Wave-functions and operator optimization for two hadrons in lattice QCD

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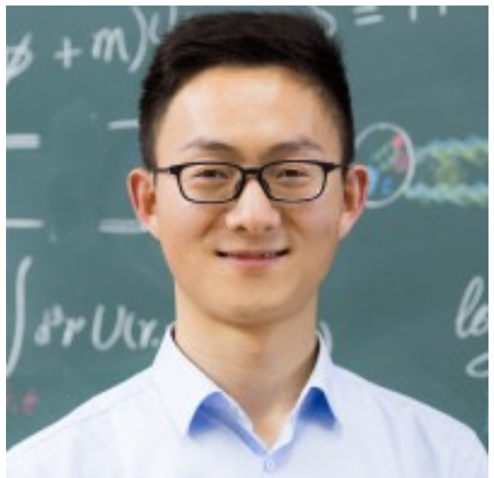
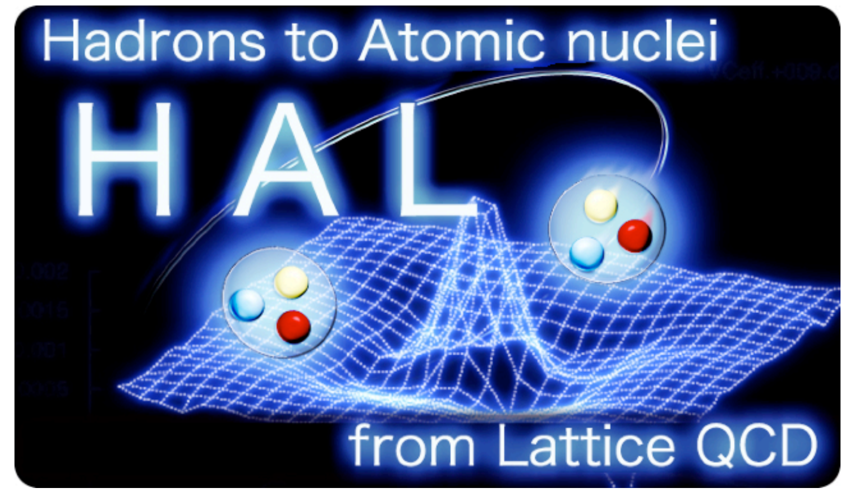
Today's topic is an application of the HAL QCD method to finite volume spectra of two baryons using spatial wavefunctions. This work has been performed mainly by Dr. Yan Lyu at RIKEN, who unfortunately cannot attend lattice2026 due to the visa problem. So I will talk on this work for him.

Yan Lyu





References

Yan Lyu, Sinya Aoki, Takumi Doi, Tetsuo Hatsuda, Kotaro Murakami, Takuya Sugiura, "Decoding Two-Particle States in QCD with Spatial Wavefunctions", Phys. Rev. D114(2026)L011503 (arXiv:2507.09930[hep-lat]).

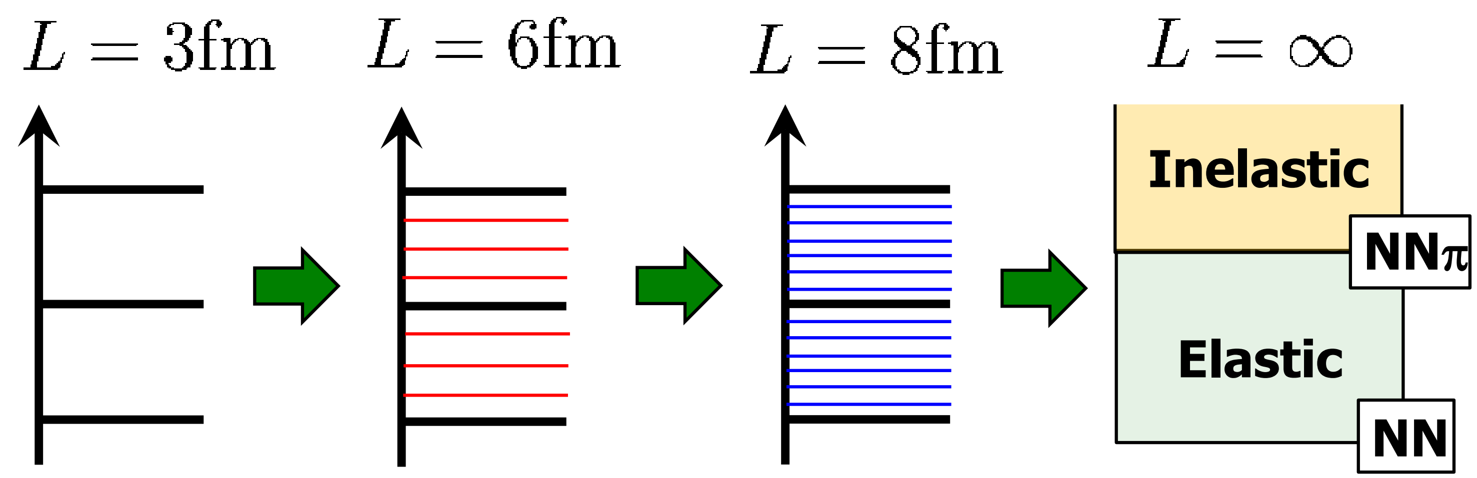
Yan Lyu, Sinya Aoki, Takumi Doi, Tetsuo Hatsuda, Kotaro Murakami, Takuya Sugiura, "Wavefunctions-based operator optimization for two-hadron systems in lattice QCD", Phys. Rev. D114(2026)014506 (arXiv:2507.09933[hep-lat]).

I. Introduction

Difficulties of two-baryon systems

Dense FV spectra

$$\Delta E \simeq \frac{1}{m_B}\left(\frac{2\pi}{L}\right)^2$$



denser as larger volume/heavier mass

We need large time $\qquad t \gg \frac{1}{\Delta E}$

bad signal-to-noise ratio

$$\frac{S(t)}{N(t)} \sim \exp\left[-2\left(m_B - \frac{3m_{\mathrm{PS}}}{2}\right)t\right]$$

Signal becomes worse for larger time.

Dilemma !

variational methods of various types

A. Francis et al., PRD99(2019)074505. (arXiv:1805.03966[hep-lat])

J.R. Green et al., PRL127(2021)242003. (arXiv:2103.01054[hep-lat])

S. Amarasinghe et al., PRD107(2023)094508. (arXiv:2108.10835[hep-lat])

J. Bulava et al., PRC113(2-26)024002. (arXiv:2505.05547[hep-lat])

It is still hard to validate correctness of results.

our proposal: optimized two-baryon operators

Flavor, spin, and angular momentum of two-baryons have already been used to disentangle elastic states.

