Lectures on Lattice QCD study of Hadron interactions (II)

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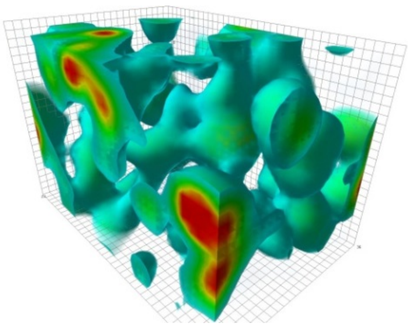
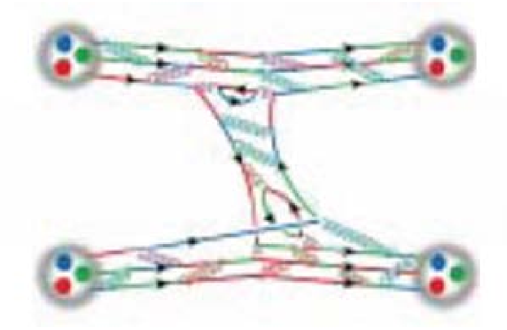
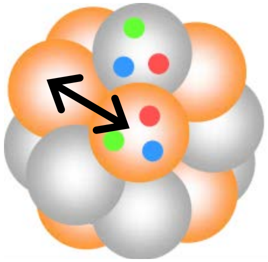
(RIKEN iTHEMS)







- **Outline**
  - Introduction
  - Brief review of scattering theory
  - Scattering on the lattice
    - Luscher’s finite volume method
    - HAL QCD method
  - S/N problem
  - More on HAL QCD method
  - Reliability issue and NN controversy
  - Summary

The Challenge

Myth of ground state saturation

(example w/ Luscher's method)

- Calculate the energy spectrum of 2-hadron on finite V lattice
  - Temporal correlation in Euclidean time ➔ energy

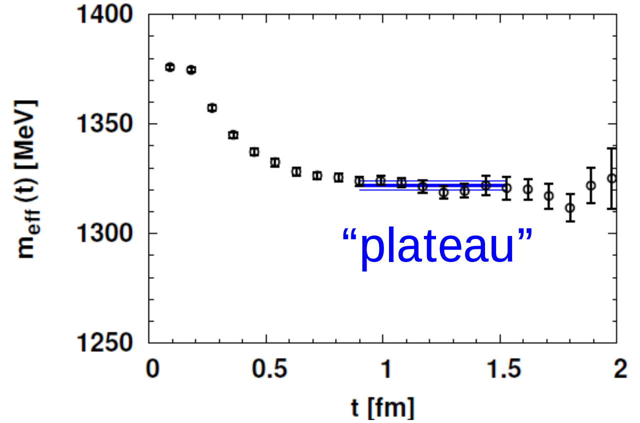
$$G(t) = \langle 0|\mathcal{O}(t)\overline{\mathcal{O}}(0)|0|\rangle = \sum_n A_n e^{-E_n t} \to A_0 e^{-E_0 t} \quad (t \to \infty)$$

- Convert the energy shift to phase shift by Luscher's formula

$$E \to \Delta E = E - 2m \text{ (effect of int.)} \to k \text{ (asymp. mom.)} \to \delta_E$$

  - Determination of energies
    - Take $t \gg 1/(E_1 - E_0)$ and find a "plateau" (G.S. saturation)

$$E_{\text{eff}}(t) = \ln\left[\frac{G(t)}{G(t+1)}\right] \xrightarrow[t\to\infty]{} E_0$$



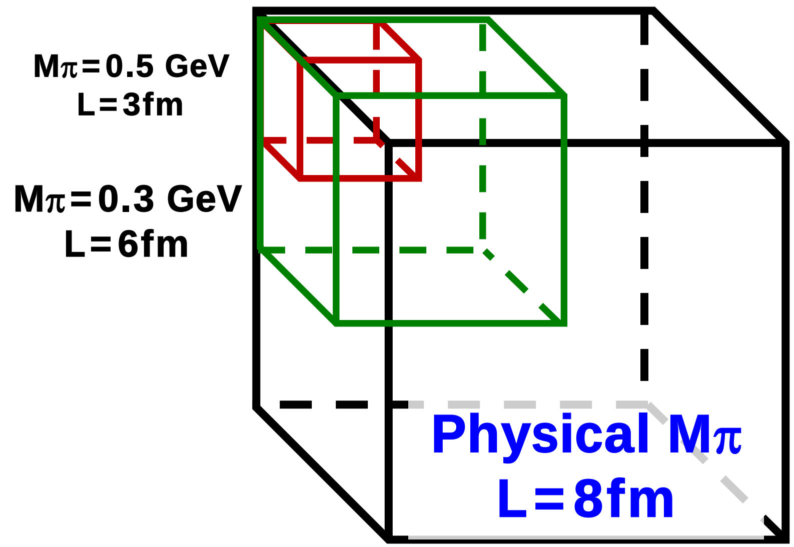
In the old (time-independent) HAL QCD method,
similar procedure is necessary
to obtain NBS w.f. for the ground state

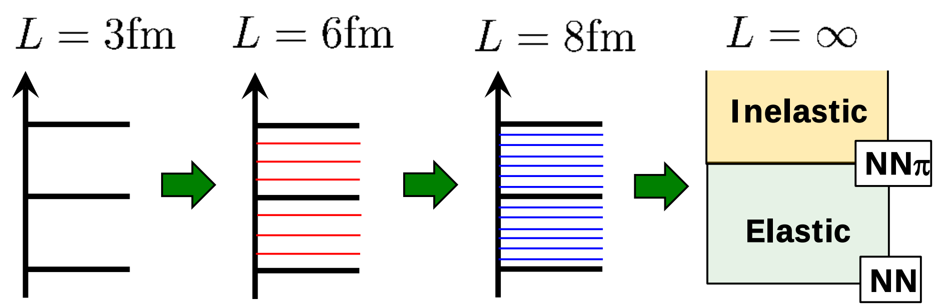
Challenges in multi-baryons on the lattice

- Excitation energy ~ binding energy or finite V effect

(very small)

$$E_1 - E_0 \simeq \frac{\vec{p}^2}{m_N} \simeq \frac{1}{m_N}\frac{(2\pi)^2}{L^2}$$





System ~w/o Gap

New Challenge for multi-body systems

The Challenge in multi-baryons on the lattice

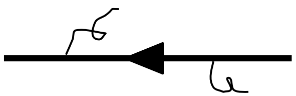
- Signal / Noise issue

Parisi ('84), Lepage ('89)

  - G.S. saturation by t ➔ ∞ required in LQCD

$$G(r,t) = \langle 0|\mathcal{O}(r,t)\overline{\mathcal{O}}(0)|0|\rangle = \sum_n \alpha_n \psi_n(r) e^{-E_n t} \xrightarrow[t\to\infty]{} \alpha_0 \psi_0(r) e^{-E_0 t}$$

quark

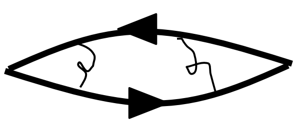


each (dressed) quark propagator carries info of pions, nucleons, ...

$$\sim \exp(-1/2\,\mathbf{m_\pi t}) + \exp(-1/3\,\mathbf{m_N t}) + \cdots$$

a la D. Kaplan (via A. Walker-Loud)

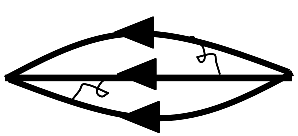
pion



signal from the lowest (=dominant) mode

$$\frac{\text{Signal}}{\text{Noise}} \sim \frac{\langle \pi(t)\pi(0)\rangle}{\sqrt{\langle \pi\pi(t)\pi\pi(0)\rangle}} \sim \frac{\exp(-\mathbf{m_\pi t})}{\sqrt{\exp(-2\mathbf{m_\pi t})}} \sim \text{const.}$$

nucleon



small signal after the cancellation of dominant modes

$$\frac{\text{Signal}}{\text{Noise}} \sim \frac{\langle N^{\mathbf{A}}(t)\bar{N}^{\mathbf{A}}(0)\rangle}{\sqrt{\langle |N^{\mathbf{A}}(t)\bar{N}^{\mathbf{A}}(0)|^2\rangle}} \sim \frac{\exp(-\mathbf{A m_N t})}{\sqrt{\exp(-3\mathbf{A m_\pi t})}}$$

$$\to \exp[-\mathbf{A}(\mathbf{m_N} - \mathbf{3/2 m_\pi})\mathbf{t}]$$

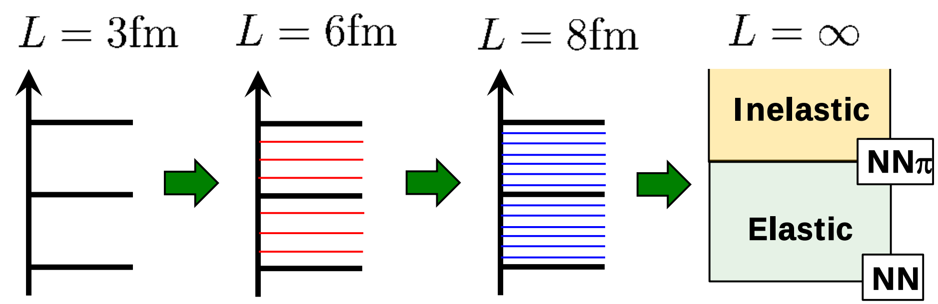
(A: mass number)

The Challenge in multi-baryons on the lattice

Existence of elastic scatt. states

➔ (almost) No Excitation Energy

➔ LQCD method based on G.S. saturation impossible



Signal/Noise issue

"Sign Problem"

$$S/N \sim \exp[-\mathbf{A} \times (\mathbf{m_N} - \mathbf{3/2m_\pi}) \times \mathbf{t}]$$

Parisi('84), Lepage('89)

L=8fm @ physical point $(E_1 - E_0) \simeq 25\text{MeV} \Longrightarrow t > 10\text{fm}$

$$S/N \sim 10^{-32}$$

Naïve plateau fitting at t ~ 1fm is unreliable ("mirage" of true signal)

T. Iritani et al. (HAL) JHEP1610(2016)101
T. Iritani et al. (HAL) PRD96(2017)034521

The solution in HAL method

We cannot avoid the excited states.

We have to confront them !

Time-dependent HAL QCD method

N.Ishii et al. (HAL QCD Coll.) PLB712(2012)437

E-indep of potential U(r,r') ➔ *(excited) scatt states share the same U(r,r')*

*They are **not contaminations**, **but signals***

Original (t-indep) HAL method

$$G_{NN}(\vec{r},t) = \langle 0|N(\vec{r},t)N(\vec{0},t)\overline{\mathcal{J}_{\rm src}(t_0)}|0\rangle$$

$$R(\boldsymbol{r},t) \equiv G_{NN}(\boldsymbol{r},t)/G_N(t)^2 = \sum A_{W_i}\psi_{W_i}(\boldsymbol{r})e^{-(W_i-2m)t}$$

← Many states contribute

$$\int d\boldsymbol{r}' U(\boldsymbol{r},\boldsymbol{r}')\underline{\psi_{W_0}(\boldsymbol{r}')} = (\underline{E_{W_0}} - H_0)\underline{\psi_{W_0}(\boldsymbol{r})}$$

$$\int d\boldsymbol{r}' U(\boldsymbol{r},\boldsymbol{r}')\underline{\psi_{W_1}(\boldsymbol{r}')} = (\underline{E_{W_1}} - H_0)\underline{\psi_{W_1}(\boldsymbol{r})}$$

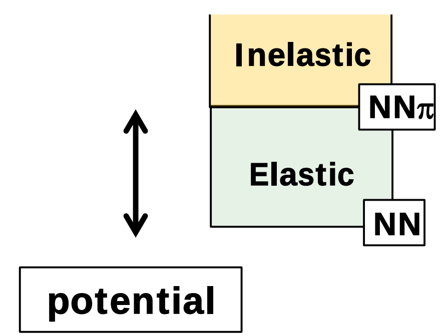
...

