP)

$$C_0(t + t_0) + \alpha C(t) = 0$$

$$\alpha = -e^{-E_0 t_0}$$

$$E_0 = -\frac{1}{t_0} \ln \frac{C(t + t_0)}{C(t)}$$



Single nucleon correlator

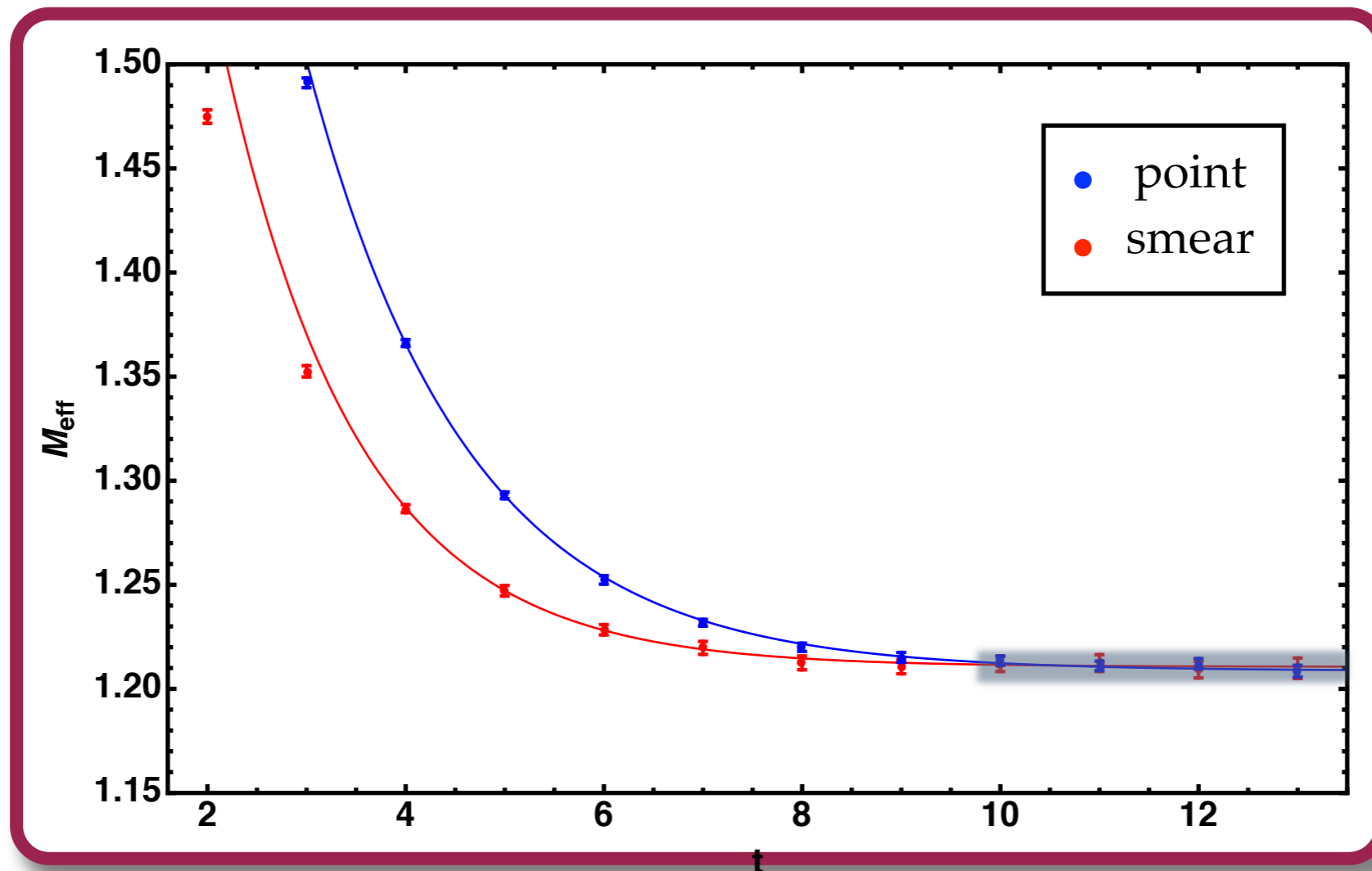
Reducing single nucleon inelastic states: Matrix Prony (poor man's GEVP)

$$MC(t + t_0) - VC(t) = 0$$

$$C(t) = \sum_{n=1}^N \alpha_n u_n \lambda_n^{-t} \quad \lambda = e^{E_n}$$

$$Mu = \lambda^{t_0} Vu$$

$$M = \left[\sum_{\tau=t}^{t+t_W} C(\tau + t_0) C(\tau)^T \right]^{-1} \quad V = \left[\sum_{\tau=t}^{t+t_W} C(\tau) C(\tau)^T \right]^{-1}$$



Single nucleon correlator

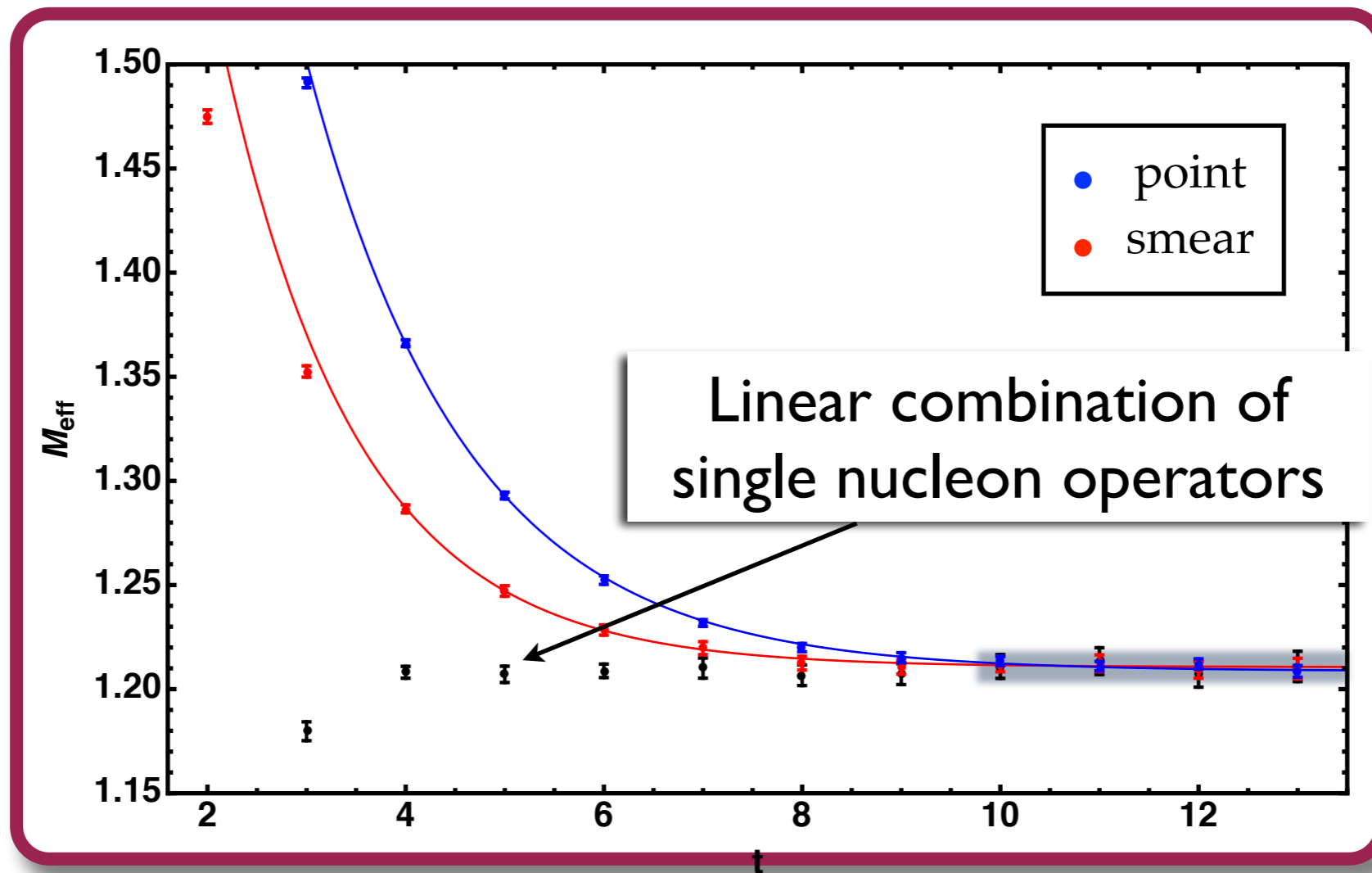
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Single nucleon correlator