⟶ As the next target, we employ spatial profiles of two baryon systems.

We construct optimized two-baryon operators using spatial wavefunctions at both sink and source

c.f. sink only

Yan Lyu, Hui Tong, Takuya Sugiura, Sinya Aoki, Takumi Doi, Tetsuo Hatsuda, Jie Meng, Takaya Miyamoto,Phys.Rev.D105(2022)7, 074512. (arXiv:2022.02782[hep-lat])

Contents

II. Optimized two-baryon operators

Yan Lyu, Sinya Aoki, Takumi Doi, Tetsuo Hatsuda, Kotaro Murakami, Takuya Sugiura,
PRD114(2026)L011503, PRD114(2026)L014506.

All-to-all two-baryon correlation function and dual basis

$$\mathcal{R}(\vec{r}_{\rm snk}, t; \vec{r}_{\rm src}) := \frac{e^{2m_B t}}{V^2} \sum_{\vec{x},\vec{y}\in\Lambda} \langle 0|B(\vec{x}+\vec{r}_{\rm snk}, t)B(\vec{x}, t)\bar{B}(\vec{y}+\vec{r}_{\rm src}, 0)\bar{B}(\vec{y}, 0)|0\rangle$$

$$= \sum_n \frac{e^{-(E_n-2m_B)t}}{V^2} \sum_{\vec{x},\vec{y}\in\Lambda} \langle 0|B(\vec{x}+\vec{r}_{\rm snk}, 0)B(\vec{x}, 0)|2B, E_n\rangle\langle 2B, E_n|\bar{B}(\vec{y}+\vec{r}_{\rm src}, 0)\bar{B}(\vec{y}, 0)|0\rangle$$

E^*:inelastic threshold

$$= \sum_{n=0}^{N} \psi_n(\vec{r}_{\rm snk})\psi_n^*(\vec{r}_{\rm src})e^{-\Delta E_n t} + O\left(e^{-\Delta E^* t}\right)$$

inelastic contributions

NBS amplitude

ψ_n's are not orthogonal to each other.

Dual basis functions $\Psi_n(\vec{r})$ such that $\boxed{\langle \Psi_n|\psi_m\rangle := \sum_{\vec{r}\in\Lambda} \Psi_n^*(\vec{r})\psi_m(\vec{r}) = \delta_{nm}}$

$$\Psi_n(\vec{r}) = \mathcal{K}^{-1}_{nm}\psi_m(\vec{r}) \qquad \mathcal{K}_{nm} := \langle \psi_n|\psi_m\rangle := \sum_{\vec{r}\in\Lambda} \psi_n^*(\vec{r})\psi_m(\vec{r})$$

Optimized two-baryon correlation function

$$\mathcal{R}(\vec{r}_{\rm snk}, t; \vec{r}_{\rm src}, t_0) = \sum_{n=0}^{N} \psi_n(\vec{r}_{\rm snk})\psi_n^*(\vec{r}_{\rm src})e^{-\Delta E_n t}$$

Source optimization

$$\langle \Psi_n | \psi_m \rangle = \delta_{nm}$$

$$R_n(\vec{r}_{\rm snk}, t) := \frac{1}{V}\sum_{\vec{r}_{\rm src}\in\Lambda} \mathcal{R}(\vec{r}_{\rm snk}, t; \vec{r}_{\rm src}, t_0)\underline{\Psi_n(\vec{r}_{\rm src})} = \psi_n(\vec{r}_{\rm snk})e^{-\Delta E_n t}$$

dual basis

Sink-source optimization

$$R_n(t) := \frac{1}{V}\sum_{\vec{r}_{\rm snk}\in\Lambda} \underline{\Psi_n^*(\vec{r}_{\rm snk})}R_n(\vec{r}_{\rm snk}, t) = e^{-\Delta E_n t}$$

Approximated construction of dual basis

Time-dependent HAL QCD method at leading order (LO)

$$V^{(0)}(\vec{r}) = \frac{1}{R^{(0)}(\vec{r},t)}\left(\frac{\nabla^2}{m_B} - \frac{\partial}{\partial t} + \frac{1}{4m_B}\frac{\partial^2}{\partial t^2}\right)R^{(0)}(\vec{r},t)$$

LO potential

$R^{(0)}(\vec{r},t)$ correlation function with the standard source such as wall/hexaquark

Eigenfunctions and eigenvalues with the LO potential on Λ (finite L and a)

$$\left[-\frac{\nabla^2}{m_B} + V^{(0)}(\vec{r})\right]\psi_n^{(0)}(\vec{r}) = \frac{k_n^2}{m_B}\psi_n^{(0)}(\vec{r}) \qquad \Delta E_n^{(0)} = 2\left(\sqrt{m_B^2 + k_n^2} - m_B\right)$$

Eigenfunction Eigenvalue

Since the LO potential is Hermitian, $\psi_n^{(0)}$'s are orthogonal to each other.

$$\longrightarrow \boxed{\Psi_n^{(0)}(\vec{r}) = \psi_n^{(0)}(\vec{r})}$$

III. Implementation

Challenge of optimized operators at source

$$R_n(\vec{r}_{\rm snk}, t) = \frac{1}{V} \sum_{\vec{r}_{\rm src} \in \Lambda} \mathcal{R}(\vec{r}_{\rm snk}, t; \vec{r}_{\rm src}, t_0) \underline{\Psi_n(\vec{r}_{\rm src})}$$

1. Naively expensive all-to-all propagators are required for a sum of $\vec{r}_{\rm src}$.

2. A quark smearing is required to reduce inelastic contributions to one baryon.

$$q_f(\vec{x}, t_0) := \sum_{\vec{r} \in \Lambda} f(\vec{r} - \vec{x}) q(\vec{r}, t_0),$$

$$f(\vec{r}) \, : \, \text{some smearing function}$$

We reduce the numerical cost utilizing stochastic method and sparsening.

