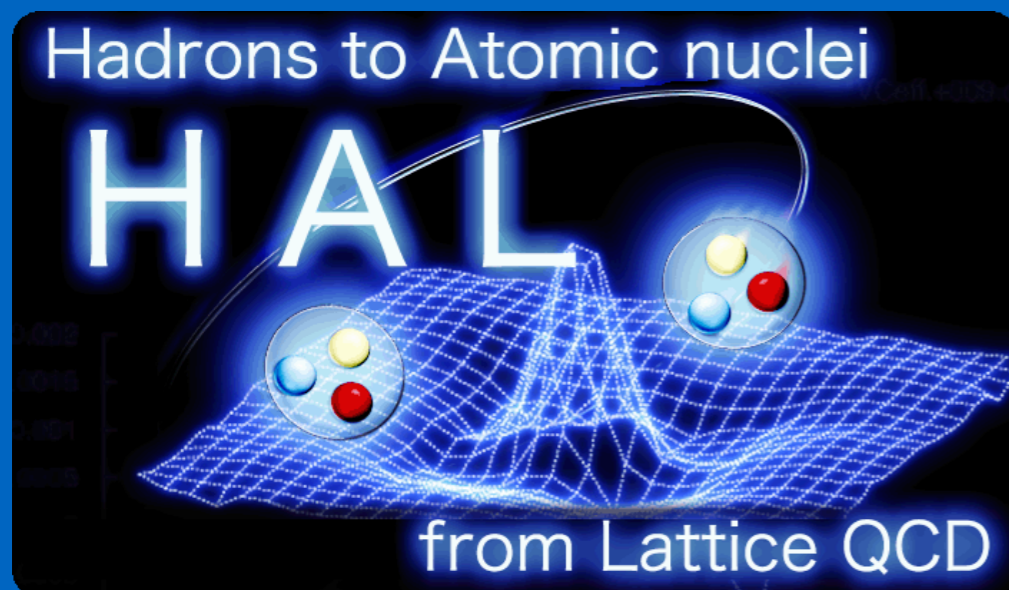


Systematics in the HAL QCD method and diagnoses of the direct method

Takumi Iritani (RIKEN)

Feb. 5-9 2018 @ INT-18-70W "Multi-Hadron Systems from Lattice QCD"



HAL QCD Collaboration

[Sinya Aoki \(Wed.\)](#), K. Sasaki, T. Aoyama,
[Daisuke Kawai \(Fri.\)](#), T. Miyamoto (YITP), T. Hatsuda,
[Takumi Doi \(Thu.\)](#), **TI**, S. Gongyo, T. M. Doi (RIKEN),
T. Inoue (Nihon Univ.), N. Ishii, Y. Ikeda,
H. Nemura, K. Murano (RCNP), F. Etminan (Univ. of
Birjand)

Contents

Intro.: Direct Method vs. HAL QCD Method

Part I: Systematics in the HAL QCD Method

Part II: Diagnoses of the Direct Method

Challenges in Multi-Baryon Systems

measurement of **ground state** from **temporal correlation**

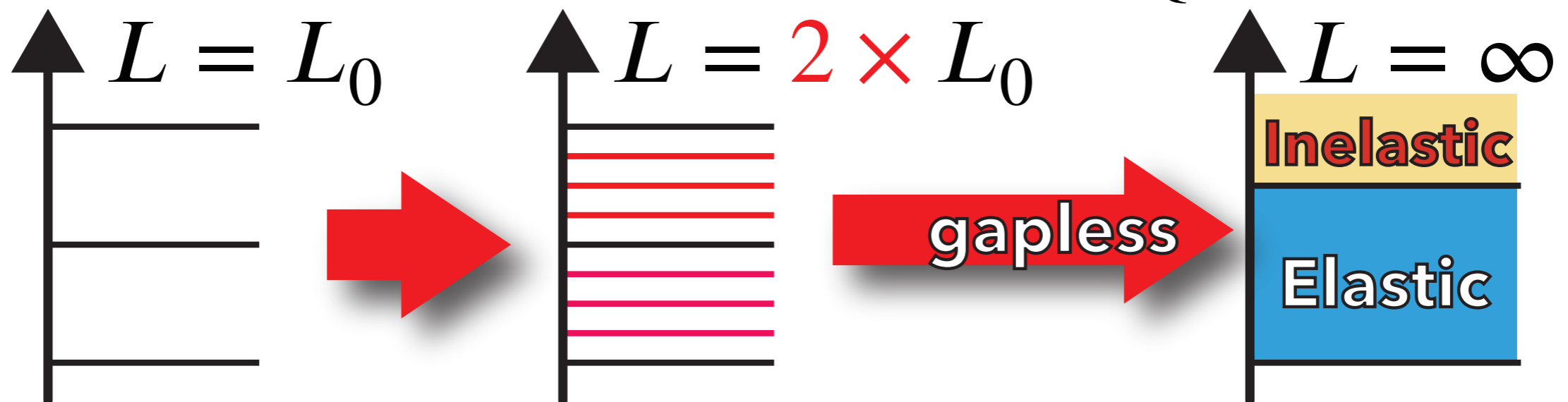
$$C_{NN}(t) = c_0 \exp(-E_0^{NN} t) + c_1 \exp(-E_1^{NN} t) + \dots \simeq c_0 \exp(-E_0^{NN} t)$$

- **S/N problem** (**A**: mass number) Parisi '84, Lepage '89

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

Scattering state contamination

$$\Delta E \sim p^2/m_N \sim \mathcal{O}(1/L^2) \ll \mathcal{O}(\Lambda_{\text{QCD}})$$



2 Hadrons in Lattice QCD (1) Direct Method

- **temporal** correlation of the two-hadron

$$R(t) \equiv C_{BB}(t) / \{C_B(t)\}^2$$

- energy shift from **plateau** of

$$\Delta E_{\text{eff}}(t) = \log \frac{R(t)}{R(t+1)} \longrightarrow E_{BB}^L - 2m_B$$

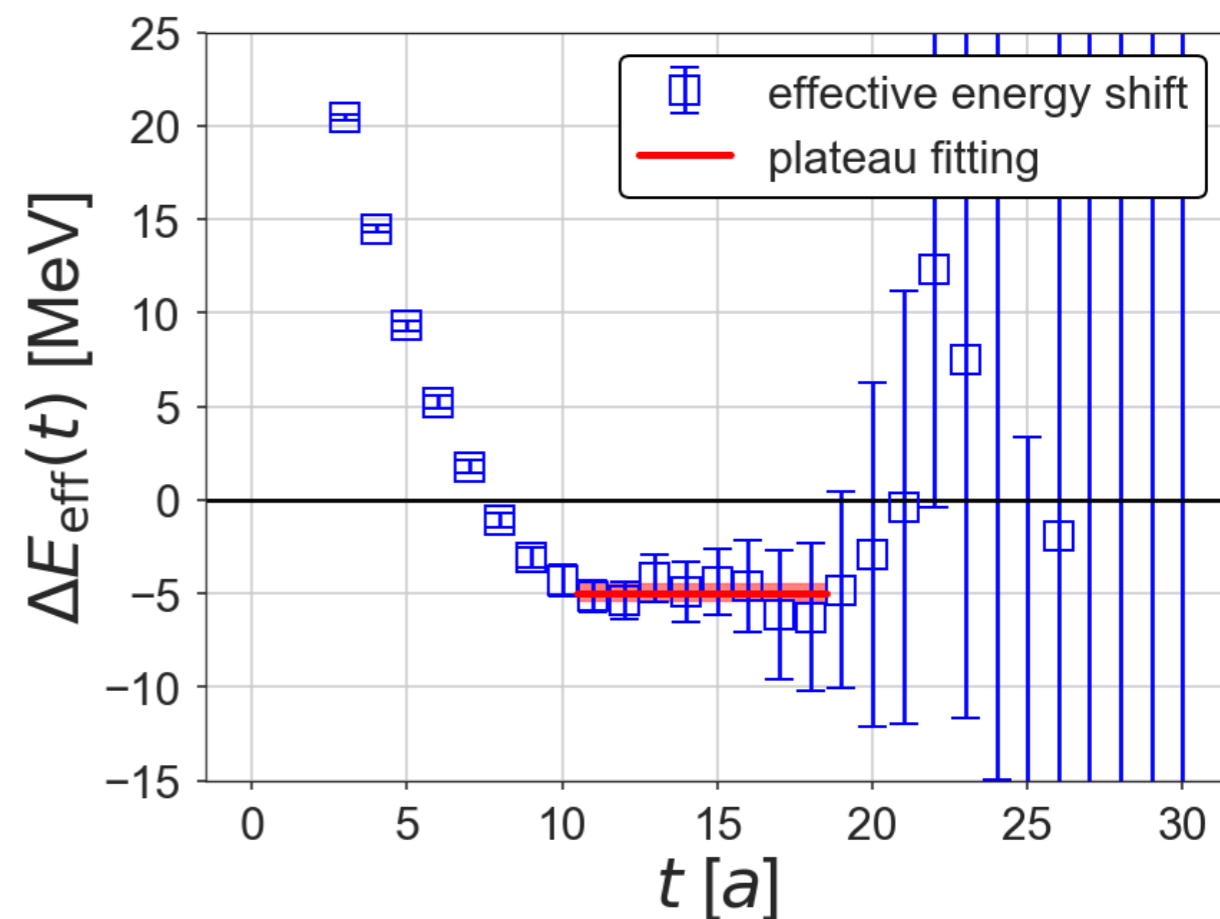
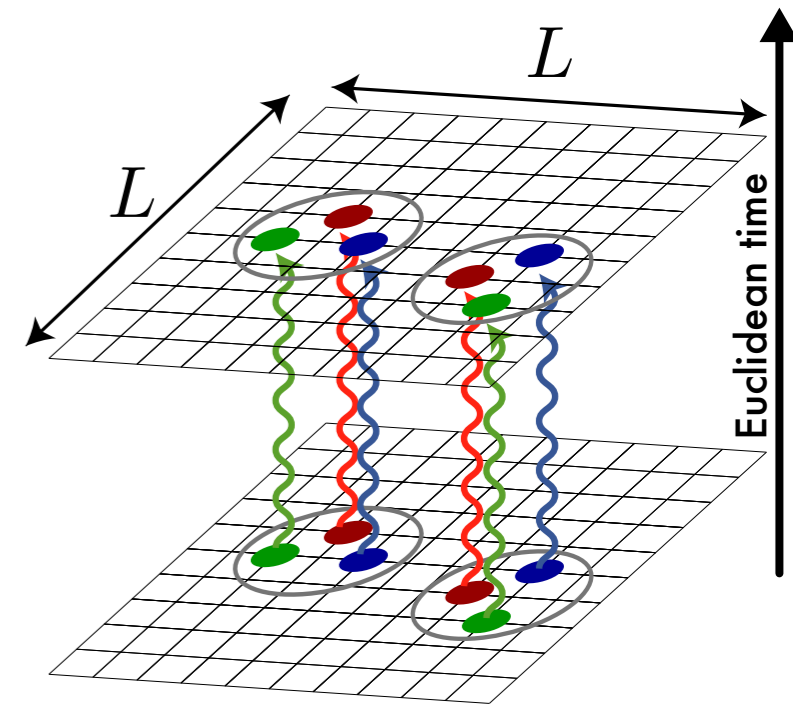
g.s. saturation is mandatory!

ex. **L = 8 fm** @ phys. mass

$\delta E_{\text{el.}} \simeq 25 \text{ MeV} \longrightarrow t > 10 \text{ fm}$

$S/N \sim \exp[-2(m_N - (3/2)m_\pi)t]$

$\longrightarrow 10^{-32}$ **extremely difficult!**



2 Hadrons in Lattice QCD (2) HAL QCD Method

Ishii-Aoki-Hatsuda '06

Hadrons to Atomic nuclei from Lattice QCD

- **spatial** correlation of the two-hadron

Nambu-Bethe-Salpeter wave func.

$$\psi_k(\vec{r}) = \langle 0 | B(\vec{r}) B(\vec{0}) | B(\vec{k}) B(-\vec{k}); \text{in} \rangle$$

- **asymptotic region** $r \gg R$

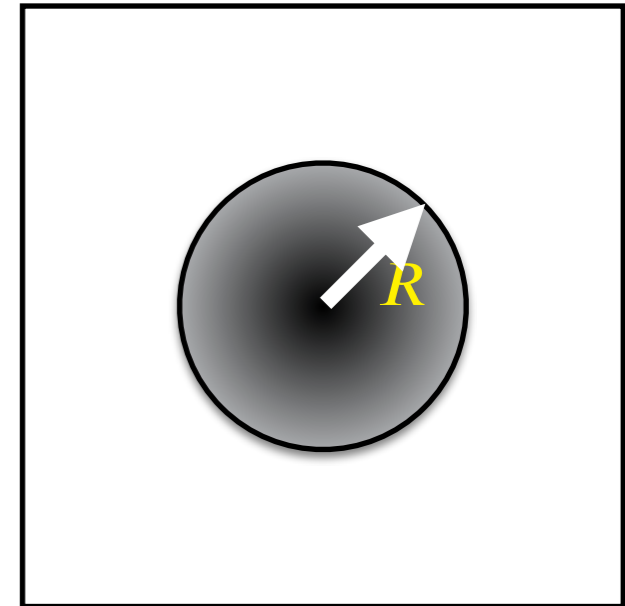
$$\psi_k(\vec{r}) \simeq C \sin(kr - l\pi/2 + \delta(k)) / (kr)$$

- **interacting region** $r < R$

$$(\nabla^2 + k^2)\psi_k(\vec{r}) = m \int d\vec{r}' U(\vec{r}, \vec{r}') \psi_k(\vec{r}')$$

energy-indep. & non-local potential & faithful to δ

$$U(\vec{r}, \vec{r}') = \sum_{|\vec{p}| \leq p_{\text{th}}} [E_p - H_0] \psi_p(\vec{r}) \psi_p^*(\vec{r}')$$



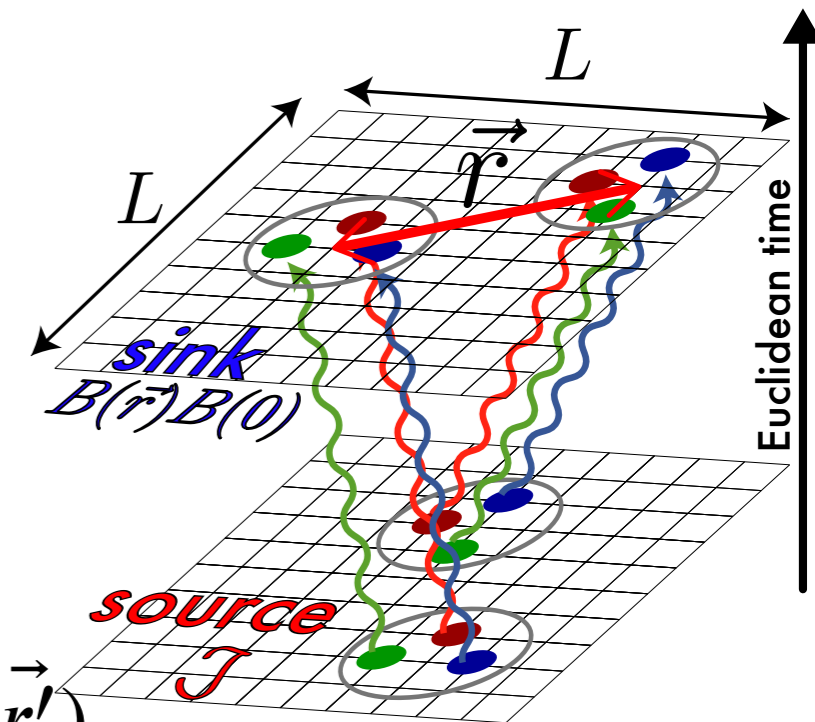
HAL QCD method: **NBS wave func.** \rightarrow $U(r, r')$ \rightarrow observables

"Time-dependent" HAL QCD Method (1)

Ishii for HAL QCD '12

$$R(\vec{r}, t) \equiv \langle 0 | T \{ B(\vec{x} + \vec{r}, t) B(\vec{x}, t) \} \bar{J}(0) | 0 \rangle / \{ C_B(t) \}^2$$

$$= \sum_n a_n \psi_{W_n}(\vec{r}) e^{-(W_n - 2m_B)t} + \mathcal{O}(e^{-\Delta W_{\text{th}}t})$$



g.s. & scattering state NBS funcs. satisfy

$$[E_{W_0} - H_0] \psi_{W_0}(\vec{r}) = \int d\vec{r}' U(\vec{r}, \vec{r}') \psi_{W_0}(\vec{r}')$$

$$[E_{W_1} - H_0] \psi_{W_1}(\vec{r}) = \int d\vec{r}' U(\vec{r}, \vec{r}') \psi_{W_1}(\vec{r}')$$

⋮

$$\mathcal{O}(e^{-\delta E_{\text{inel}}t}) \ll \mathcal{O}(e^{-\delta E_{\text{el}}t})$$

they are signals

with **elastic saturation (exponentially easier than g.s. saturation!)**

$$\Rightarrow \left[\frac{1}{4m_B} \frac{\partial^2}{\partial t^2} - \frac{\partial}{\partial t} - H_0 \right] R(\vec{r}, t) = \int d\vec{r}' U(\vec{r}, \vec{r}') R(\vec{r}', t)$$

“Time-dependent” HAL QCD Method (2)

$$\left[\frac{1}{4m_B} \frac{\partial^2}{\partial t^2} - \frac{\partial}{\partial t} - H_0 \right] R(\vec{r}, t) = \int d\vec{r}' U(\vec{r}, \vec{r}') R(\vec{r}', t)$$

local pot. by *velocity expansion* of **E-indep.** & **non-local pot.** $U(\mathbf{r}, \mathbf{r}')$

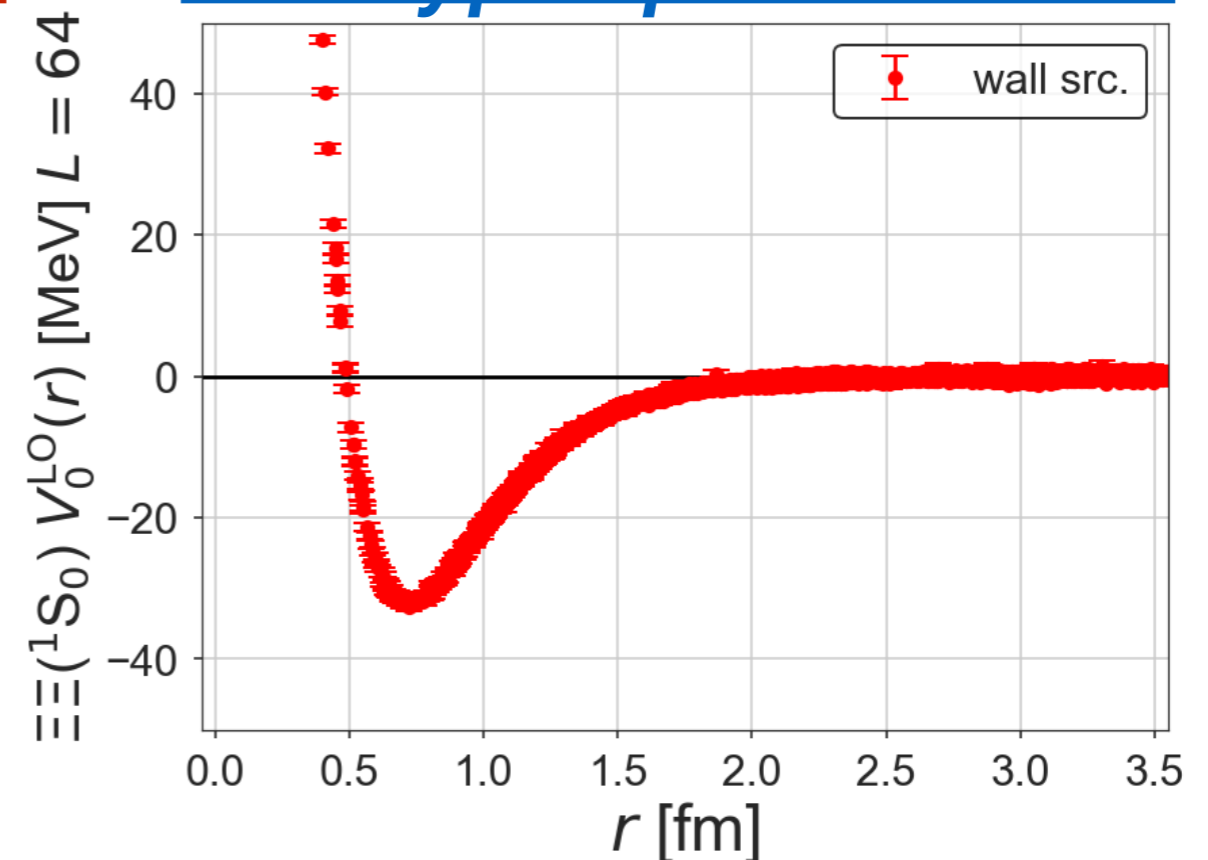
$$U(\vec{r}, \vec{r}') = \left[V_0(\vec{r}) + V_1(\vec{r}) \mathbf{L} \cdot \mathbf{S} + V_2(\vec{r}) \nabla^2 + \dots \right] \delta(\vec{r} - \vec{r}')$$

previous results by **HAL QCD** mainly employ

“leading order approximation” of wall-type quark source

$$U(\vec{r}, \vec{r}') \simeq V_0^{\text{LO}}(\vec{r}) \delta(\vec{r} - \vec{r}')$$

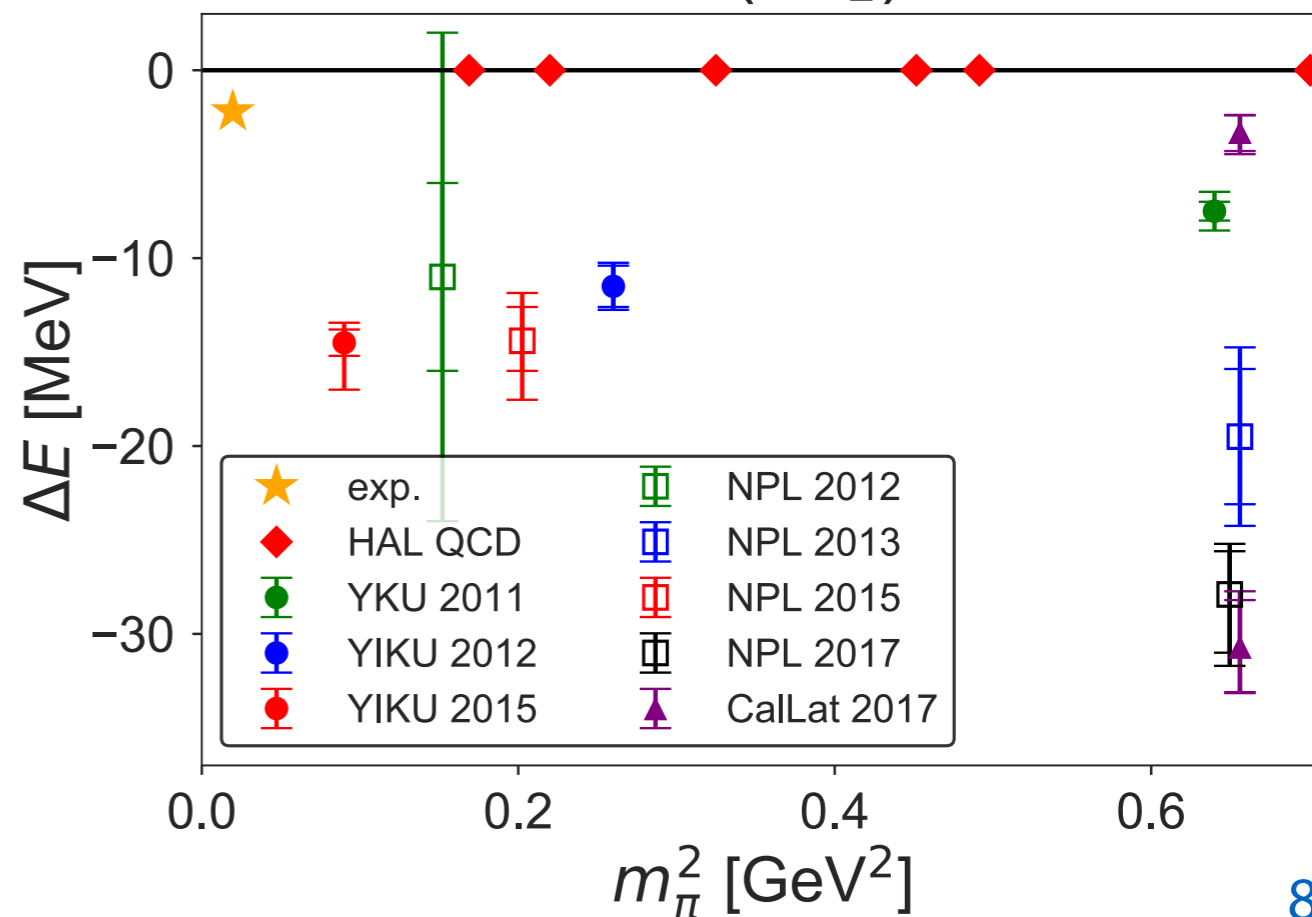
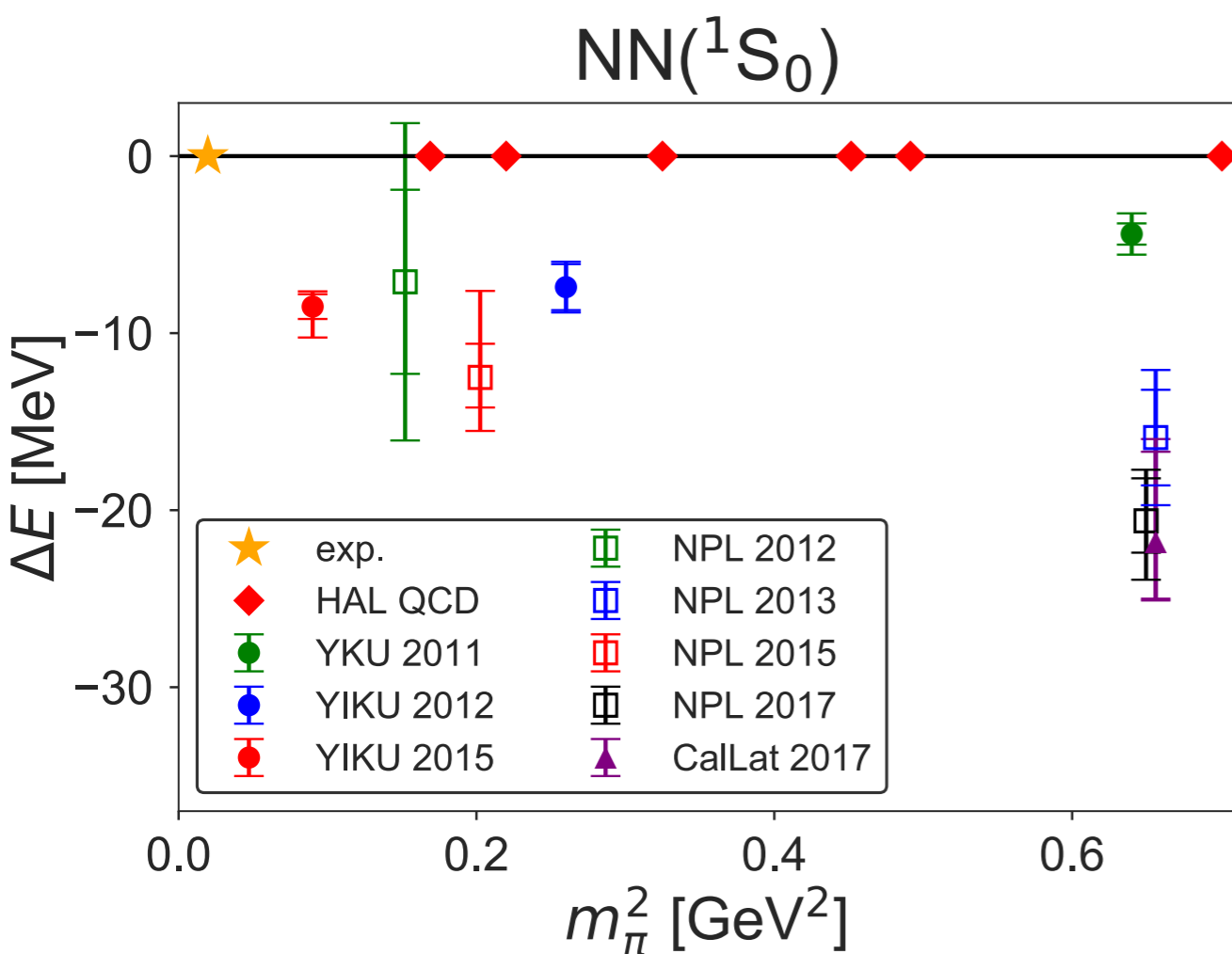
Q: Is this expansion reasonable & converged?