New t-dep HAL method

All equations can be combined as

$$\int d\boldsymbol{r}' U(\boldsymbol{r},\boldsymbol{r}')\underline{R(\boldsymbol{r}',t)} = (\underline{-\frac{\partial}{\partial t} + \frac{1}{4m}\frac{\partial^2}{\partial t^2}} - H_0)\underline{R(\boldsymbol{r},t)}$$

System w/ Gap



~~G.S. saturation~~ ➔ "Elastic state" saturation

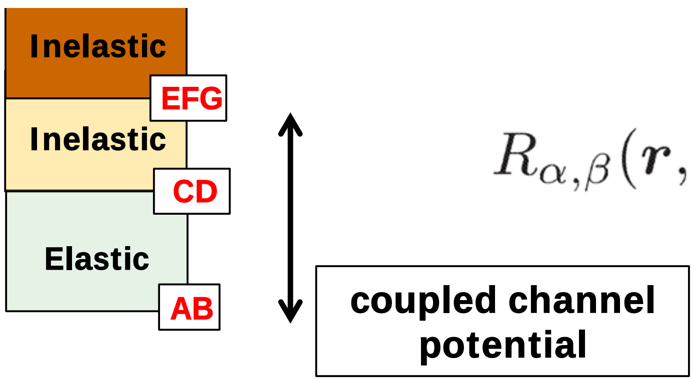
[Exponential Improvement]

Coupled Channel systems

(beyond inelastic threshold)

- Time-dep method is very useful for coupled channel
  - Interesting physics (e.g. resonances) embedded in the continuum

e.g.) AB ←→ CD coupled channel



$$\alpha, \beta = AB \text{ or } CD$$

$$\begin{aligned} R_{\alpha,\beta}(\boldsymbol{r}, t) &\equiv G_{\alpha,\beta}(\boldsymbol{r}, t) / \exp[-(m_{\alpha_1} + m_{\alpha_2})t] \\ &= \sum_i A_\beta^{W_i} \psi_\alpha^{W_i}(\boldsymbol{r}) e^{-(W_i - m_{\alpha_1} - m_{\alpha_2})t} \end{aligned}$$

$$\int d\boldsymbol{r}' U_{\alpha,\gamma}(\boldsymbol{r}, \boldsymbol{r}') \Delta_{\alpha,\gamma} R_{\gamma,\beta}(\boldsymbol{r}', t) = (-\frac{\partial}{\partial t} - H_0^\alpha) R_{\alpha,\beta}(\boldsymbol{r}, t)$$

$$\Delta_{\alpha,\beta} \equiv \exp[-(m_{\alpha_1} + m_{\alpha_2})t] / \exp[-(m_{\beta_1} + m_{\beta_2})t]$$

(relativistic term neglected for simplicity)

Examine the reliability of the HAL QCD method

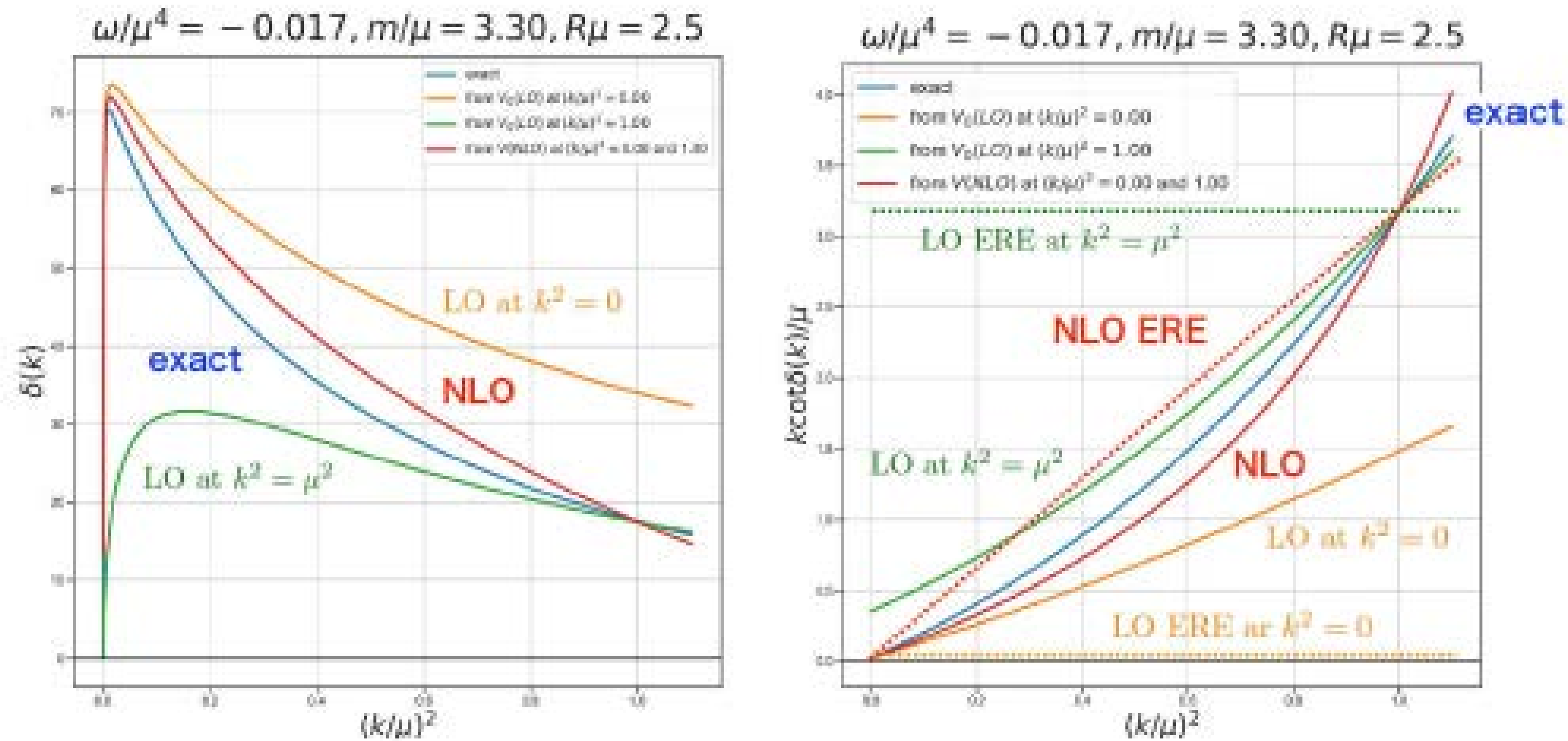
Convergence of the derivative expansion of potential

Contaminations from inelastic states

T. Iritani et al. (HAL) PRD99(2019)014514

Demonstration how derivative expansion works

Aoki-Doi, Front.Phys.8(2020)307



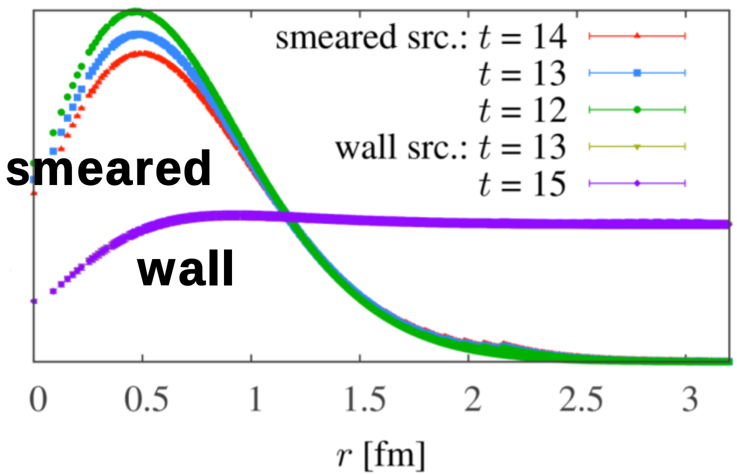
Derivative expansion
for a non-local potential

$$U(\mathbf{r}, \mathbf{r}') = \omega v(\mathbf{r}) v(\mathbf{r}'), \quad v(\mathbf{r}) \equiv e^{-\mu r}.$$

Source op. dependence in HAL

$\Xi\Xi\ (^1S_0)$

NBS correlator



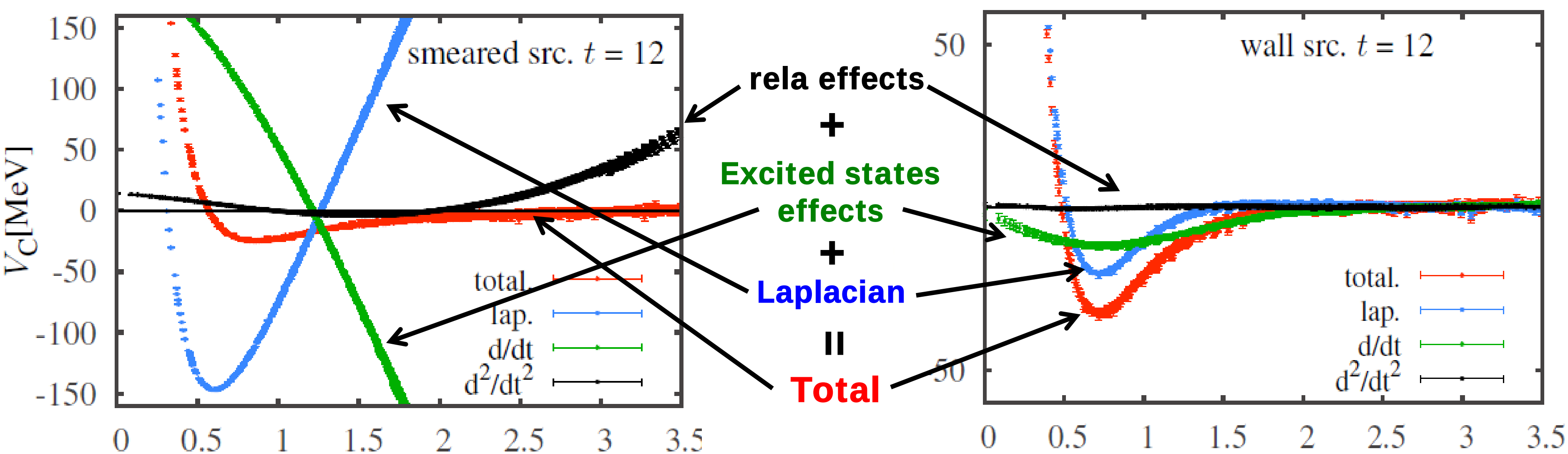
- wall src – t-dep is weak
- smeared src – t-dep exists
  - ➔ contribution from excited states

$$V_c(\vec{r}) = -\frac{H_0 R}{R} - \frac{(\partial/\partial t)R}{R} + \frac{(\partial/\partial t)^2 R}{4mR}$$

- t-dep HAL method works well
  - 🡐 O(100) MeV cancellation

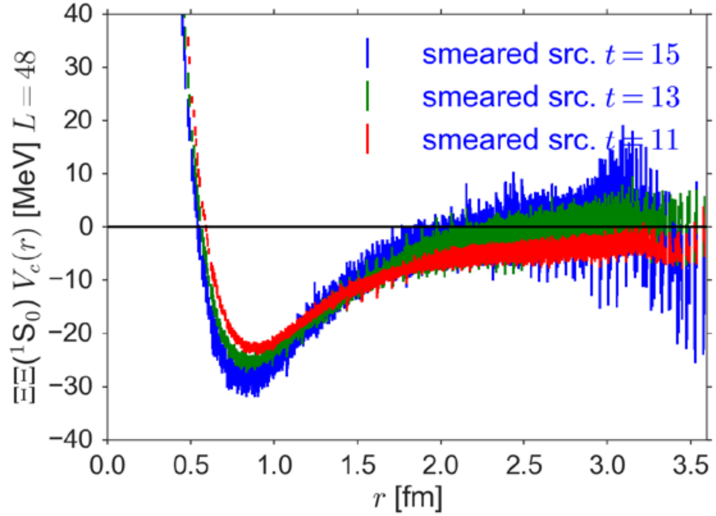
Potential

☐ smeared src. ■ wall src.