Y. Li et al., PRD103(2021)014514.

W. Detmold et al., PRD104(2021)034502.

2-types of quark source smearing functions

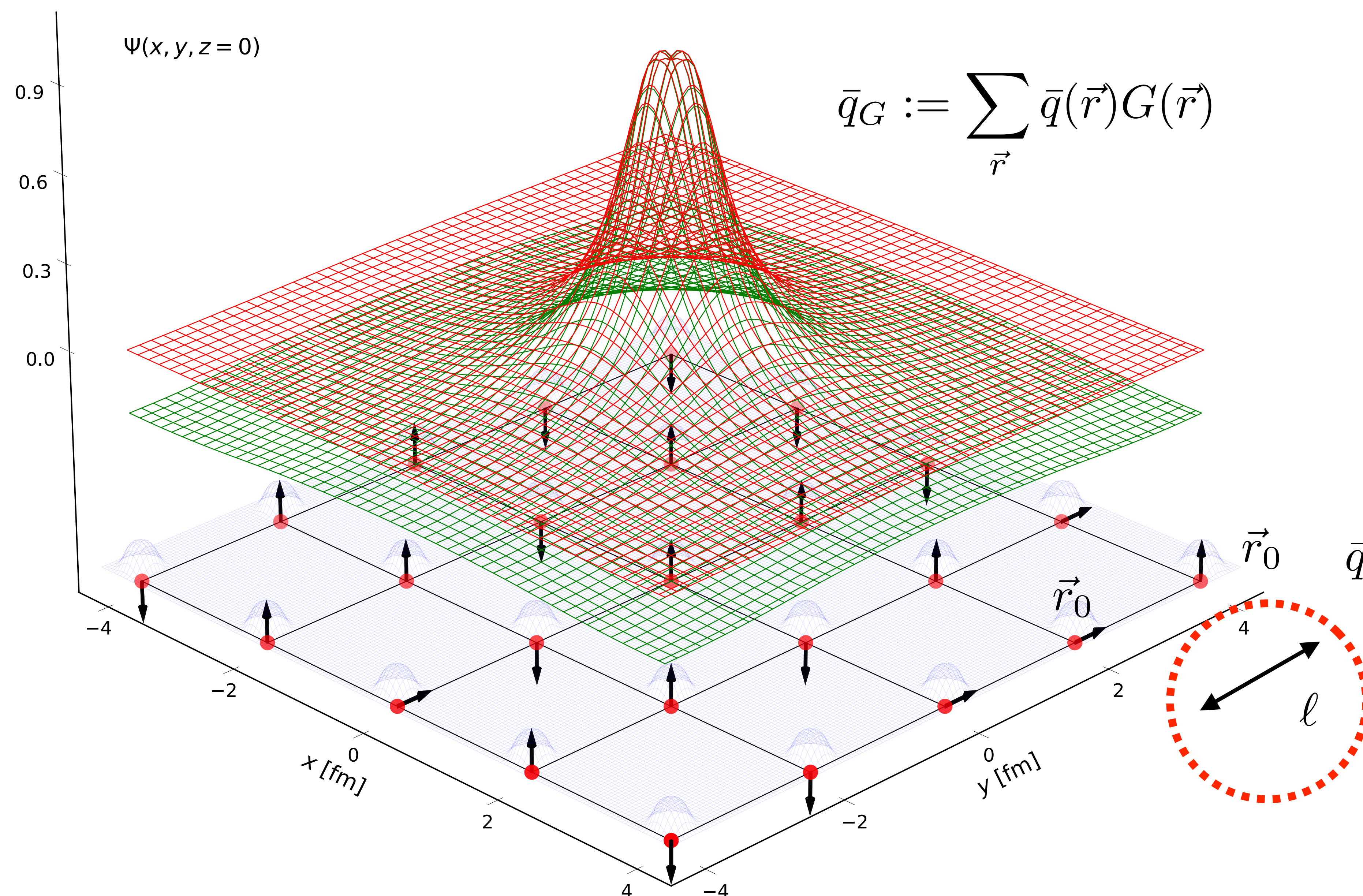
smeared source at $\vec{x}=\vec{0}$ $\qquad G(\vec{r}) = f(\vec{r}-\vec{0})$

wavefunction

sparsening source $\qquad F_n(\vec{r}) = \dfrac{1}{V_{\rm sub}^{1/3}} \displaystyle\sum_{\vec{r}_0\in\Lambda_{\rm sub}} Z_3(\vec{r}_0)\Psi_n^{1/3}(\vec{r}_0) f(\vec{r}-\vec{r}_0)$

Z_3 noise $\qquad Z_3 \in \{1, e^{i2\pi/3}, e^{i4\pi/3}\}$

sub-lattice $\qquad \Lambda_{\rm sub} = \{\ell\vec{r} \mid \vec{r}\in\mathbb{Z}^3, 0\le r_{x,y,z} < L/\ell\}$



$$\bar{q}_G := \sum_{\vec{r}} \bar{q}(\vec{r}) G(\vec{r})$$

$$\bar{q}_{F_n} := \sum_{\vec{r}} \bar{q}(\vec{r}) F_n(\vec{r})$$

Source operators after noise averages

Z_3 noises

$$\langle Z_3(\vec{r}_0) Z_3(\vec{r}_2) Z_3(\vec{r}_2)\rangle_{Z_3} = \delta(\vec{r}_0 - \vec{r}_1)\delta(\vec{r}_0 - \vec{r}_2)$$

One noise per configuration

sparsening average

$$\frac{1}{\Lambda_{\rm sub}} \sum_{\vec{r}\in\Lambda_{\rm sub}} \cdots = \frac{1}{V} \sum_{\vec{m}\in\Gamma} \sum_{\vec{r}\in\Lambda} e^{i\frac{2\pi}{\ell}\vec{m}\cdot\vec{r}} \cdots$$

$$\Gamma = \left\{\vec{m}\in\mathbb{Z}^3 \mid 0 \le m_{x,y,z} < \ell\right\}$$

extra contributions from $\vec{m} \neq \vec{0}$ momenta

$\Lambda_{\rm sub}$ should be fine enough for a good approximation while simultaneously sparse enough to reduce statistical fluctuations from Z_3 noises.

Combining two, we obtain the desired result as

$$\langle(\bar{q}_G)^3(\bar{q}_{F_n})^3\rangle_{Z_3} = \frac{1}{V_{\rm sub}} \bar{B}(\vec{0}) \sum_{\vec{r}_0\in\Lambda_{\rm sub}} \psi_n(\vec{r}_0)\bar{B}(\vec{r}_0) \simeq \frac{1}{V}\bar{B}(\vec{0}) \sum_{\vec{r}_0\in\Lambda} \psi_n(\vec{r}_0)\bar{B}(\vec{r}_0)$$

The origin ($\vec{r} = \vec{0}$) is chosen randomly configuration by configuration.