NN Systems from Lattice QCD

- *Inconsistency between these methods*
- *It was a long-standing problem in lattice QCD.*

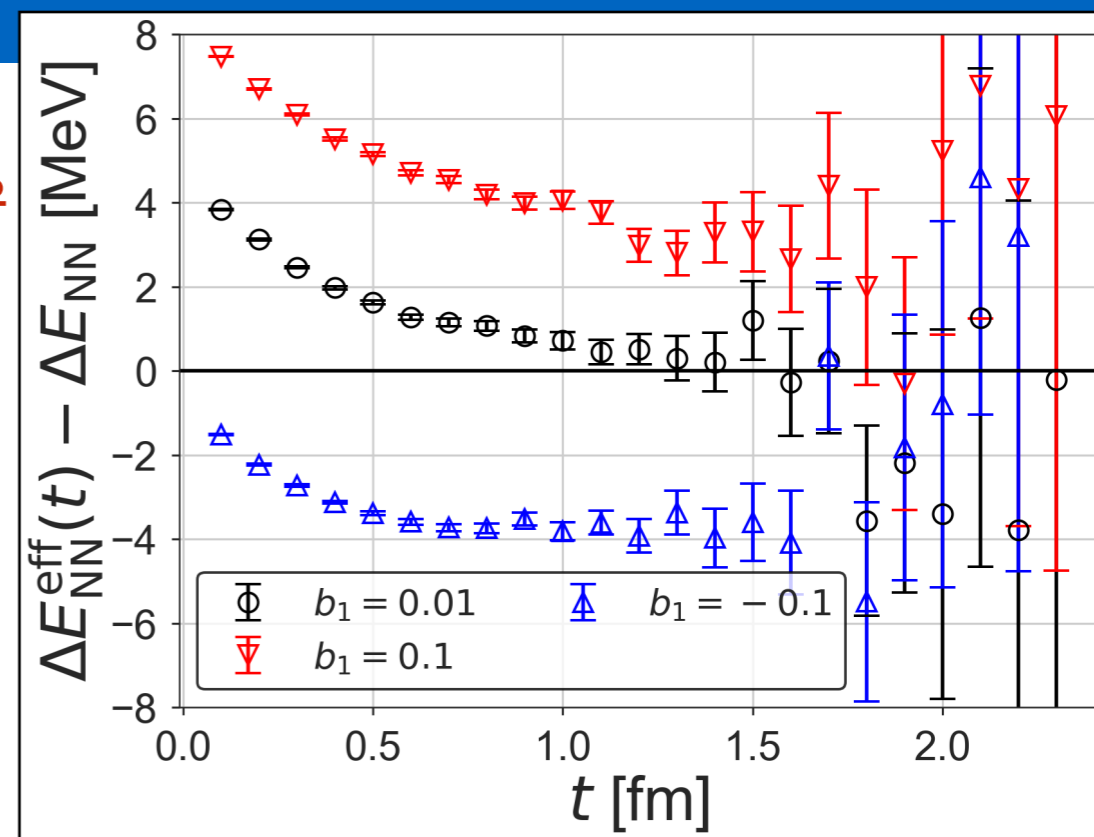
	“Direct”	HAL QCD	phys. point
Dineutron (1S_0)	bound	unbound	unbound
Deuteron (3S_1)	bound	unbound	bound



Fundamental Problem in Direct Method: Fake Plateau

Simple plateau fitting is challenging.

ground state saturation requires
huge temporal correlation

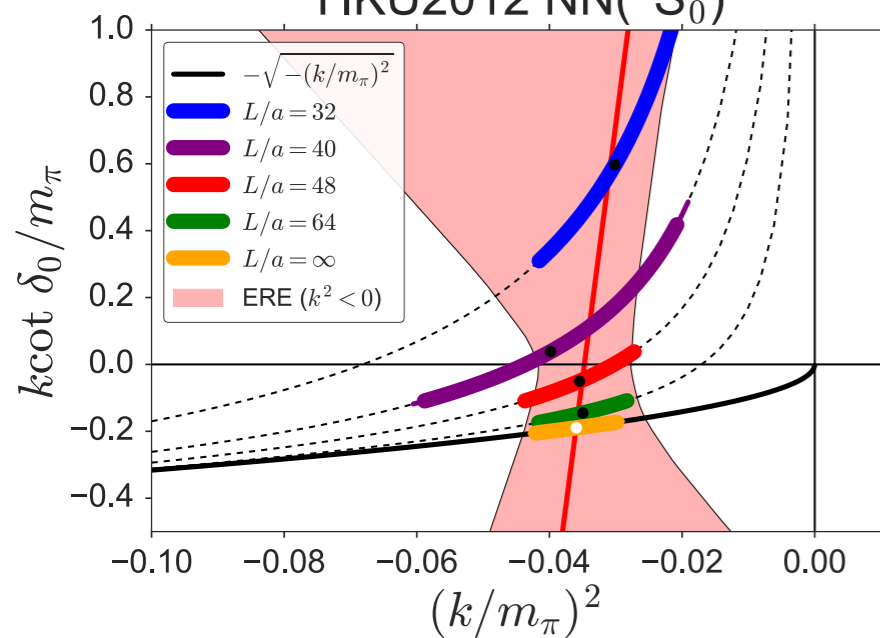


Normality Check Aoki's Talk (Wed)

previous studies show "anomalous behavior."

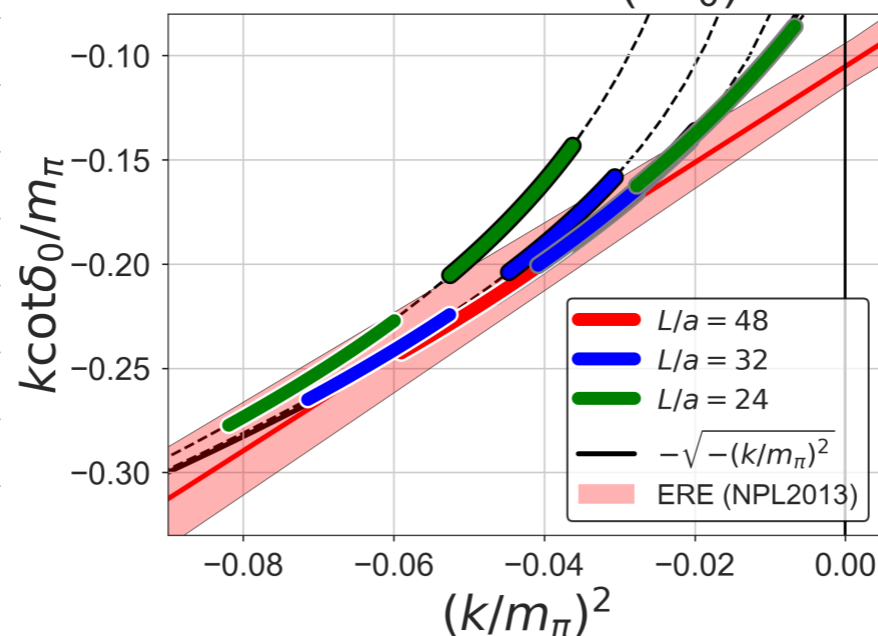
singular ERE

YIKU2012 NN(1S_0)



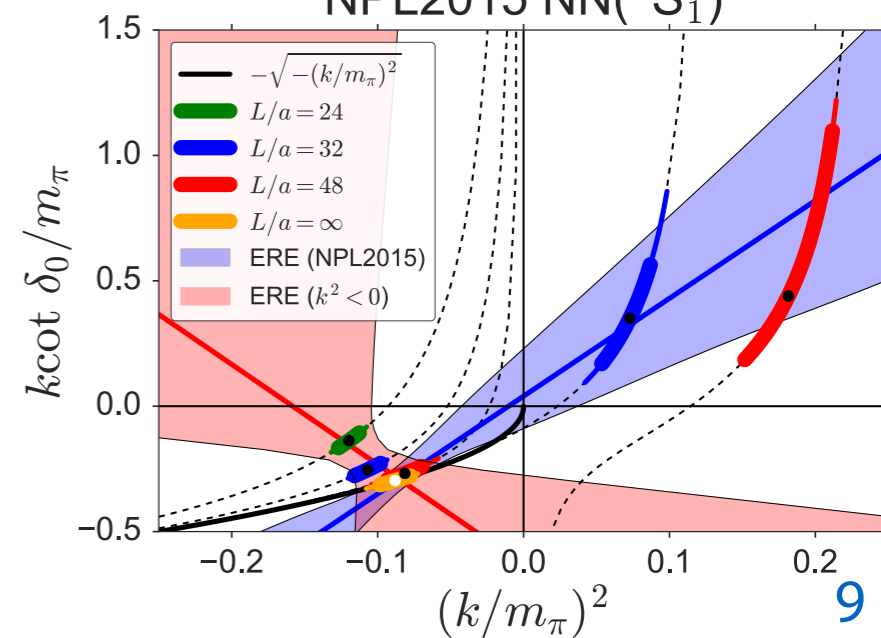
unphysical pole

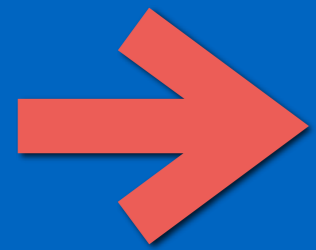
NPL2013 NN(1S_0)



unphys. & mismatch

NPL2015 NN(3S_1)





Next: Reliability of the HAL QCD Method

Part I: Systematics in the HAL QCD Method

Ref.

TI for HAL QCD Coll., PoS(Lattice 2016) 109, arXiv:1610.09763.

& in prep

1. convergence of velocity expansion

2. inelastic state contamination

Setup & Channel: $\Xi\Xi(^1S_0)$ at $m_\pi = 0.51$ GeV

better signal & the same SU(3) rep. as $NN(^1S_0)$

time-dep. HAL QCD method

$$\left[\frac{1}{4m_B} \frac{\partial^2}{\partial t^2} - \frac{\partial}{\partial t} - H_0 \right] R(\vec{r}, t) = \int d\vec{r}' U(\vec{r}, \vec{r}') R(\vec{r}', t)$$

local pot. by *velocity expansion* of **E-indep.** & **non-local pot.** $U(\mathbf{r}, \mathbf{r}')$

LO approximation (standard in previous. HAL QCD works)

$$U(\vec{r}, \vec{r}') \simeq V_0^{\text{LO}}(\vec{r}) \delta(\vec{r} - \vec{r}')$$

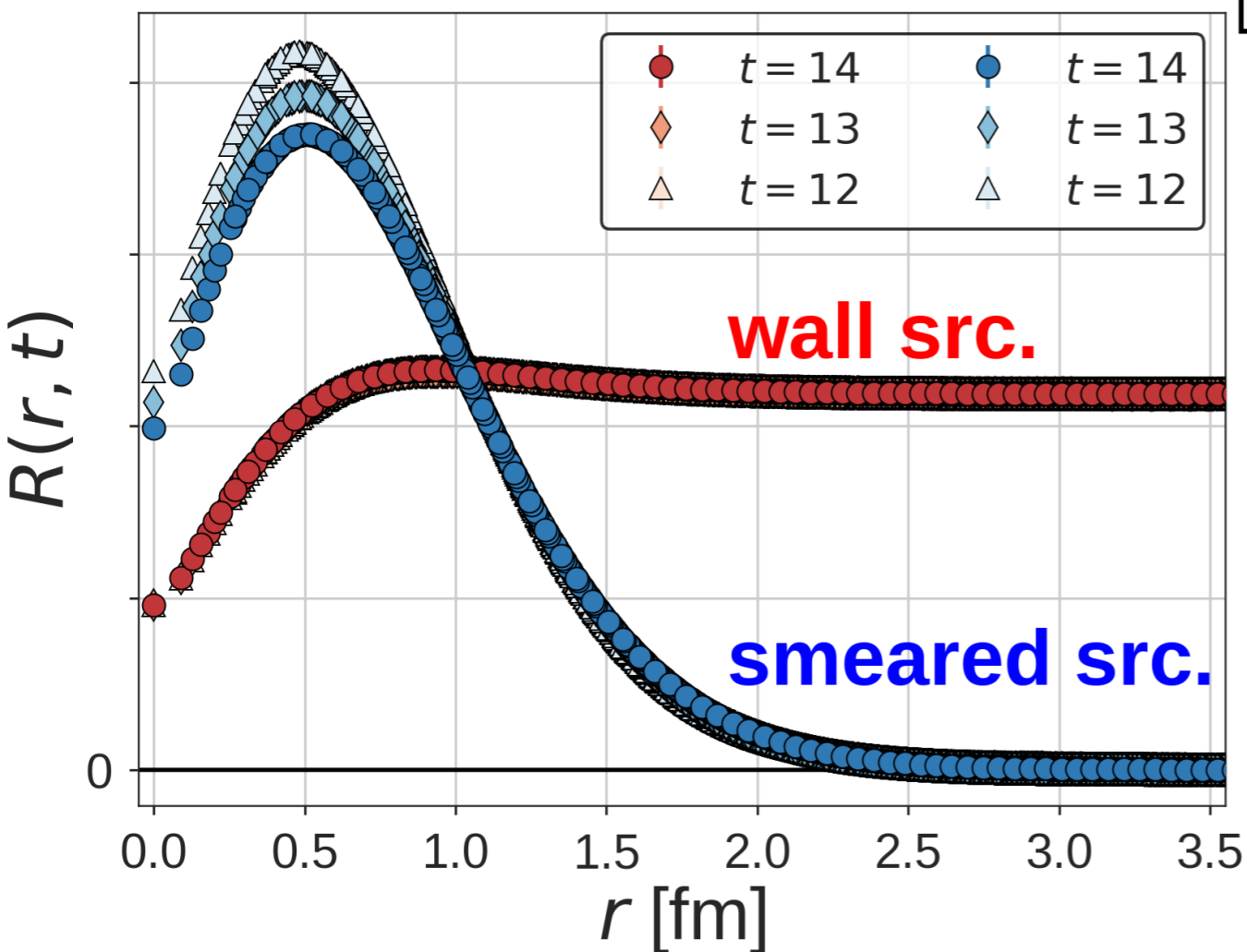
N²LO approximation & $V_2(\mathbf{r})$

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

→ **Check:** higher order correction of the HAL QCD pot.
by using wall-type & smear-type quark sources

Time Dependence of the Spatial Correlation

wall src. – delocalized & weak t-dep.
smearcd src. – localized & strong t-dep.



$$R(\vec{r}, t) \equiv C_{\text{BB}}(\vec{r}, t) / \{C_{\text{B}}(t)\}^2$$

$$= \sum_n a_n \Psi_n(\vec{r}) e^{-\Delta E_n t}$$

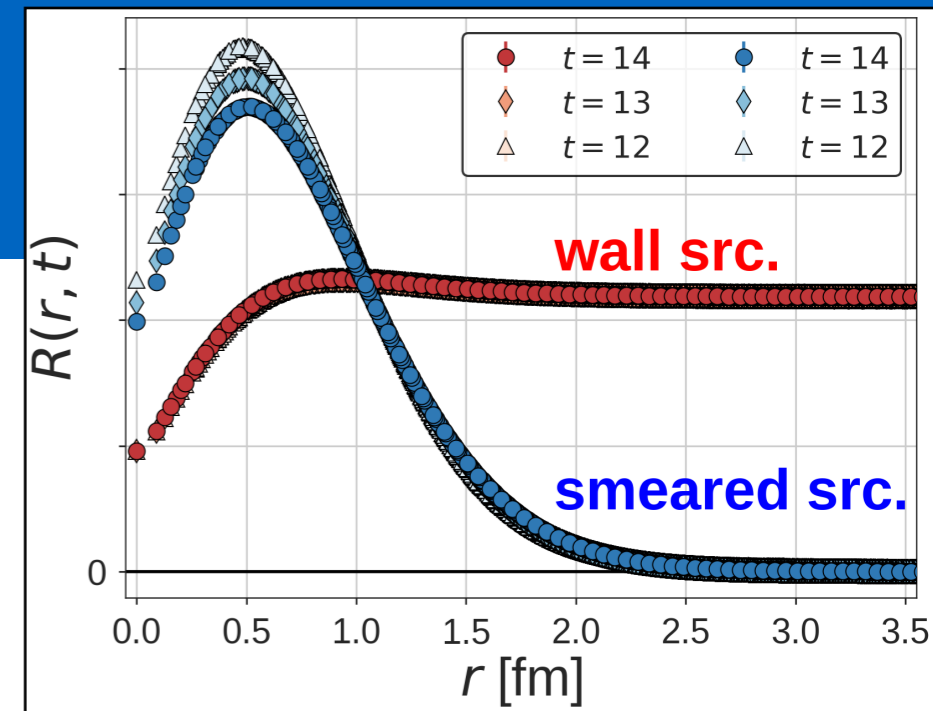
src. & time dependence

These correlators are mixtures of excited states.

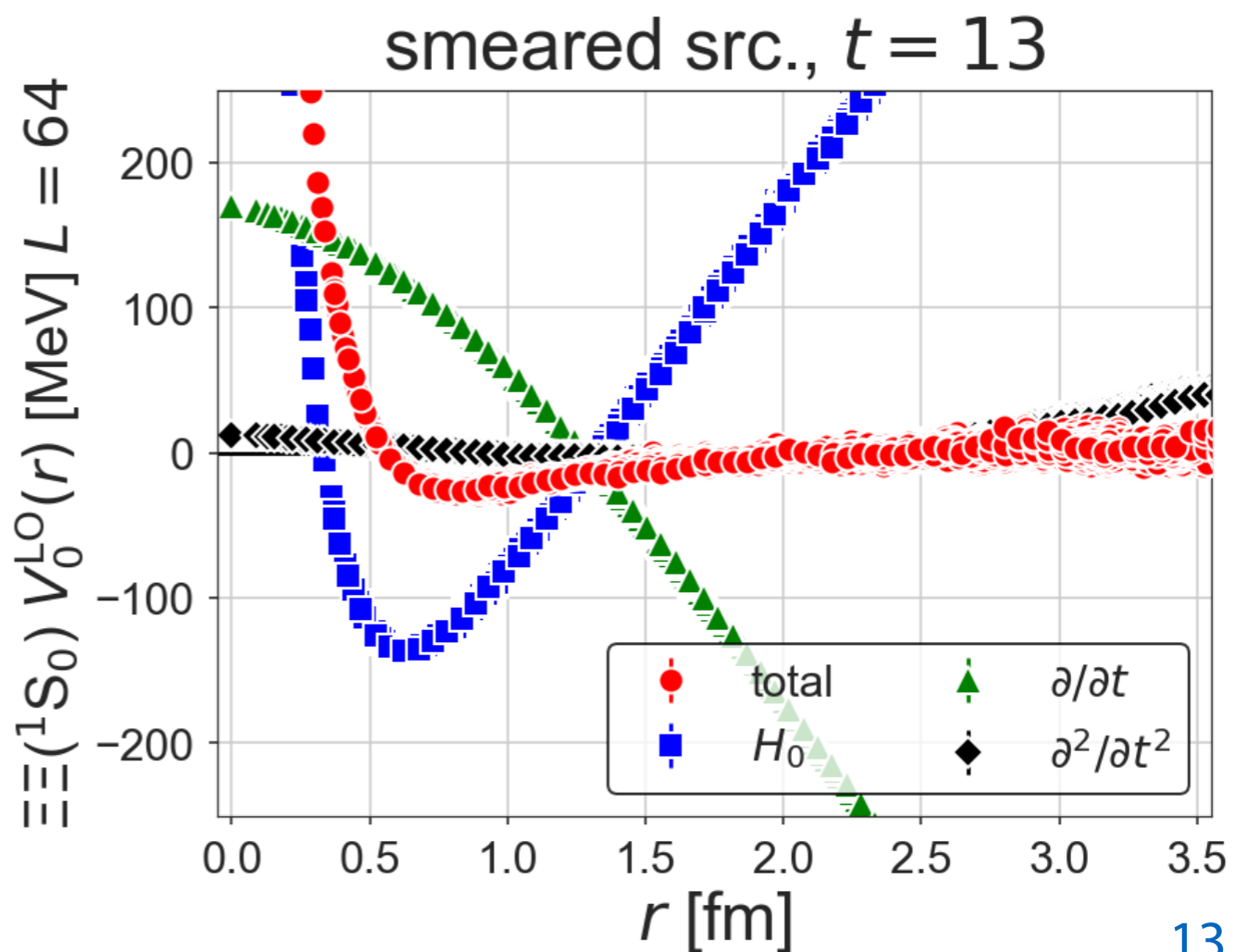
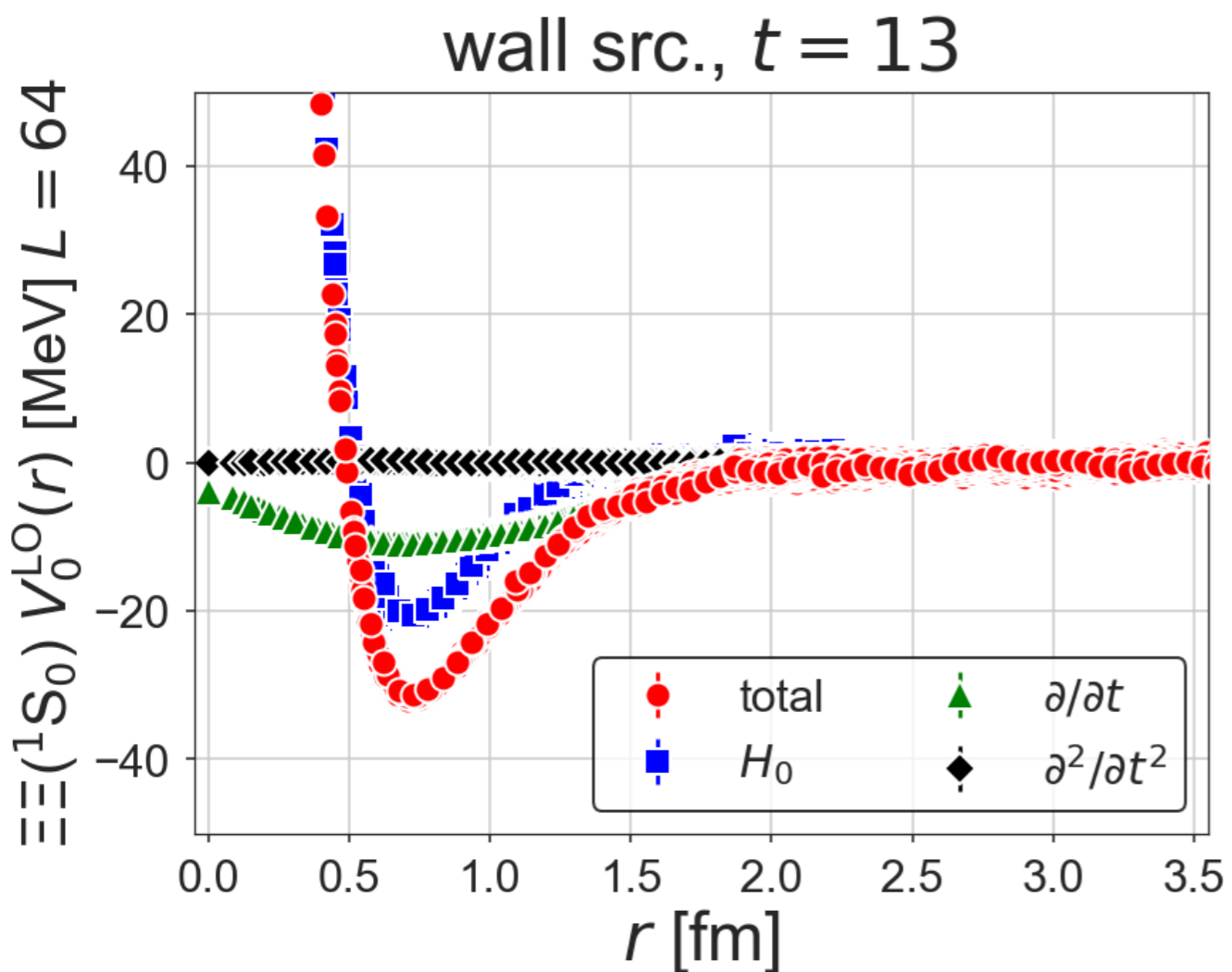
time-dep. HAL QCD method is essential!

Potential (Leading Order) (1)

$$V_0^{\text{LO}}(r) = \frac{1}{4m_B} \frac{(\partial^2/\partial t^2)R}{R} - \frac{(\partial/\partial t)R}{R} - \frac{H_0 R}{R}$$

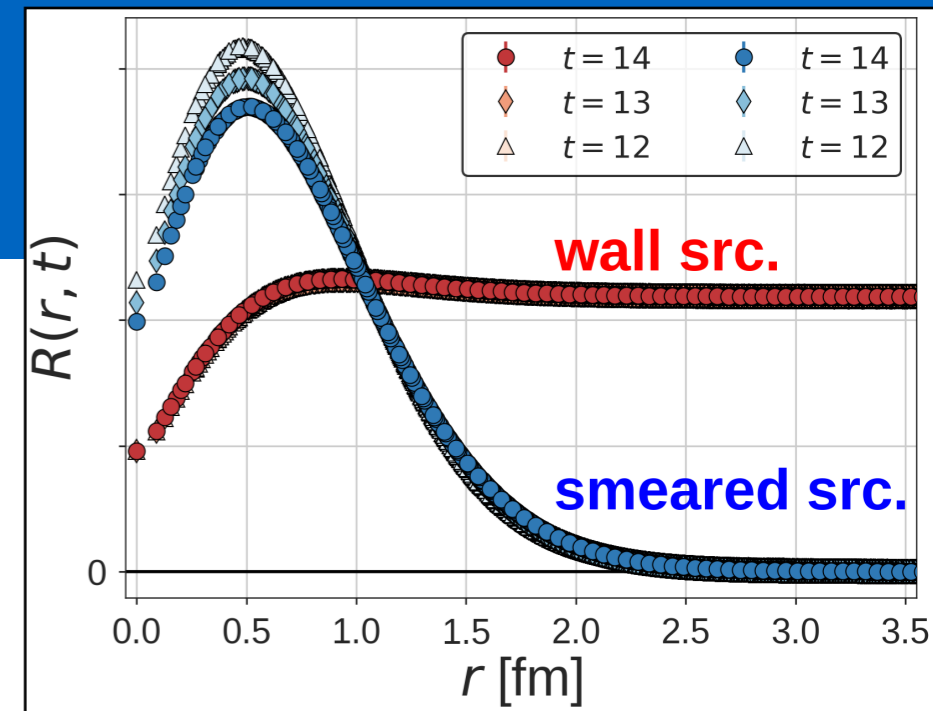


R-corr. differs, but *qualitatively* the same behavior



Potential (Leading Order) (2)

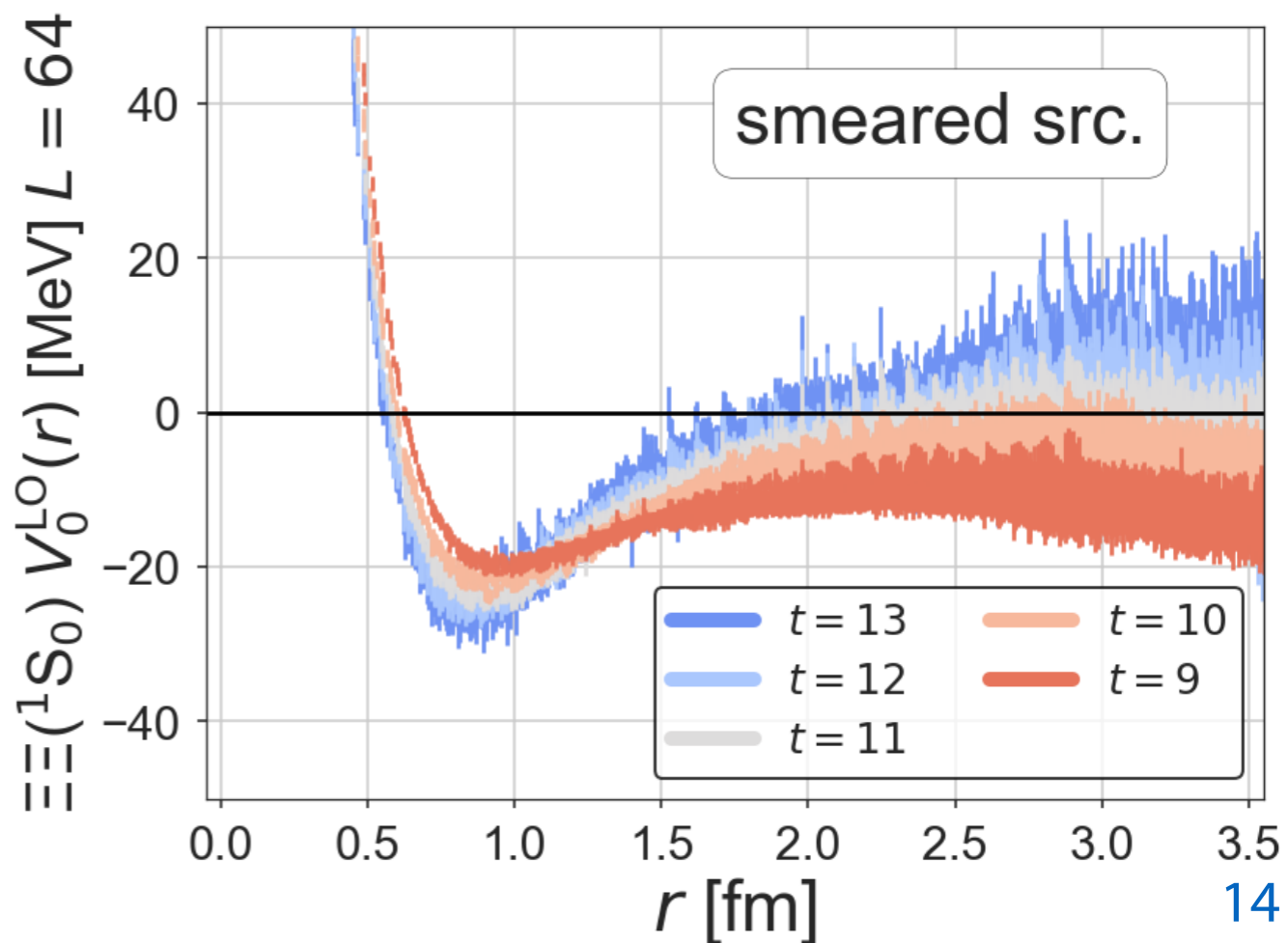
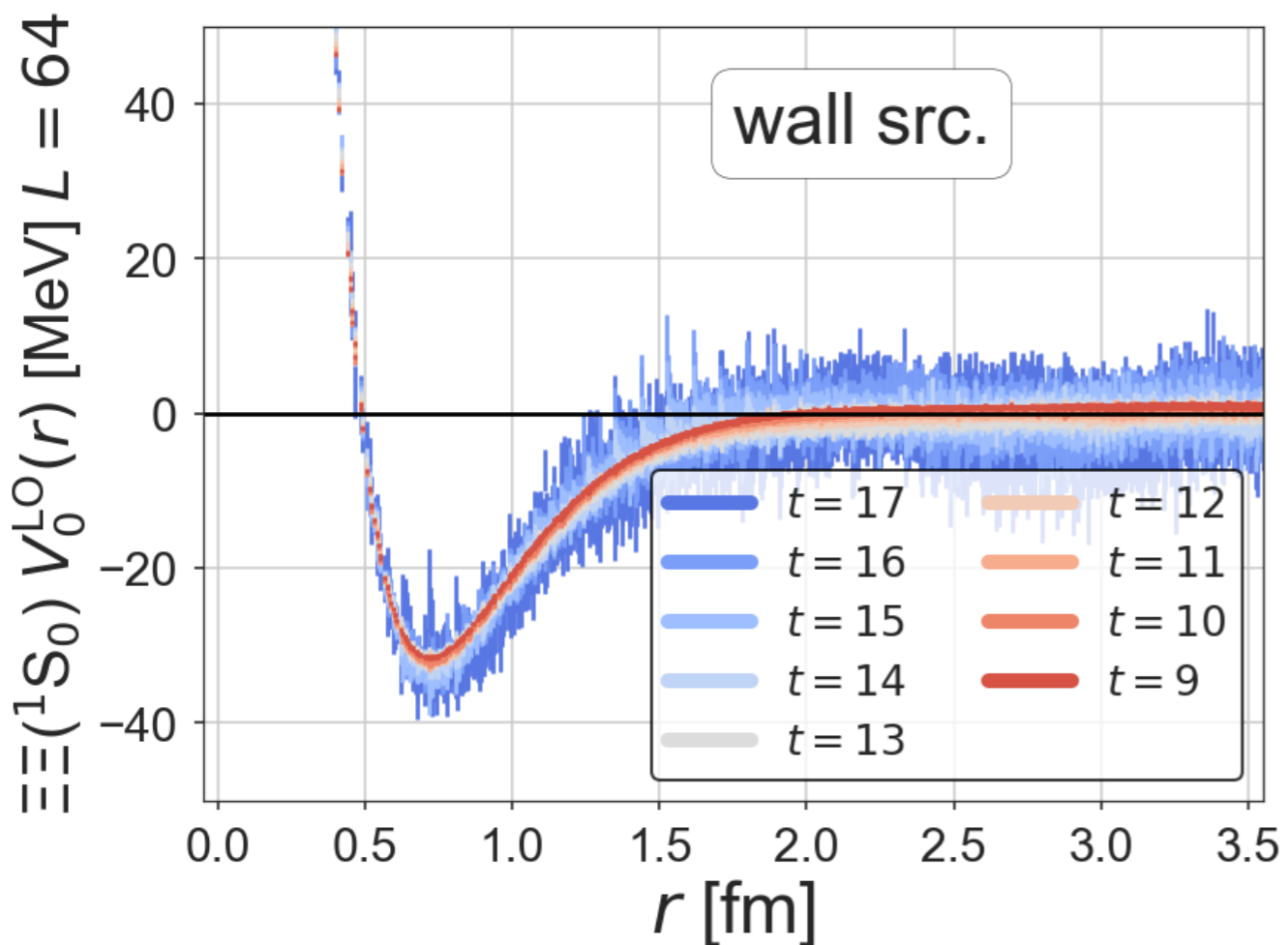
$$V_0^{\text{LO}}(r) = \frac{1}{4m_B} \frac{(\partial^2/\partial t^2)R}{R} - \frac{(\partial/\partial t)R}{R} - \frac{H_0 R}{R}$$