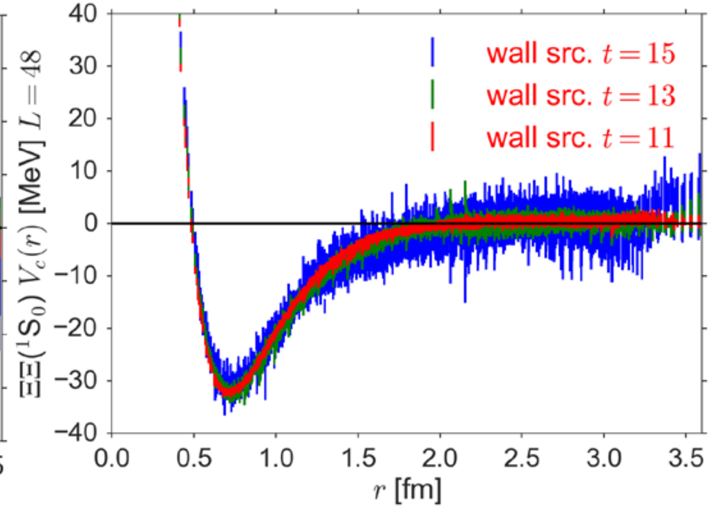


Source op. dependence in HAL

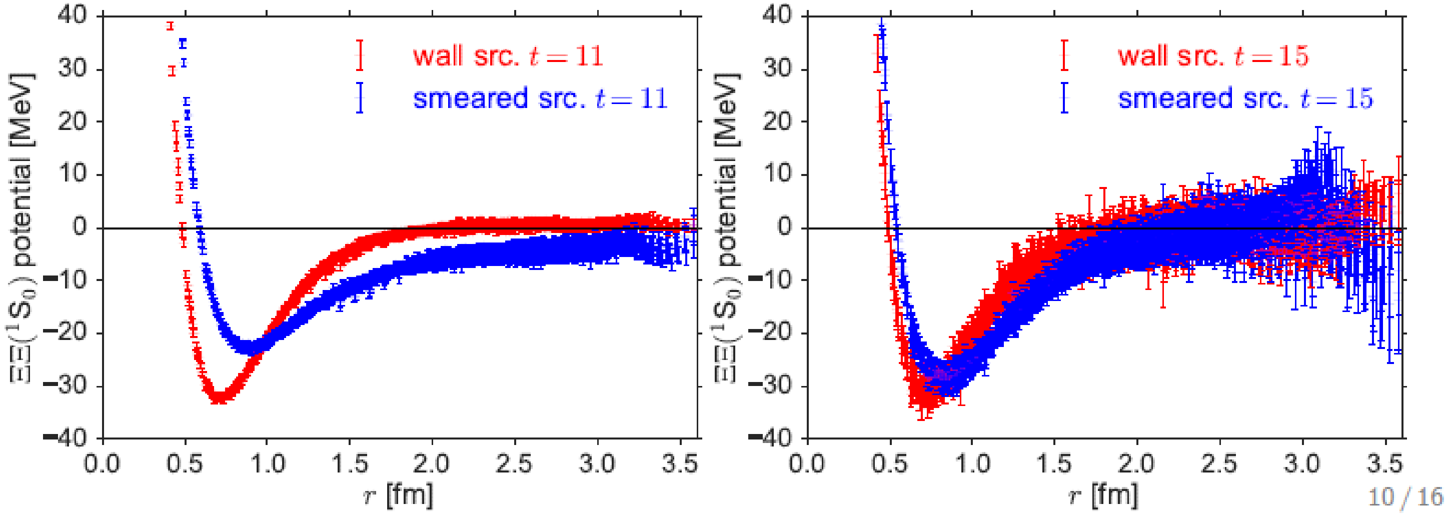
smeared: t-dep



wall : t-indep



smeared & wall in the same fig



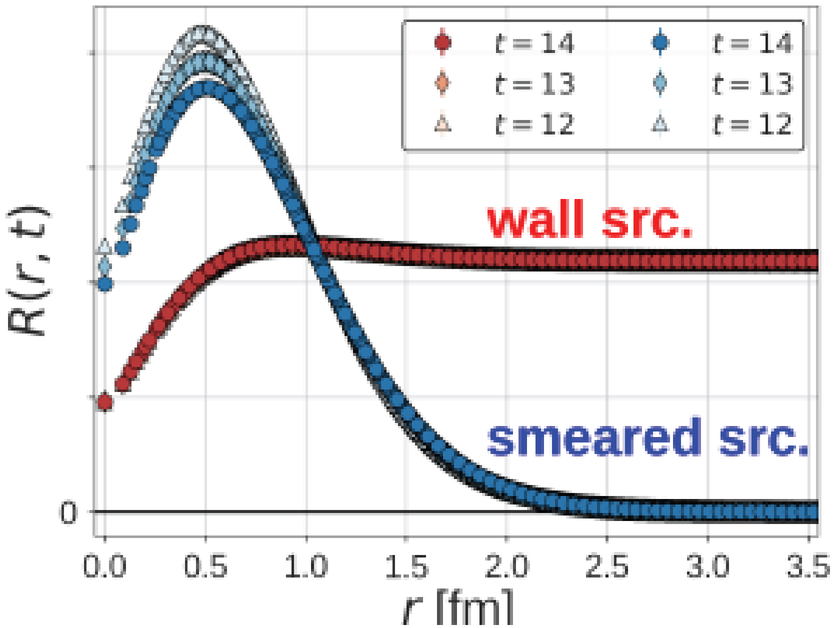
Smeared / Wall almost agree : t-dep HAL method works excellently

Smeared tends to converge to Wall w/ larger t, but deviation still exists

Higher Order Approximation (N²LO) (1)

$$U(r,r') \simeq \left[V_0^{\mathrm{N^2LO}}(r) + V_2^{\mathrm{N^2LO}}(r)\nabla^2\right]\delta(r-r')$$

$$\begin{cases} \frac{1}{4m_B}\frac{(\partial^2/\partial t^2)R^{\mathrm{wall}}}{R^{\mathrm{wall}}} - \frac{(\partial/\partial t)R^{\mathrm{wall}}}{R^{\mathrm{wall}}} - \frac{H_0 R^{\mathrm{wall}}}{R^{\mathrm{wall}}} = V_0^{\mathrm{N^2LO}}(r) + V_2^{\mathrm{N^2LO}}(r)\frac{\nabla^2 R^{\mathrm{wall}}}{R^{\mathrm{wall}}} \\ \frac{1}{4m_B}\frac{(\partial^2/\partial t^2)R^{\mathrm{smear}}}{R^{\mathrm{smear}}} - \frac{(\partial/\partial t)R^{\mathrm{smear}}}{R^{\mathrm{smear}}} - \frac{H_0 R^{\mathrm{smear}}}{R^{\mathrm{smear}}} = V_0^{\mathrm{N^2LO}}(r) + V_2^{\mathrm{N^2LO}}(r)\frac{\nabla^2 R^{\mathrm{smear}}}{R^{\mathrm{smear}}} \end{cases}$$



$V_0^{\mathrm{N^2LO}}(r)$ and $V_2^{\mathrm{N^2LO}}(r)$

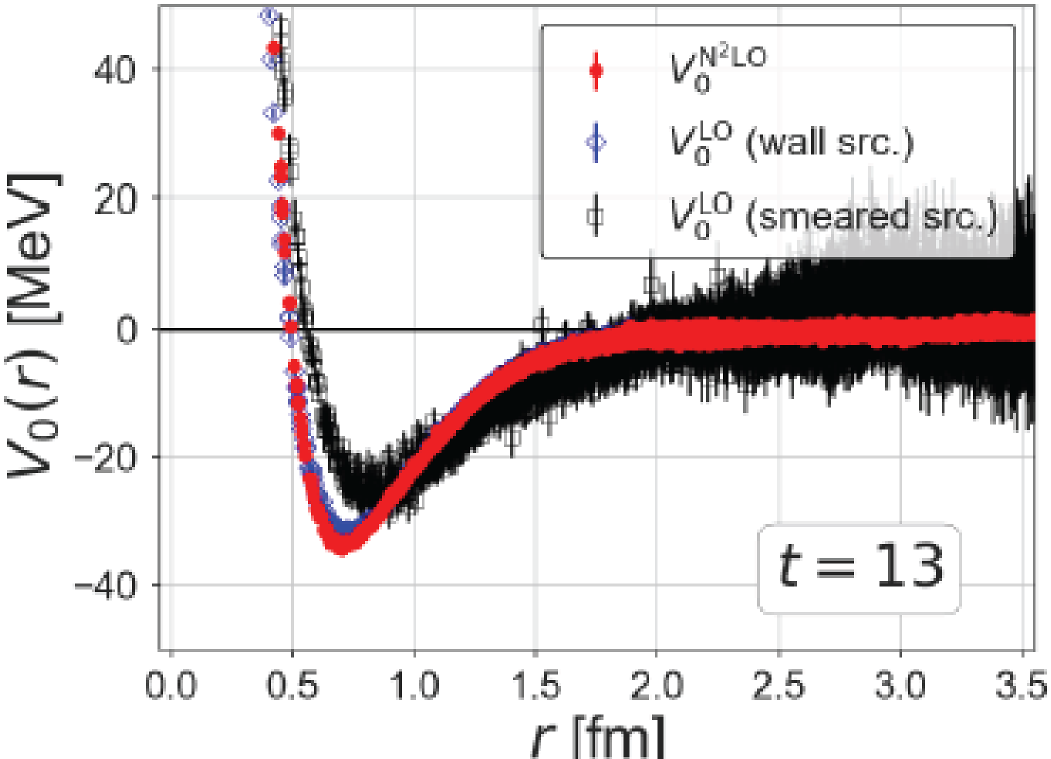
Higher Order Approximation (N²LO) (2)

$$U(r,r') \simeq \left[V_0^{\mathrm{N^2LO}}(r) + V_2^{\mathrm{N^2LO}}(r)\nabla^2\right]\delta(r-r')$$

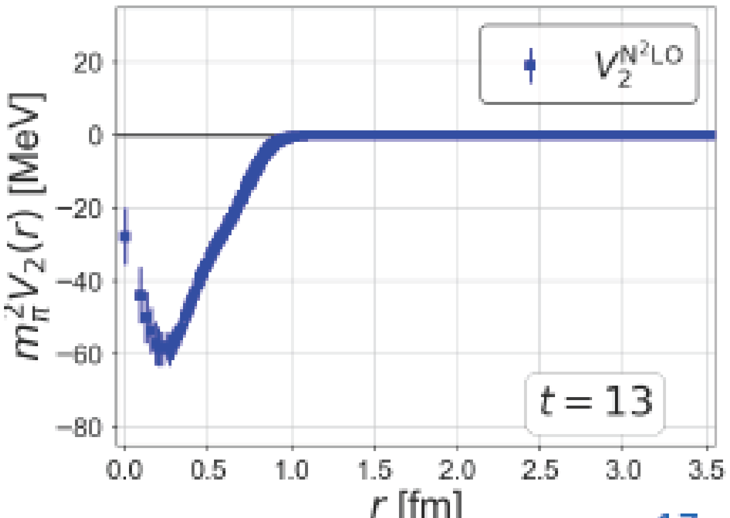
wall src. –> small $\mathbf{V_2\nabla^2}$ **correction**
smeared src. –> large $\mathbf{V_2\nabla^2}$ **correction**