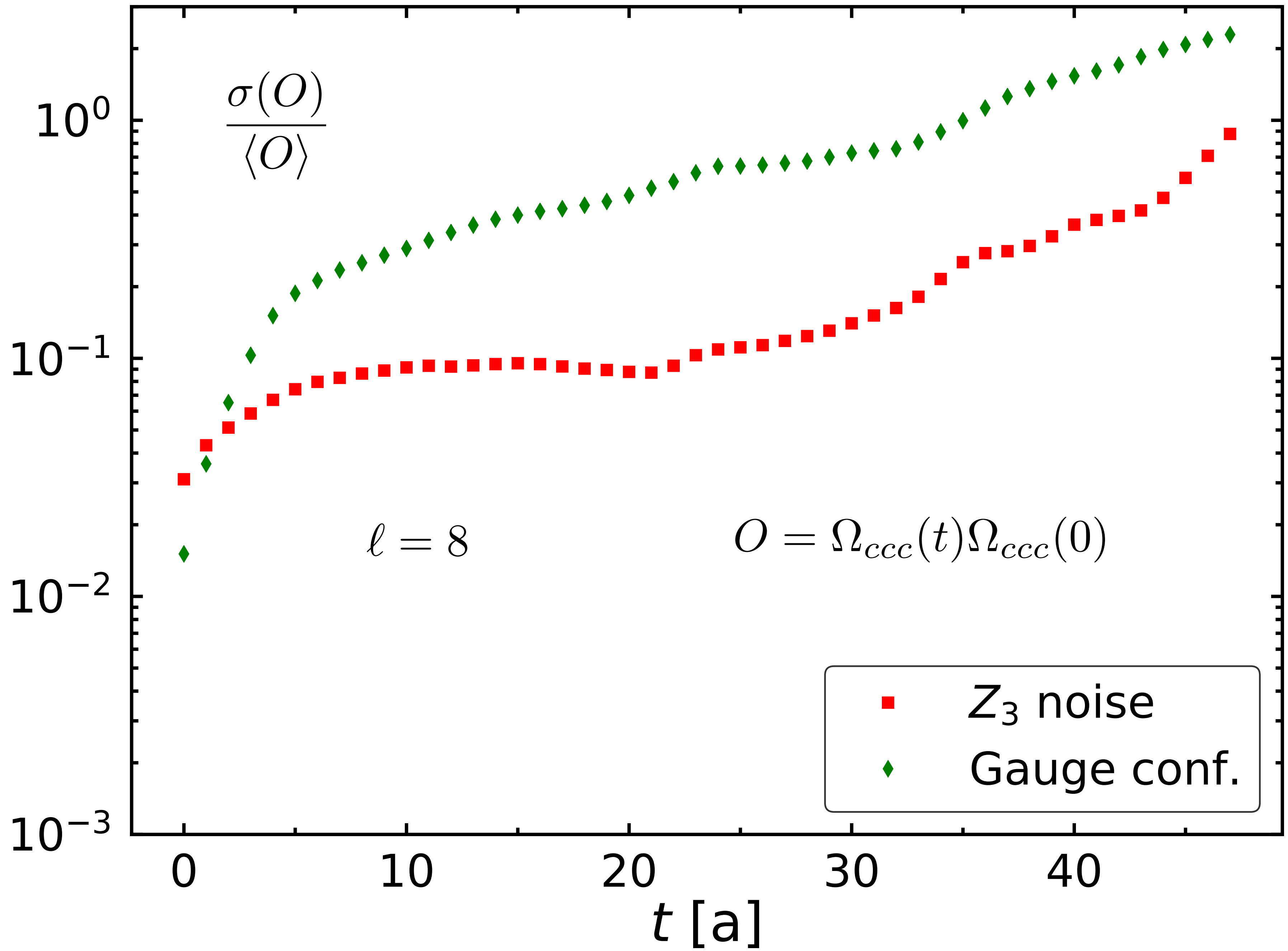
Choice of sparsening parameters

total error

$$\epsilon = \sqrt{\frac{\sigma^2_{\text{gauge}}}{N_{\text{gauge}}} + \frac{\sigma^2_{Z_3}}{N_{Z_3} N_{\text{gauge}}}}$$

σ_X: variance

comparison of variances



$\ell = 8, N_{Z_3} = 1$

seems OK.

IV. Application

Spectra of the $\Omega_{ccc}\Omega_{ccc}$ system

Yan Lyu, Sinya Aoki, Takumi Doi, Tetsuo Hatsuda, Kotaro Murakami, Takuya Sugiura,
PRD114(2026)L011503, PRD114(2026)L014506.

Physical point configurations

T. Aoyama, T.M. Doi, T. Doi, E. Itou, Y. Lyu, K. Murakami, T. Sugiura, PRD110(2024)094502 ,

2+1 flavor QCD with Iwasaki gauge + NP $O(a)$ improved clover quark

a [fm]	L	m_π [MeV]	m_K [MeV]	La [fm]	$m_\pi L$
0.0844(1)	96	137.1(3)	501.8(7)	8.10(1)	5.63(1)

relativistic heavy quark action (Tsukuba-type) for quenched charm quark

Aoki-Kuramashi-Tominaga, PTEP 109(2003) 383.