R-corr. differs, but *qualitatively* the same behavior

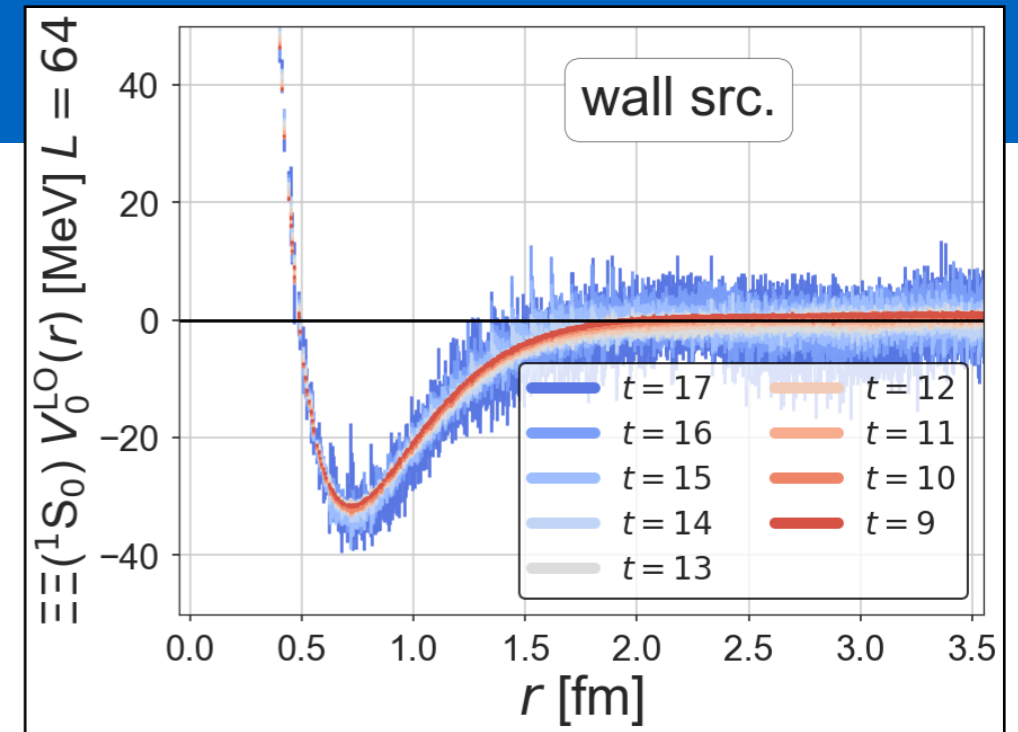
wall src. – t-independent

smeared src. – t-dependent

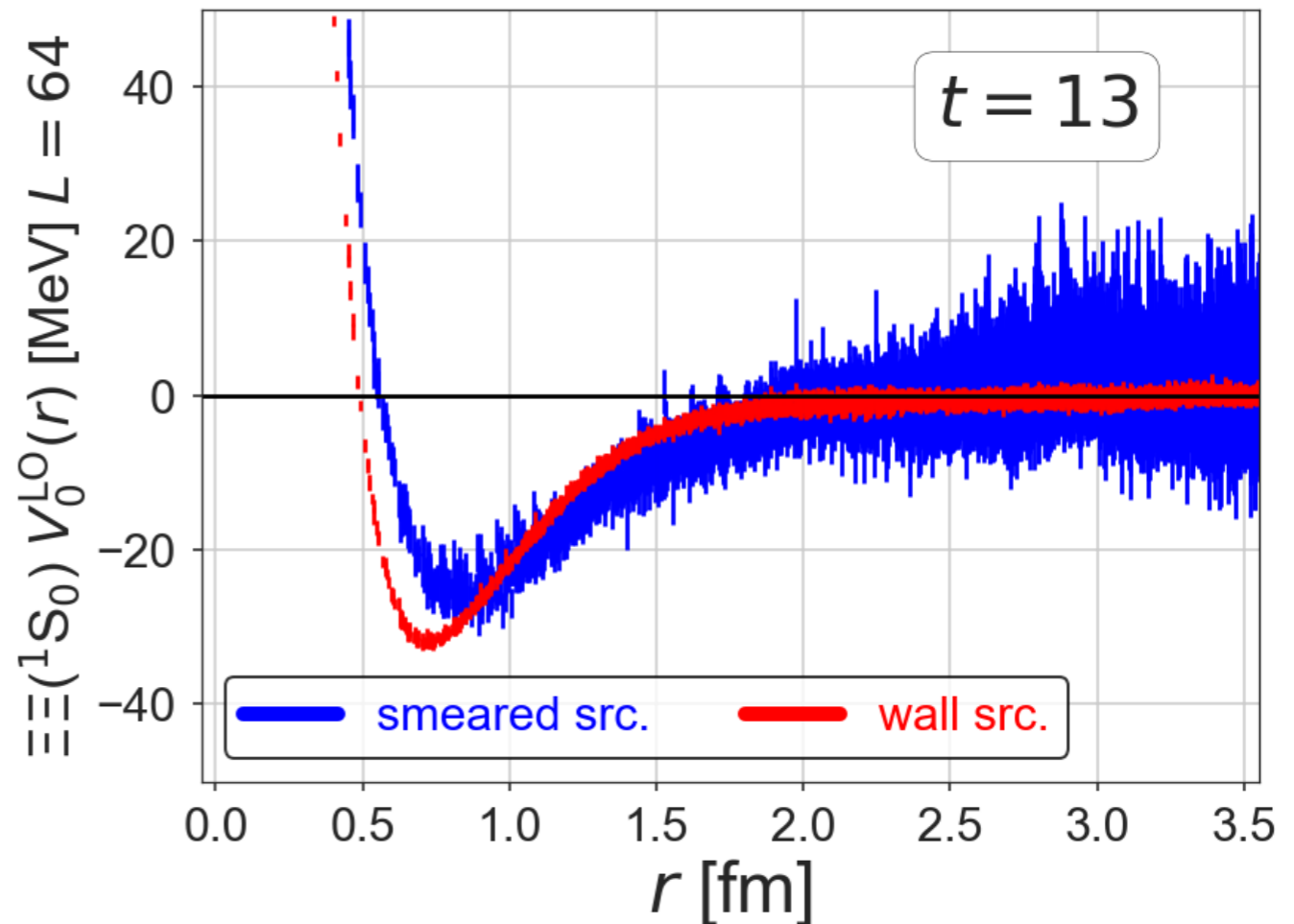
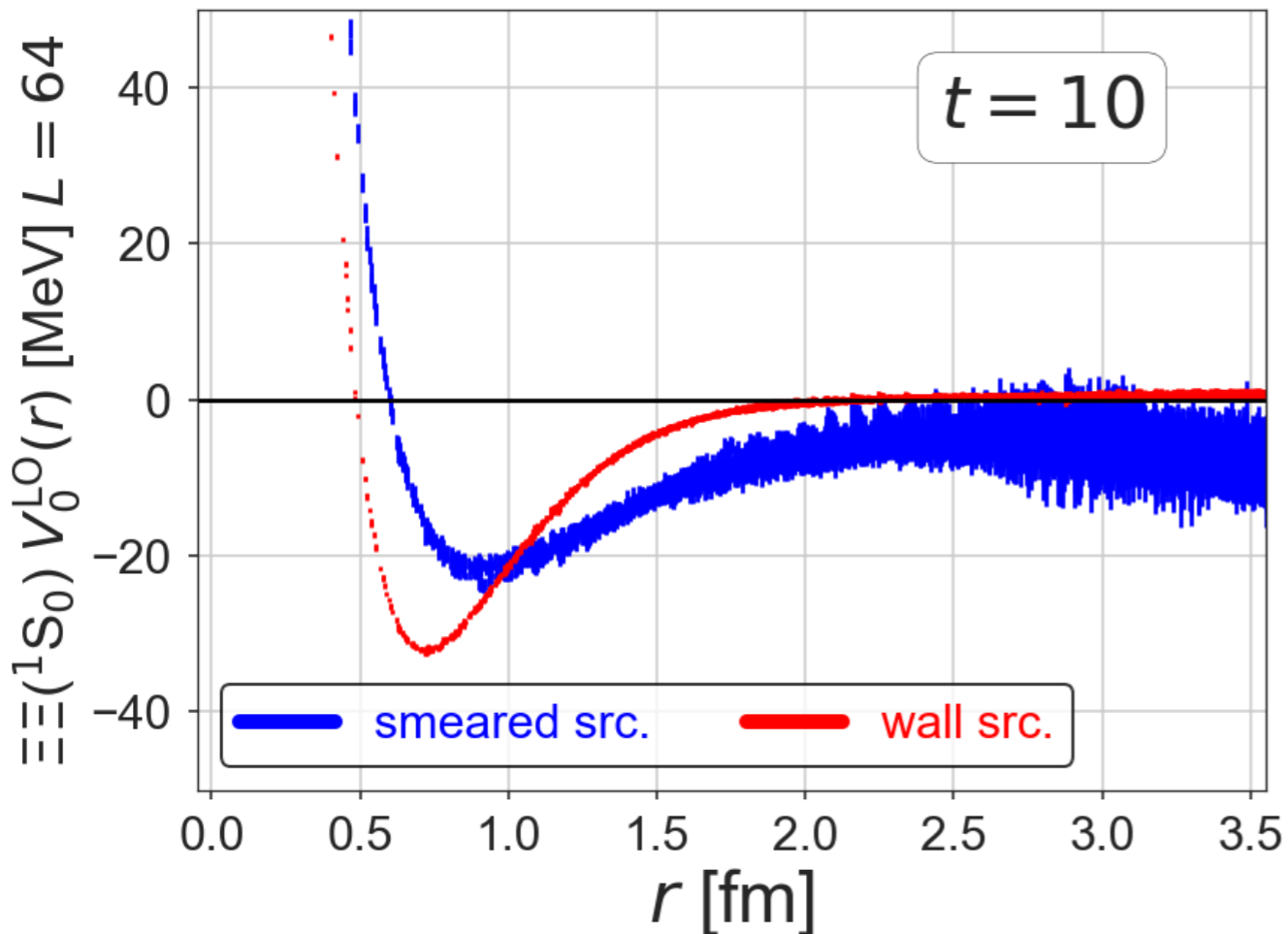


Systematic in LO Potential

- **Wall** src. = time-indep.
- **Smear**ed src. \rightarrow **Wall** src.



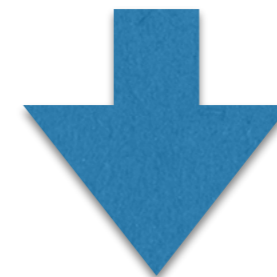
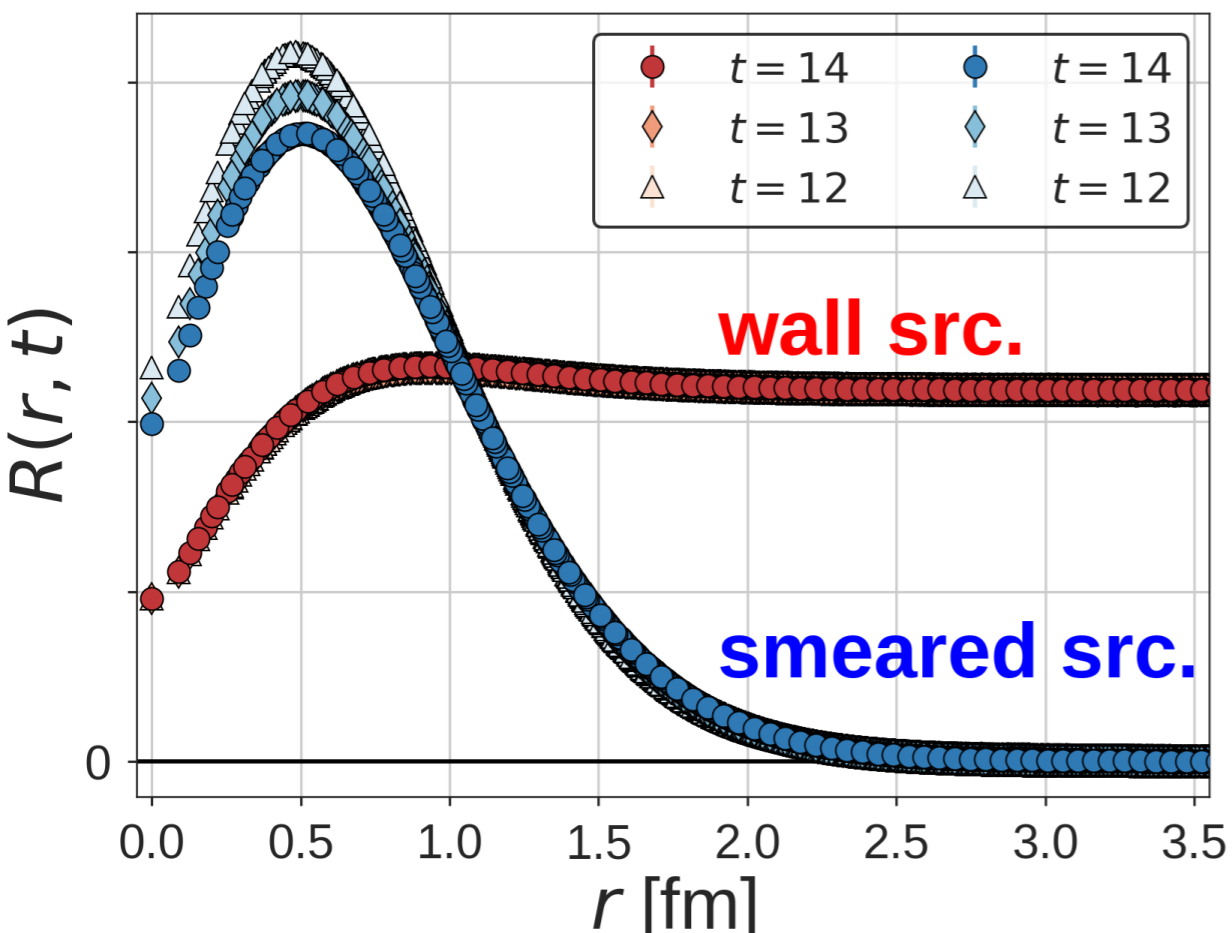
t-dep. implies systematics from truncation



Higher Order Approximation (N²LO) (1)

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

$$\left\{ \begin{array}{l} \frac{1}{4m_B} \frac{(\partial^2 / \partial t^2) R^{\text{wall}}}{R^{\text{wall}}} - \frac{(\partial / \partial t) R^{\text{wall}}}{R^{\text{wall}}} - \frac{H_0 R^{\text{wall}}}{R^{\text{wall}}} = V_0^{\text{N}^2\text{LO}}(r) + V_2^{\text{N}^2\text{LO}}(r) \frac{\nabla^2 R^{\text{wall}}}{R^{\text{wall}}} \\ \frac{1}{4m_B} \frac{(\partial^2 / \partial t^2) R^{\text{smear}}}{R^{\text{smear}}} - \frac{(\partial / \partial t) R^{\text{smear}}}{R^{\text{smear}}} - \frac{H_0 R^{\text{smear}}}{R^{\text{smear}}} = V_0^{\text{N}^2\text{LO}}(r) + V_2^{\text{N}^2\text{LO}}(r) \frac{\nabla^2 R^{\text{smear}}}{R^{\text{smear}}} \end{array} \right.$$



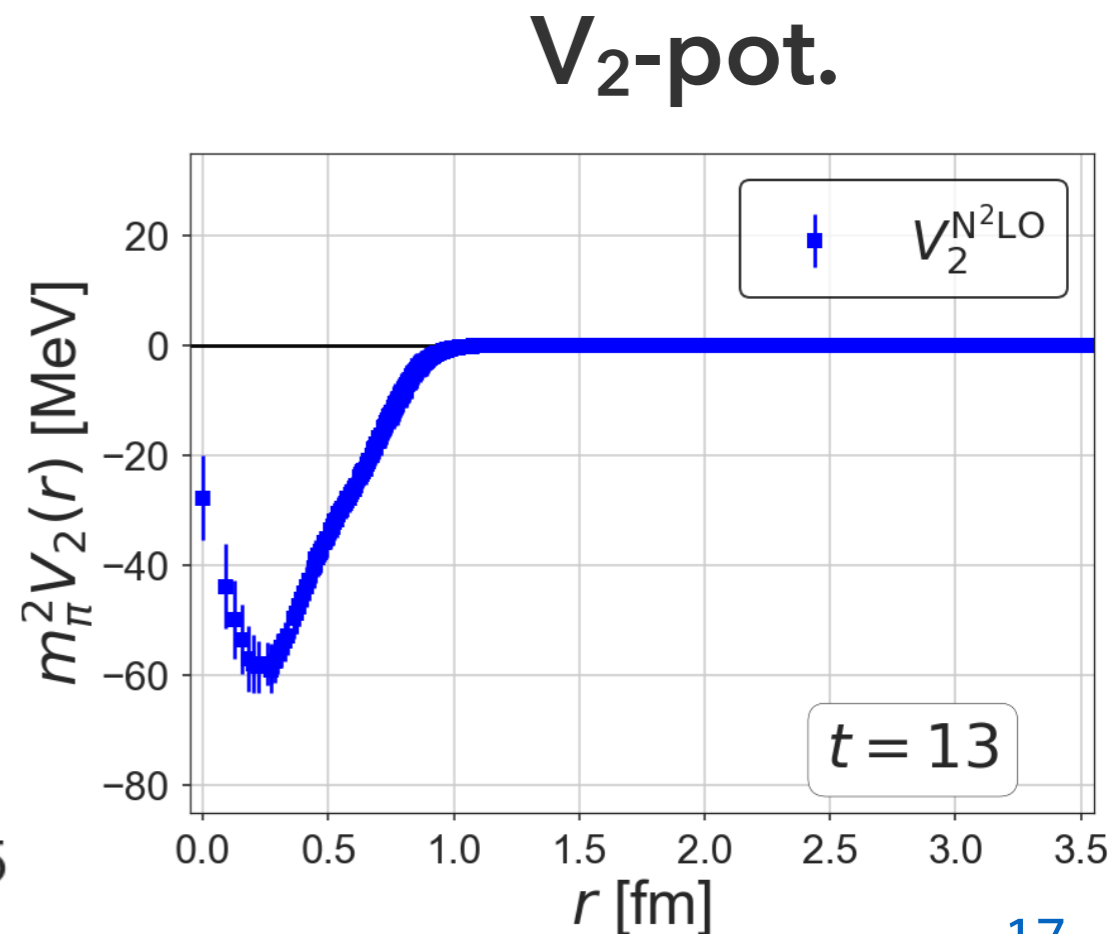
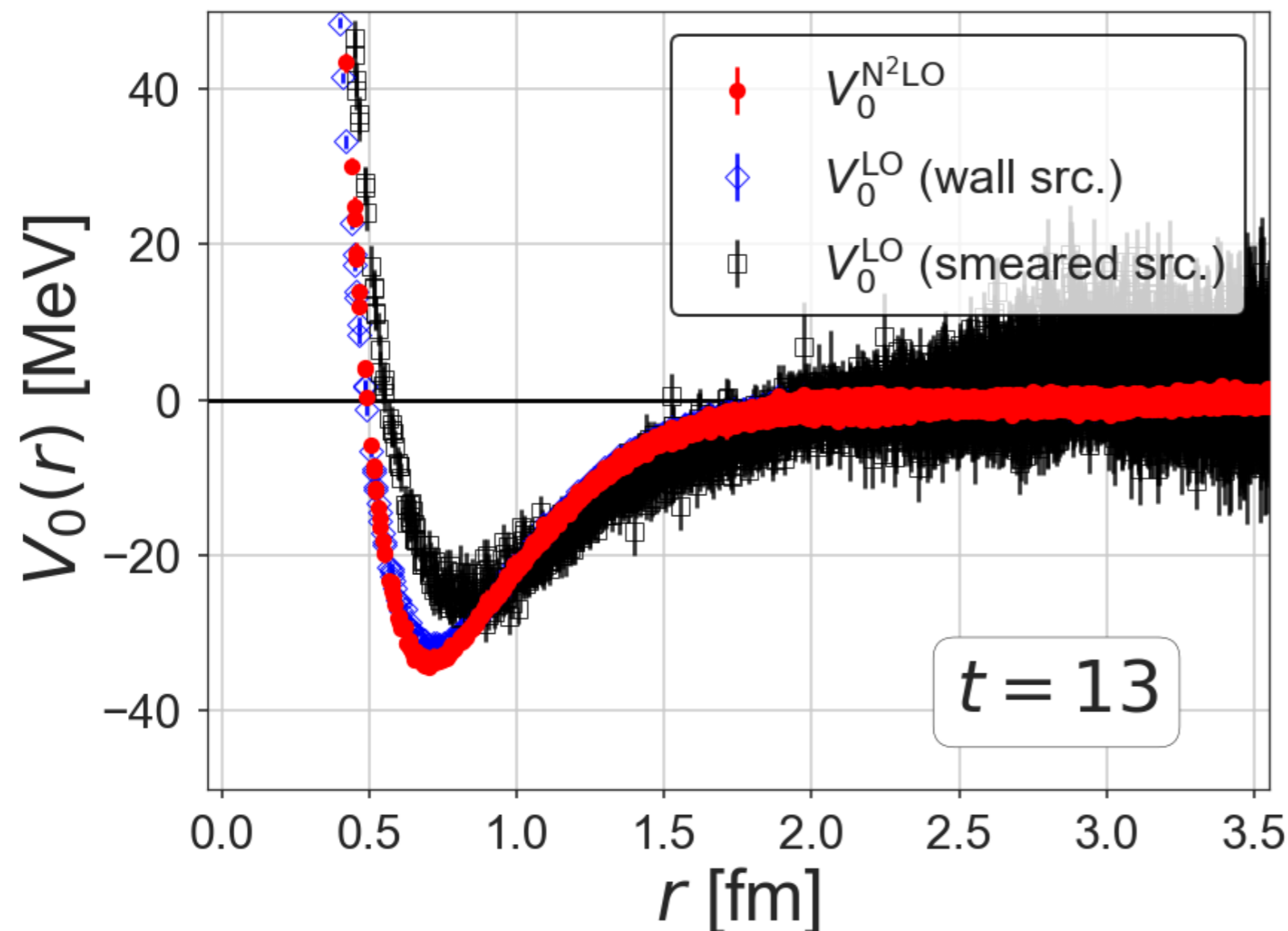
$V_0^{\text{N}^2\text{LO}}(r)$ and $V_2^{\text{N}^2\text{LO}}(r)$

Higher Order Approximation (N²LO) (2)

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

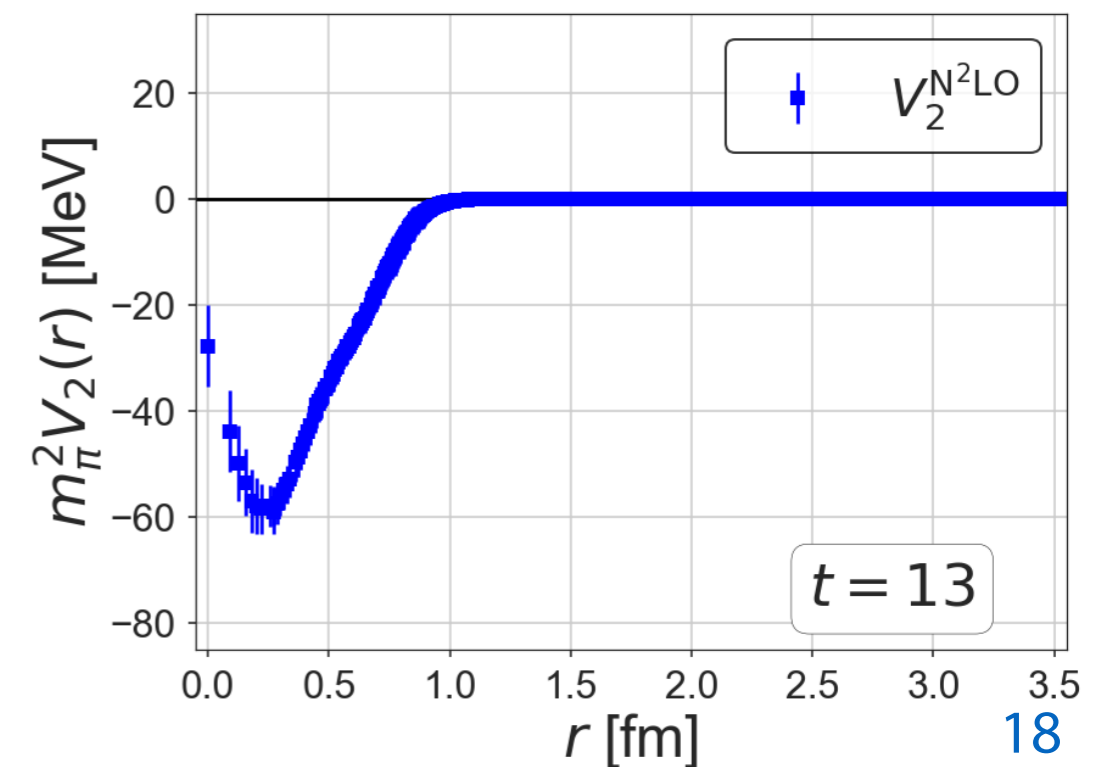
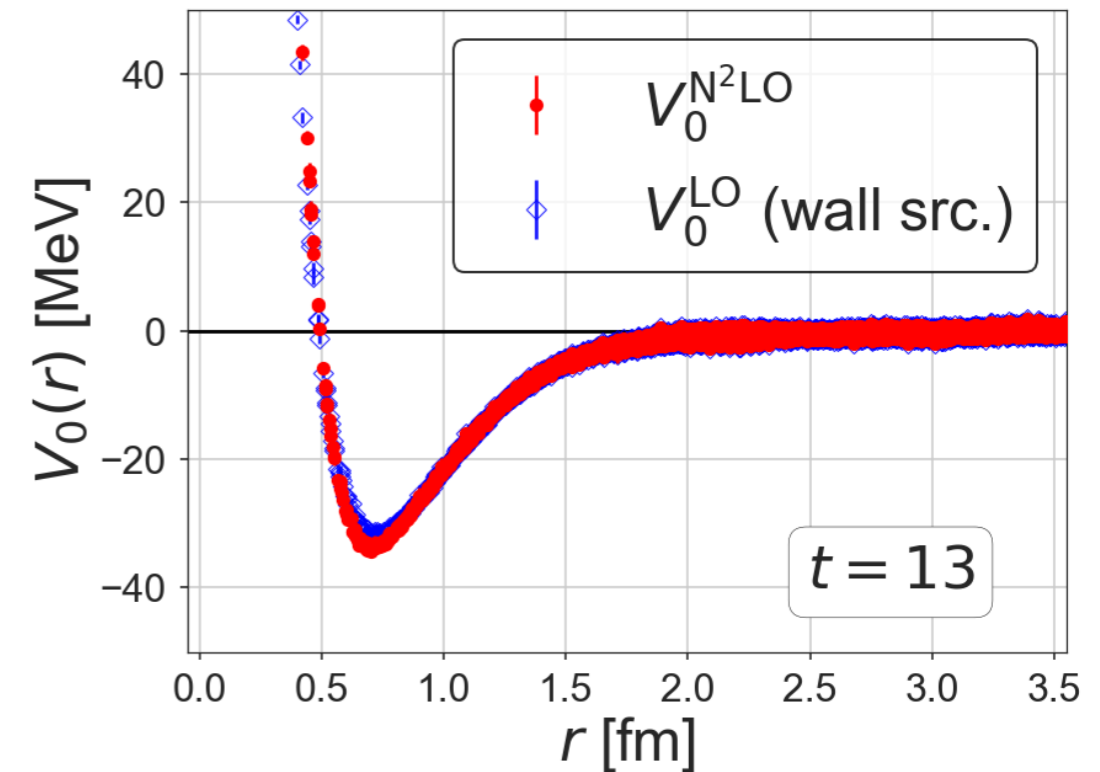
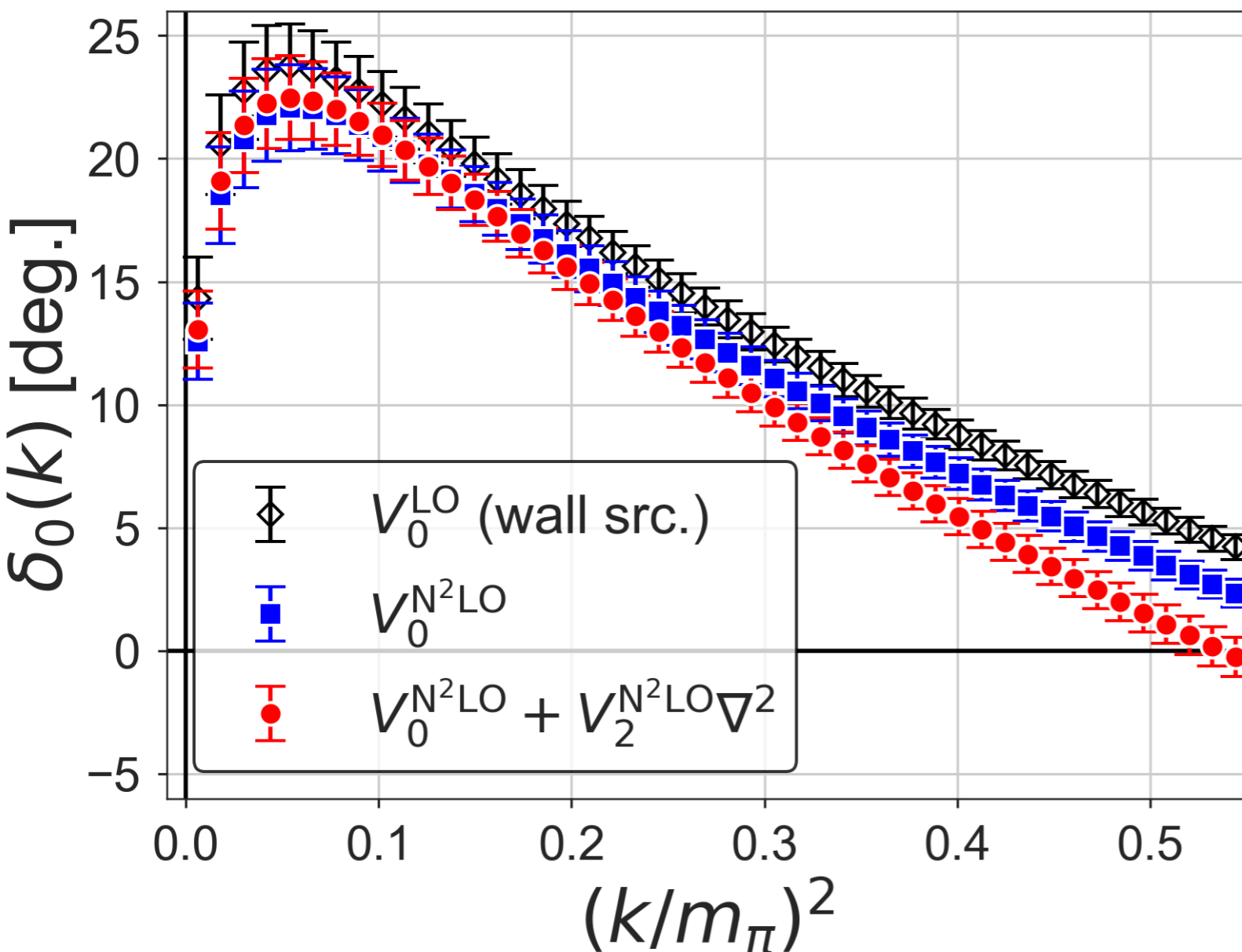
wall src. → small $V_2 \nabla^2$ correction
smearred src. → large $V_2 \nabla^2$ correction