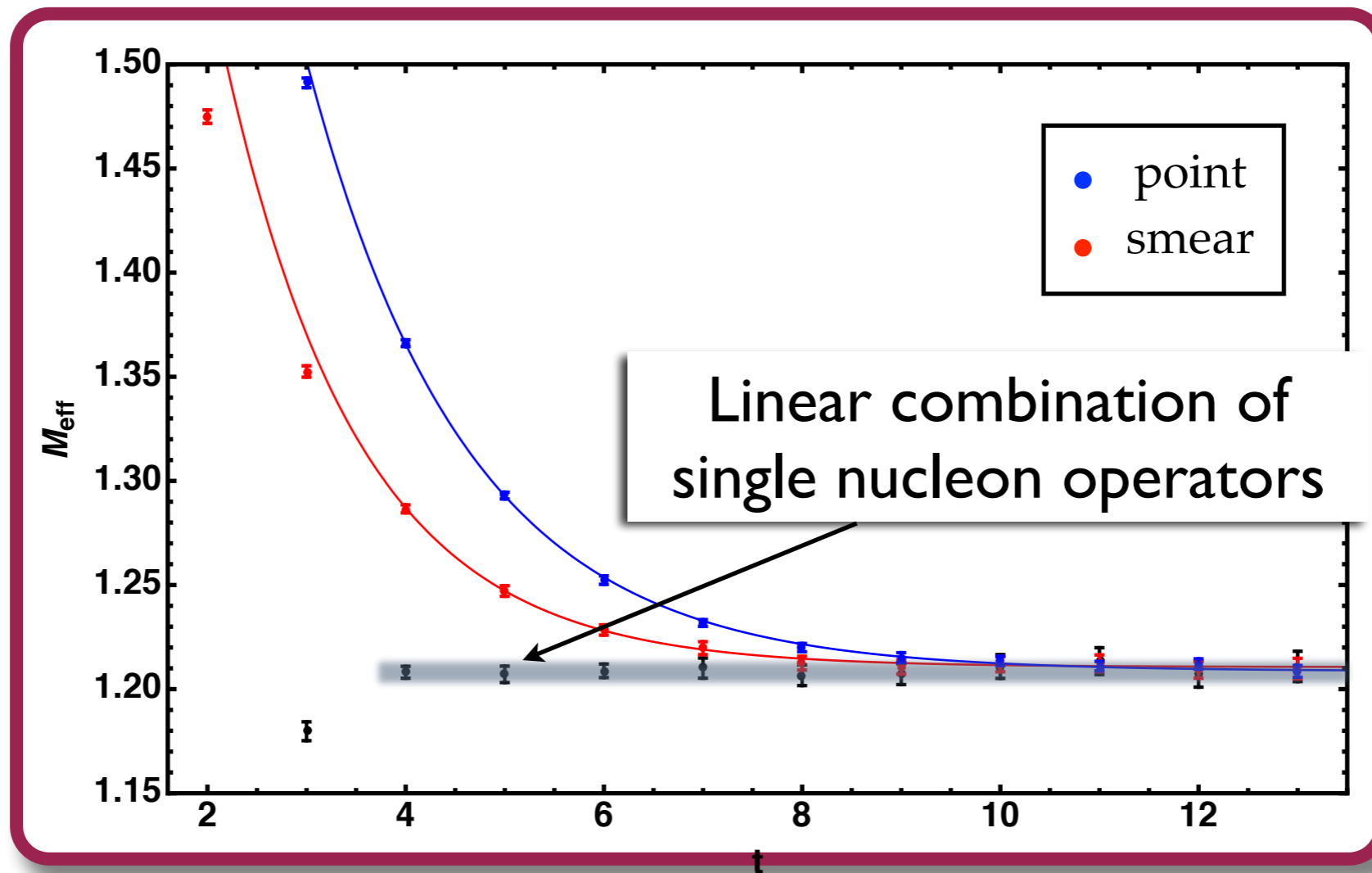
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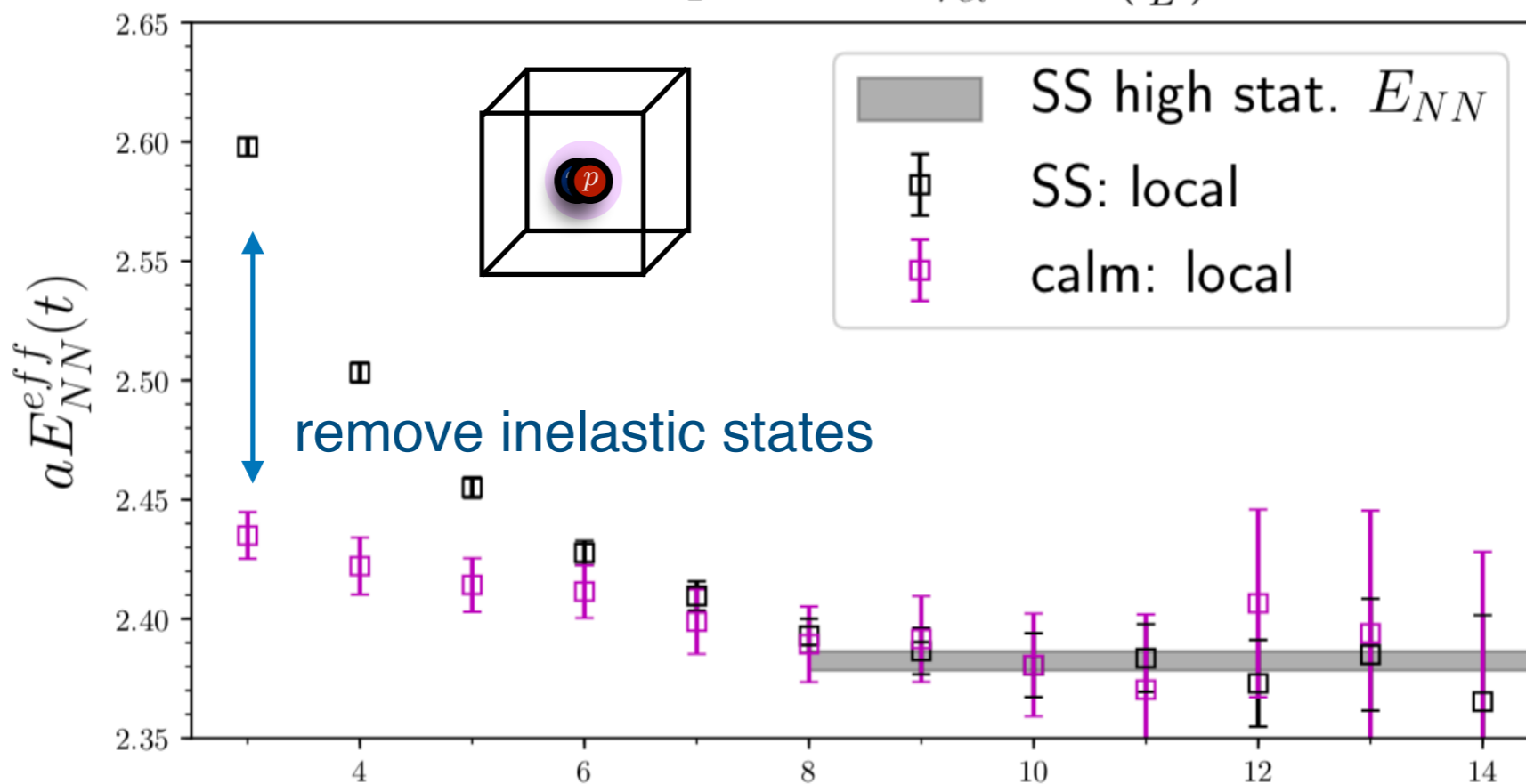
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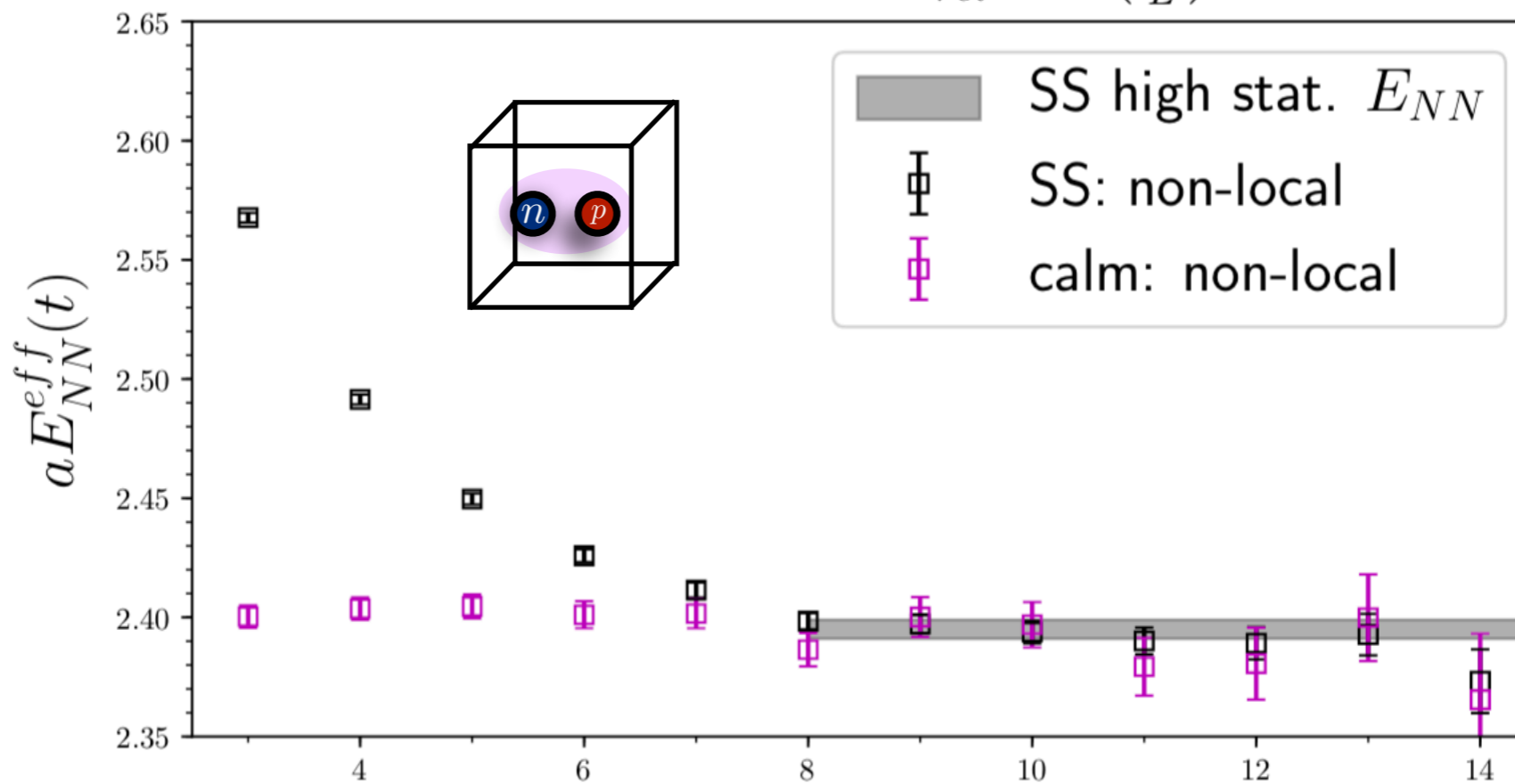