→ $V_2(r)\nabla^2 R^{\mathrm{wall/smear}}(r)$

dep. on shape of **R**

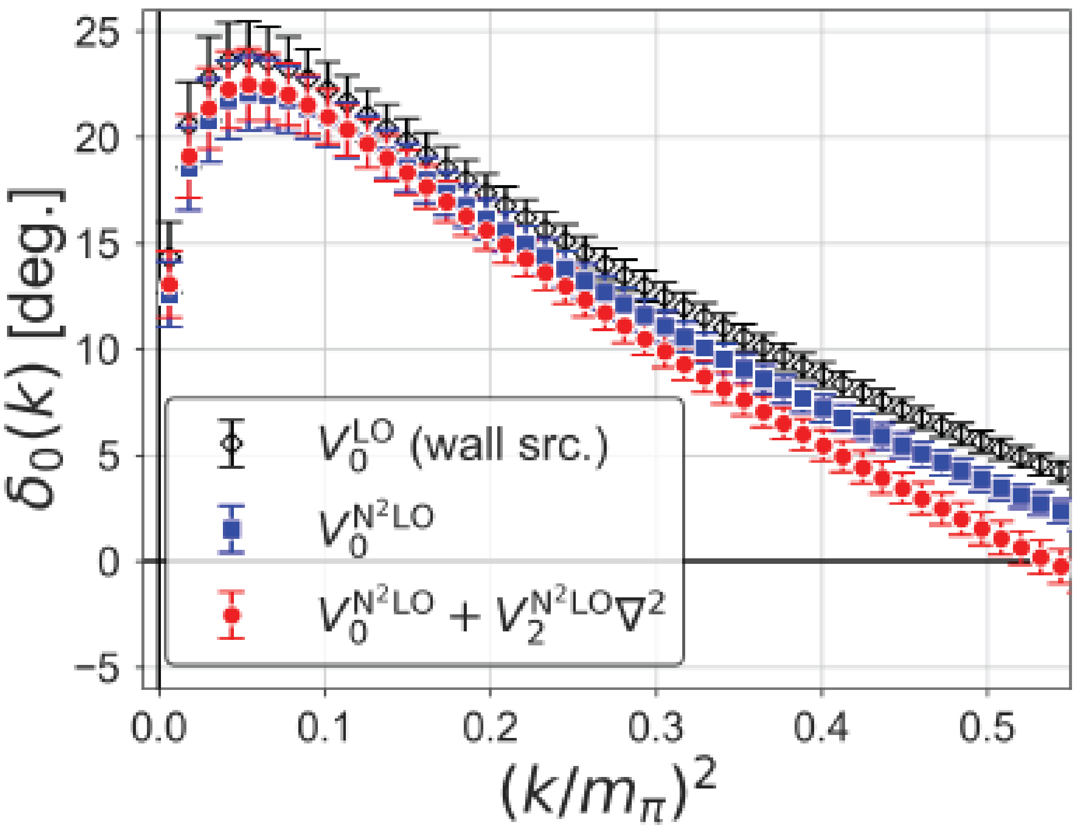


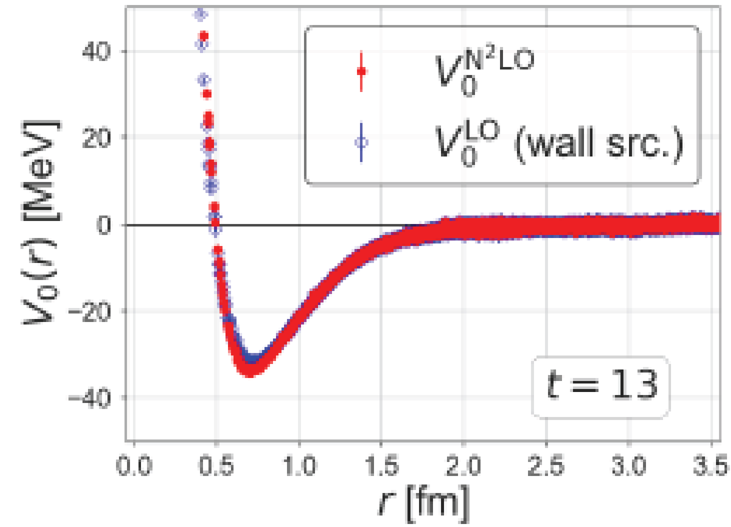
V₂-pot.

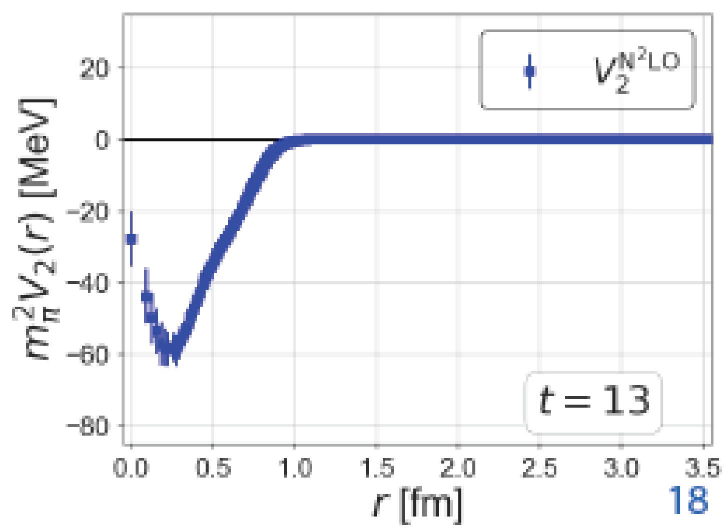


Phase Shift and Uncertainties in Velocity Expansion

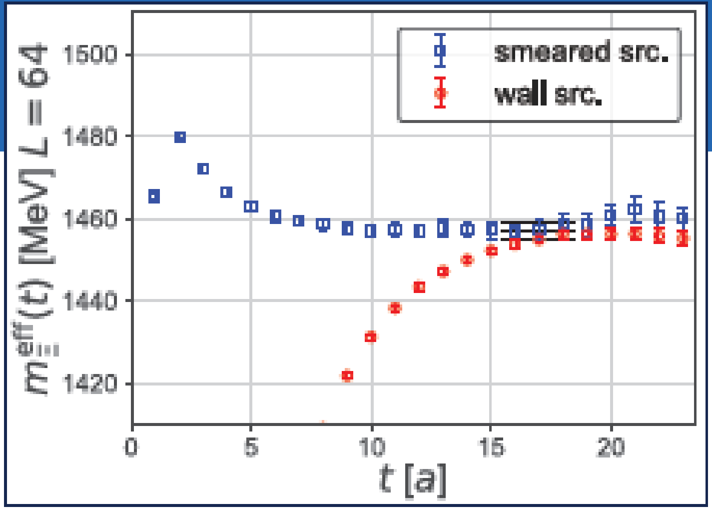
- **Wall src.** **LO approx.** (standard of HAL QCD studies) **works well at low energy.**
- **V_2 correction** at high energy





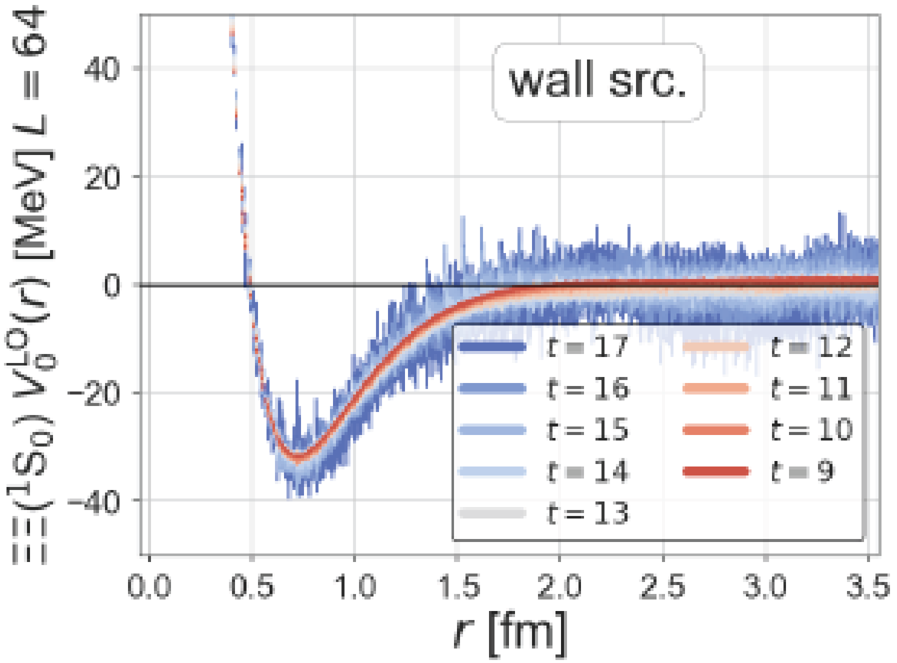


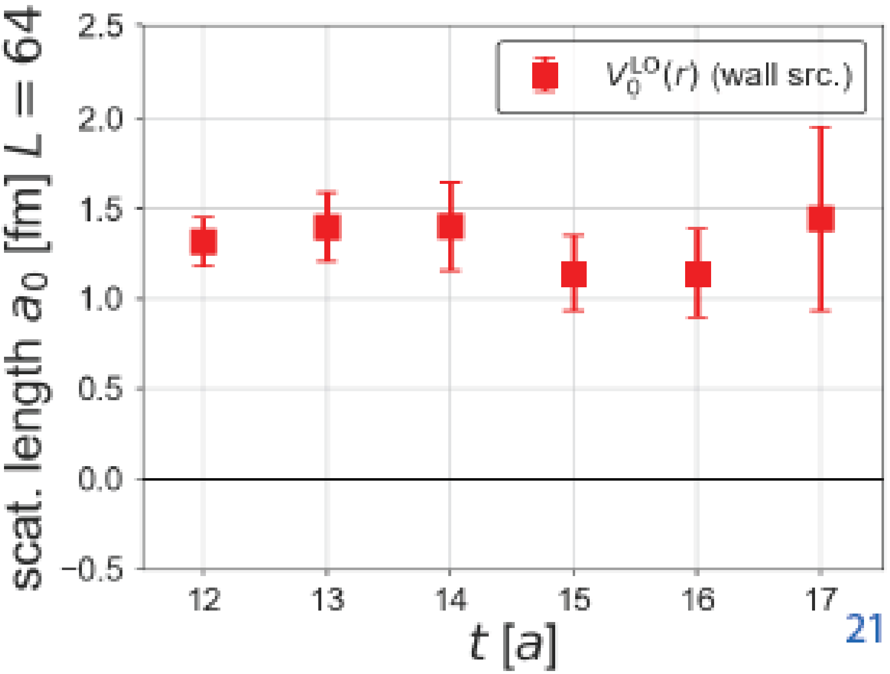
t-dep. of the Wall src.



single saturation is later than smeared src.

potential & observable are stable even at early time





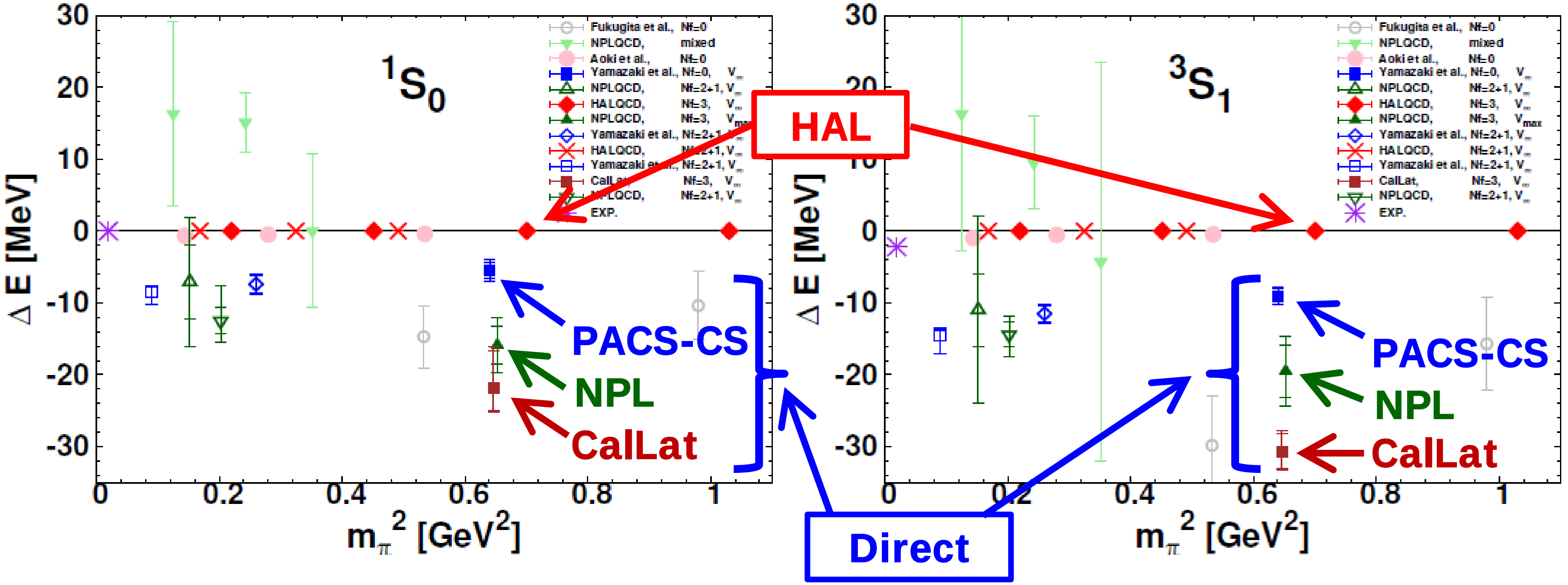
On the NN controversy in Lattice QCD

Direct method vs HAL method
(NN @ heavy quark masses)