→ $V_2(r) \frac{\nabla^2 R^{\text{wall/smear}}(r)}{\text{dep. on shape of R}}$



Phase Shift and Uncertainties in Velocity Expansion

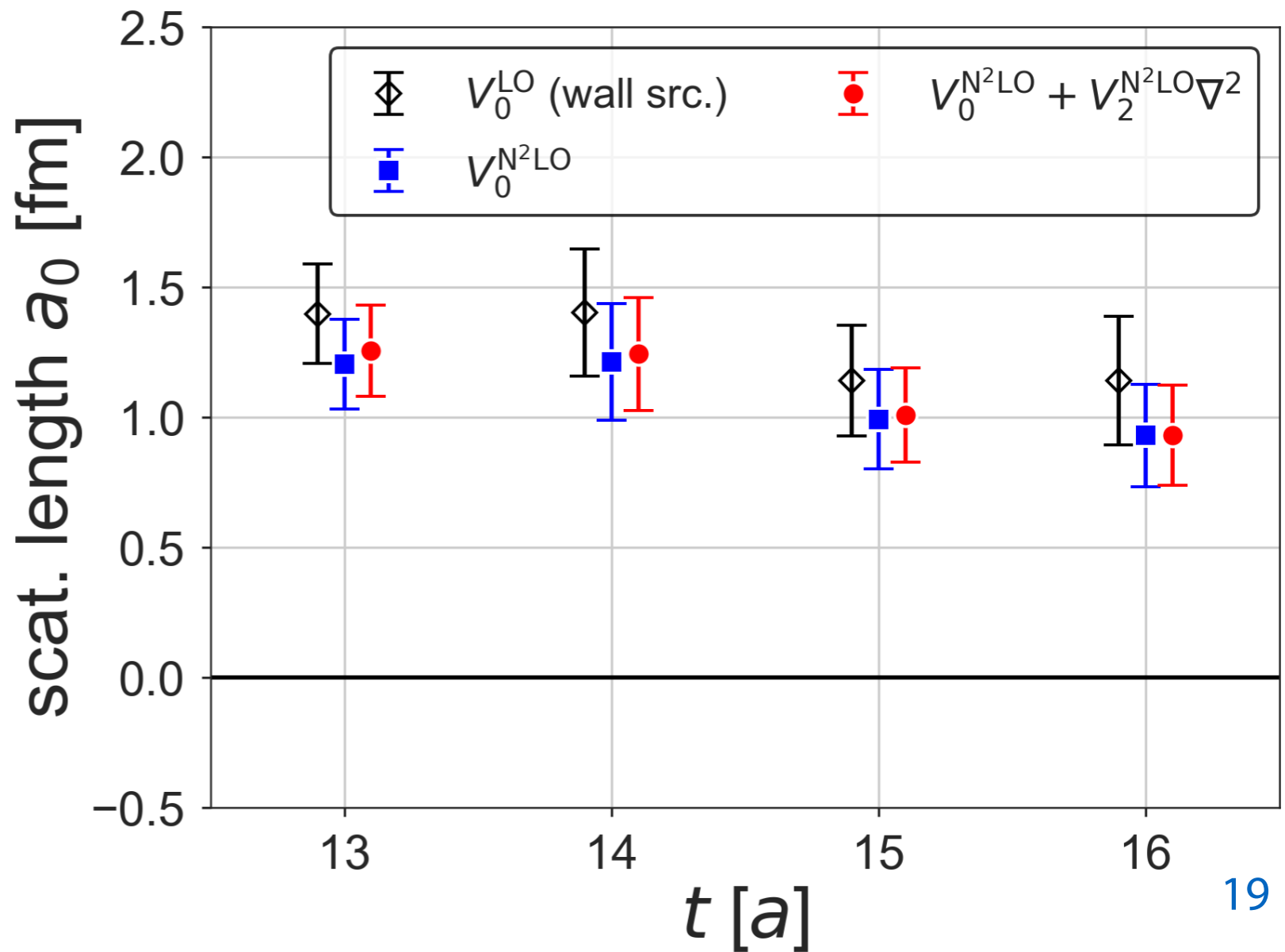
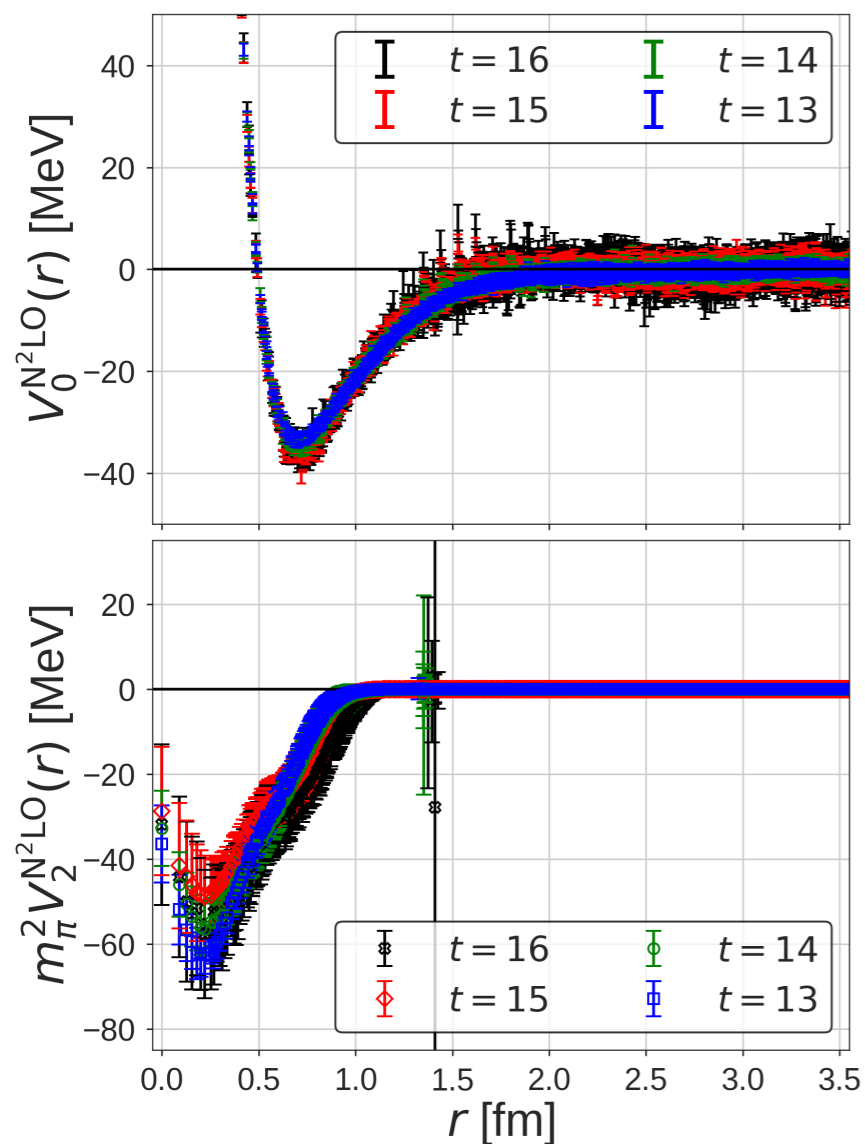
- **Wall src. LO approx.** (standard of HAL QCD studies) works well at low energy.
- **V_2 correction** at high energy



Time-dependence of Potential (N²LO)

- **N²LO** velocity expansion $U(r, r') \simeq \left[V_0^{\text{N}^2\text{LO}}(r) + V_2^{\text{N}^2\text{LO}}(r) \nabla^2 \right] \delta(r - r')$
t-indep. => convergence of the velocity expansion up to **N²LO**

Systematics in velocity expansion are under control.



Part I: Systematics in the HAL QCD Method

Ref.

TI for HAL QCD Coll., PoS(Lattice 2016) 109, arXiv:1610.09763.

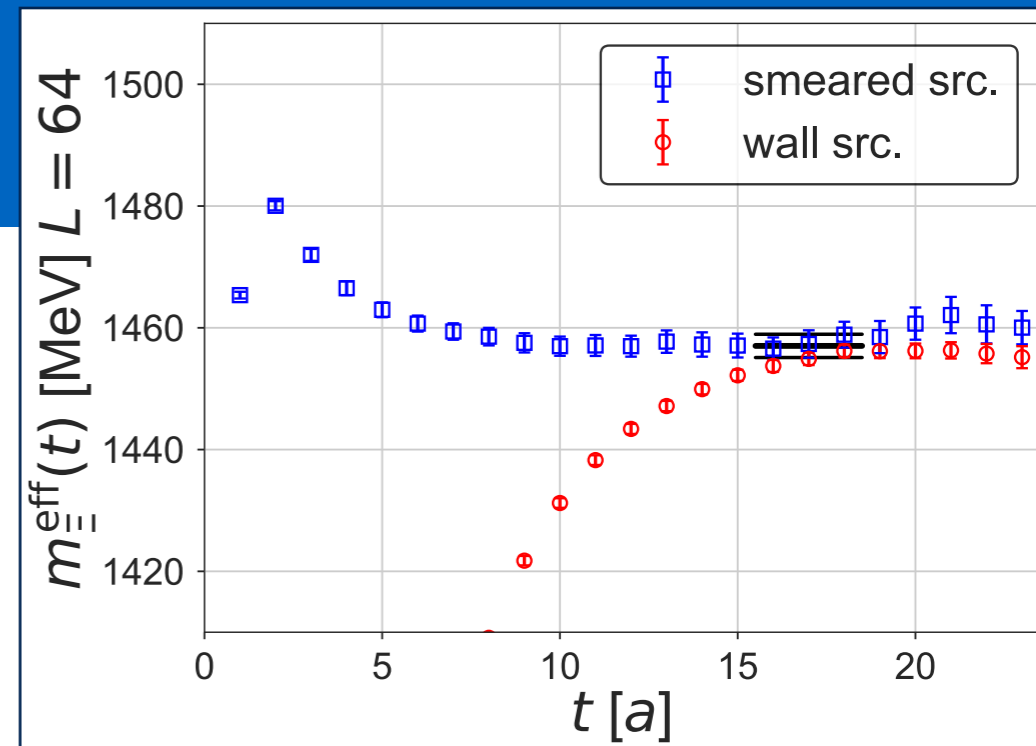
& in prep

1. convergence of velocity expansion

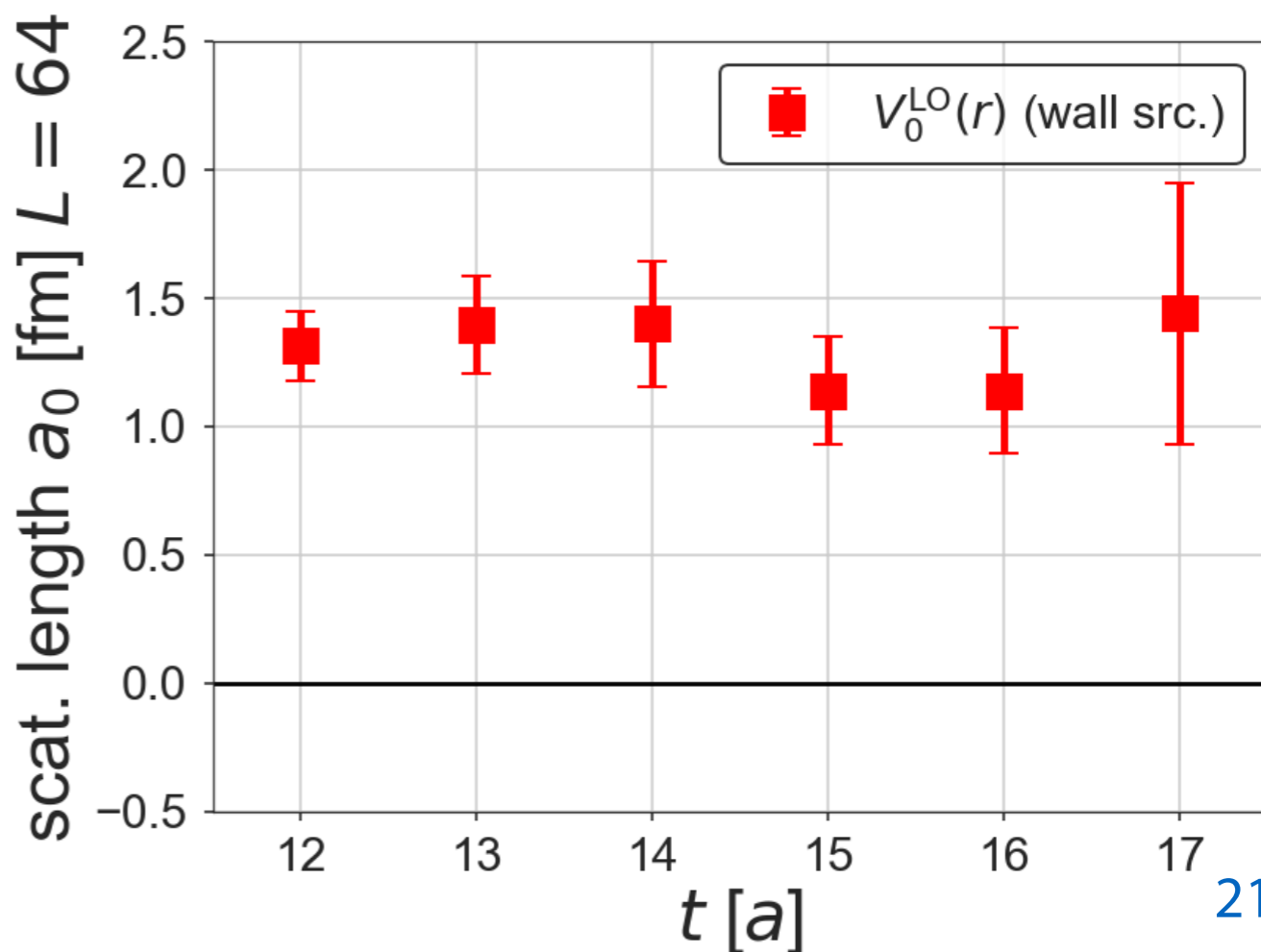
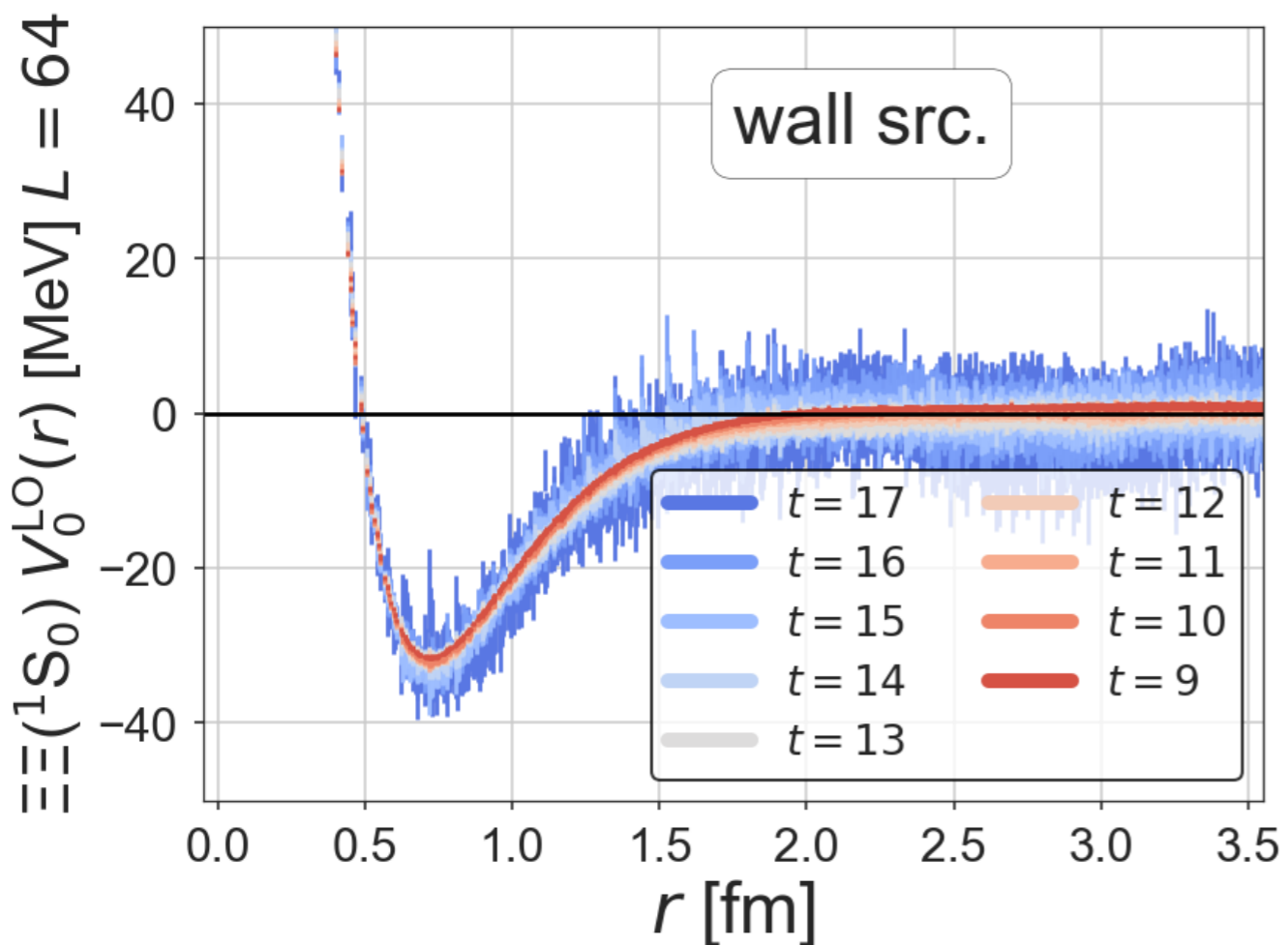
2. inelastic state contamination

t-dep. of the Wall src.

single saturation is later
than smeared src.



potential & observable are stable even at early time



Intermission:

**“Correct” finite volume method
analysis for two-baryon
in lattice QCD**

Lüscher's Method from HAL QCD: G.S. Energy

- **eigenvalue** at **finite box** L^3 with **HAL QCD pot.**

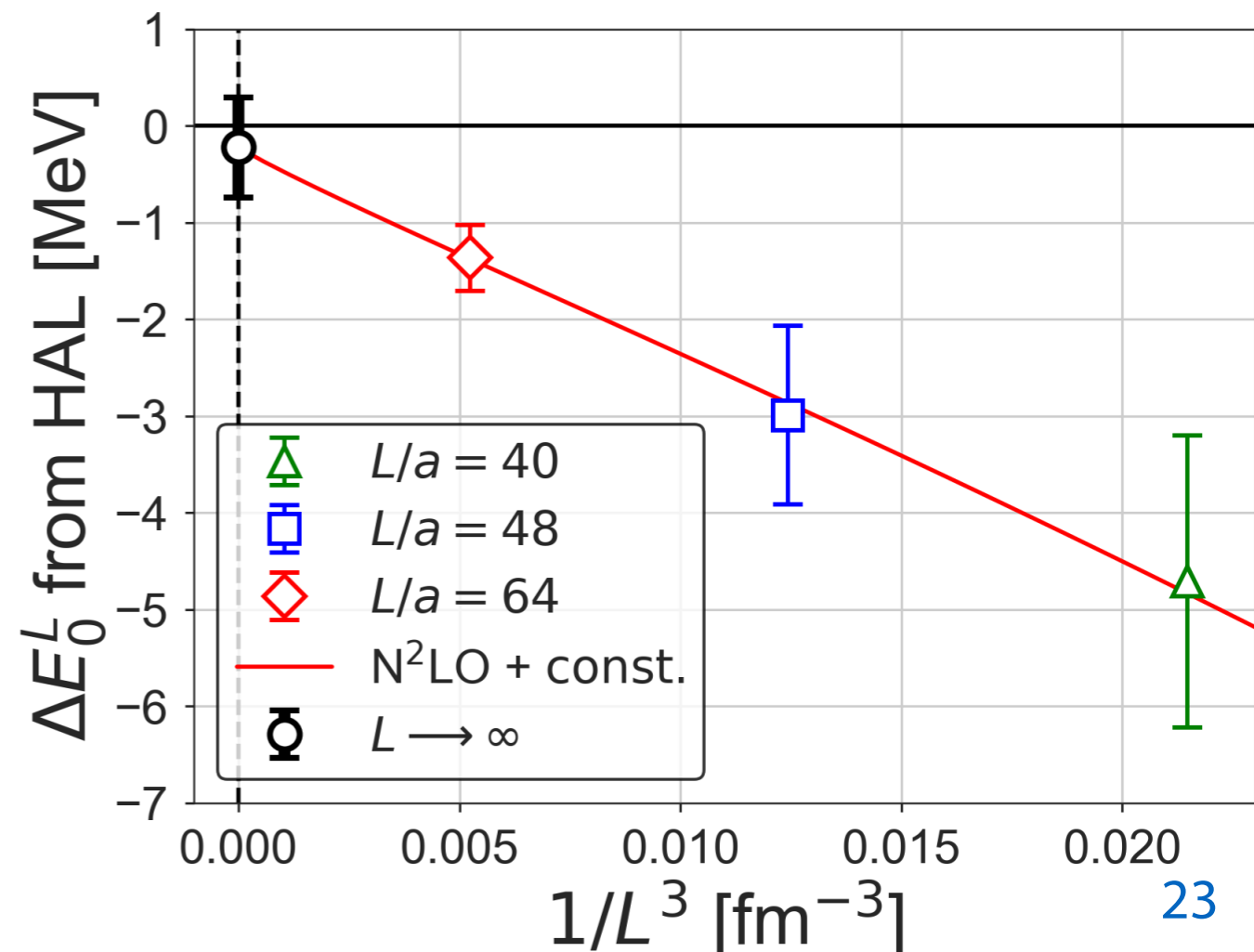
$$[H_0 + V_0(r) + V_2(r)\nabla^2]\Psi = \Delta E\Psi$$

$$\Delta E_0^L \simeq -\frac{2\pi a_0}{\mu L^3} \left[1 + c_1 \frac{a_0}{L} + c_2 \left(\frac{a_0}{L} \right)^2 \right]$$

→ **attractive** but **unbound**

scattering length

$$a_0 \equiv \lim_{k \rightarrow 0} \frac{\tan \delta(k)}{k}$$
$$= 0.93(29) \text{ fm}$$

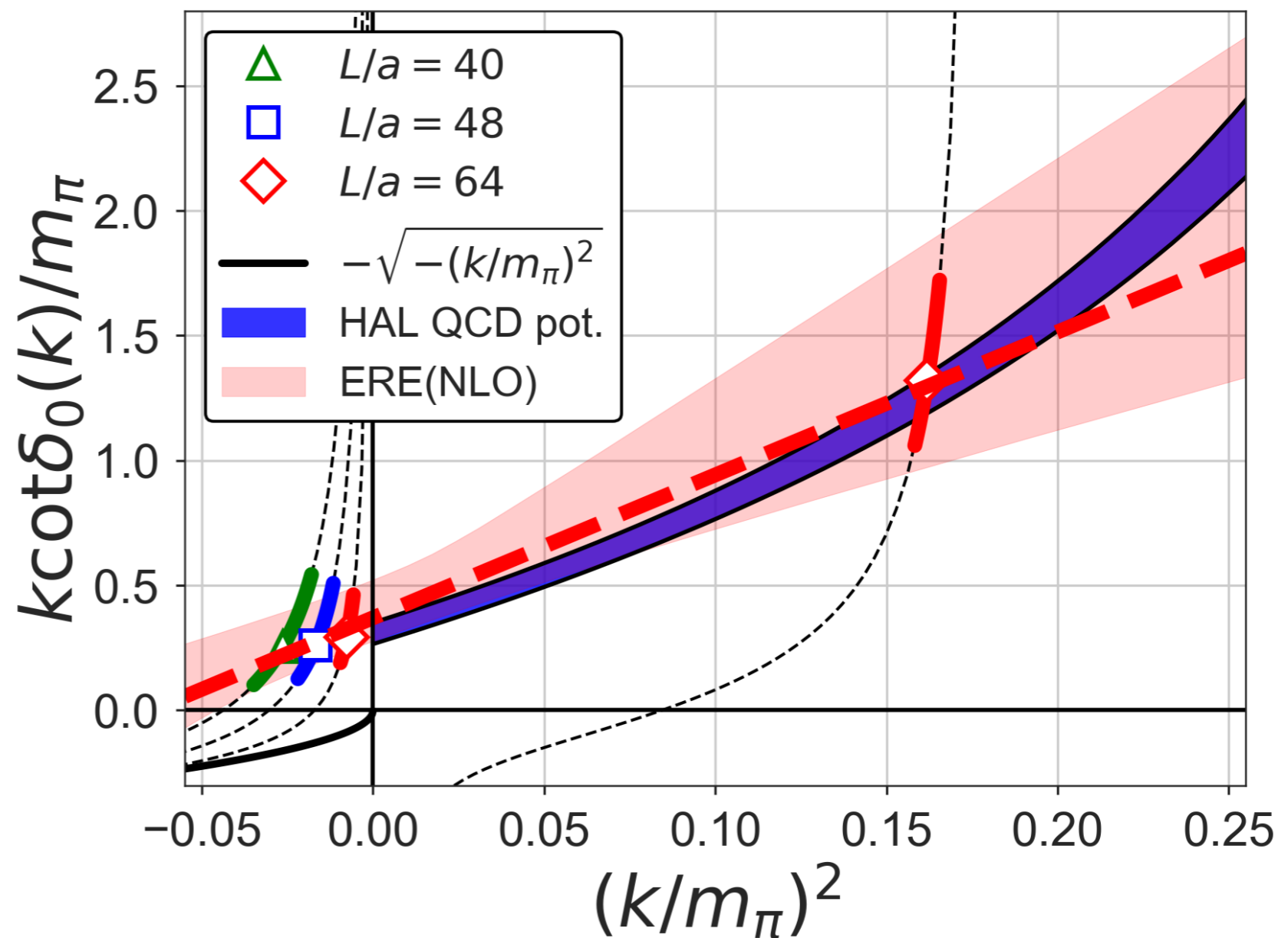
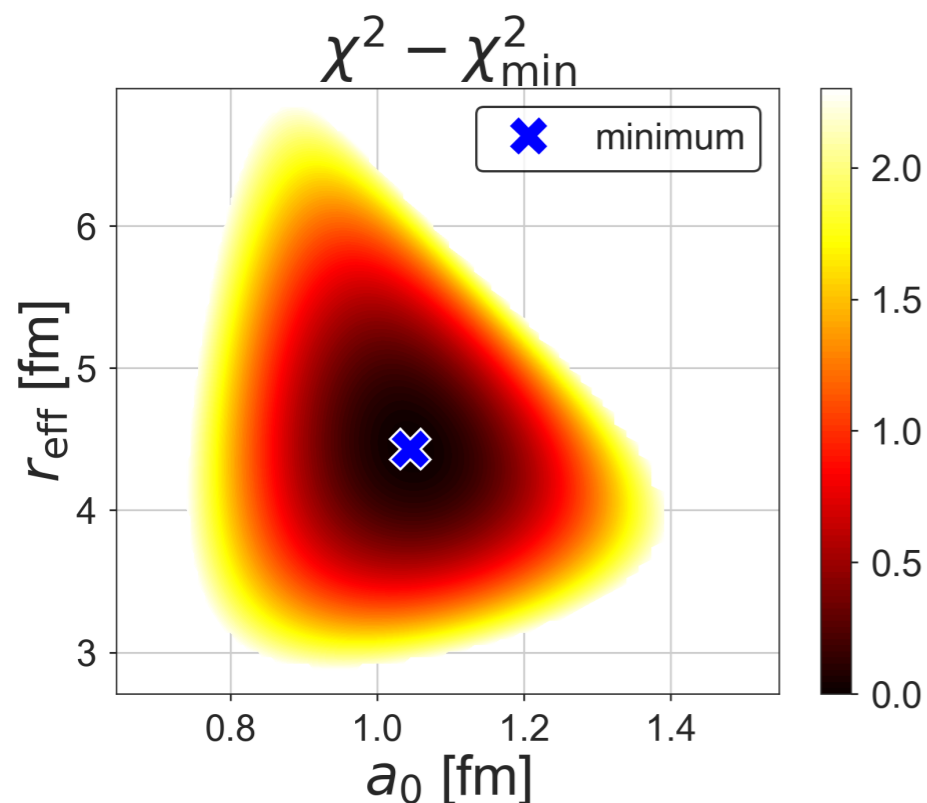


Lüscher's Method from HAL QCD: ERE Analysis

finite vol. energy shift $\Delta E_L \longrightarrow k \cot \delta(k)$ by Lüscher's formula

ERE(NLO) works well

$$k \cot \delta_0 = \frac{1}{a_0} + \frac{1}{2} r_{\text{eff}} k^2$$



Part II: Diagnosis of the Fake Plateaux in the Direct Method

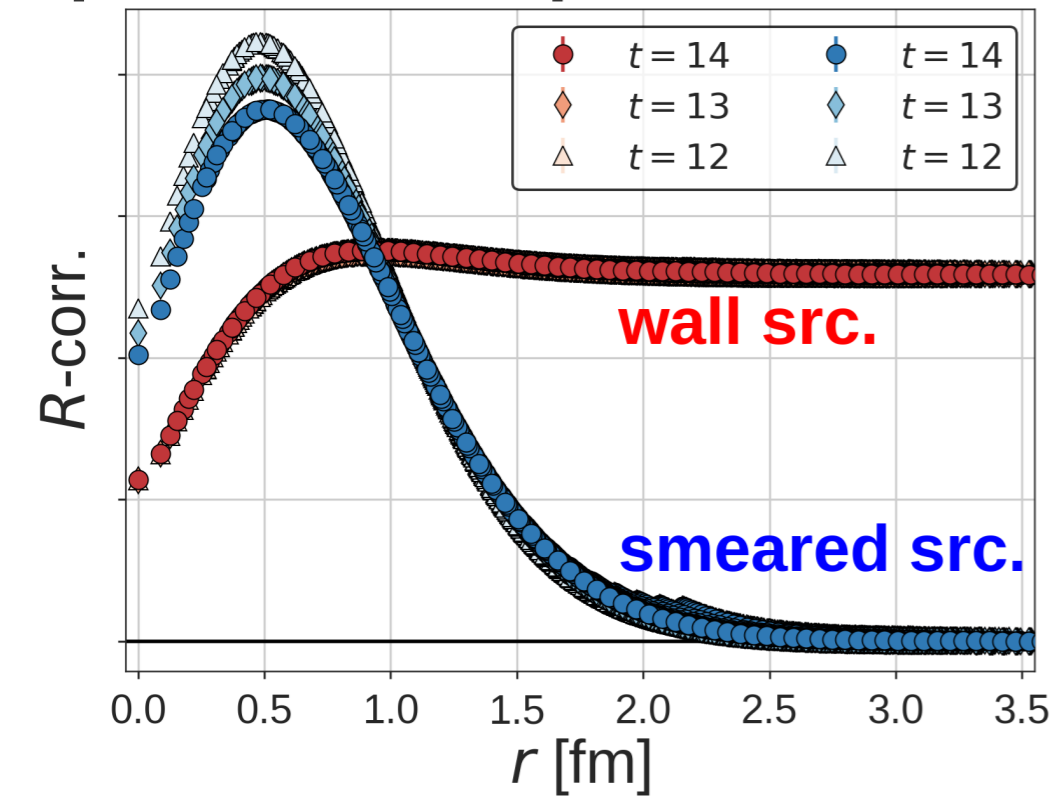
Ref.