Single nucleon correlator

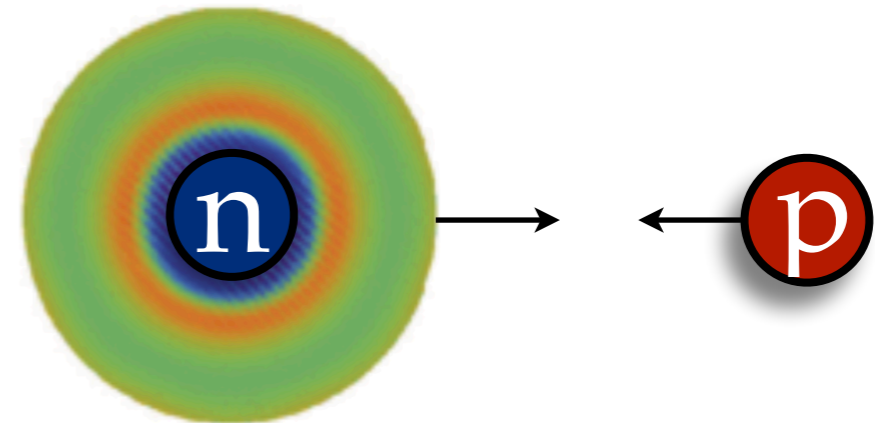
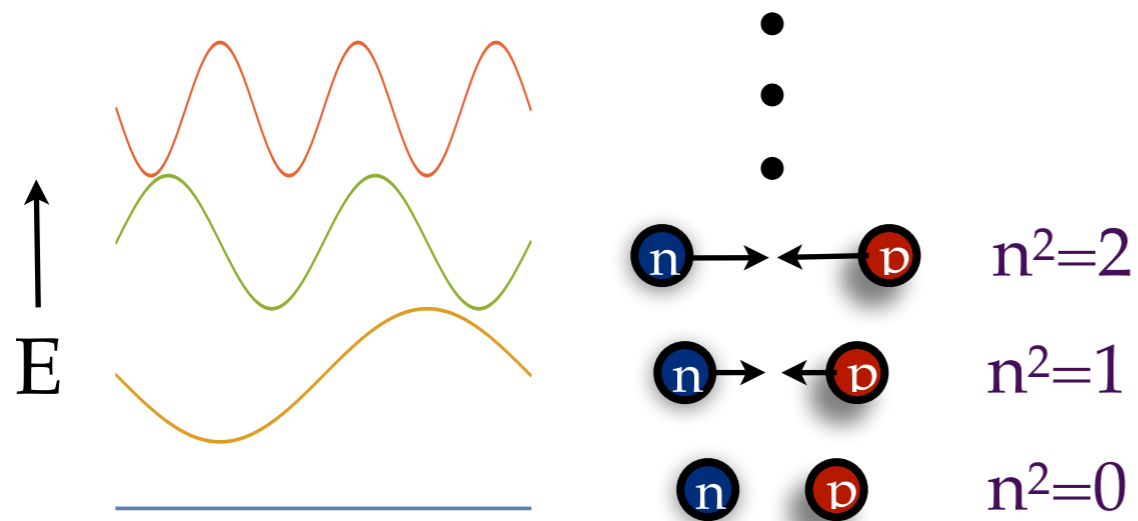
$$NN : T_1^+ : {}^3S_1 : p_{rel}^2 = 0 \left(\frac{2\pi}{L}\right)^2$$



$$NN : T_1^+ : {}^3S_1 : p_{rel}^2 = 0 \left(\frac{2\pi}{L}\right)^2$$



MP method for NN



- NPLQCD first used MP directly on NN correlators
- Works best as a two-step process: determine single-nucleon op, then minimize two-body elastic excited states
- Prony often doesn't work well for more than 2 ops:
 - excited states extracted are unreliable
 - may be able to do two stages of Prony to further reduce elastic excited states