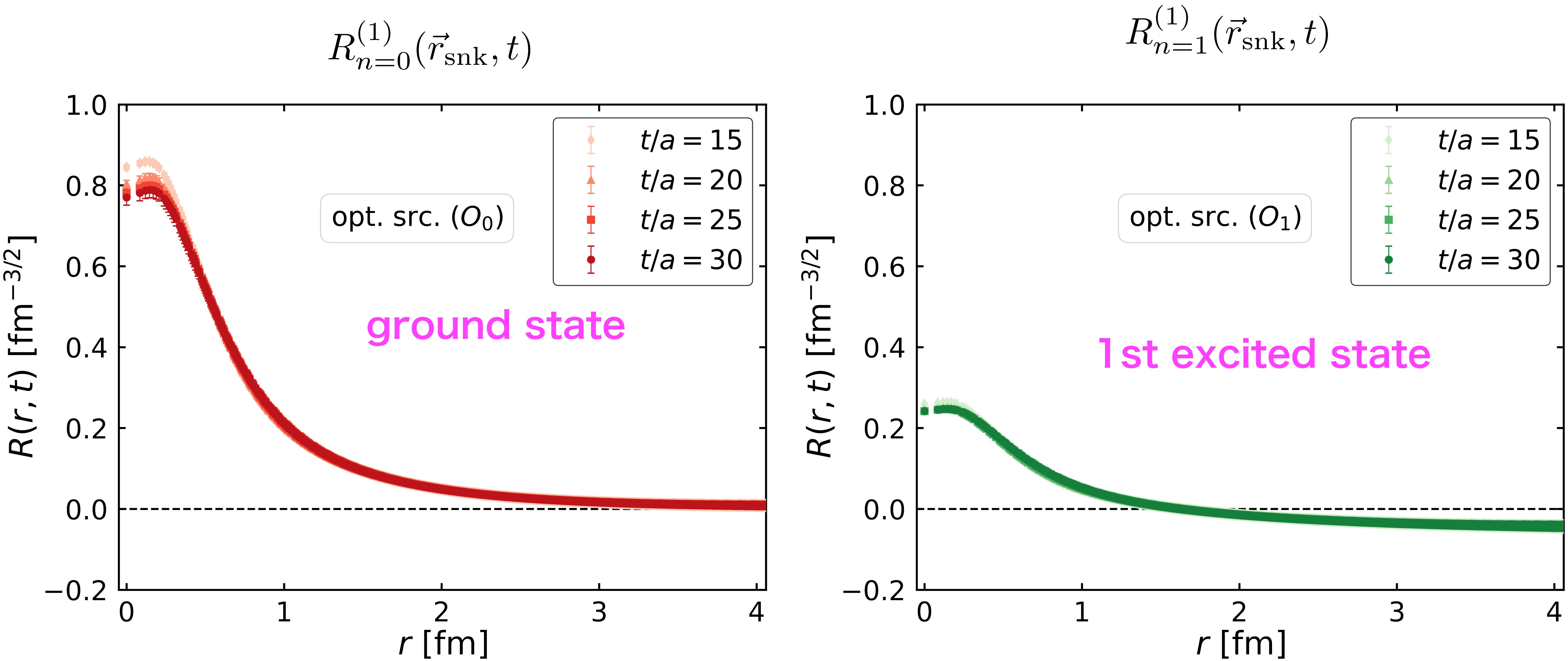
charm quark mass

$$M_{\rm av} := \frac{m_{\eta_c} + m_{J/\psi}}{4} \simeq 3102\,\mathrm{MeV} \qquad M_{\rm av}^{\rm exp} = 3068.5(0.1)\ \mathrm{MeV}$$

$$m_{\Omega_{ccc}} = 4847.3(1)\ \mathrm{MeV} \longrightarrow \Delta E \simeq \frac{1}{m_{\Omega_{ccc}}}\left(\frac{2\pi}{L}\right)^2 \simeq 5\ \mathrm{MeV}$$

We naively need $t \gg 40$ fm to resolve 5 MeV difference (out of $2m_{\Omega_{ccc}} \simeq 9700$ MeV).

Correlation functions with optimized operators

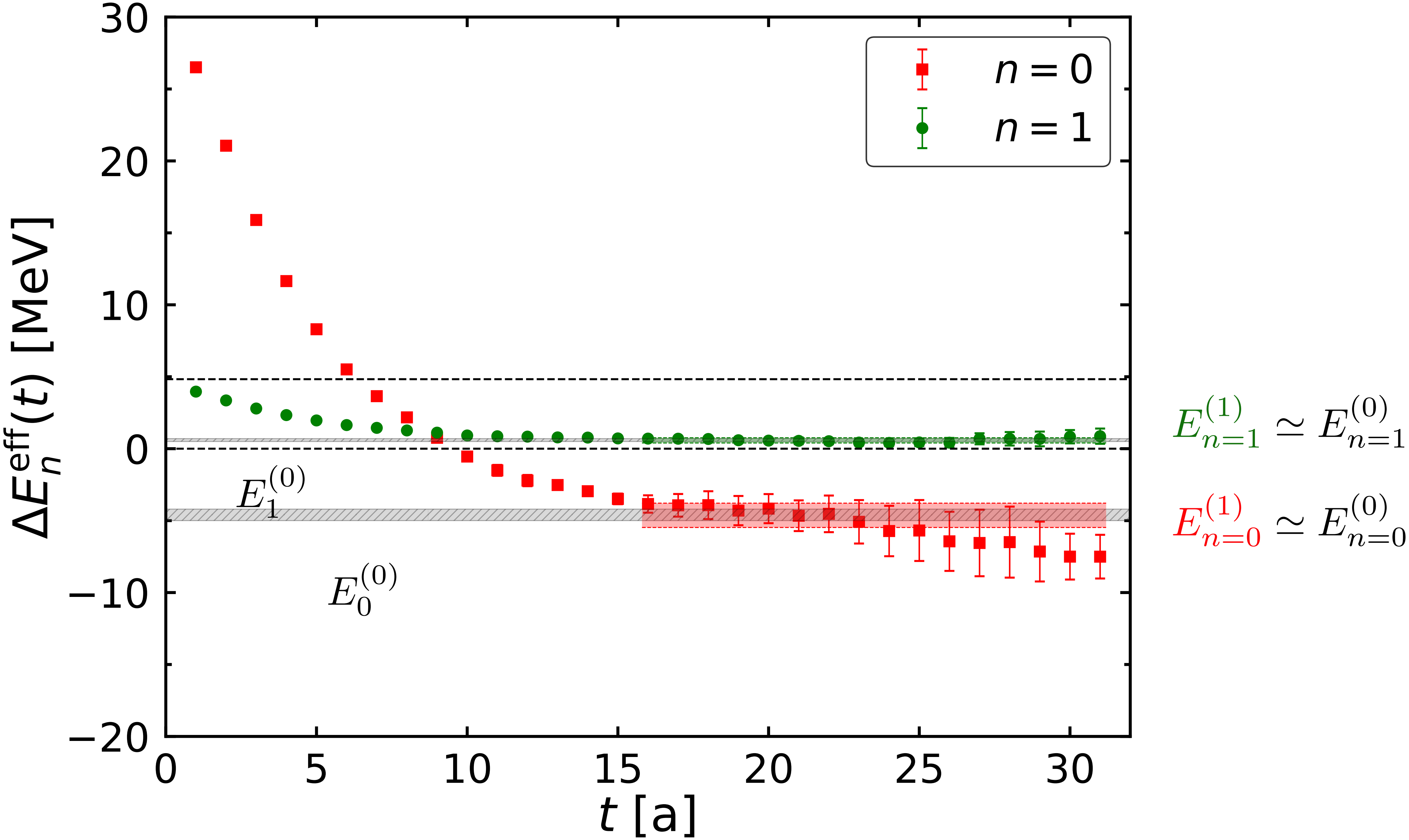


Time dependences are small.