HAL method (HAL) : **unbound**
Direct method (PACS-CS (Yamazaki et al.) / NPL / CalLat): **bound**

Direct method = naïve plateau fitting + Luscher's formula

"di-neutron" / "deuteron"



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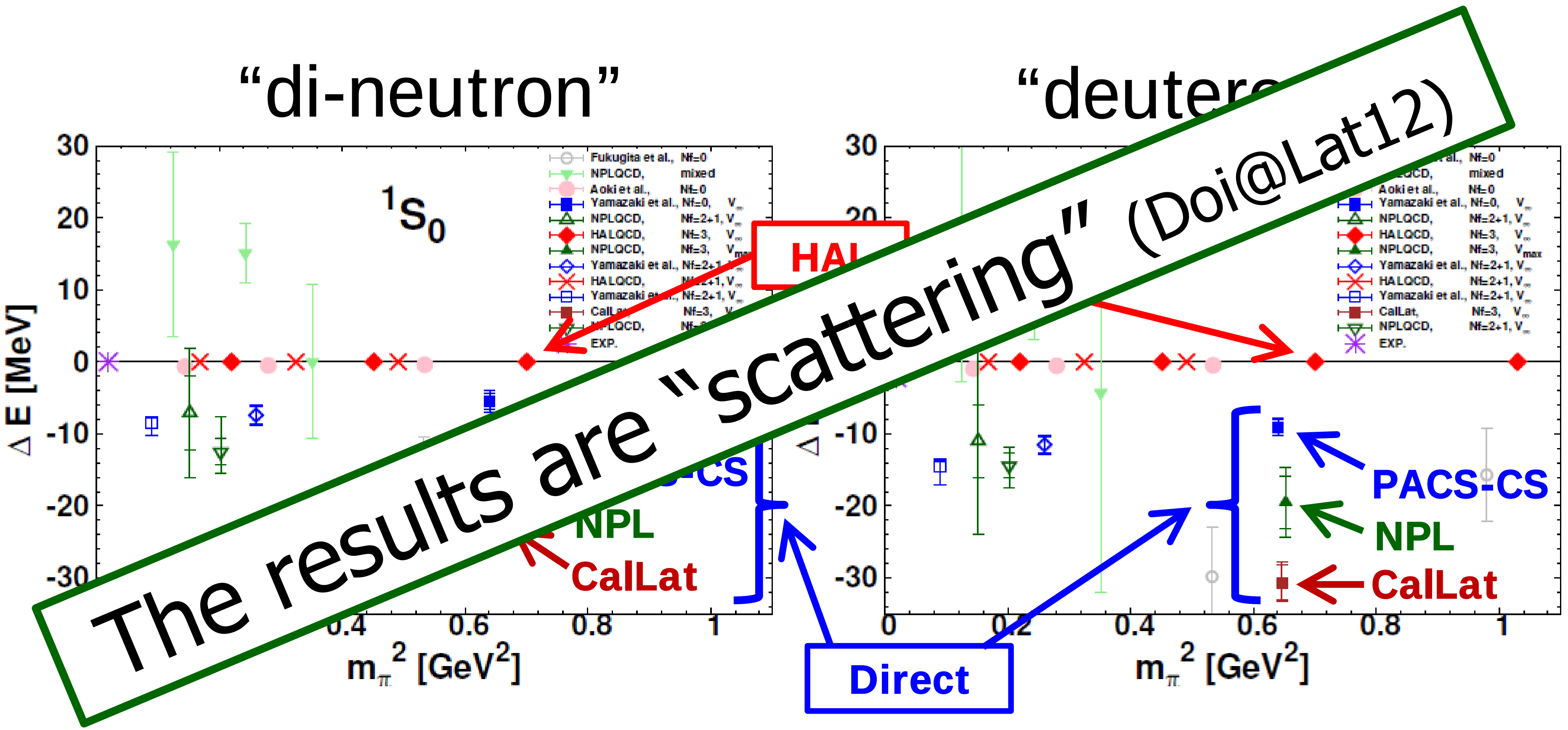
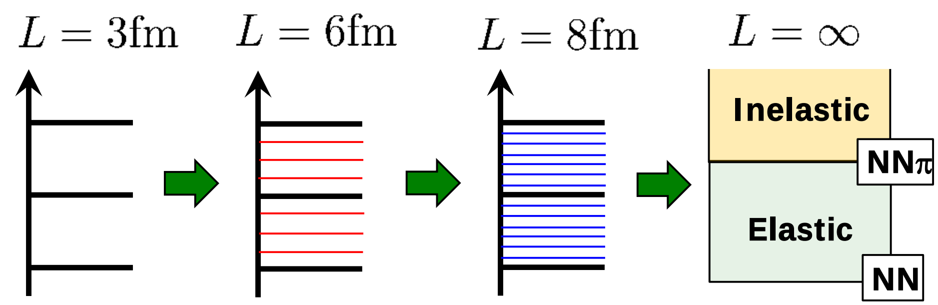


The Challenge in multi-baryons on the lattice

Existence of elastic scatt. states

➔ (almost) No Excitation Energy

➔ LQCD method based on G.S. saturation impossible



Signal/Noise issue

"Sign Problem"

$$S/N \sim \exp[-\mathbf{A} \times (\mathbf{m_N} - \mathbf{3/2m_\pi}) \times \mathbf{t}]$$

Parisi('84), Lepage('89)

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Naïve plateau fitting at t ~ 1fm is unreliable ("mirage" of true signal)

T. Iritani et al. (HAL) JHEP1610(2016)101
T. Iritani et al. (HAL) PRD96(2017)034521

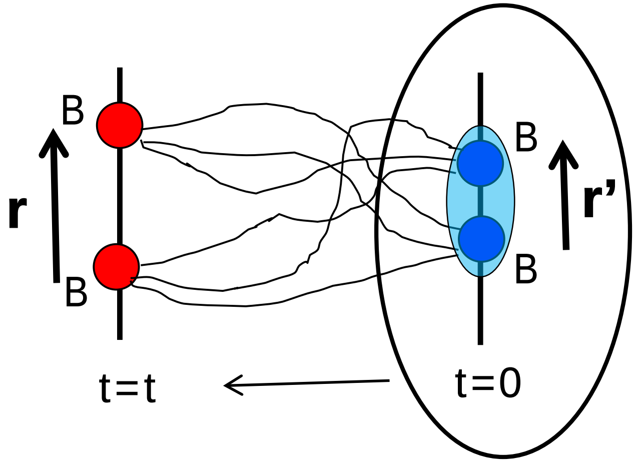
Anatomy of the Direct method
and
the consistency between
Luscher’s formula and HAL method

T. Iritani et al. (HAL) JHEP03(2019) 007

Ideal and real of “optimized” smeared src

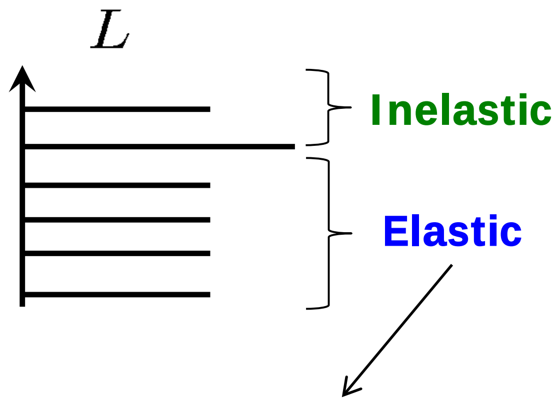
Smeared src:

Optimized to suppress **1-body inelastic states**



Recall the real challenge for two-baryon systems:

➔ Noises from **2-body elastic excited states**

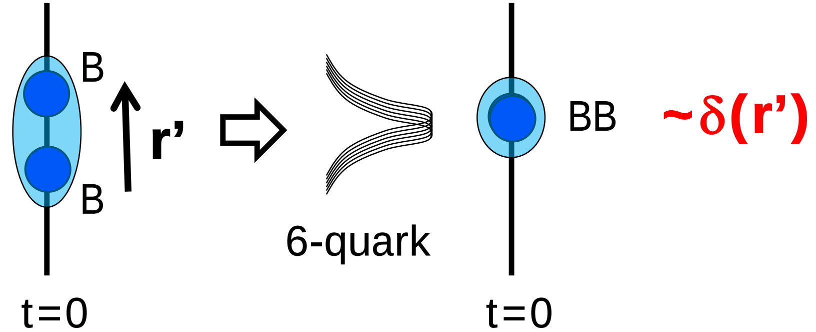


$$\sim B(\vec{p'})B(-\vec{p'}), \ \vec{p'} = (2\pi/L)\vec{n}$$

➔ Traditional smeared src is NOT optimized for two-body systems !

Detailed implementation of smeared src

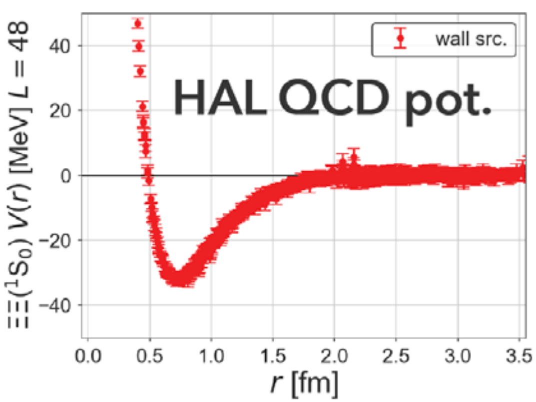
all 6-quarks are smeared at the same spacial point



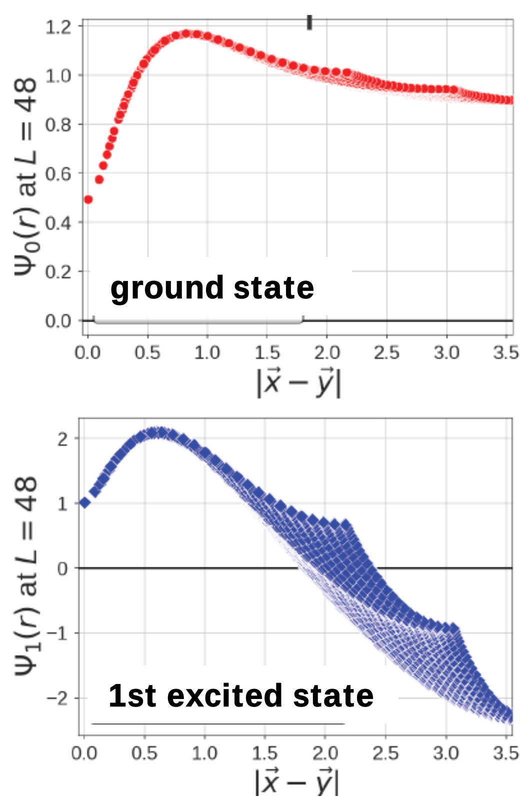
➔ Large contaminations from 2-body elastic excited states are “rather natural”