The future? GEVP approaches

Variational basis of interpolating operators: $O_i(x_0)$

Define the states: $|\tilde{\phi}_i\rangle = \hat{O}_i|0\rangle$ and $|\phi_i\rangle = e^{-t_0 \hat{H}/2}|\tilde{\phi}_i\rangle$

The future? GEVP approaches

Variational basis of interpolating operators: $O_i(x_0)$

Define the states: $|\tilde{\phi}_i\rangle = \hat{O}_i|0\rangle$ and $|\phi_i\rangle = e^{-t_0 \hat{H}/2} |\tilde{\phi}_i\rangle$

Variational principle ($t > t_0$):

$$\lambda_1(t, t_0) = \text{Max}_{\{\alpha_i\}} \frac{\langle \phi | e^{-(t-t_0)\hat{H}} | \phi \rangle}{\langle \phi | \phi \rangle}, \quad |\phi\rangle = \sum_{i=1}^N \alpha_i |\phi_i\rangle$$

Eigenvalue: $\lambda_1(t, t_0) \approx e^{-E_1(t-t_0)}$

The future? GEVP approaches

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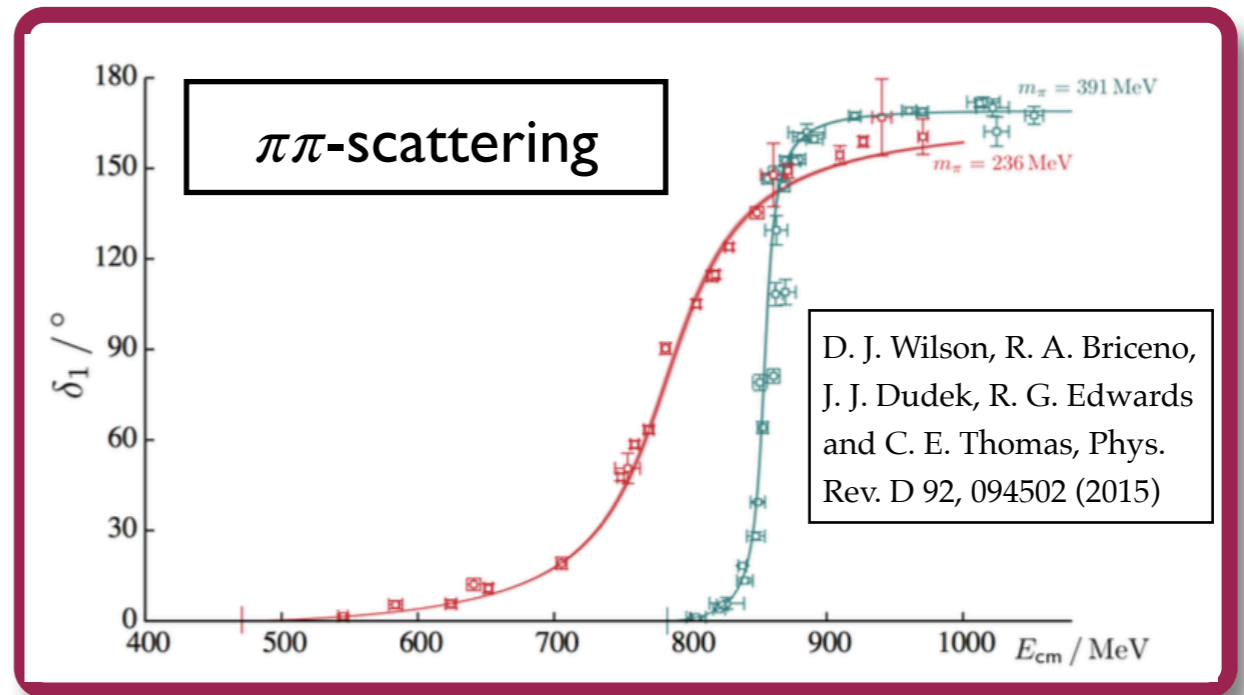
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Eigenvalue: $\lambda_1(t, t_0) \approx e^{-E_1(t-t_0)}$

Largest eigenvalue of a
GEVP, which can be used to
determine multiple states:

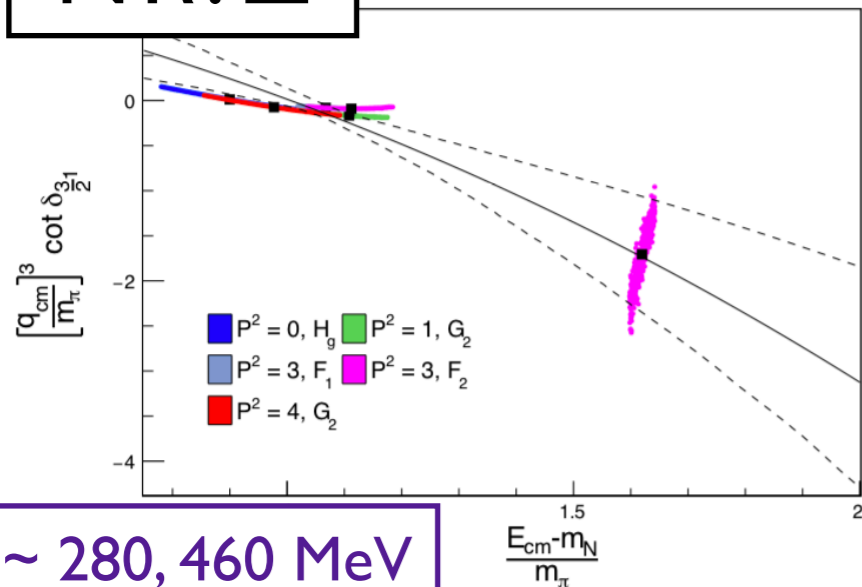
$$C_{ij}(t) = \langle \hat{O}_i(t) \hat{O}_j^\dagger(0) \rangle$$
$$C(t) v_n(t, t_0) = \lambda_n(t, t_0) C(t_0) v_n(t, t_0)$$
$$n = 1, \dots, N$$