→ A single state dominates in each correlation function.

optimized operator $$O_n(t) := \frac{1}{V^2}\sum_{\vec{x},\vec{r}\in\Lambda} B(\vec{x}+\vec{r},t)B(\vec{x},t)\Psi^*_n(\vec{r})$$

Effective energies



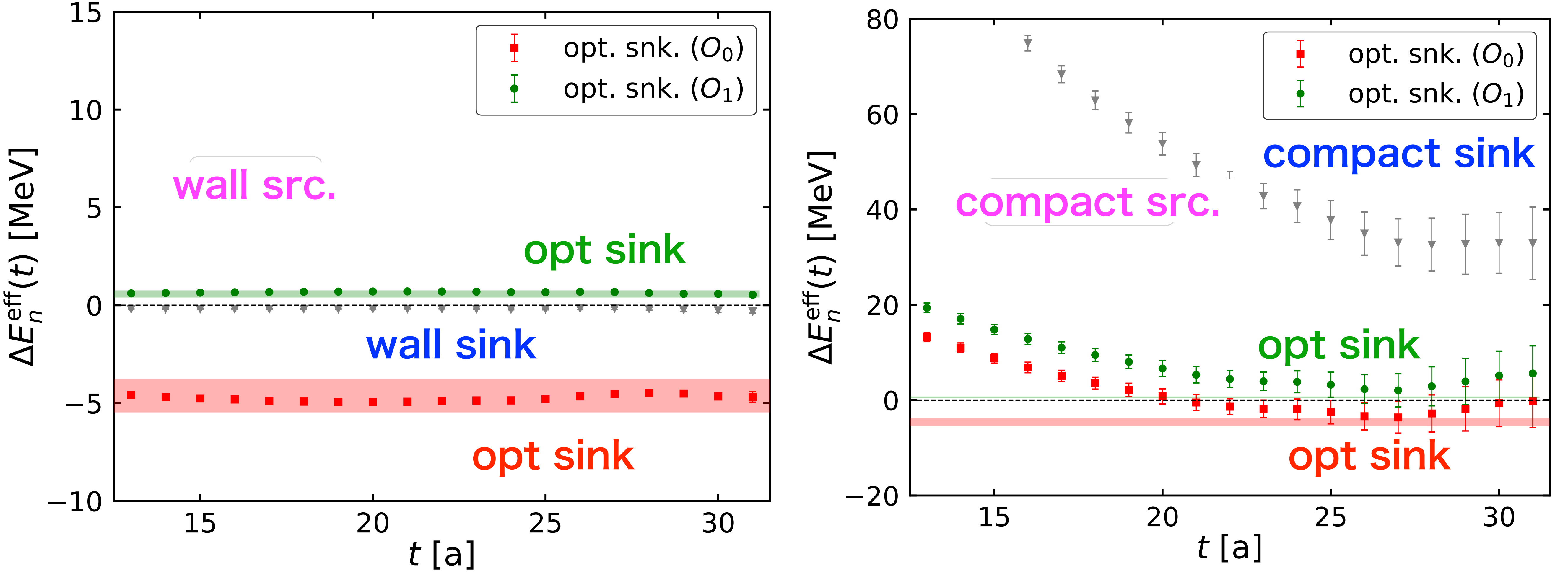
The optimized operators resolve the 5 MeV splitting in energies.

Smaller errors and less time variation in the 1st excited state, probably

(1) all points contribute to signals. (2) profile is more stable in t .

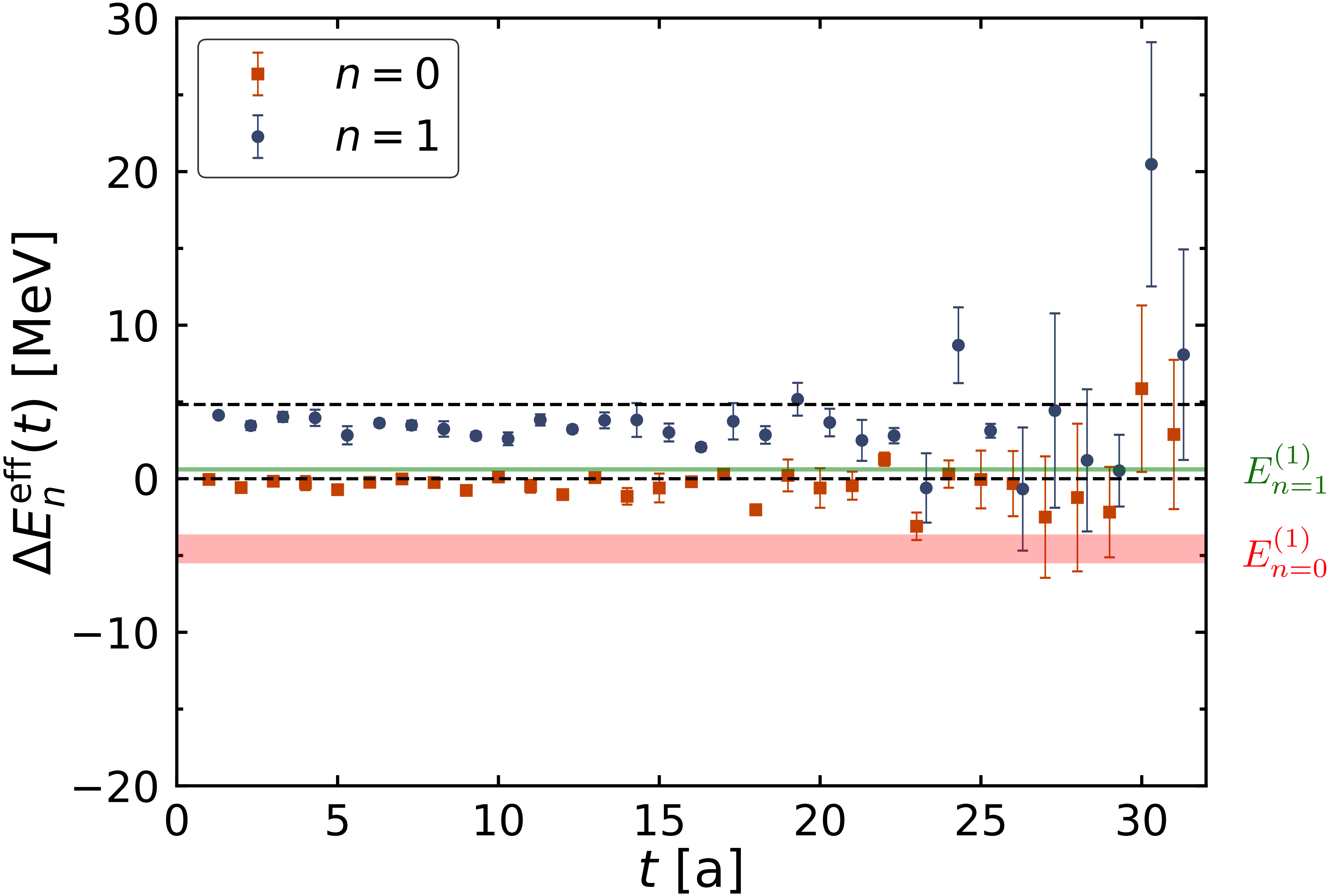
\# of points $\propto r^2$

Optimized sink operators



Optimized sink operators also work well, while non-optimized ones lead to “fake plateaux”.