Operator optimized for 2-body system by HAL

- HAL method ➔ HAL pot ➔ 2-body wave func. @ finite V
- 2-body wave func. ➔ optimized operator
  - Applicable for sink and/or src op : Here we apply for sink op
- While utilizing info by HAL, formulation is Luscher's formula

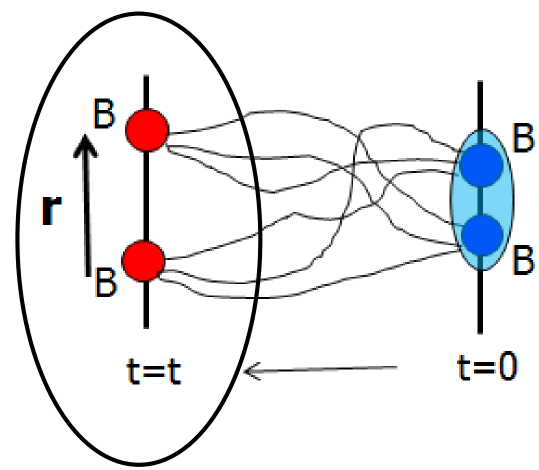


wave func. ψ(r)



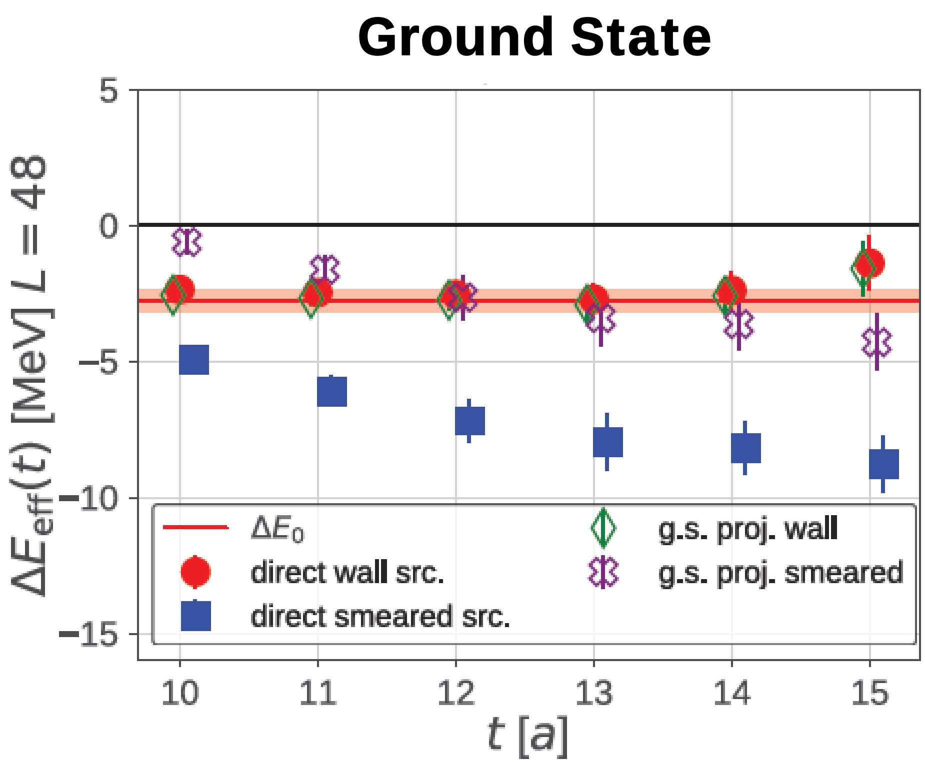
HAL-optimized sink op

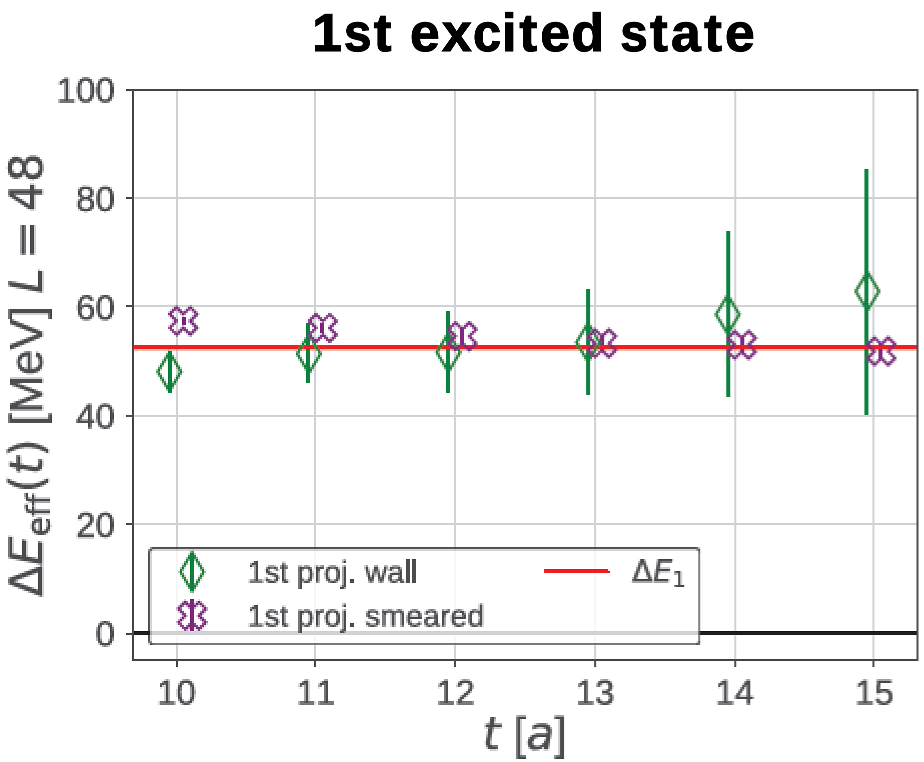
$$\mathcal{J}^{2B}_{\rm sink} = \sum_{\vec{r}} \psi^\dagger(r) \sum_{\vec{x}} B(\vec{r}+\vec{x})B(\vec{x})$$



Effective energy shift ΔE from “HAL-optimized op”

HAL-optimized sink op ➔ projected to each state ➔ “True” plateaux



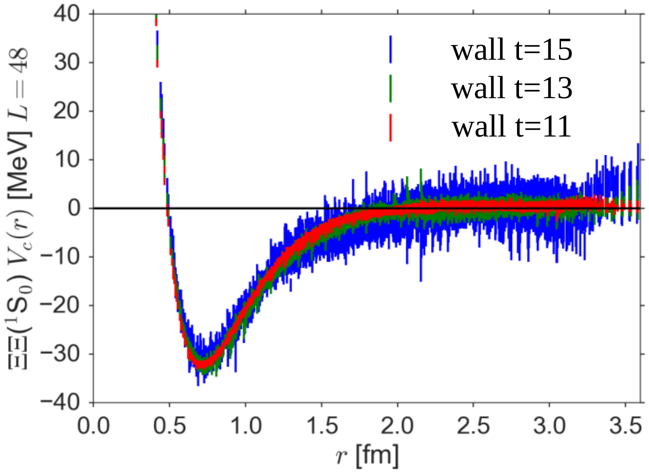


HAL QCD pot = Lushcer’s formula w/ proper projection

≠ Direct method w/ naïve plateau fitting

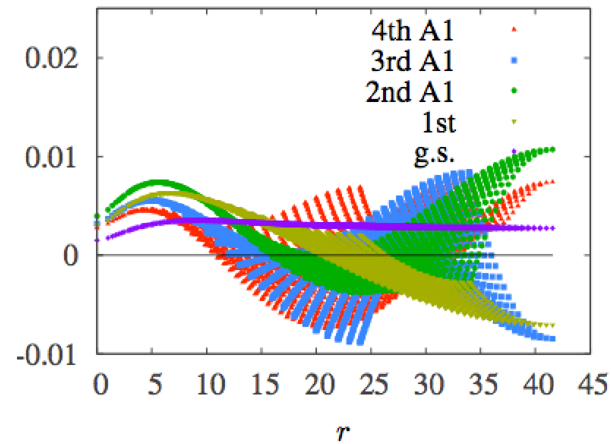
Understand the origin of "pseudo-plateaux"

Potential



Solve Schrodinger eq. in Finite V

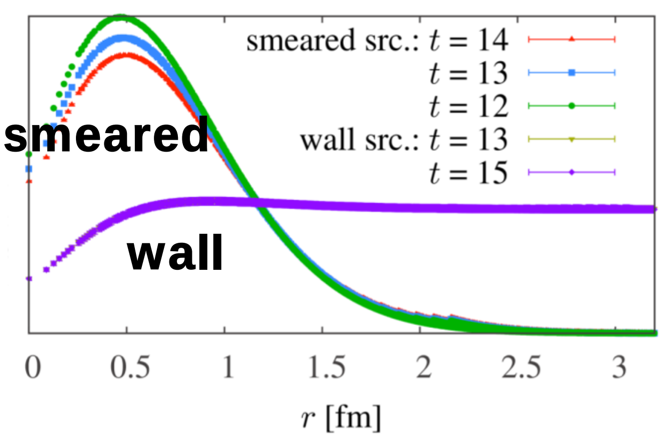
Eigen-wave functions



Eigen-energies

n-th A1	ΔE_n [MeV]
0	-2.58(1)
1	52.49(2)
2	112.08(2)
3	169.78(2)
4	224.73(1)

NBS correlator R(r,t)



Decompose NBS correlator to each eigenstates

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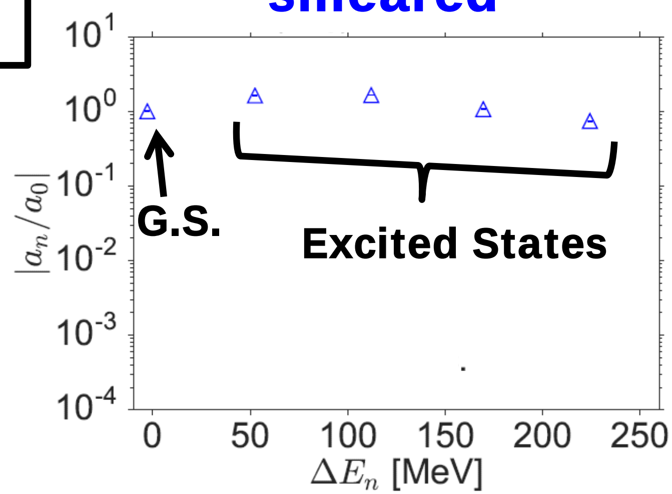
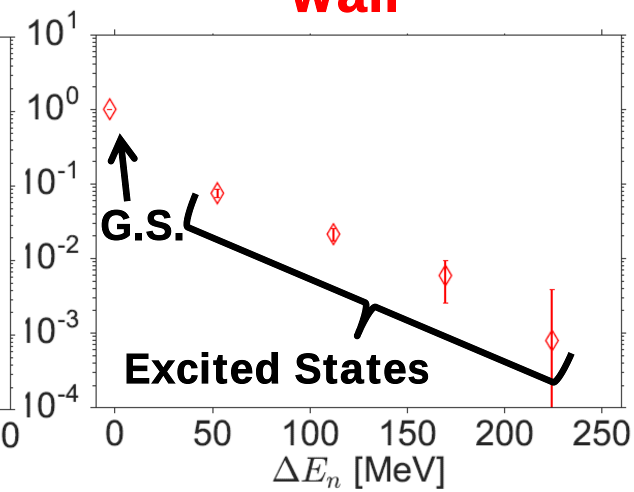
NBS correlator R(r,t)