The future? GEVP approaches

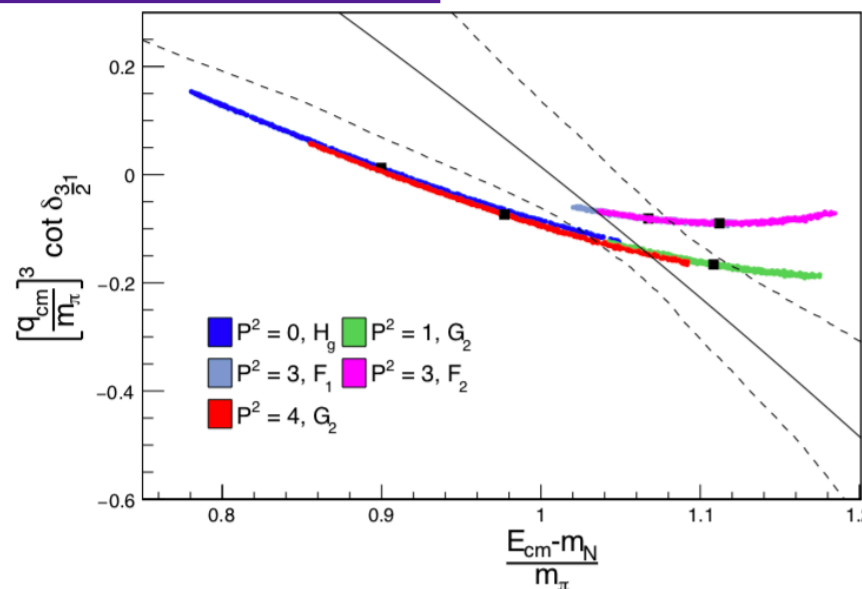


The future? GEVP approaches

$N\pi: \Delta$

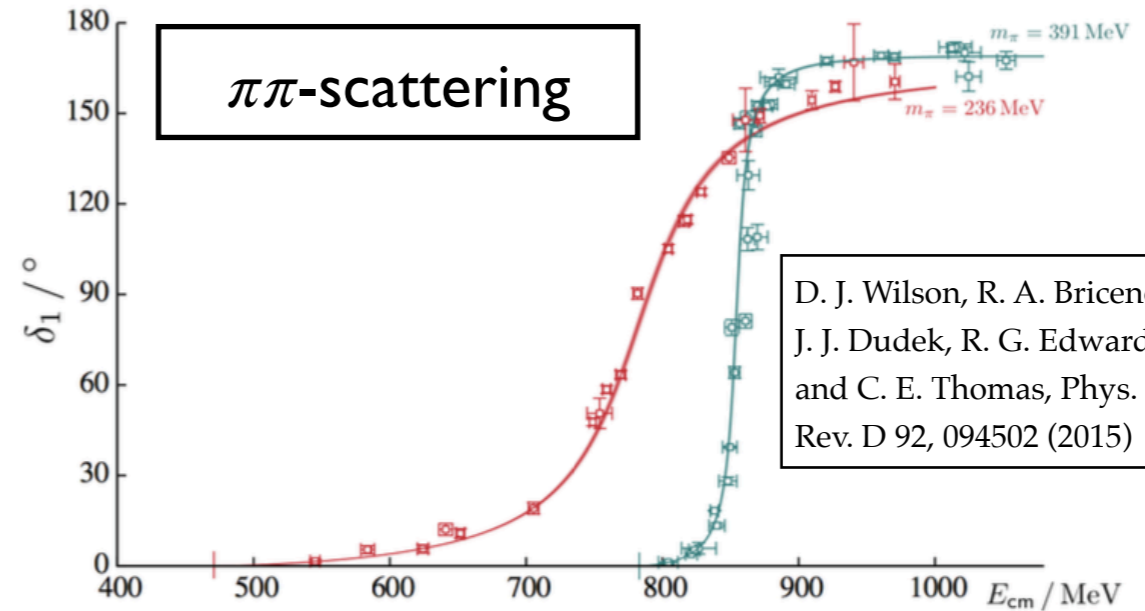


$m_\pi \sim 280, 460 \text{ MeV}$



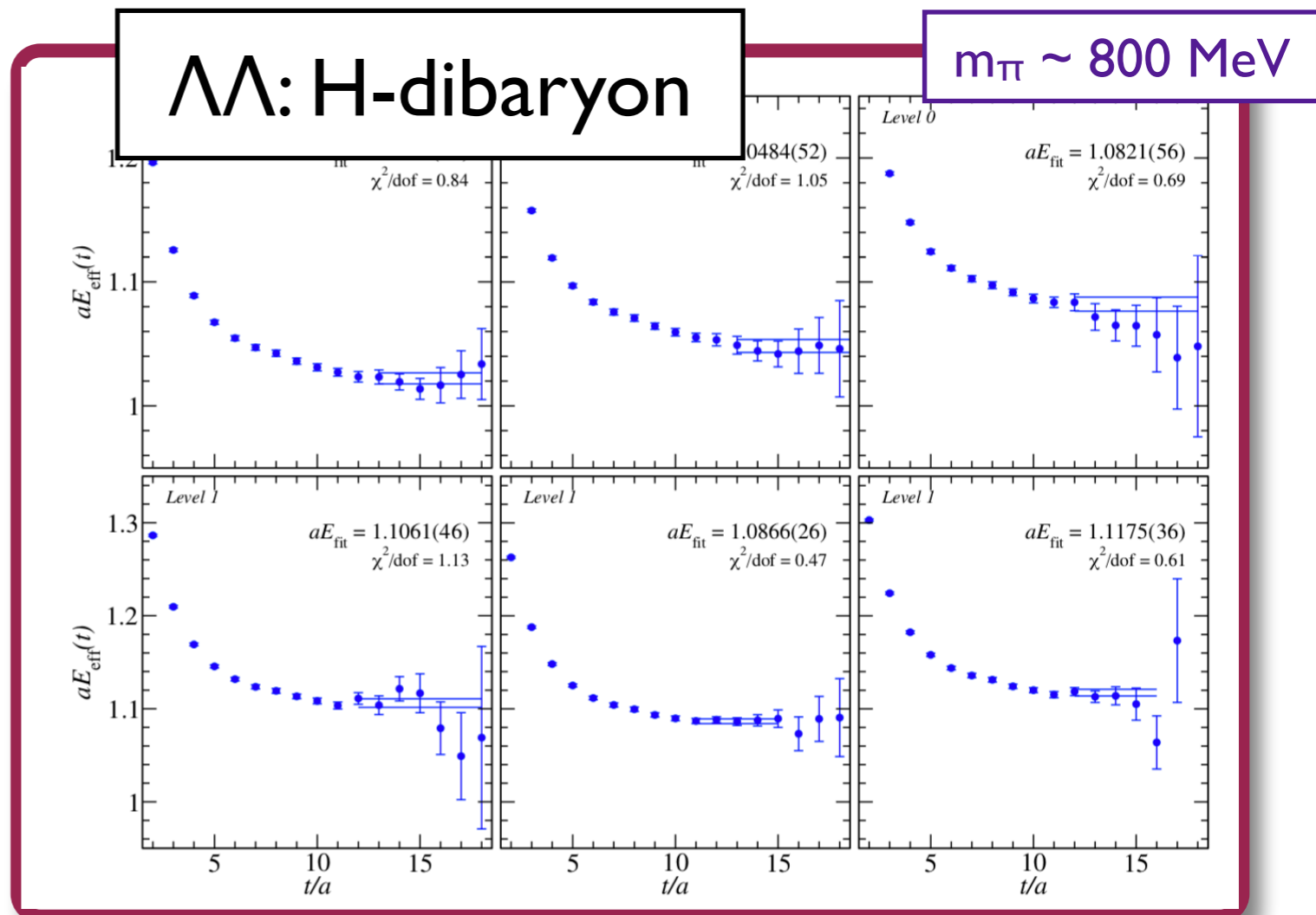
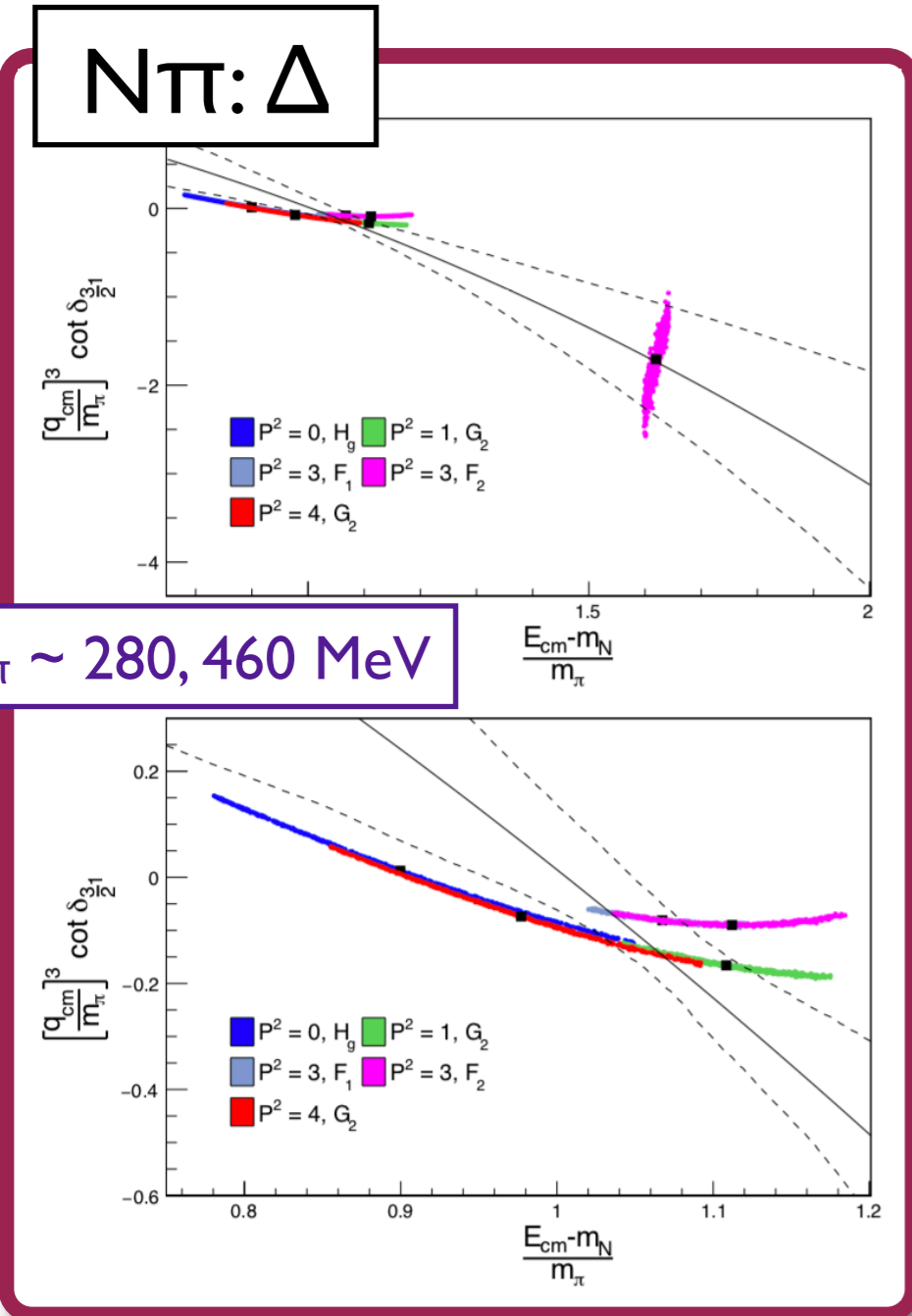
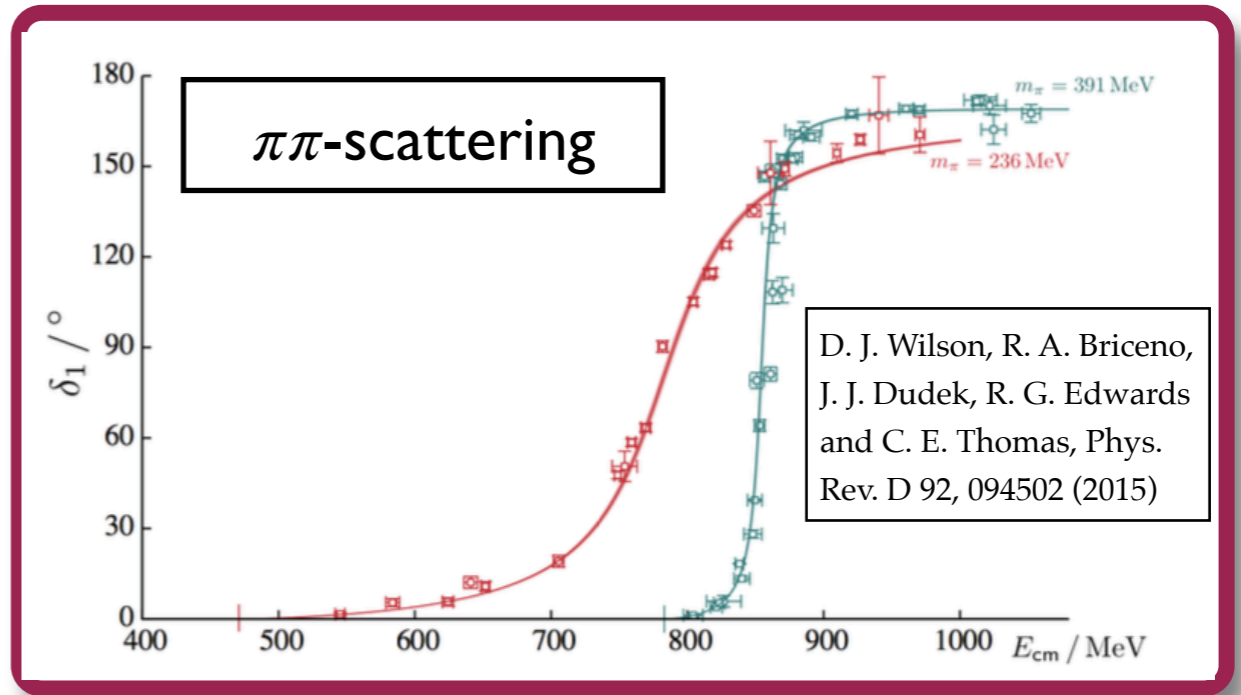
Andersen, Bulava, Horz, Morningstar (2018)