2x2 variational analysis by plain-waves vs. optimized operators



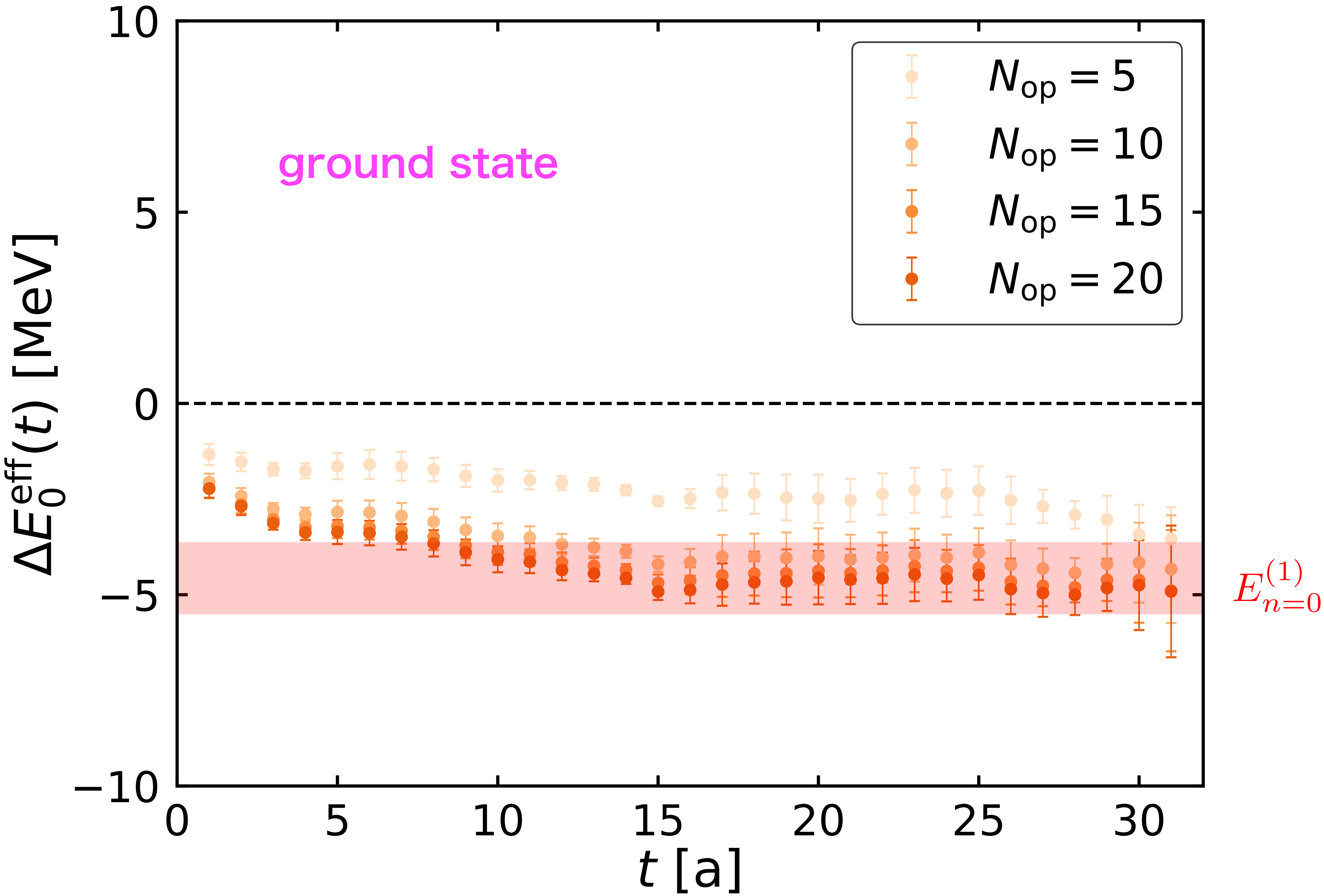
As expected, 2x2 plain-waves fail.

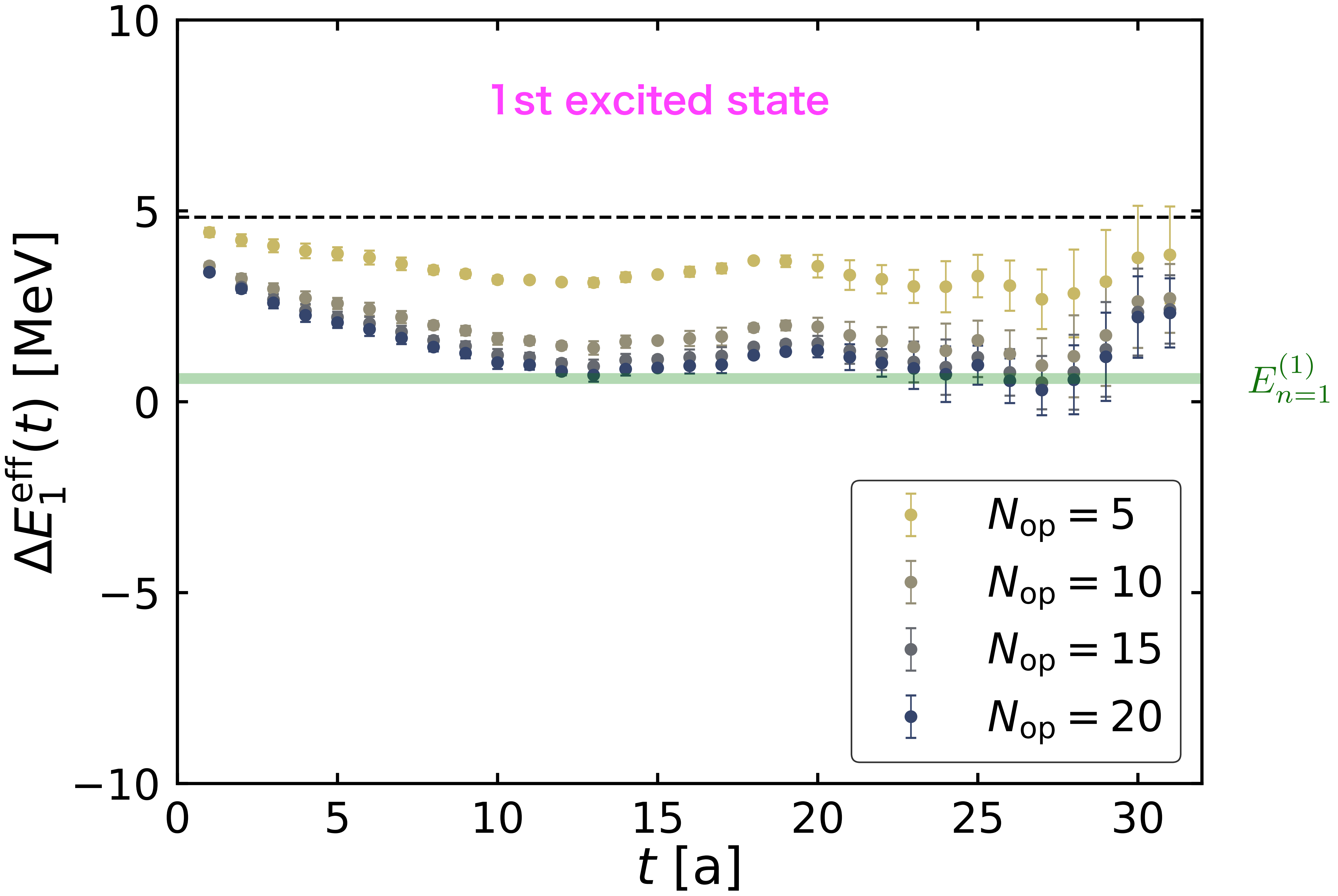
plain-wave approximation for (effective) optimized operators