Contribution from each (excited) states (@ t=0)

smeared



wall



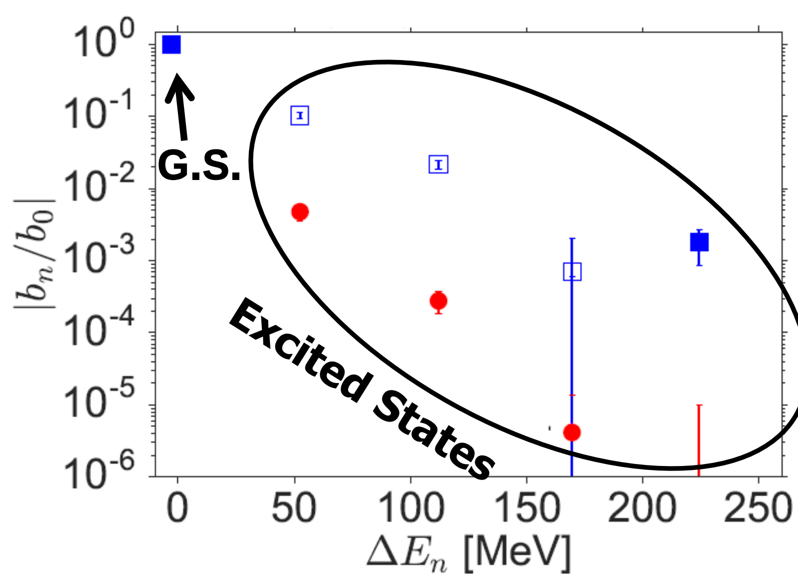
excited states NOT suppressed

excited states suppressed

Temporal-correlator R(t) = Σ_r R(r,t)

(R(t) w/ smeared has been used in the Direct method)

Contribution from each (excited) states (@ t=0)

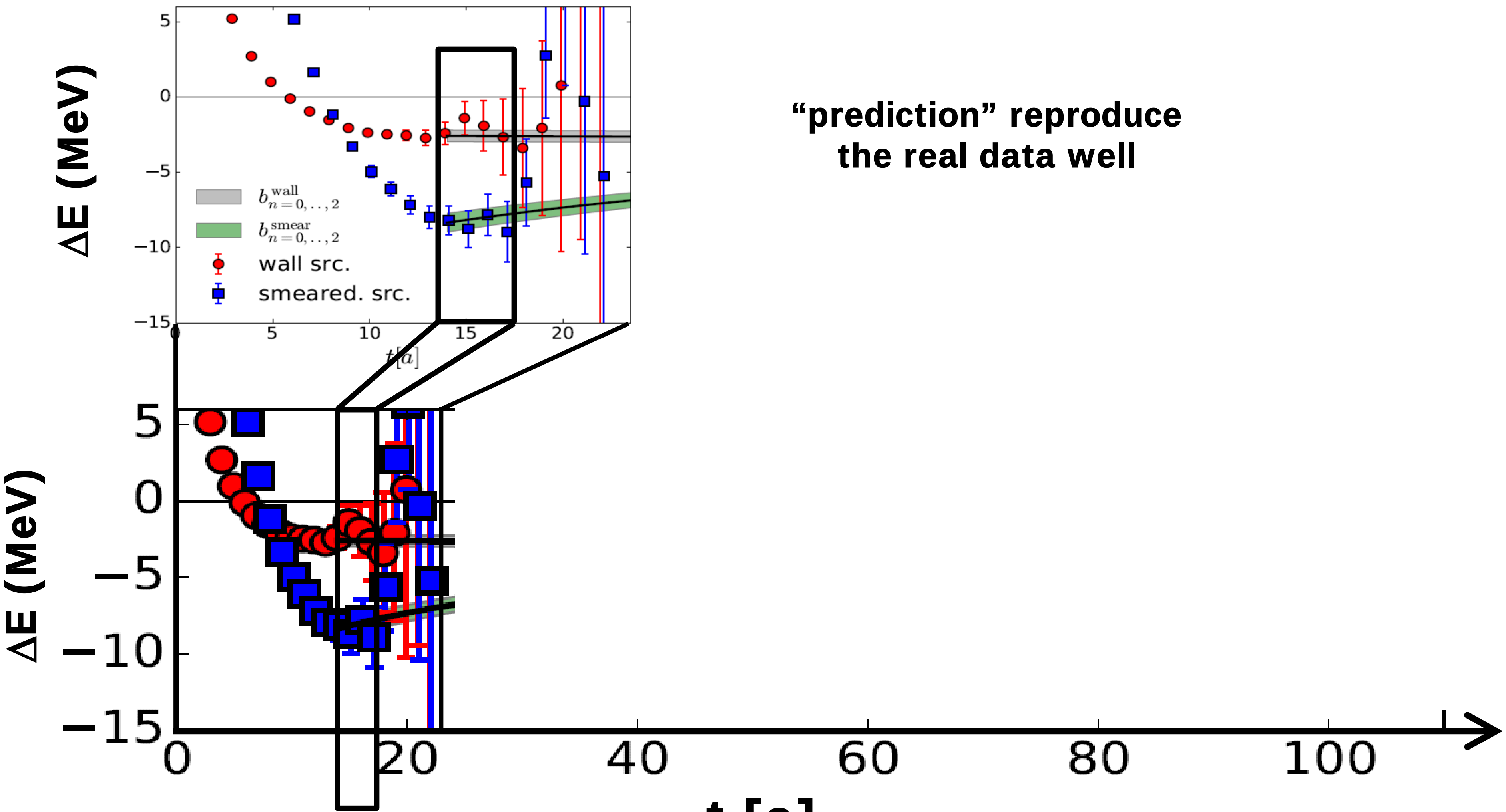


Blue: smeared

Red: wall

Understand the origin of "pseudo-plateaux"

We are now ready to "predict" the behavior of m(eff) of ΔE at any "t"



"prediction" reproduce the real data well

"pseudo-plateaux" at t ~ 1fm

"real plateau" at t ~ 10fm

(E_1-E_0=50MeV)

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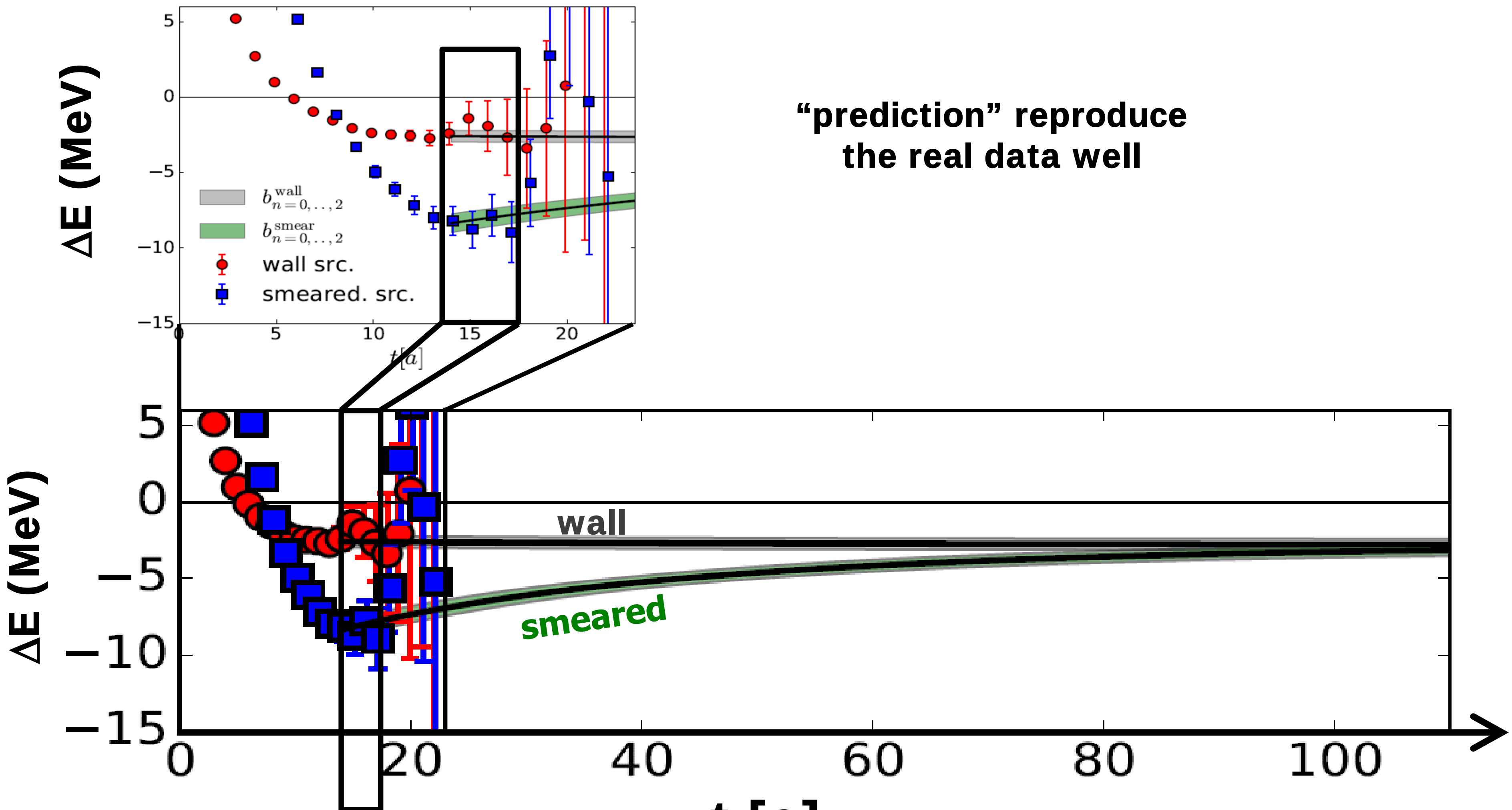

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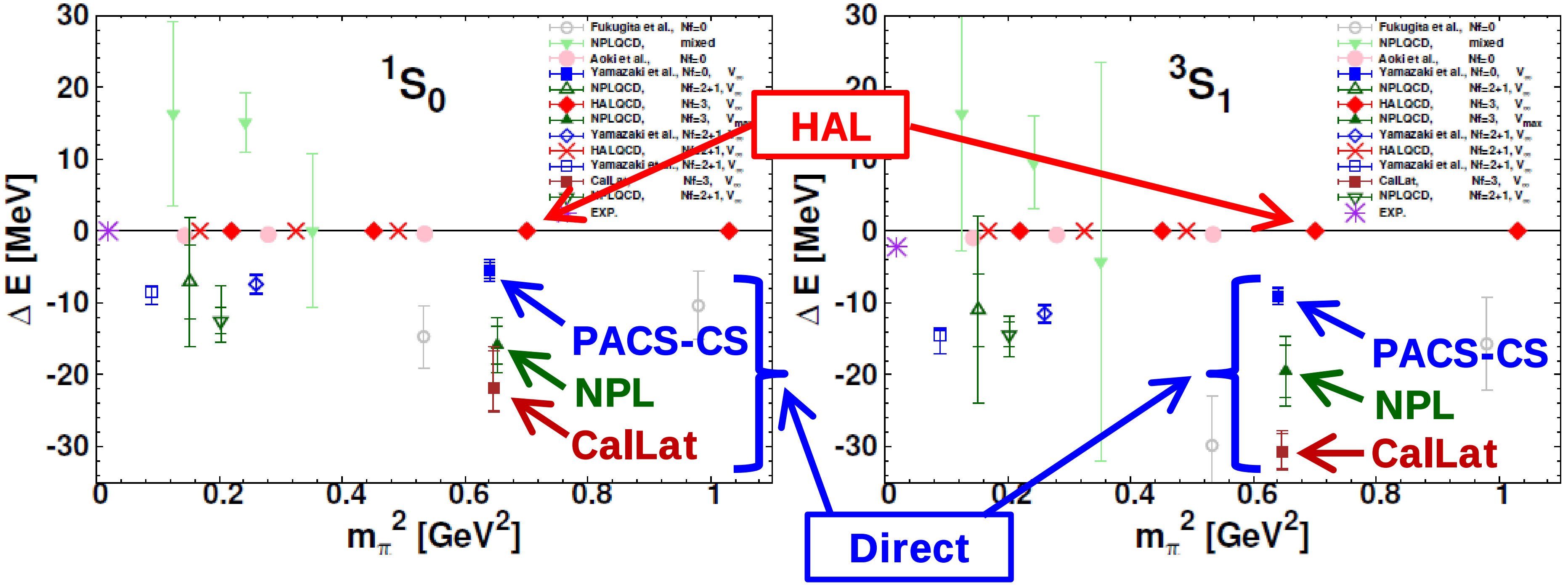
Direct method vs HAL method
(NN @ heavy quark masses)