TI for HAL QCD Coll., PoS(Lattice 2016) 109, arXiv:1610.09763.

& in prep.

Contamination and Fake Plateaux

Spatial(&Temporal) Correlation



$$R(\vec{r}, t) = \frac{C_{BB}(\vec{r}, t)}{\{C_B(t)\}^2}$$

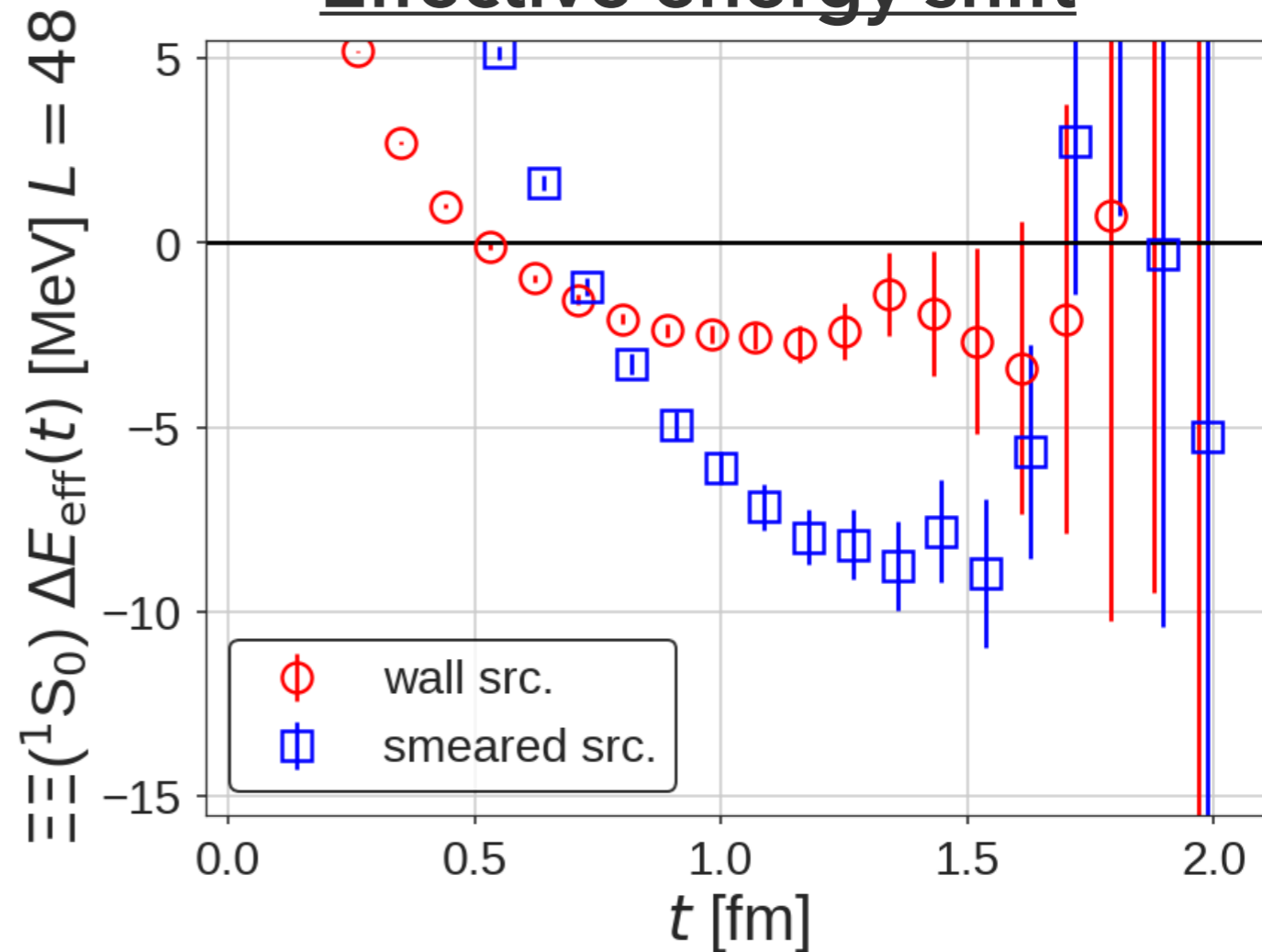
$$= \sum_n a_n \Psi_n(\vec{r}) e^{-\Delta E_n t}$$

↑



$$\Delta E_{\text{eff}}(t) = \log \frac{\sum_{\vec{r}} R(\vec{r}, t)}{\sum_{\vec{r}} R(\vec{r}, t+1)}$$

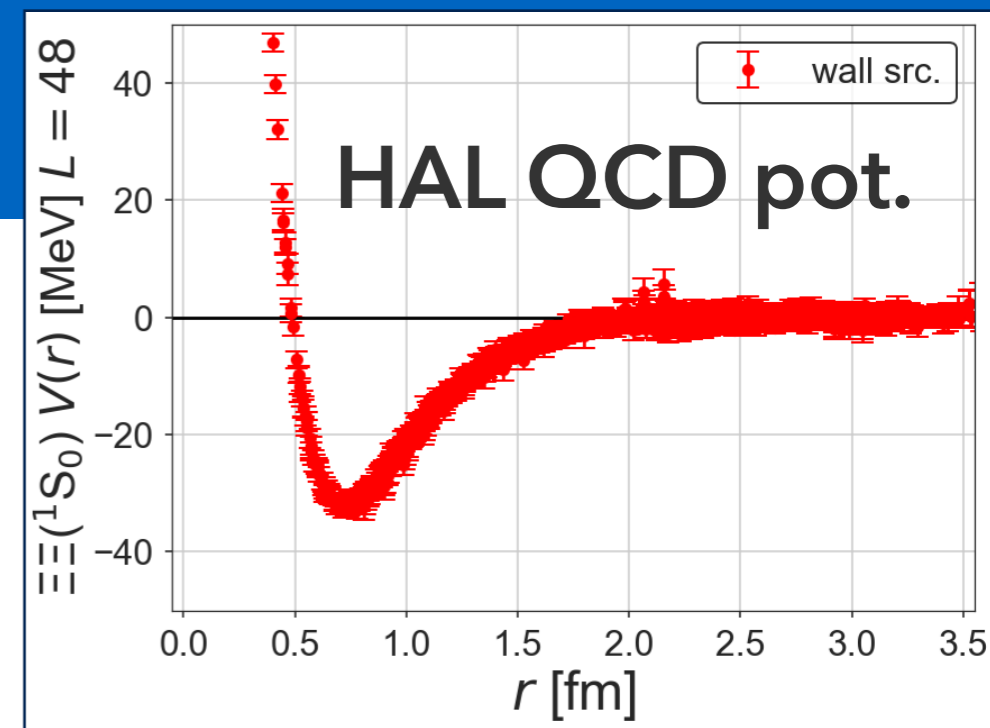
Effective energy shift



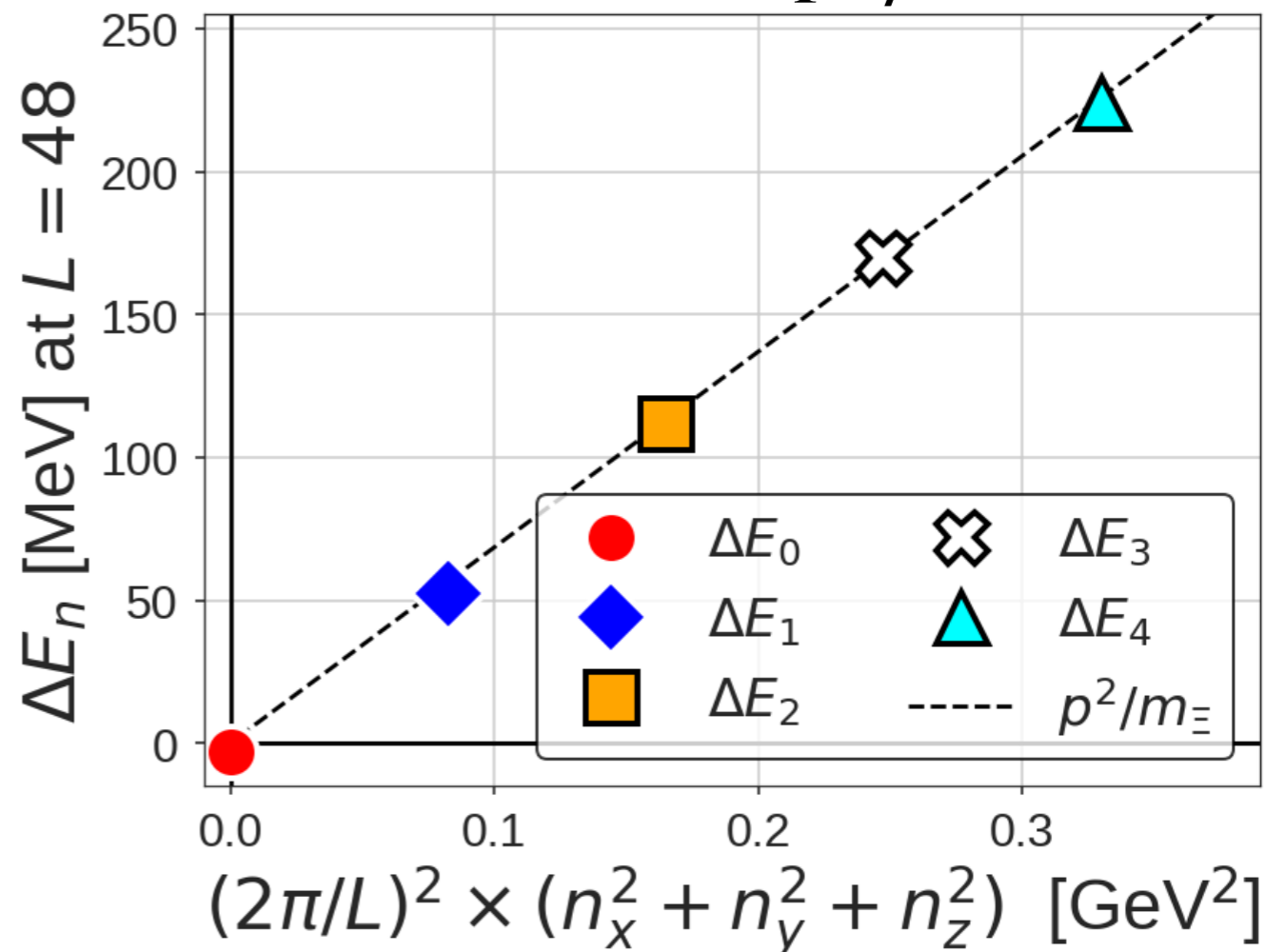
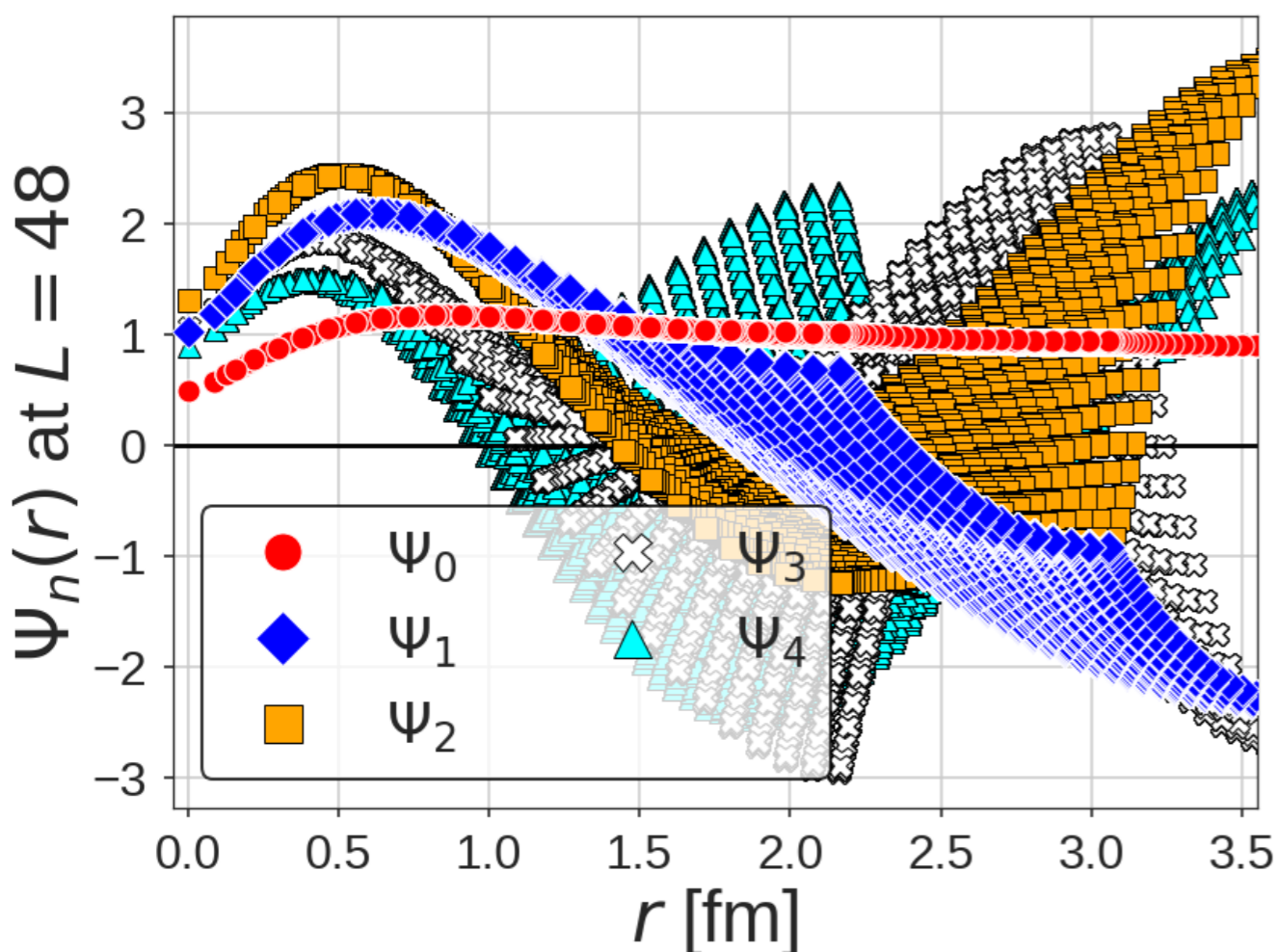
Final Check: magnitudes of the **contamination** & origin of the fake plateaux

Eigenfunctions & Eigenvalues

Solving $\underline{H_0 + V(r)}$ in the finite box



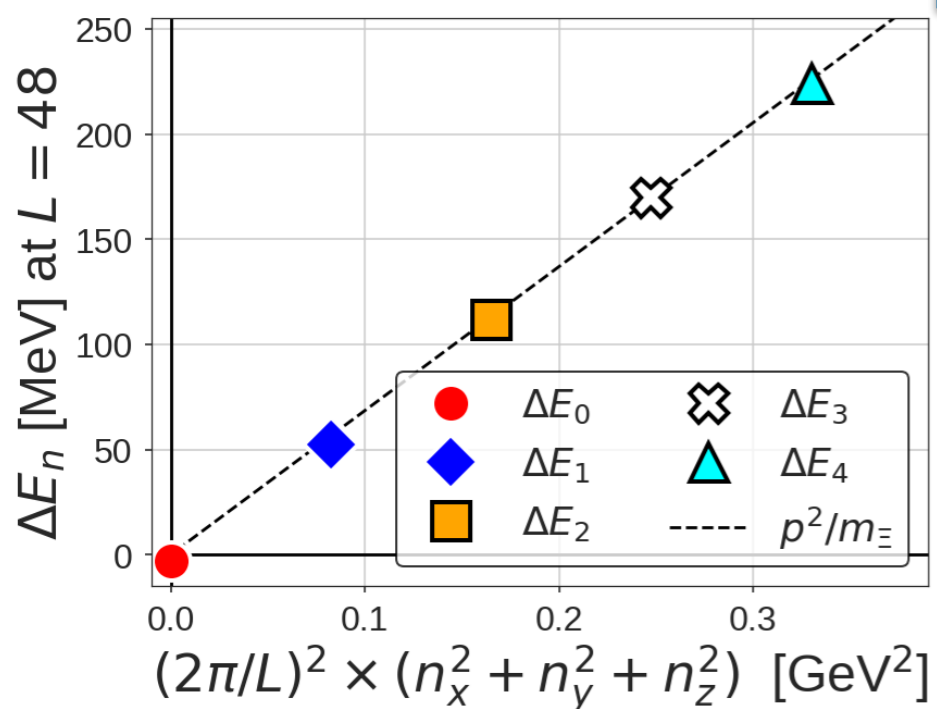
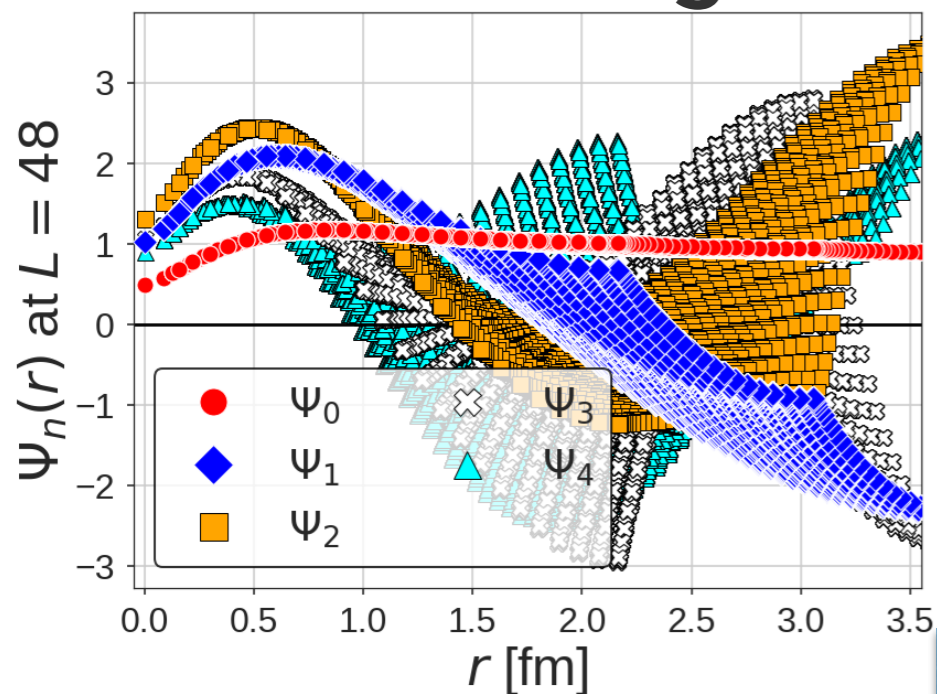
Low-lying eigenfunctions & eigenvalues $\sim p^2/m$



normalization $\sum |\Psi_n(r)|^2 = 1$

Eigenmode Decomposition of the Spatial Correlator

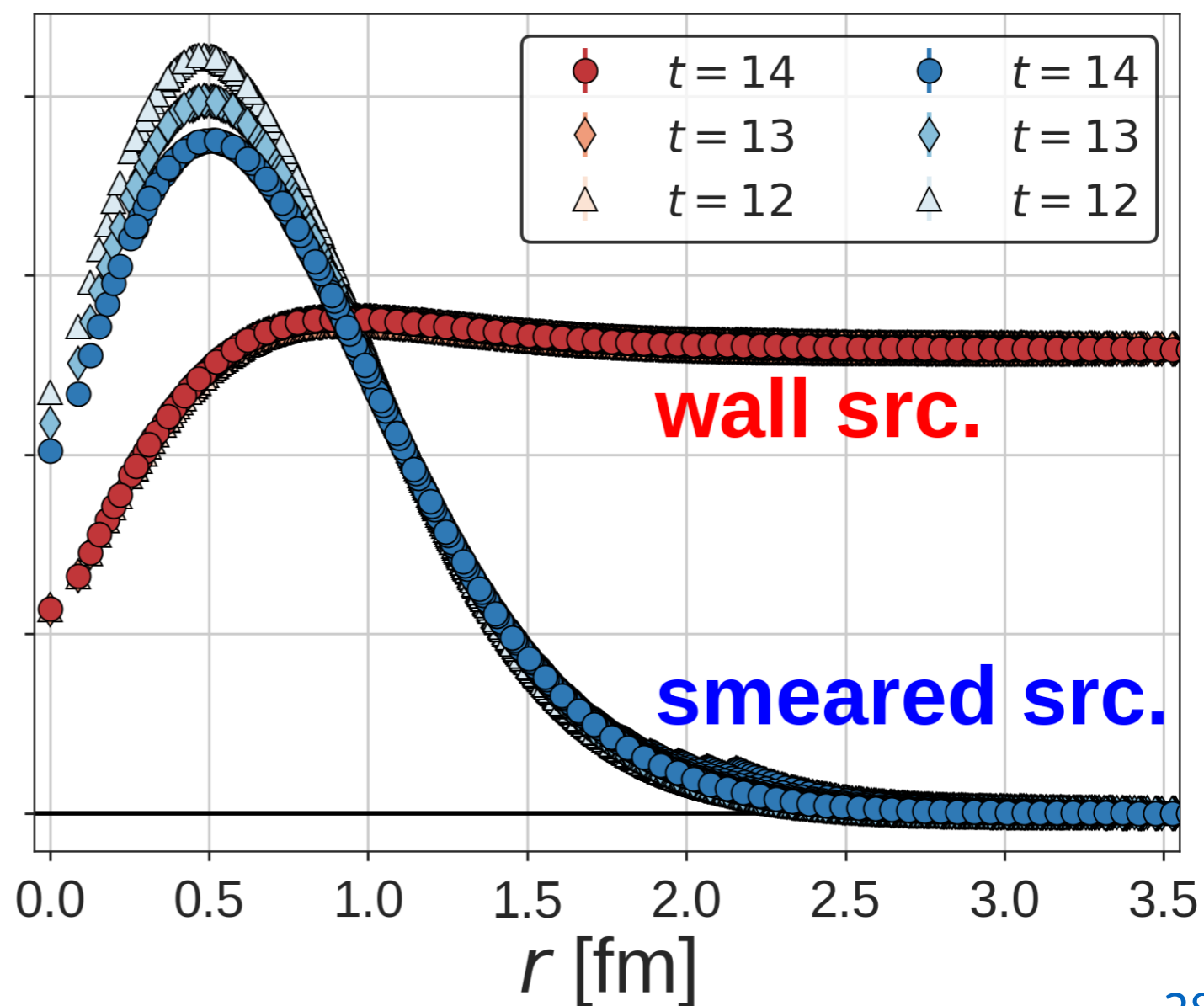
finite volume eigenstates



determine overlap coeff.

$$R^{\text{wall/smear}}(\vec{r}, t) = \sum_n a_n^{\text{wall/smear}} \Psi_n(\vec{r}) e^{-\Delta E_n t}$$

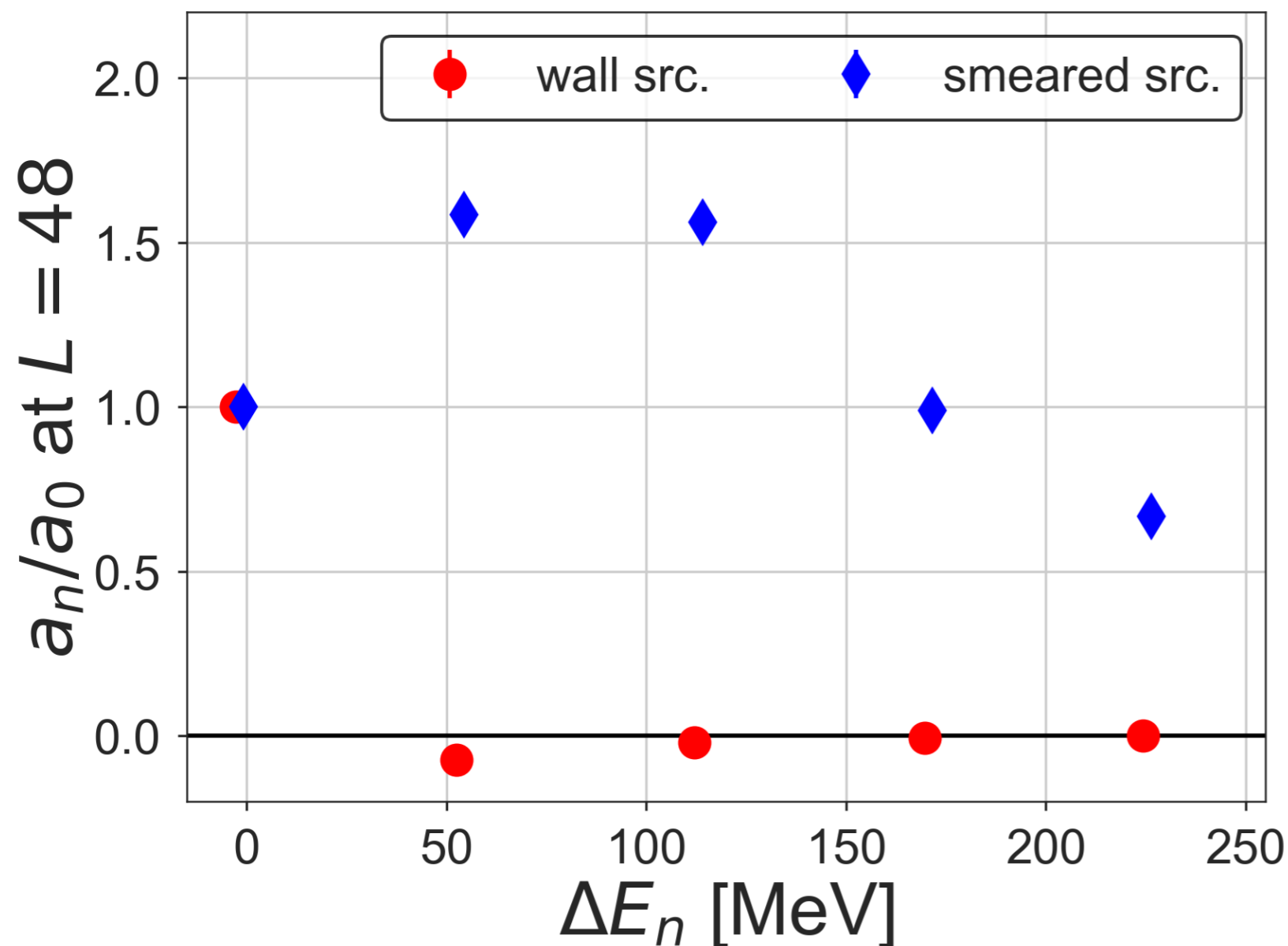
R-corr.



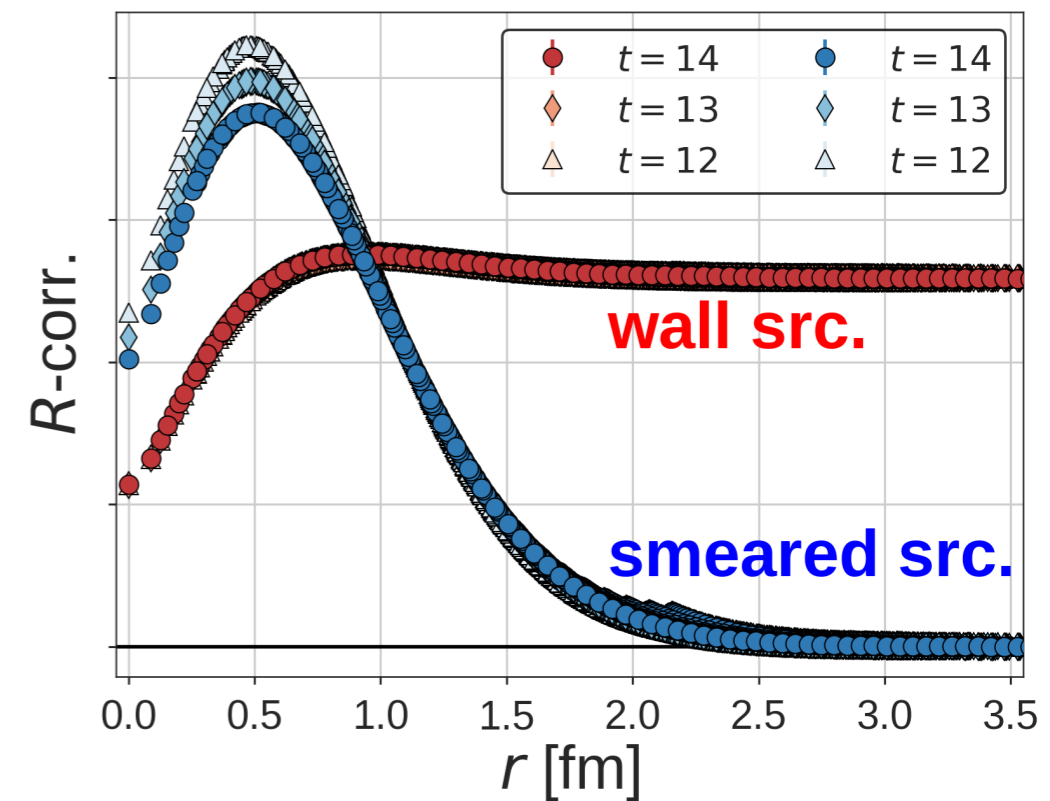
Overlap of Excited States

$$R^{\text{wall/smear}}(\vec{r}, t) = \sum_n a_n^{\text{wall/smear}} \Psi_n(\vec{r}) e^{-\Delta E_n t}$$

"smeared src." has large overlaps with **scat. states**.