$\pi\pi$ -scattering



D. J. Wilson, R. A. Briceno,
J. J. Dudek, R. G. Edwards
and C. E. Thomas, Phys.
Rev. D 92, 094502 (2015)

The future? GEVP approaches



The future?
GEVP approaches
NN?



The future? GEVP approaches NN?



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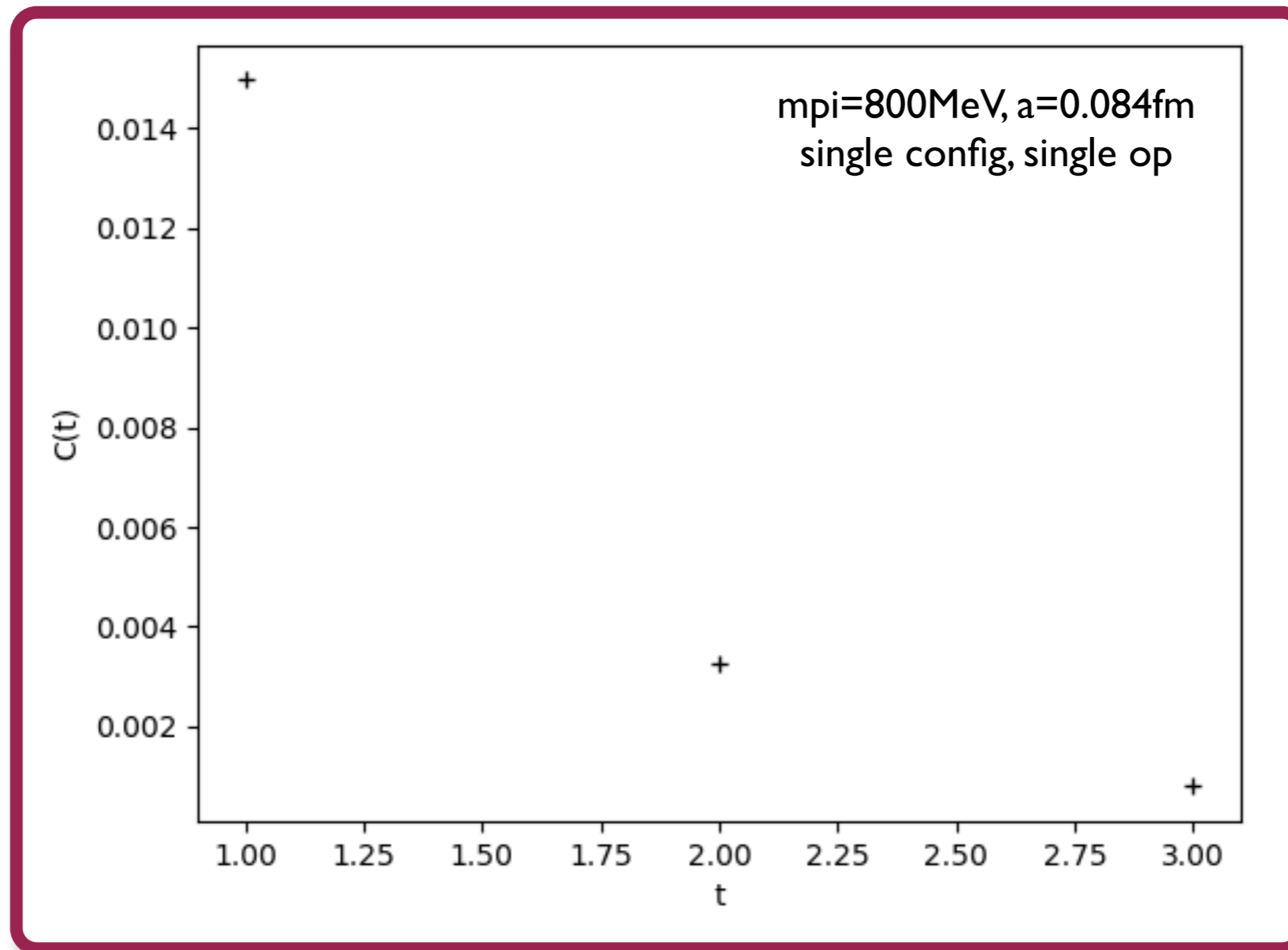
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 - sLapH stochastically projects onto low momentum states, easing this scaling with V