HAL method (HAL) : **unbound**

Direct method (PACS-CS (Yamazaki et al.) / NPL / CalLat): **bound**

Direct method = naïve plateau fitting + Luscher's formula

“di-neutron” “deuteron”



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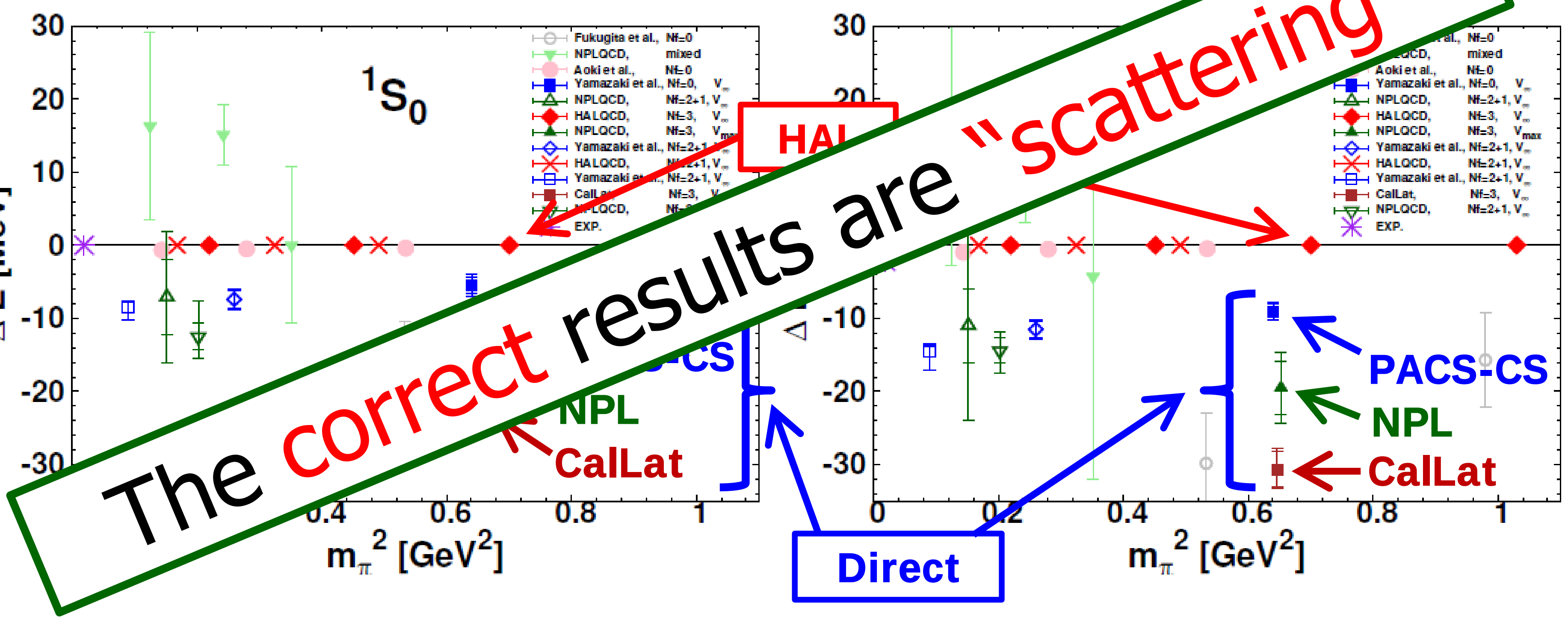


New LQCD calc also confirms our HAL results

New calc w/ Luscher's FV formula
does not use naïve plateau fitting
(variational study is used)

A. Walker-Loud @ Lat2023
"I believe the old results are wrong
(including those I was involved with)"

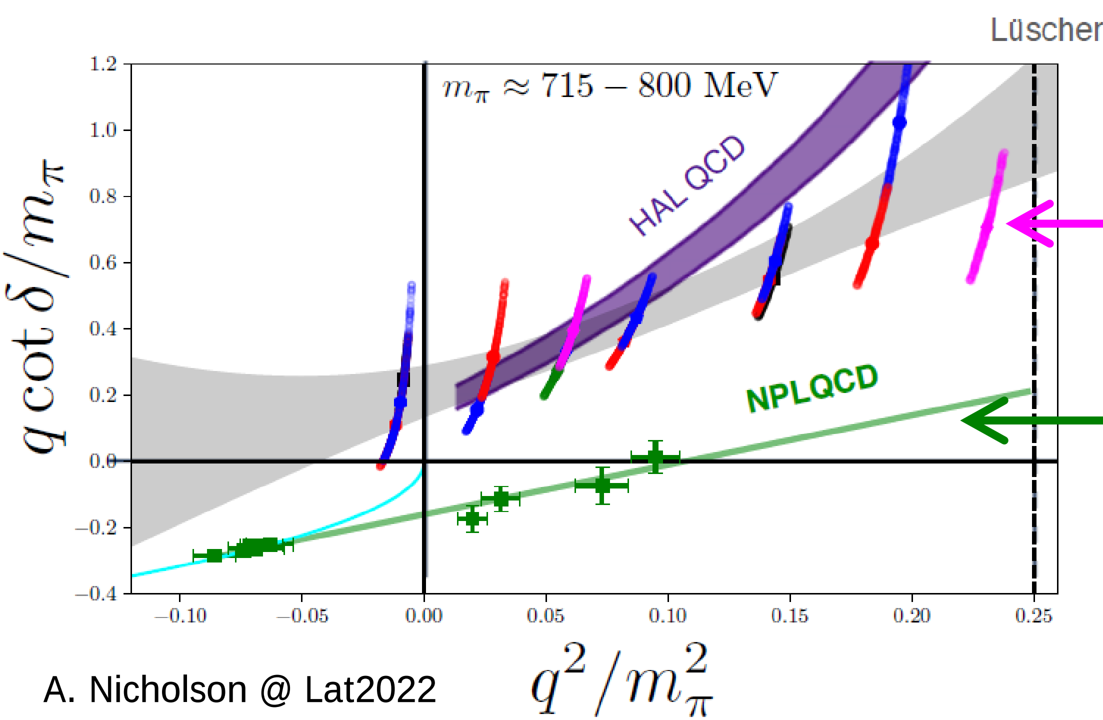
LQCD Results with (deeply) bound di-nucleons

2006	NPLQCD - first dynamical LQCD calculations of NN	
2011	NPLQCD	$M\pi \simeq 390$ MeV
2012	Yamazaki et al.	$M\pi \simeq 510$ MeV
2012	NPLQCD	$M\pi \simeq 800$ MeV
2015	Yamazaki et al.	$M\pi \simeq 310$ MeV
2015	CalLat	$M\pi \simeq 800$ MeV + P,D,F waves
2015	NPLQCD	$M\pi \simeq 450$ MeV
2020	NPLQCD	$M\pi \simeq 450$ MeV

LQCD Results without bound di-nucleons (or inconclusive)

2012	HAL QCD	$M\pi \simeq 710$ MeV
2012	HAL QCD	$M\pi \simeq 469$ — 1171 MeV
2019	"Mainz"	$M\pi \simeq 960$ MeV
2020	CoSMoN	$M\pi \simeq 714$ MeV
2021	NPLQCD	$M\pi \simeq 800$ MeV

A. Walker-Loud @ Lat2023



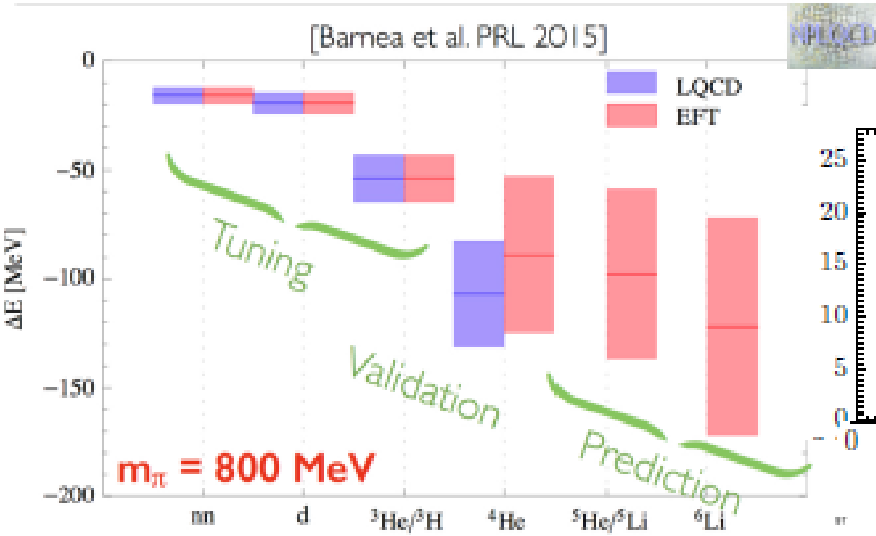
New FV results

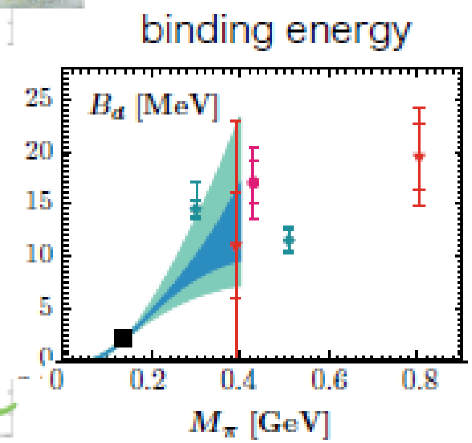
Old FV results

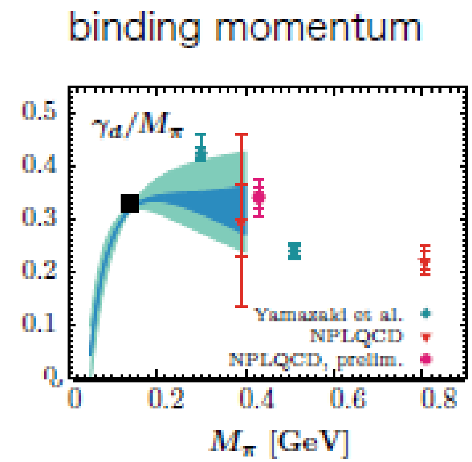
A. Nicholson @ Lat2022

Could (chiral) effective theories invalidate old finite volume data ?

Unfortunately, the answer seems “No”.







pionless EFT Beane@CD15

ChPT Baru@CD15

The chiral EFTs and old lattice data seemed consistent if EFT parameters were fixed by the same lattice data.

It is hard for EFTs to tell whether lattice data are correct or not.

S. Aoki @ CD2024

In my opinion,
NN controversy was over

but with some lessons
which may be useful for young researchers...

- Hadron Forces from LQCD — Ishii-Aoki-Hatsuda (PRL99)
- Exponentially better S/N — Ishii et al. (PLB712)
- Coupled channel systems — Aoki et al. (Proc.Jpn.Acad.Ser.B87)

[Theory] = HAL QCD method

Hadron Interactions from Lattice QCD simulations

[Software]

= Unified Contraction Algorithm

- Exponential speedup — Doi-Endres (CPC184)

$$^{3}\mathrm{H}/^{3}\mathrm{He} \quad : \quad \times 192$$
$$^{4}\mathrm{He} \quad : \quad \times 20736$$
$$^{8}\mathrm{Be} \quad : \quad \times 10^{11}$$

[Hardware]

= Supercomputers

- Monte Carlo Integration w/ 10^9 dof
- Extensive use of top supercomputers

Summary

- Hadron forces: Bridge between particle/nuclear/astro-physics
- LQCD study of Hadron forces is the frontier!
  - Luscher's finite volume method
  - HAL QCD method
    - Energy-indep non-local potential useful for reliable calc
  - We can calculate phase shifts (in infinite V) from simulations on finite V
  - Systematic error carefully investigated
- LQCD results @ phys point will make huge impact