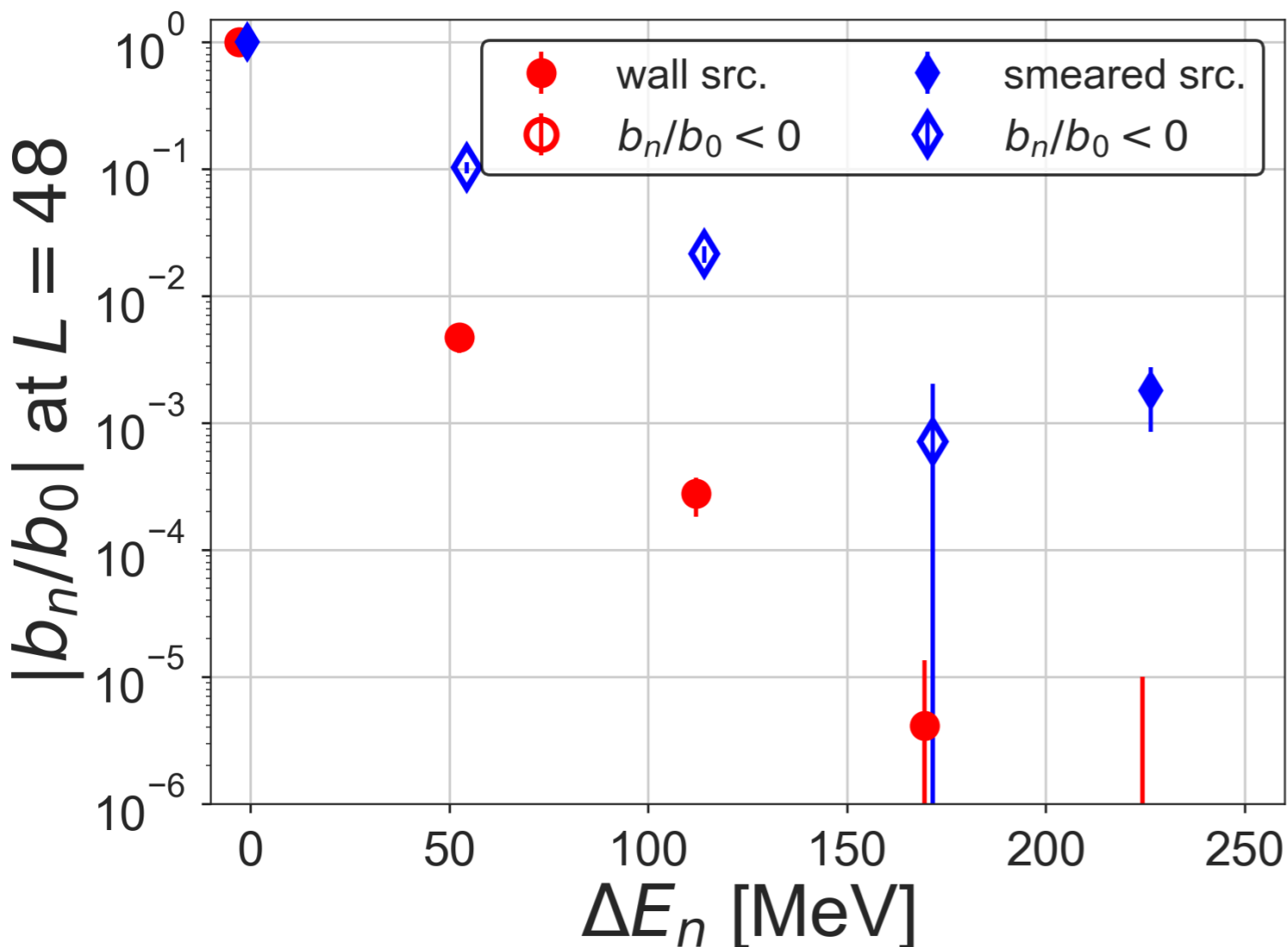
$$\mathcal{O}(a_0^{\text{smear}}) \sim \mathcal{O}(a_n^{\text{smear}})$$



Contaminations of Excited States

$$R(t) = \sum_n b_n^{\text{wall/smear}} e^{-\Delta E_n t} \quad \text{with} \quad b_n^{\text{wall/smear}} = a_n^{\text{wall/smear}} \sum_{\vec{r}} \Psi_n(\vec{r})$$

b_n : magnitude of contamination in $\Delta E_{\text{eff}}(t)$



ex.

- **wall source**

$$b_1/b_0 \ll 1 \%$$

- **smeared source**

$$|b_1/b_0| \simeq 10 \%$$

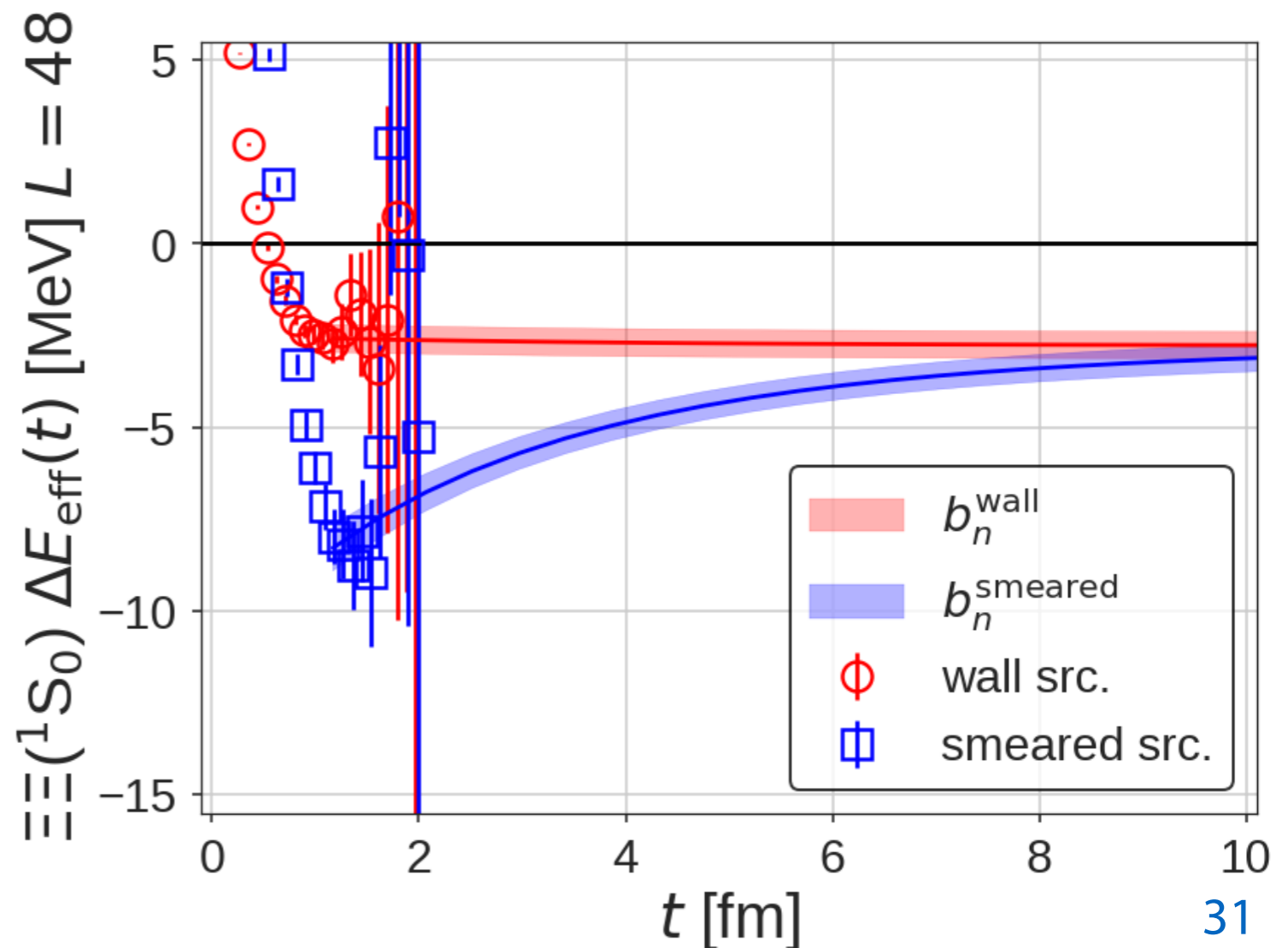
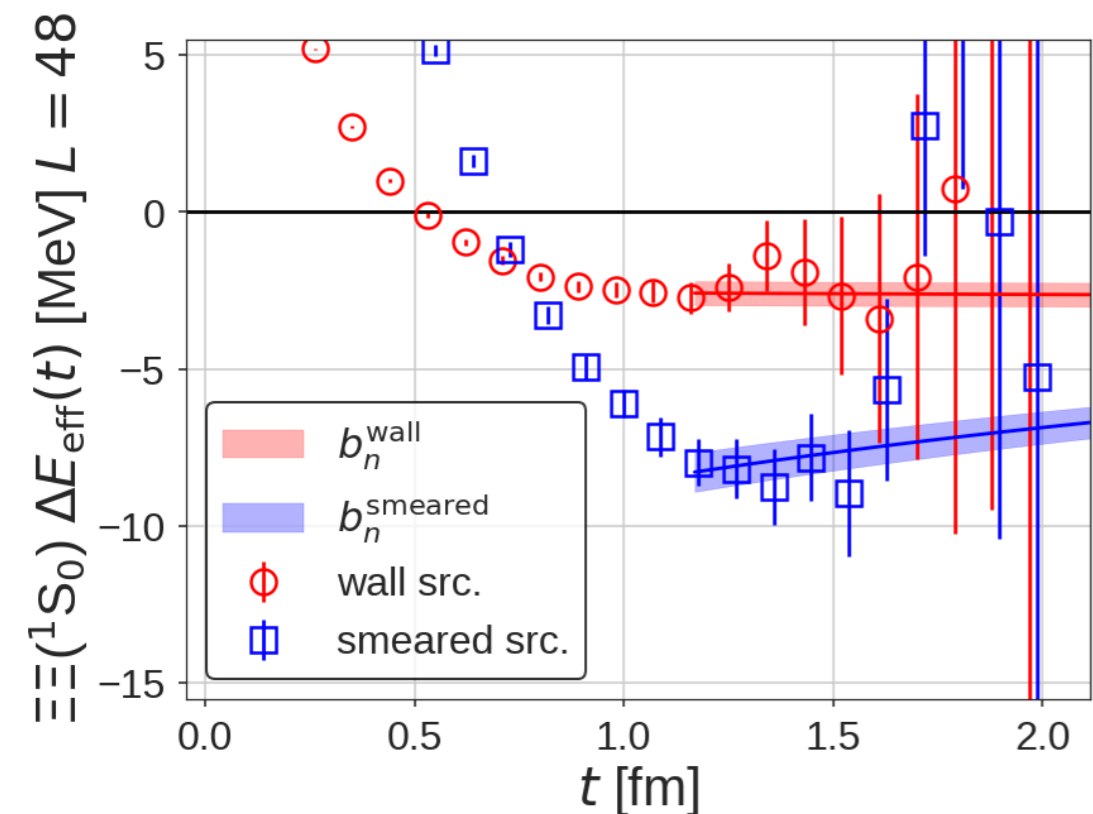
Origin of Fake Plateaux and Saturation

$$\Delta E_{\text{eff}}^{\text{wall/smear}}(t) \equiv \log \frac{R(t)}{R(t+1)} = \log \frac{\sum_n b_n^{\text{wall/smear}} \exp(-\Delta E_n t)}{\sum_n b_n^{\text{wall/smear}} \exp(-\Delta E_n (t+1))}$$

- "direct measurement" is reproduced by **low-modes**

g.s. saturation for **smear**ed src. \sim **10 fm !!!**

naïve expectation
 $1/\delta E_{\text{el.}} \sim 10 \text{ fm}$

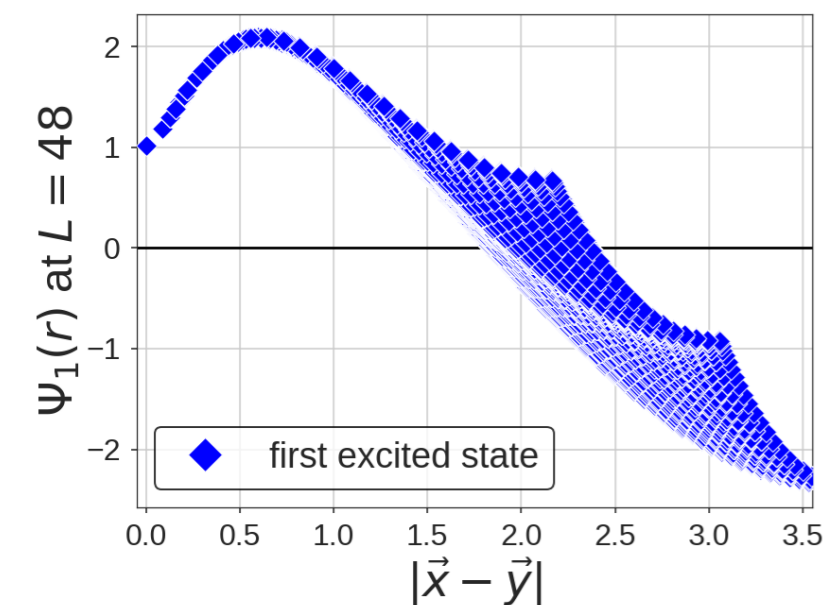
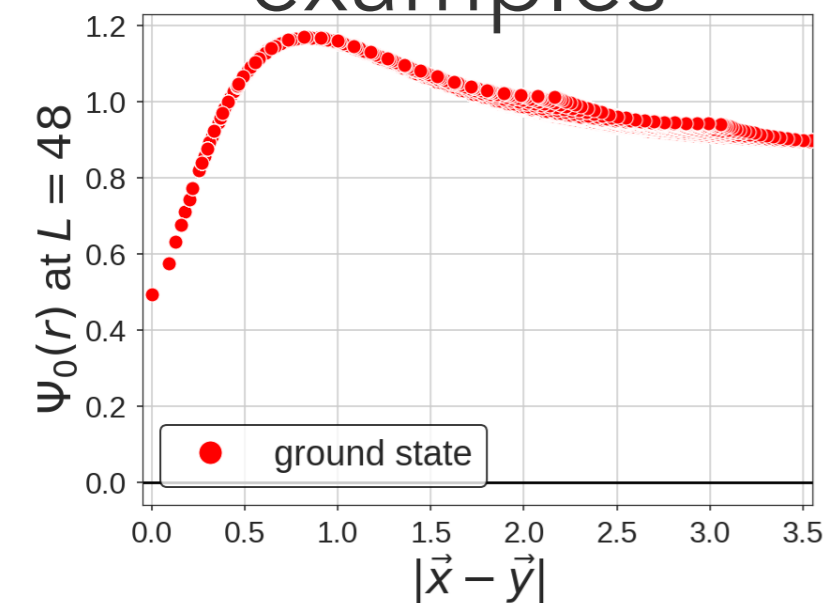


Sink Op. Projection with Proper Eigenmode (1)

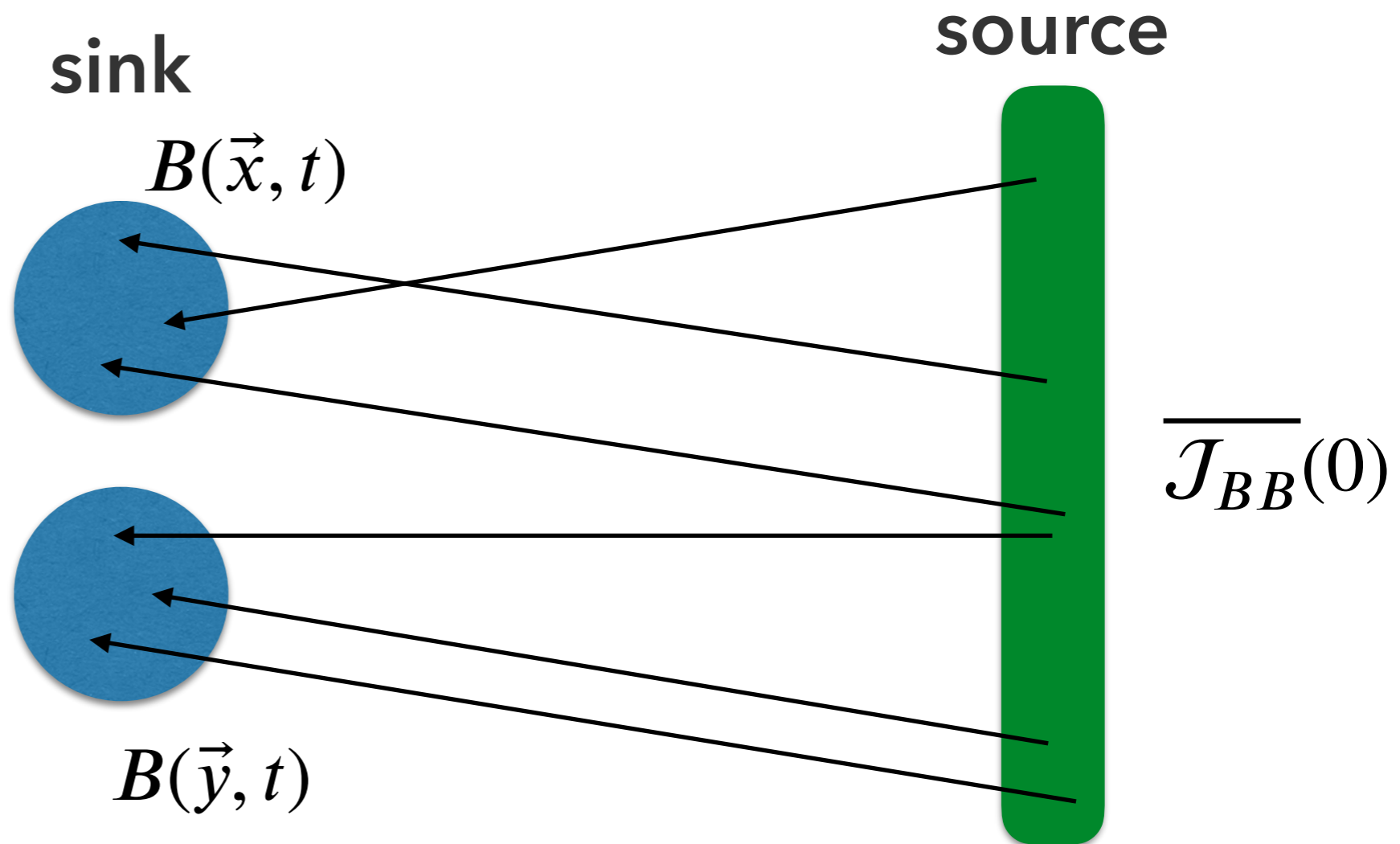
- "correct sink operator"

$$R^{(n)}(t) = \sum_{\vec{x}, \vec{y}} \Psi_n(|\vec{x} - \vec{y}|) \langle B(\vec{x}, t) B(\vec{y}, t) \overline{\mathcal{J}_{BB}(0)} \rangle / \{C_B(t)\}^2$$

examples



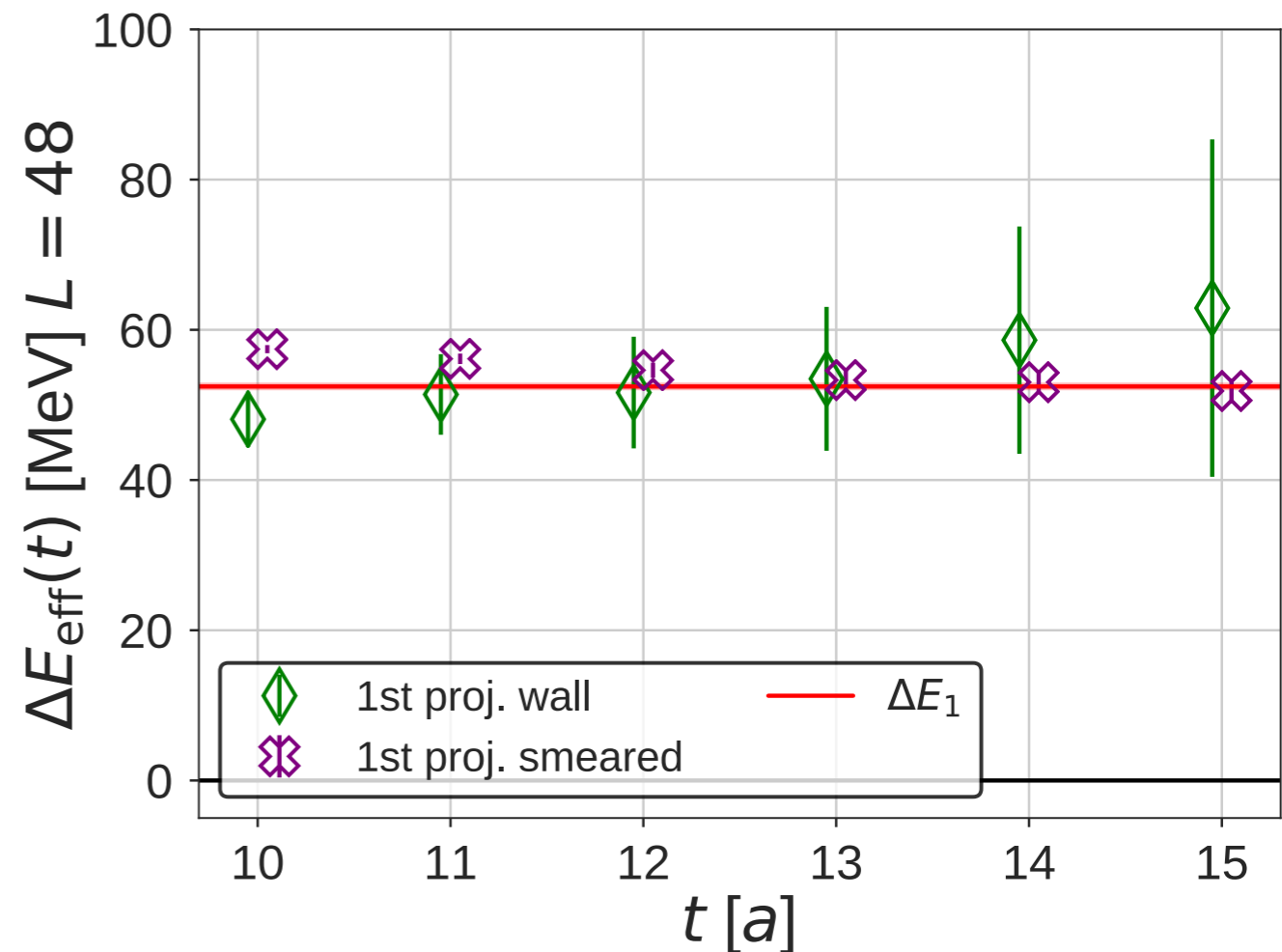
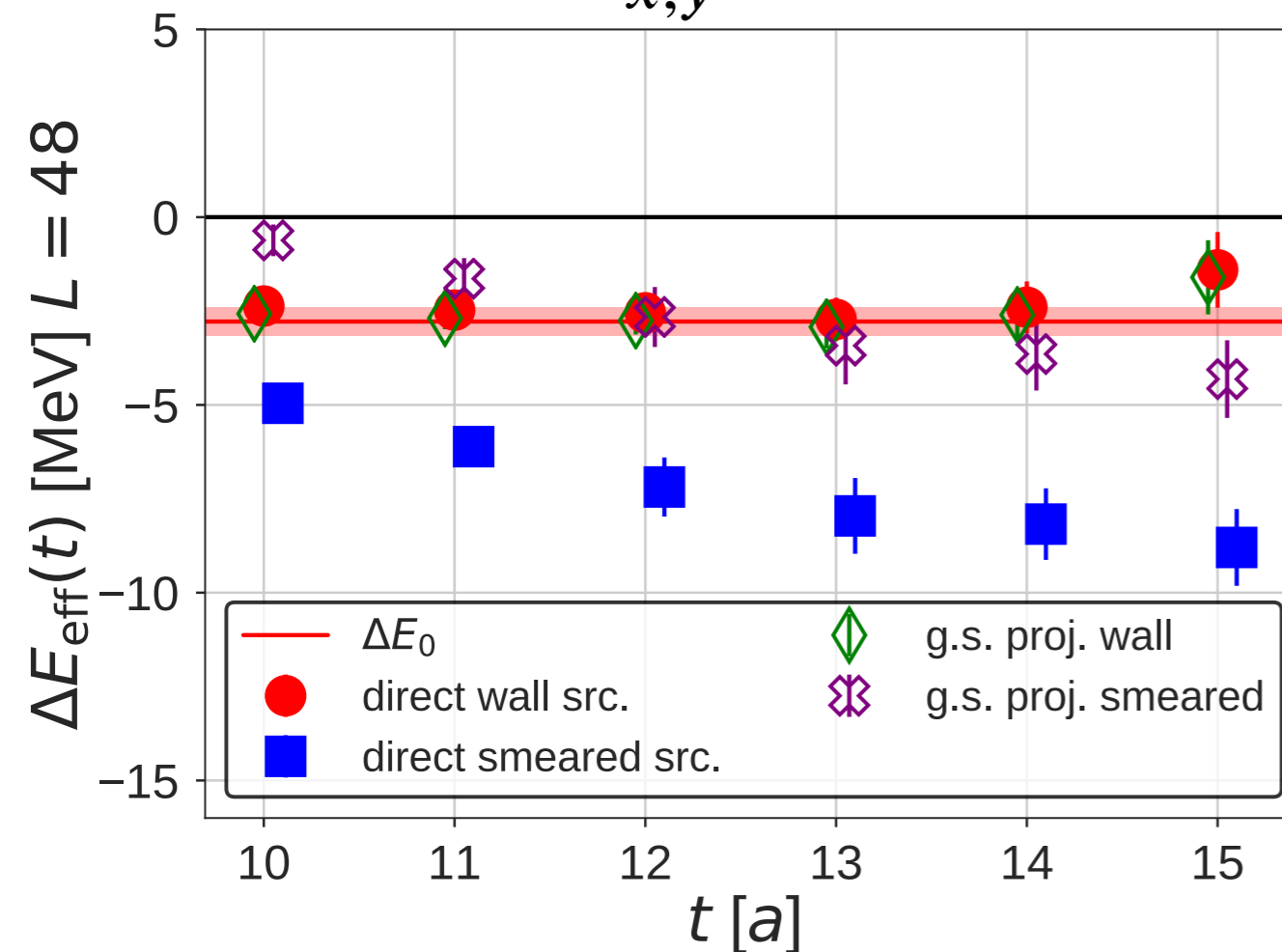
$\Psi(|\vec{x} - \vec{y}|)$



Sink Op. Projection with Proper Eigenmode (2)

- “correct sink operator” \rightarrow “true plateau” appears

$$R^{(n)}(t) = \sum_{\vec{x}, \vec{y}} \Psi_n(|\vec{x} - \vec{y}|) \langle B(\vec{x}, t) B(\vec{y}, t) \overline{\mathcal{J}_{BB}(0)} \rangle / \{C_B(t)\}^2$$



HAL QCD = Lüscher's method with *proper projection*
≠ naive plateau fitting

Summary

Direct Method vs. HAL QCD Method

- HAL QCD method can control **scattering states**.
- We checked
 - **The velocity expansion of non-local pot.** has **good convergence at low energies**.
 - **Leading order expansion of the wall src.**
(standard of HAL QCD studies) **works well**.
 - **The inelastic state contamination** is **under control**.
- We show the origin of the fake plateau in the direct method comes from the scattering state contamination.
- **HAL QCD** results at (almost) **physical point**