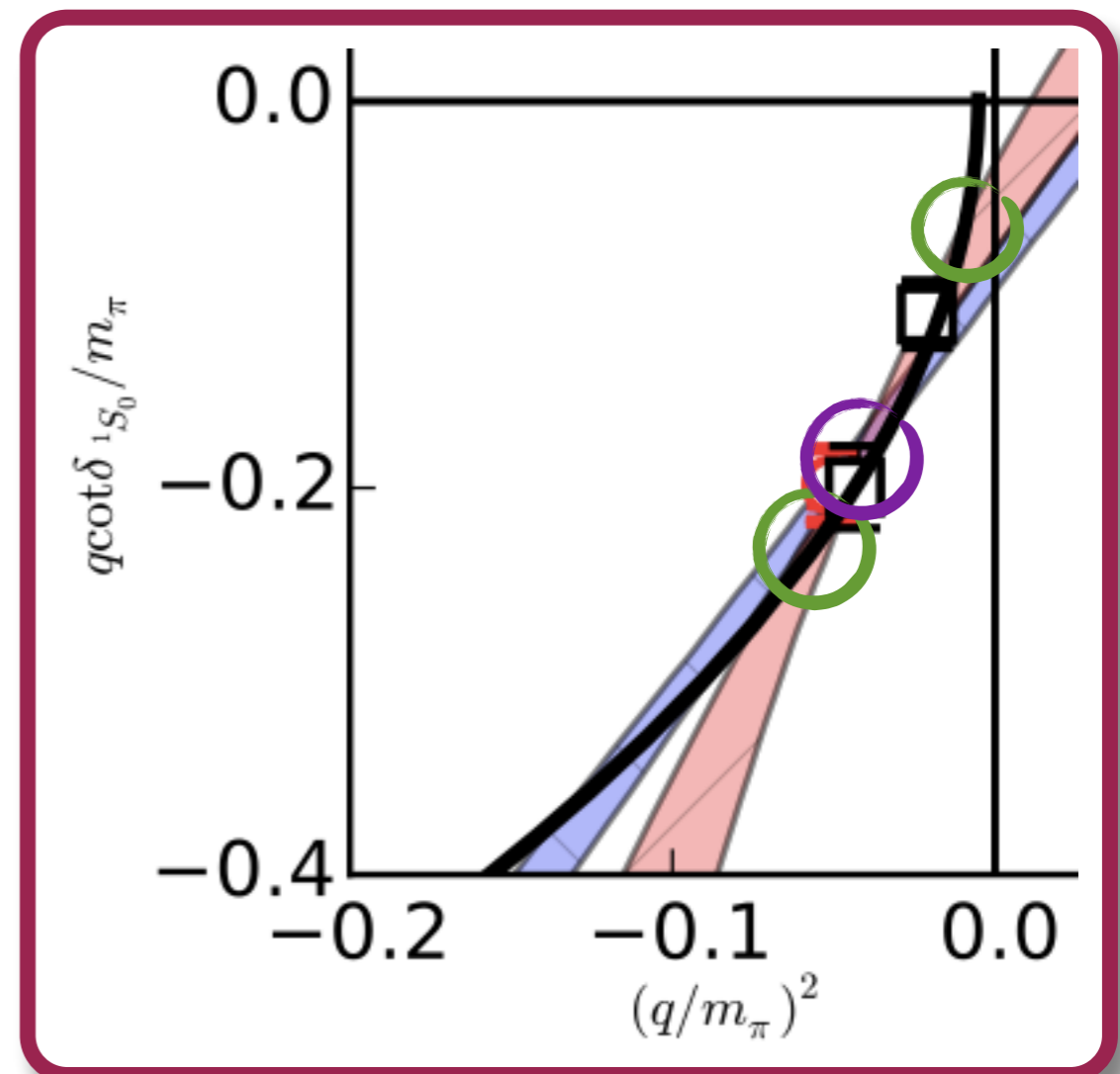
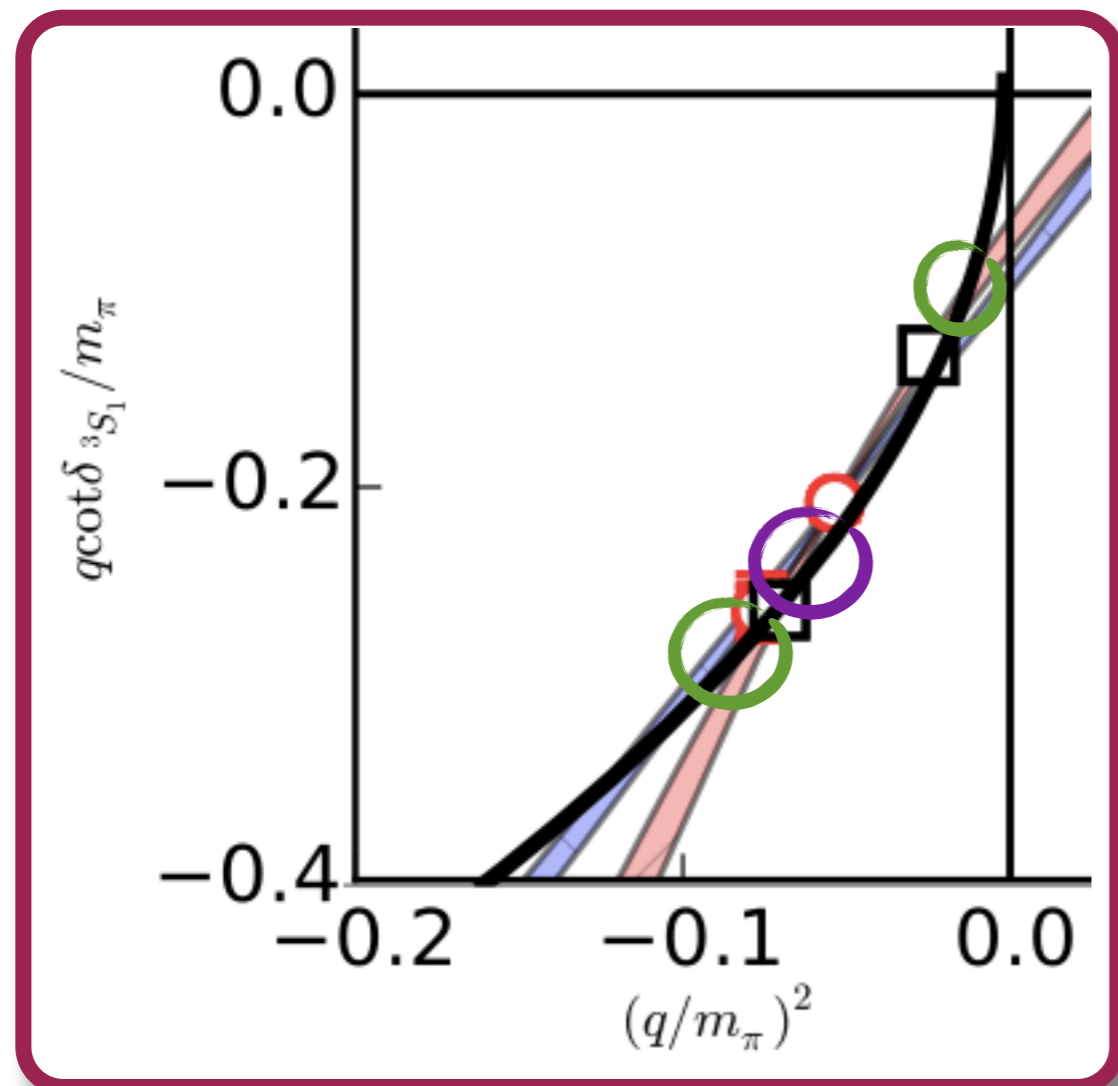
NN scattering with sLapH