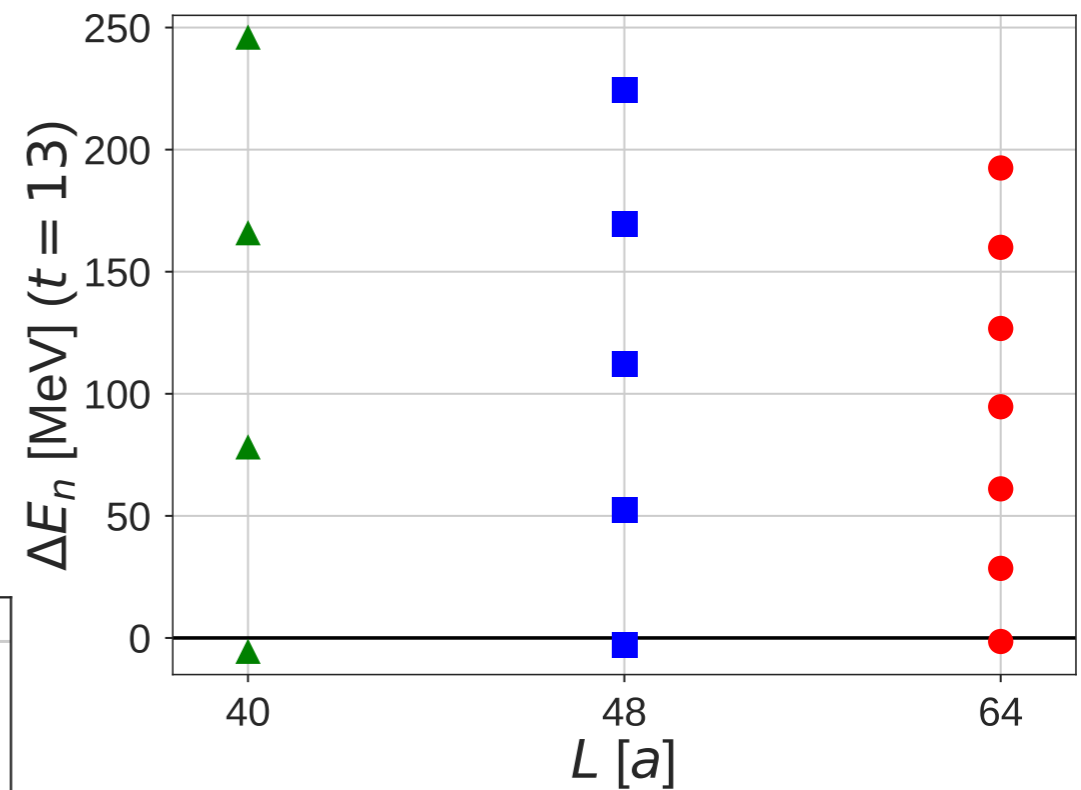
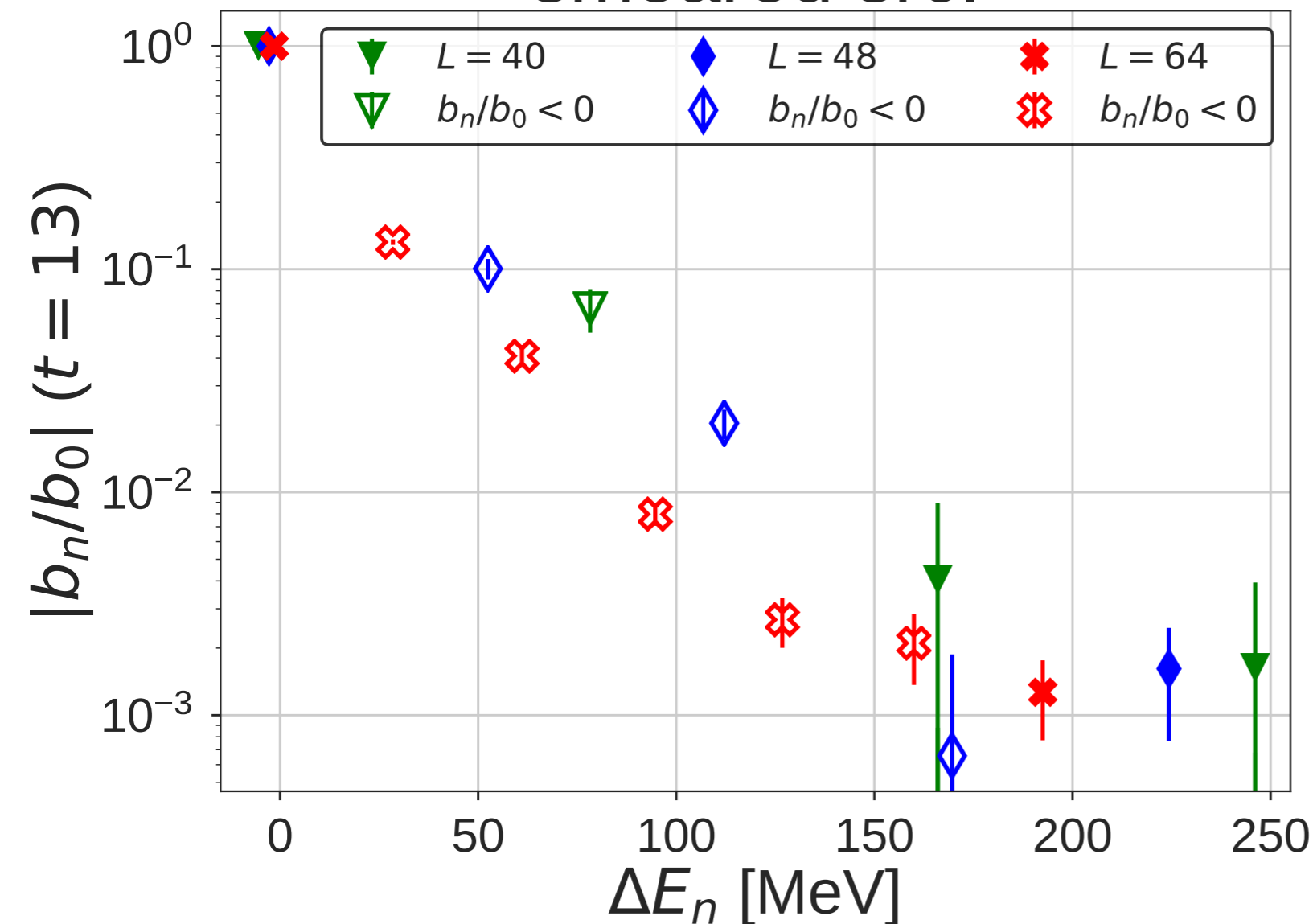
Next Talk by Takumi Doi

BACKUPS

Volume Dep. of the Fake Plateaux (1)

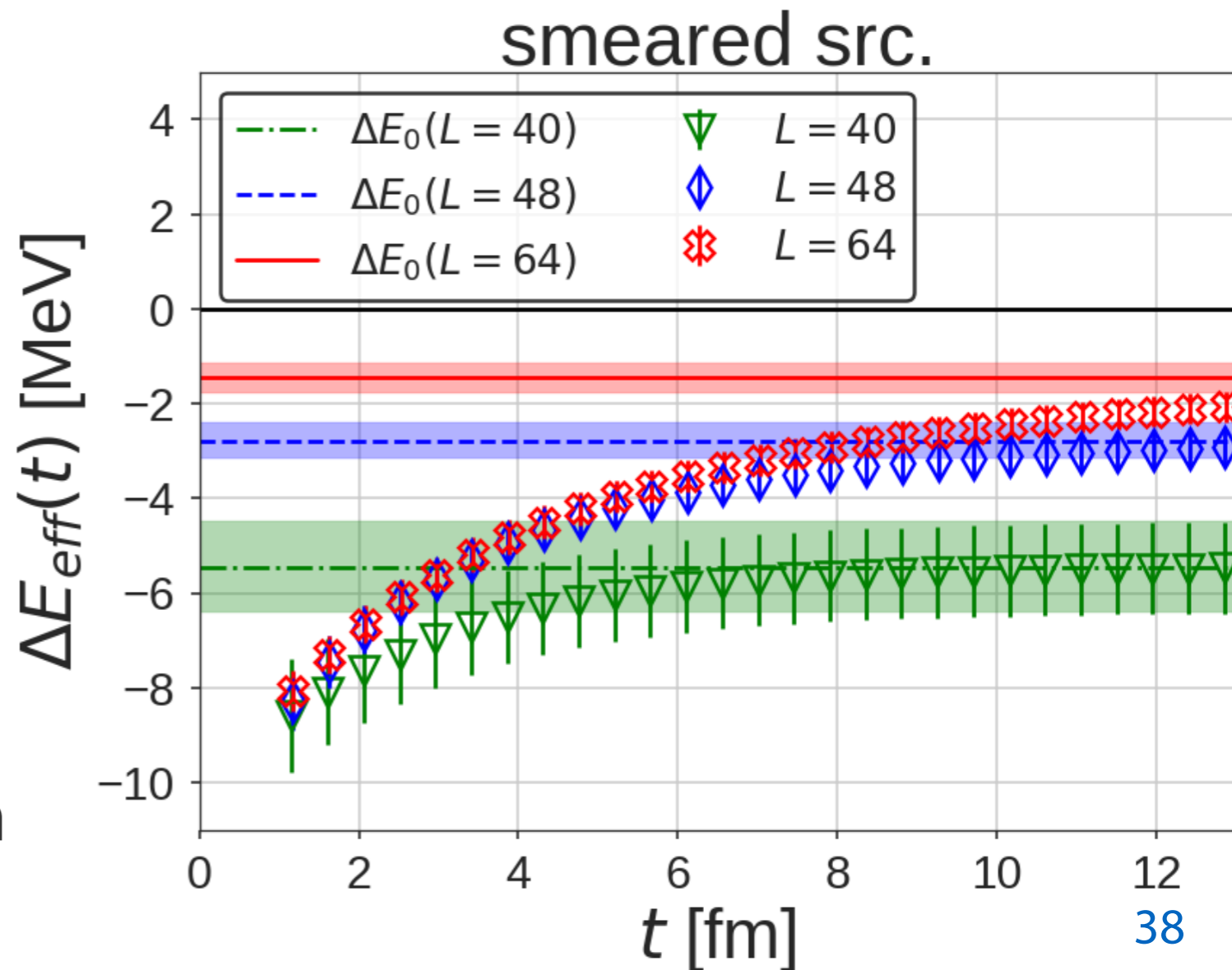
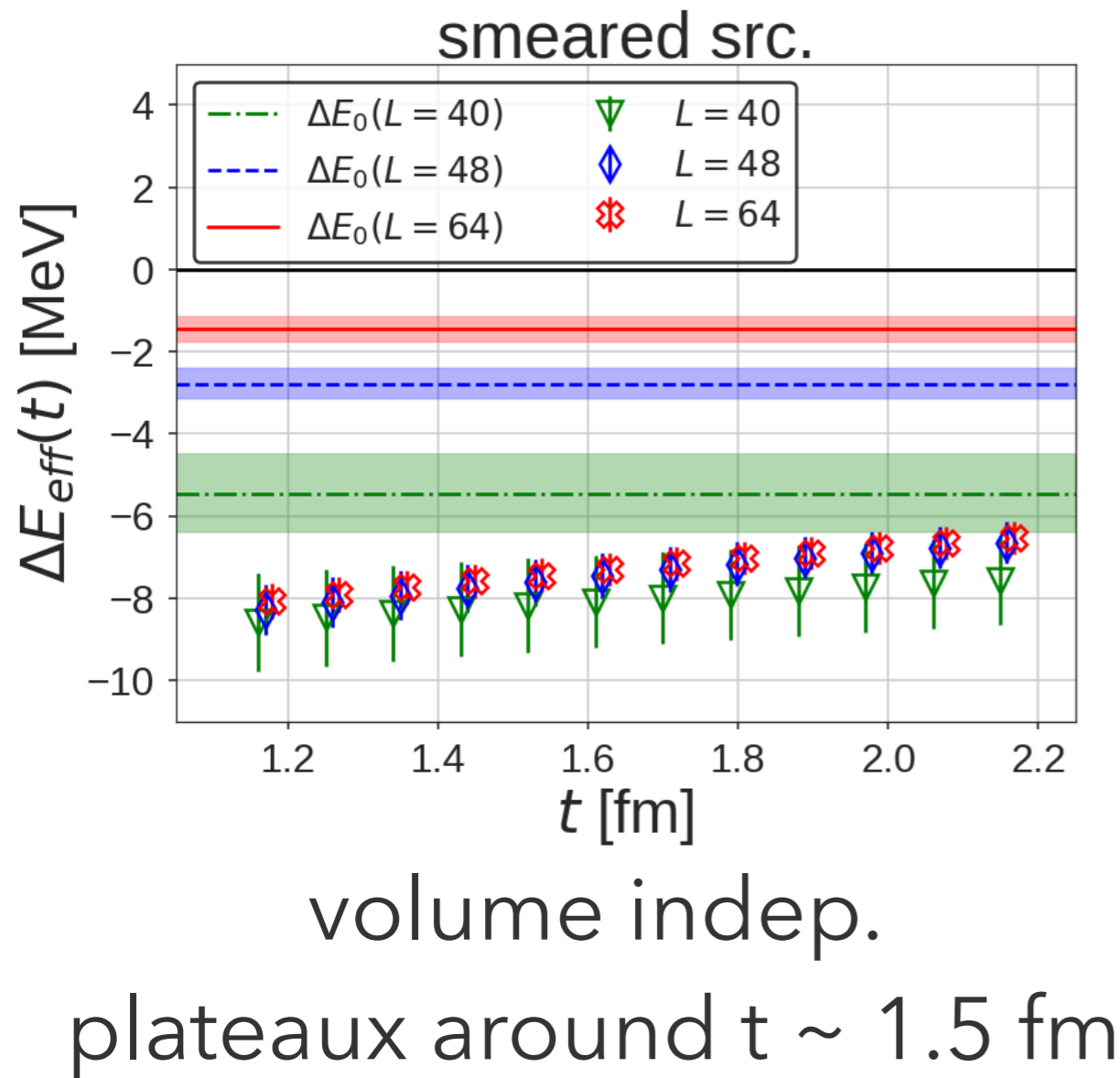
- **Scattering state gap** – $1/L^2$
- scat. states becomes severe for a larger volume

smearred src.



Volume Dep. of the Fake Plateaux (2)

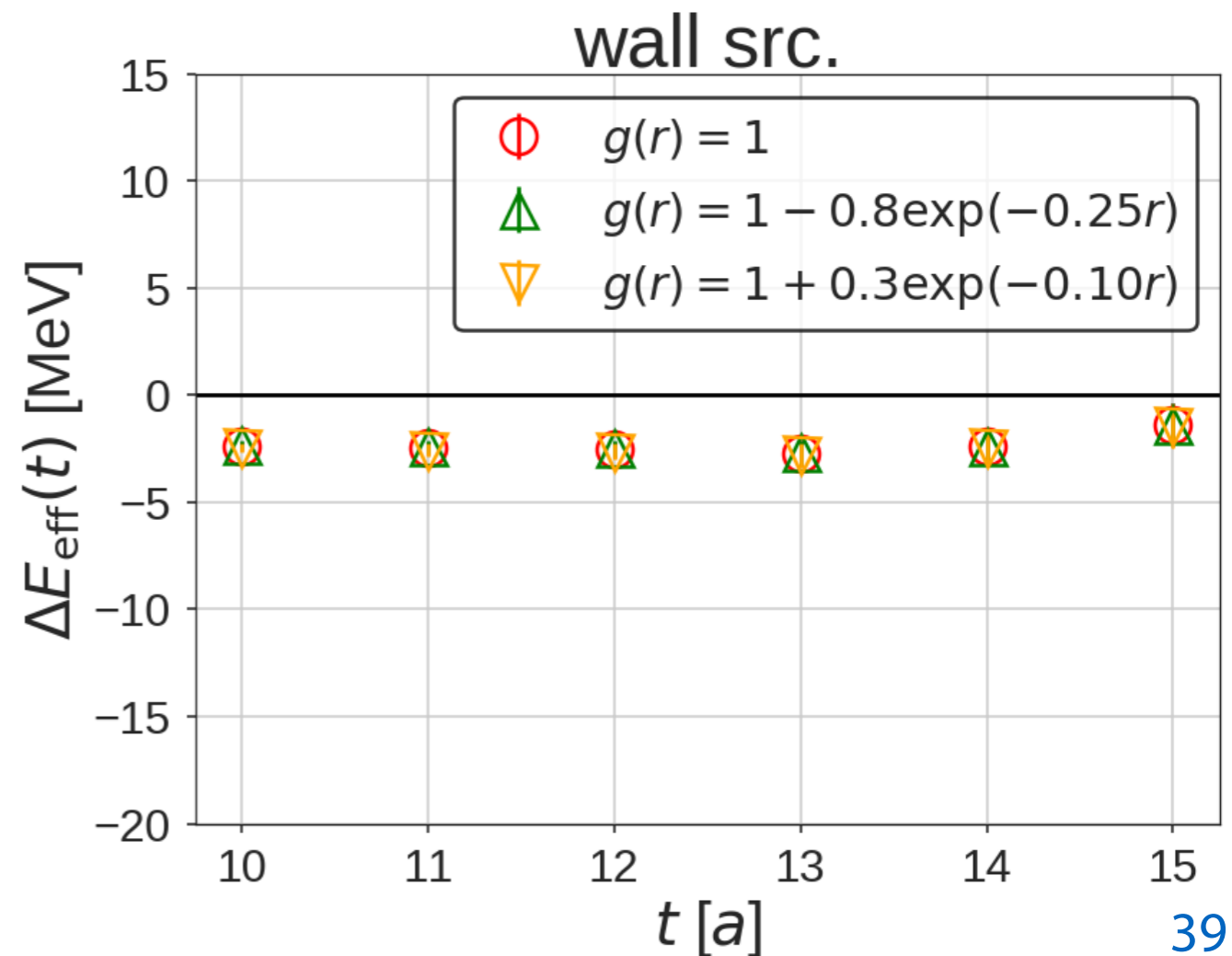
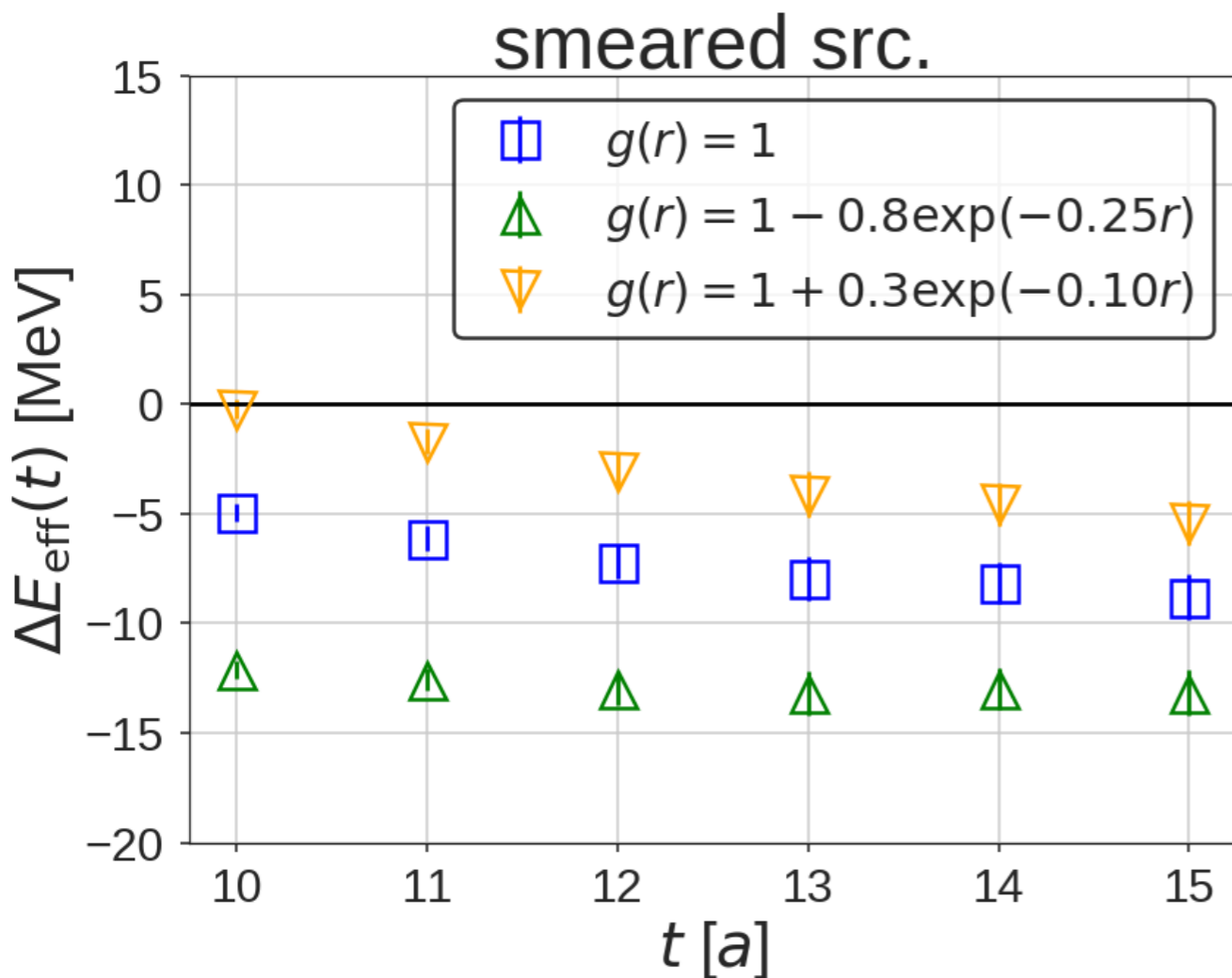
- **Volume indep.** does not mean **ground state saturation**.
- **Volume dep.** appears at later time.



Sink Operator Dependence of the Plateaux

- **smear**ed src. depend on “sink”
- **w**all src. is stable

$$C_{BB}(t) = \sum_{\vec{x}, \vec{y}} g(|\vec{x} - \vec{y}|) \langle B(\vec{x}, t) B(\vec{y}, t) \overline{\mathcal{J}_{BB}(0)} \rangle$$



Lüscher's Finite Volume Method & Bound State

1. Lüscher's formula $k \cot \delta_0(k) = \frac{1}{\pi L} \sum_{\mathbf{n} \in \mathbb{Z}^3} \frac{1}{|\mathbf{n}|^2 - (kL/2\pi)^2}$
2. Effective Range Expansion (**ERE**)

$$k \cot \delta_0(k) \simeq \frac{1}{a_0} + \frac{1}{2} r_{\text{eff}} k^2 + \dots$$

ex. physical quark mass
 NN(3S_1) finite volume

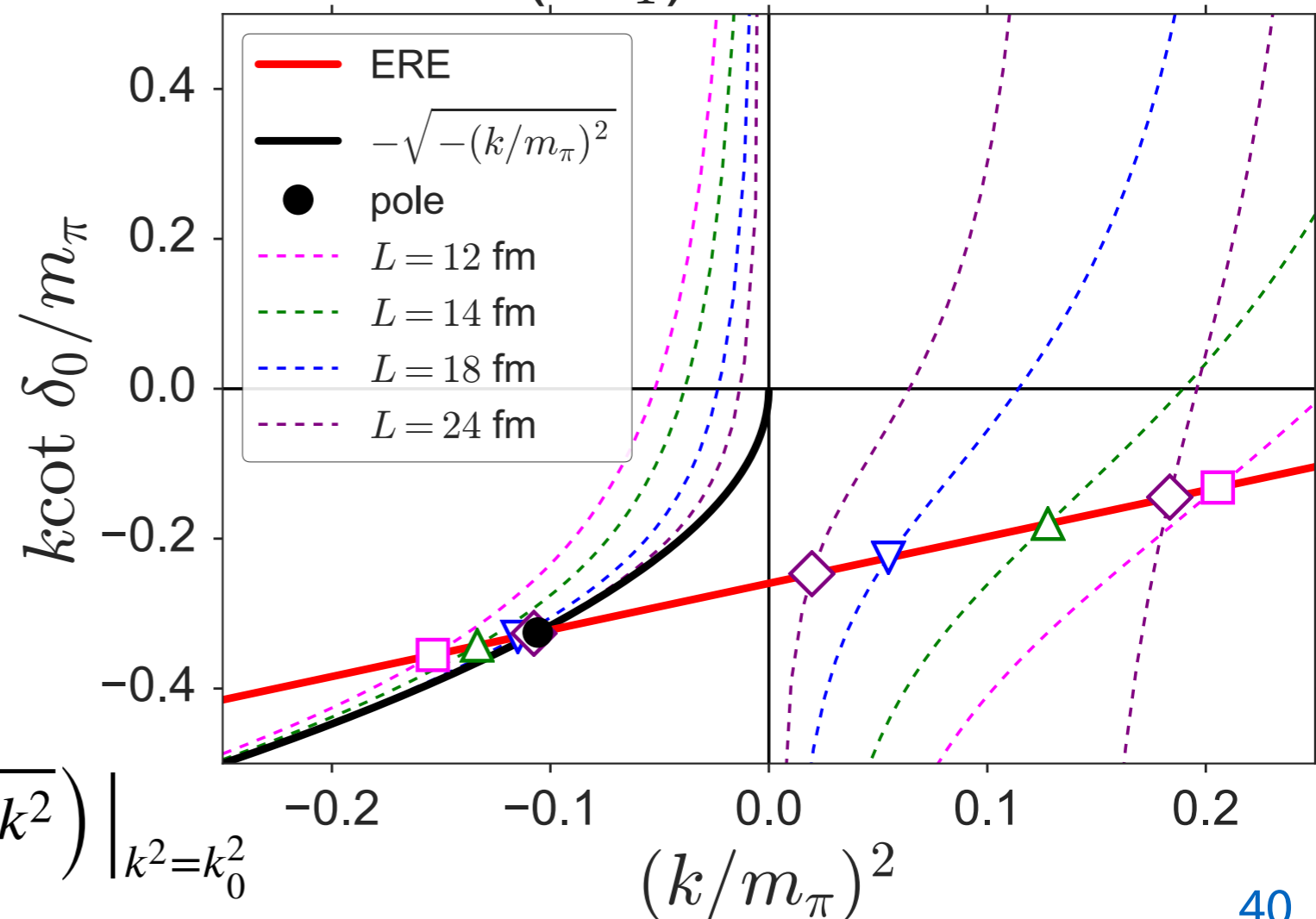
3. Search **bound state**

@ S-matrix's pole

$$k_0 \cot \delta_0(k_0) = -\sqrt{-k_0^2}$$

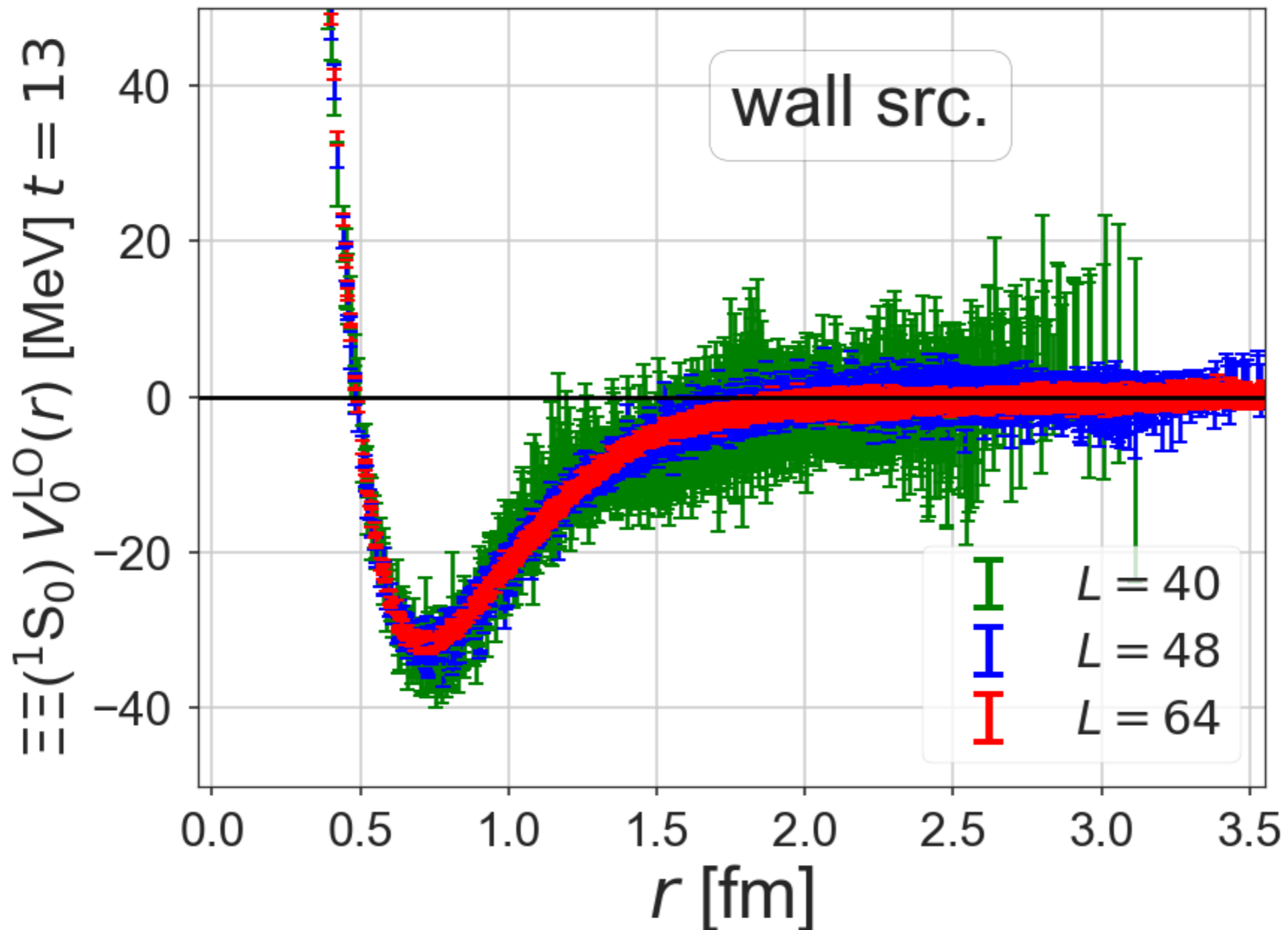
& physical pole cond.

$$\left. \frac{d}{dk^2} (k \cot \delta_0(k)) \right|_{k^2=k_0^2} < \left. \frac{d}{dk^2} \left(-\sqrt{-k^2} \right) \right|_{k^2=k_0^2}$$



Volume Independence of the Potential

- The potential from $L = 40, 48$ and 64 are consistent.