+ C. Andersen, J. Bulava, A. Hanlon, D. Howarth, B. Hörz, C. Morningstar

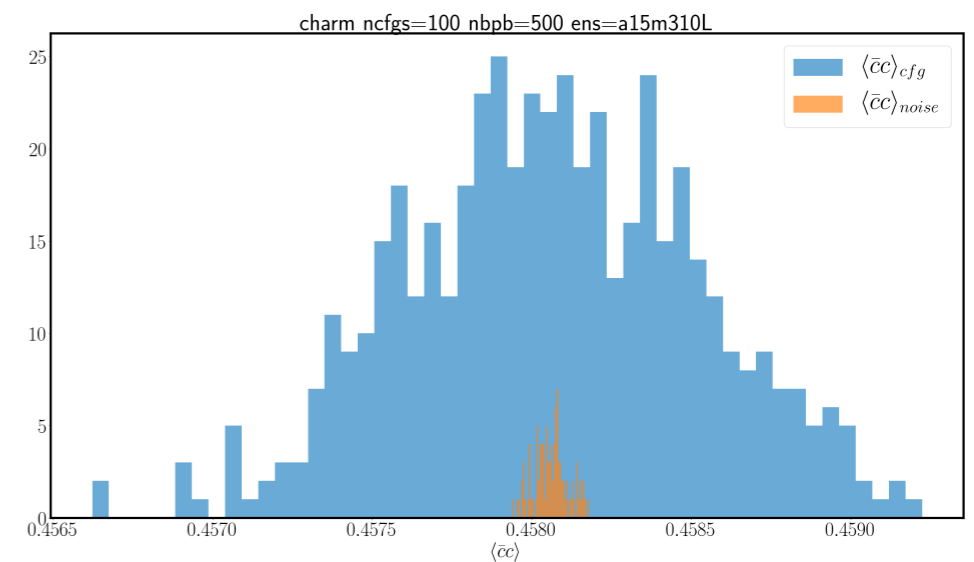
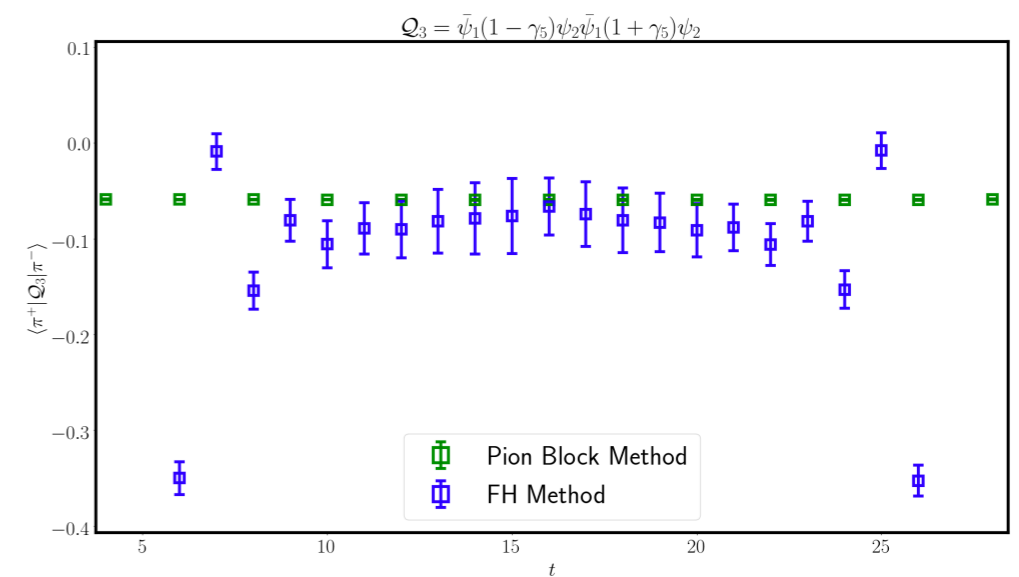
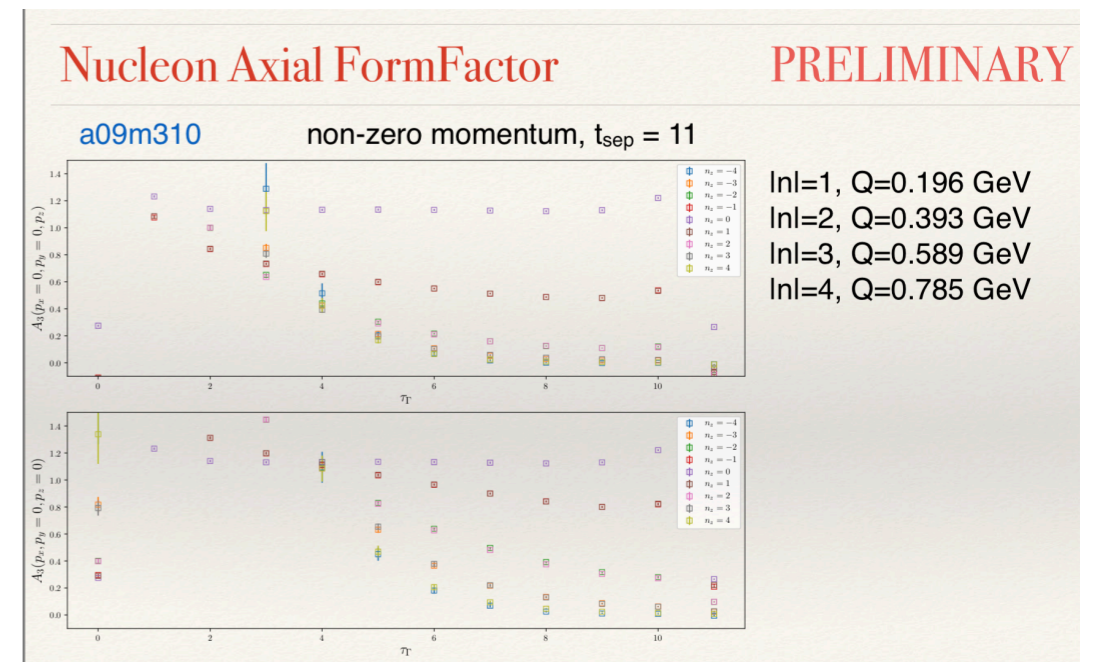
Fully resolving this puzzle likely requires GEVP including both momentum space and local ops

We are currently performing a comparison of methods (HAL potential, Luscher using both MP and sLapH) on same ensembles at 800 MeV



Other progress

- Nucleon axial form factors
- Feynman-Hellmann method for computing 4-quark MEs
- Charm content of the nucleon (DM MEs) $\langle N | \bar{c}c | N \rangle$



- RIKEN / LBL: C.C. Chang
- RIKEN: E. Rinaldi
- NERSC: T. Kurth
- nVidia: M.A. Clark
- LBL / UCB: A. Walker-Loud, B. Hörz
- Glasgow: C. Bouchard
- LLNL: P. Vranas, D. Howarth
- Carnegie Mellon: C. Morningstar
- SDSU: J. Bulava, C. Andersen
- UMD: E. Berkowitz
- Mainz: A. Hanlon
- UNC: H. Monge-Camacho, AN