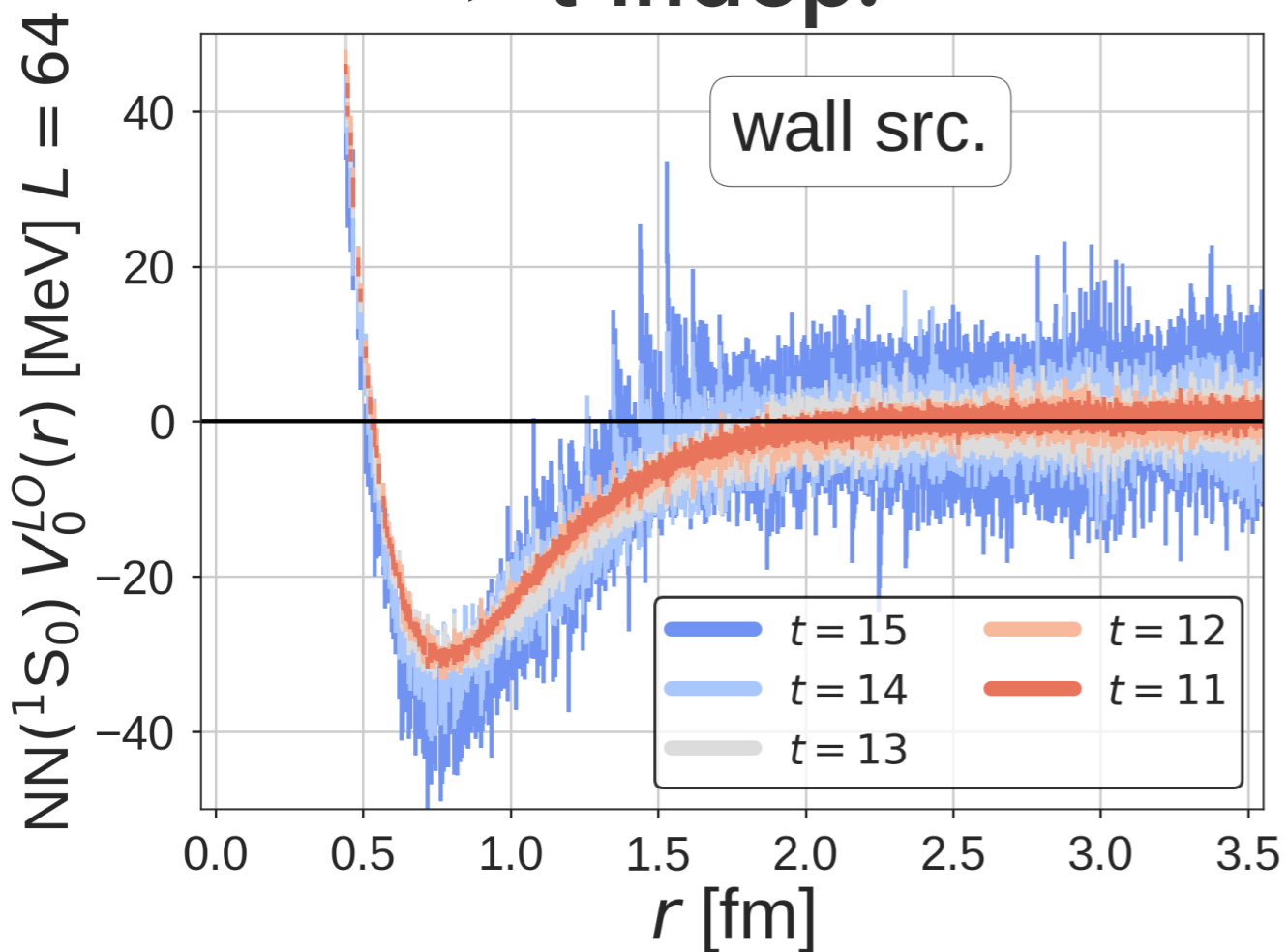
NN(1S_0) System at $M_{\text{PI}} = 510 \text{ MeV}$ (1) LO Approx.

$$U(r, r') \simeq V_0^{\text{LO}}(r)\delta(r - r')$$

- Quantitatively, the same as $\Xi\Xi$ (1S_0)

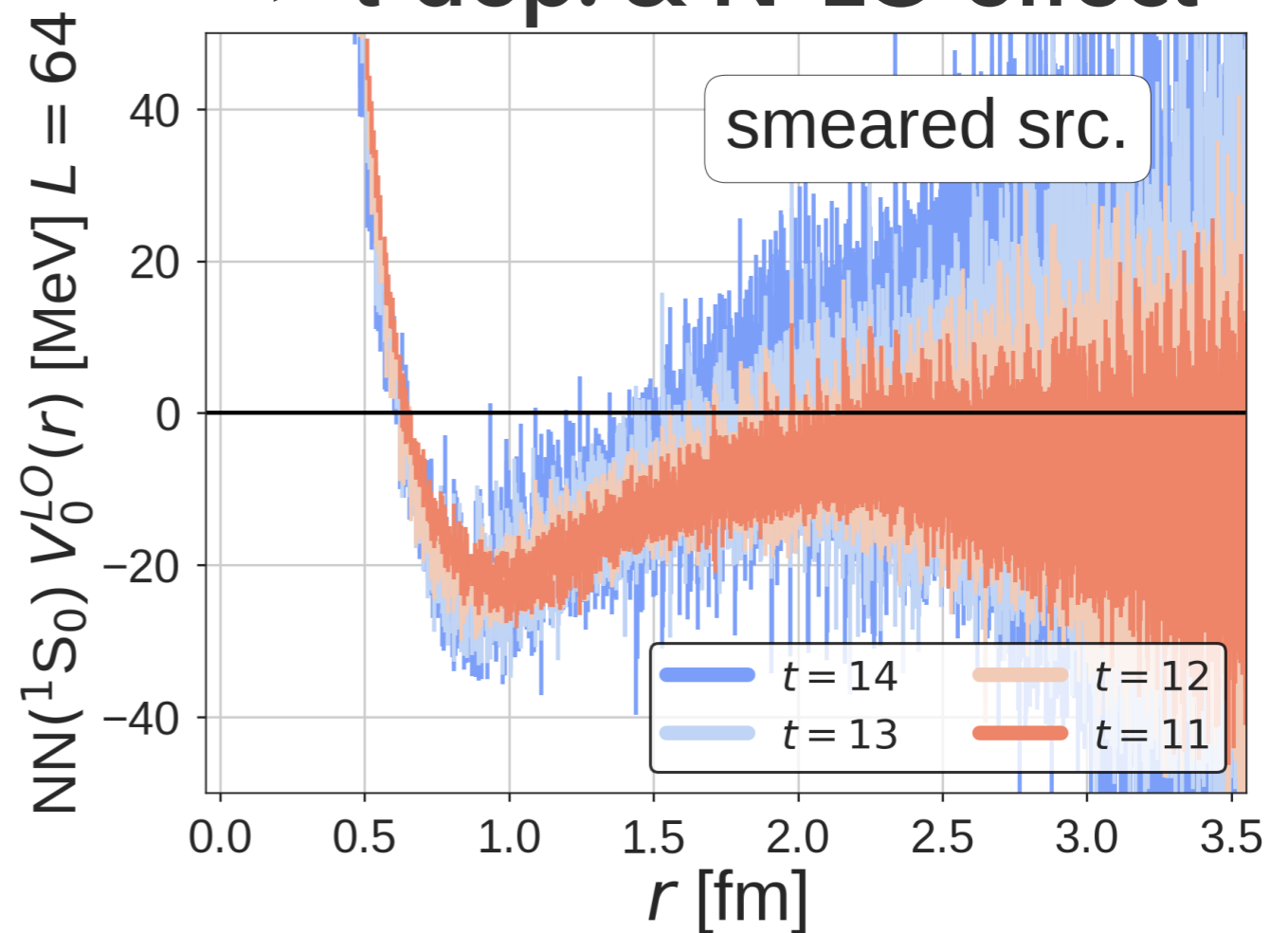
wall src.

\rightarrow t-indep.



smearred src.

\rightarrow t-dep. & N²LO effect

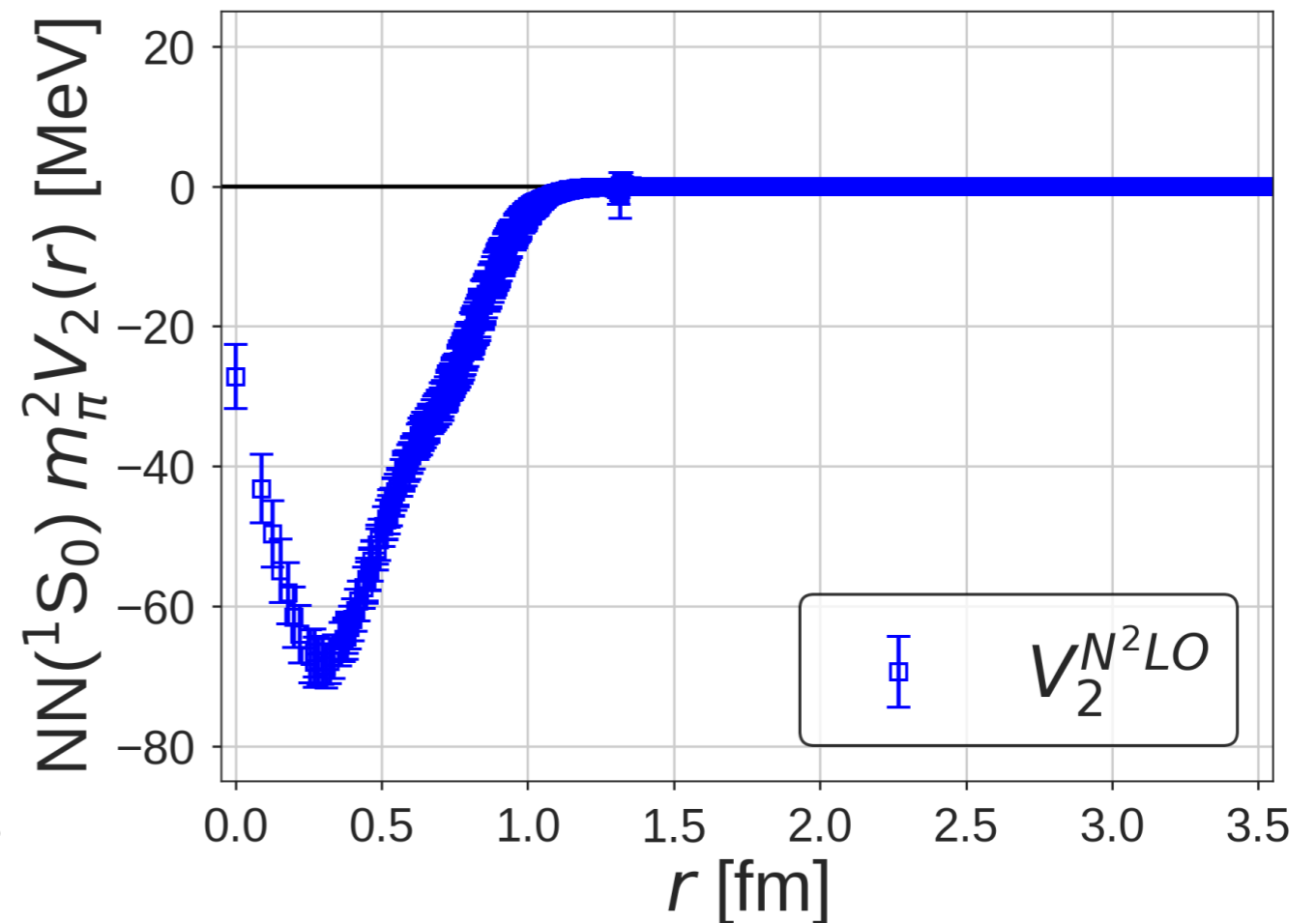
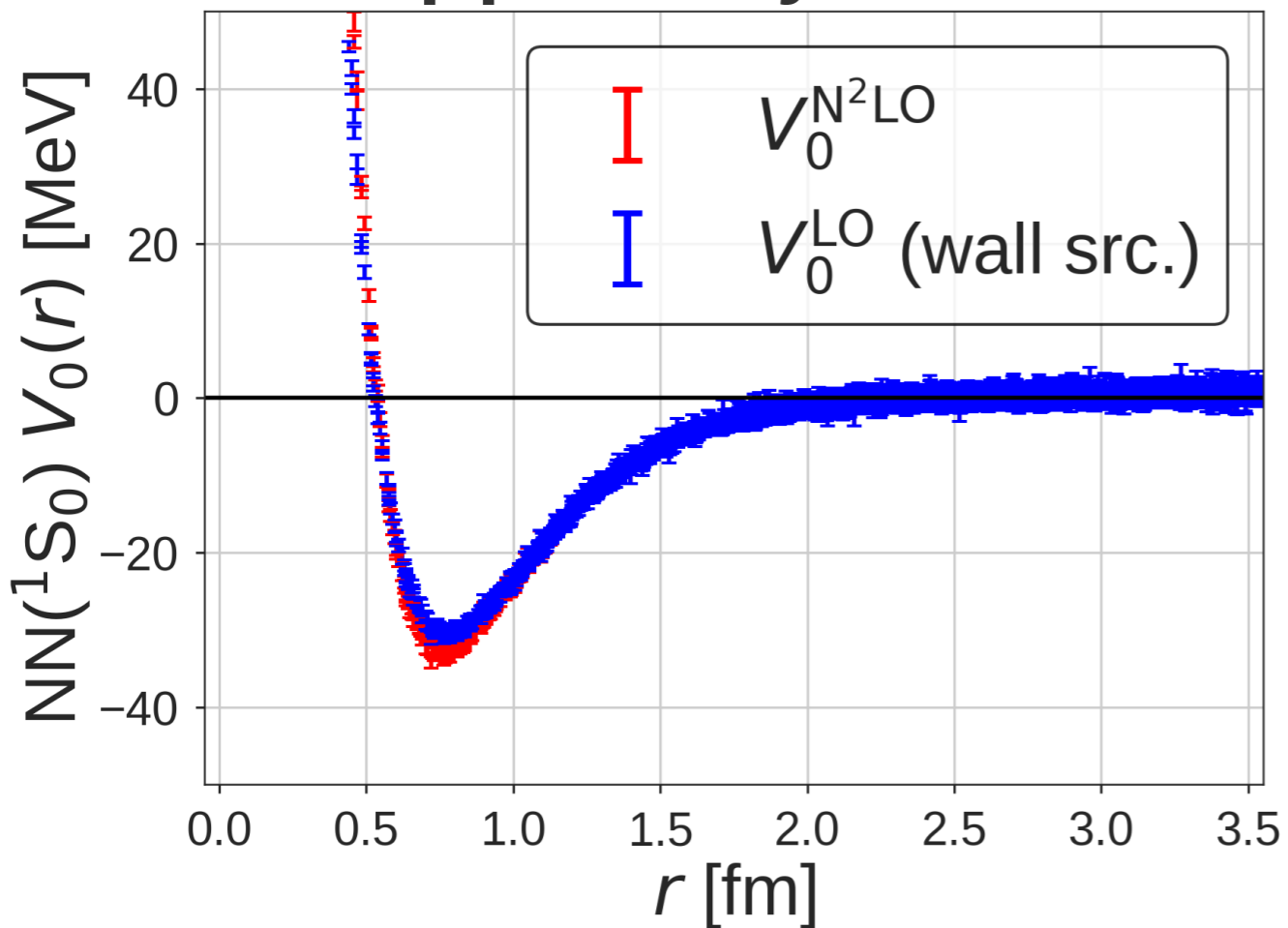


NN(1S_0) System at $M_{\text{Pl}} = 510 \text{ MeV}$ (2) $N^2\text{LO}$ Approx.

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

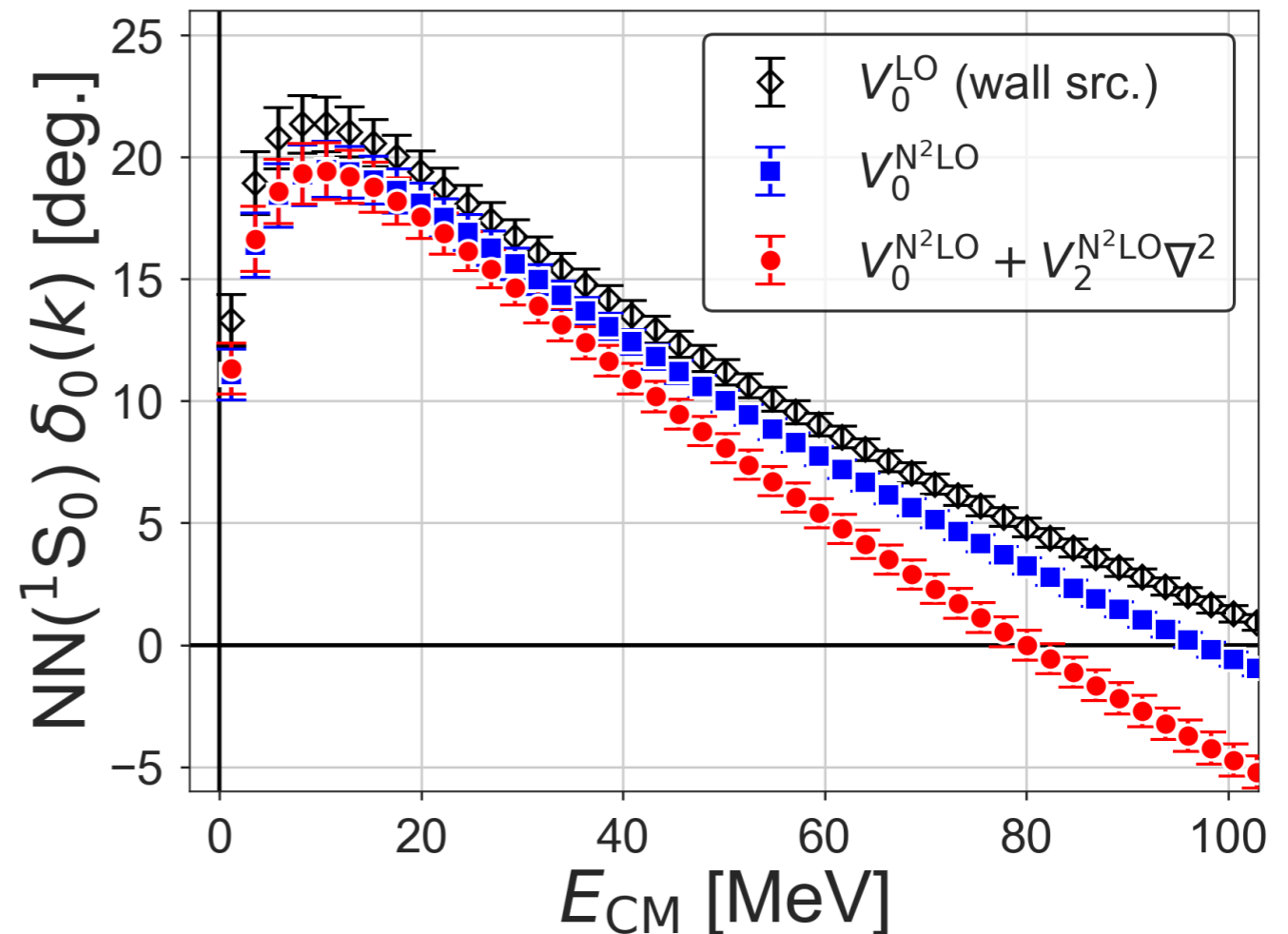
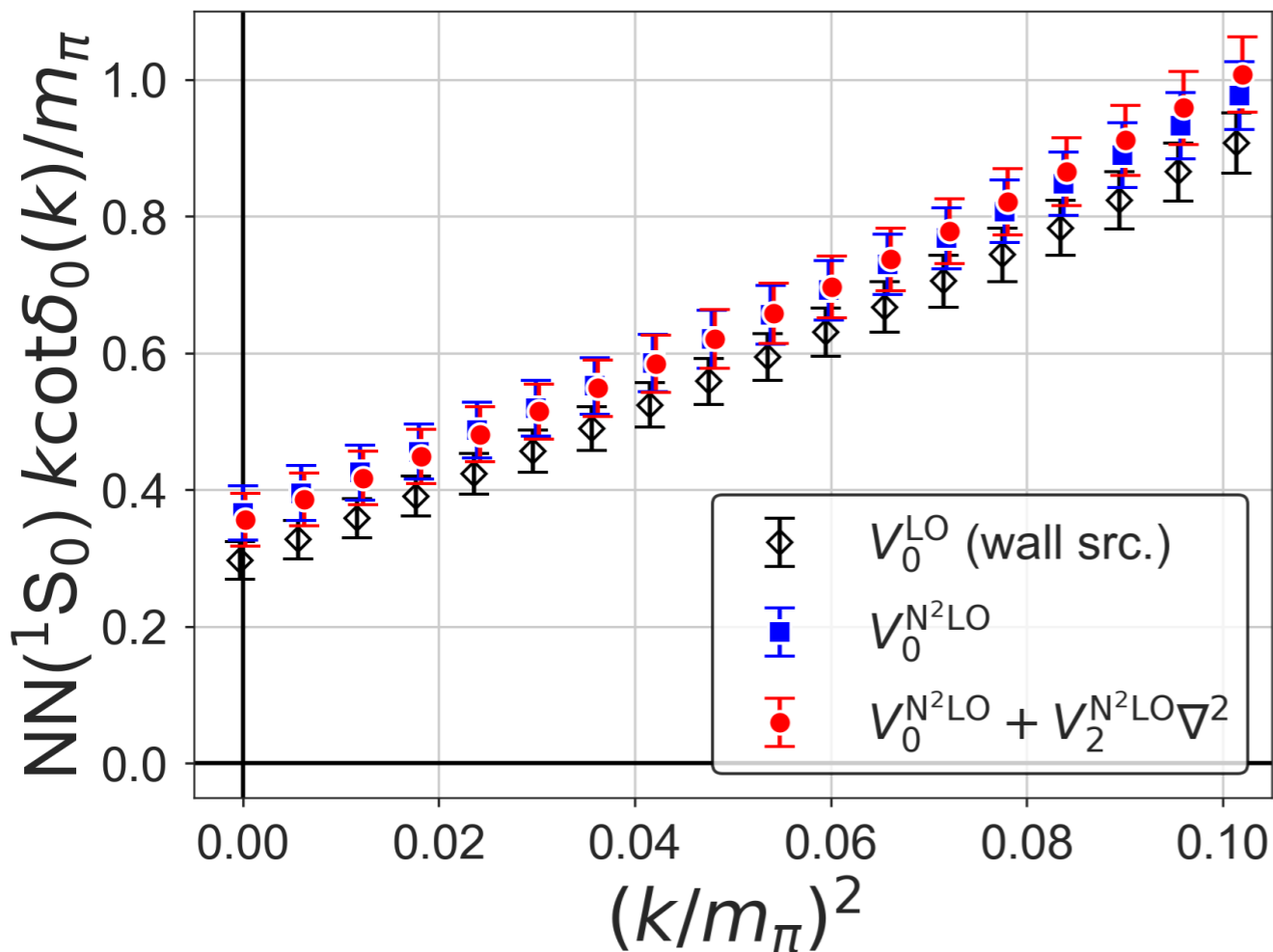
- Quantitatively, the same as $\Xi\Xi$ (1S_0)

good convergence of
LO approx. by wall src.



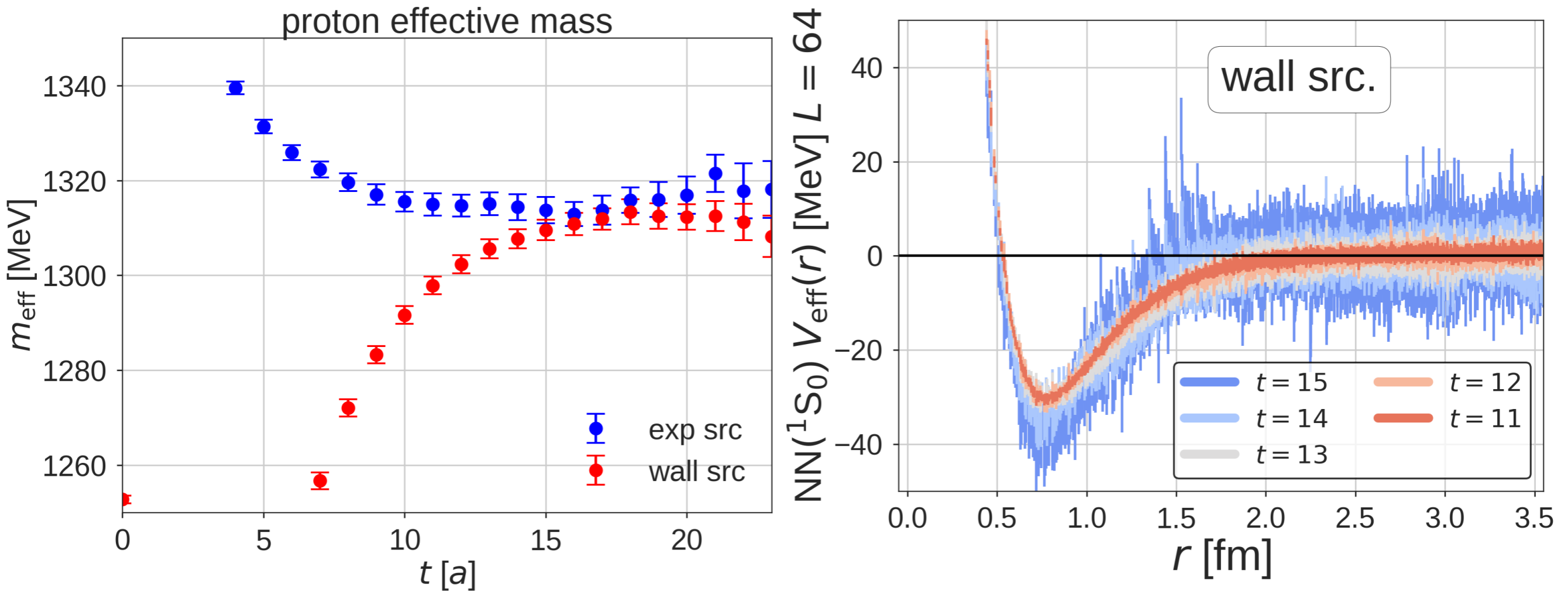
NN(1S_0) System at $M_{\pi} = 510$ MeV (3) Phase Shift

- Quantitatively, the same as $\Xi\Xi$ (1S_0)
- NN(1S_0) is **unbound** at this pion mass.
- **Wall src. LO approx.** is consistent at low energy



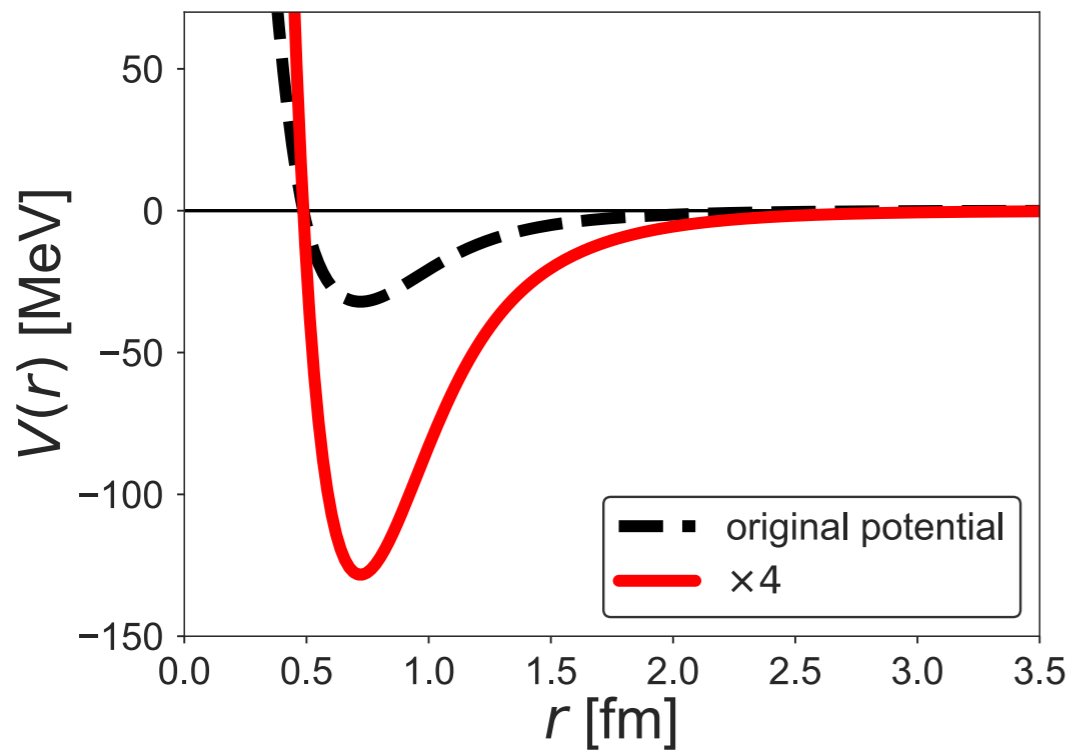
NN(1S_0) System at $M_{\text{Pl}} = 510 \text{ MeV}$ (4) Proton Mass

- LO approx. wall src. potential is stable against time.
- Inelastic contamination is under control.

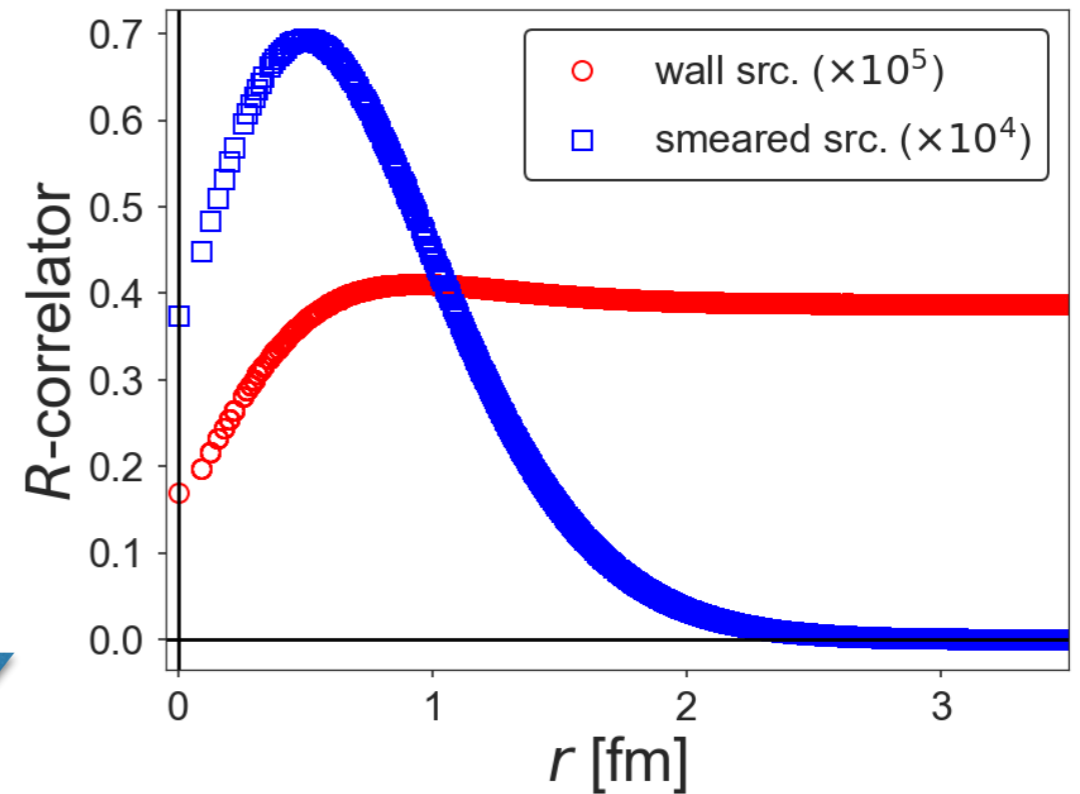


Fake Plateaux for Binding System

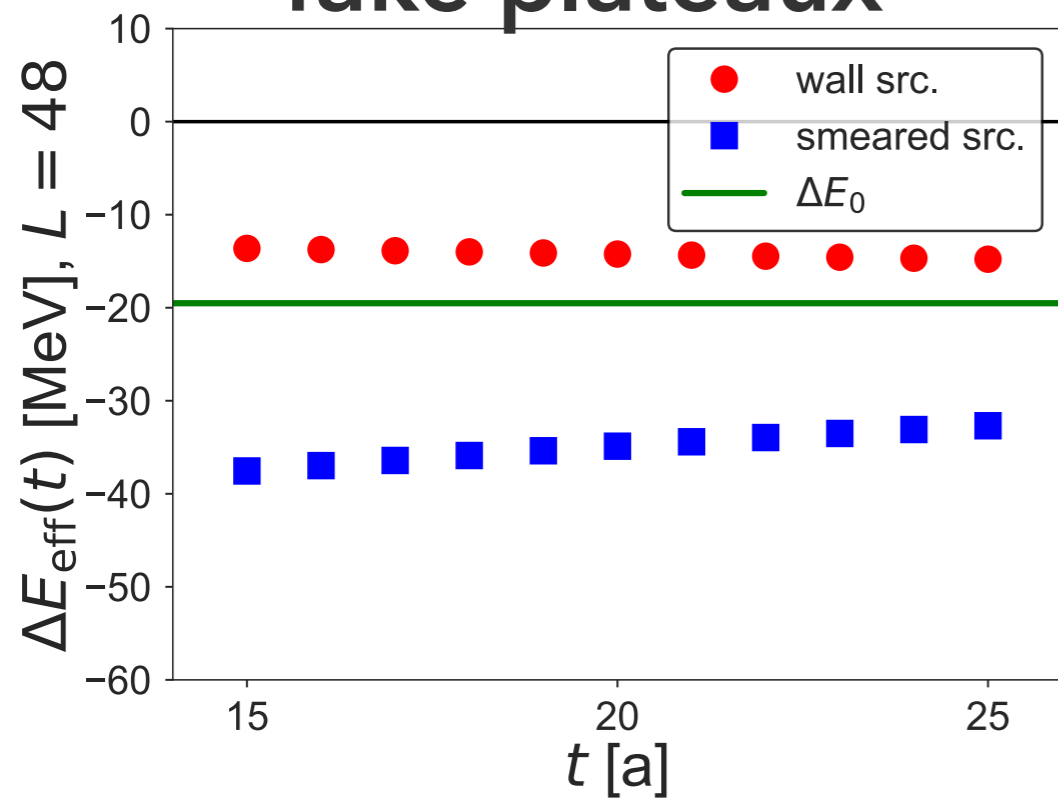
mock potential w/ bound state



mock wave func.



fake plateaux



g.s. convergence