dual basis in p-space

$$O^{\text{eff}}_{0,1}(t, n = N_{\text{op}}) := \sum_{|\vec{p}| \leq p_n} \bar{O}(\vec{p}, t)\tilde{\Psi}^*(\vec{p})$$

plain-wave op





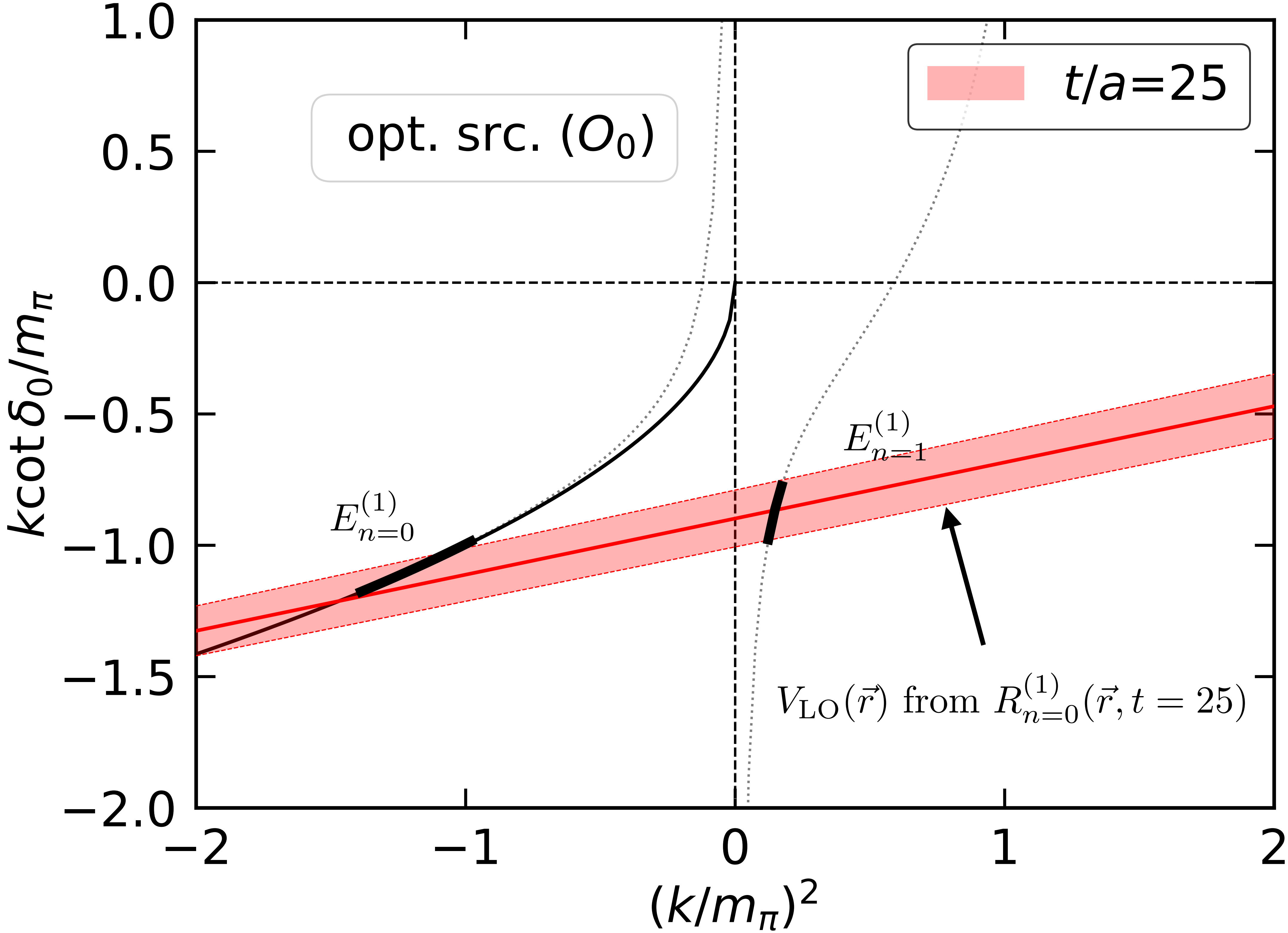
Momentum operators of $O(10)$ levels are needed to construct good operators.

V. Summary

Summary

- A systematic framework for constructing optimized two-hadron operators using spatial wave function is proposed.
- An explicit implementation of optimized operators at source is considered.
  - quark smearing to reduce excited state contaminations for 1 baryon
  - spatial summation by Z_3 noises avoiding costly all-to-all propagators
  - sparsening technique to tame fluctuations from Z_3 noises
- Application to the $\Omega_{ccc}\Omega_{ccc}$ system at $m_\pi \simeq 137$ MeV
  - our method successfully resolves the 5 MeV energy splitting
  - finite volume spectra agrees with phase shifts from LO potential (next slide)
- Optimized operators can be also used to construct variational bases.

Scattering phase shifts via potential from O_0



Scattering phase shifts from finite volume spectra and the LO potential with the optimized operator are consistent.

Future projects

- Apply new method to various systems
  - NN at various pion masses
  - exotic states such as $\Lambda(1405), \kappa, \cdots$
  - More

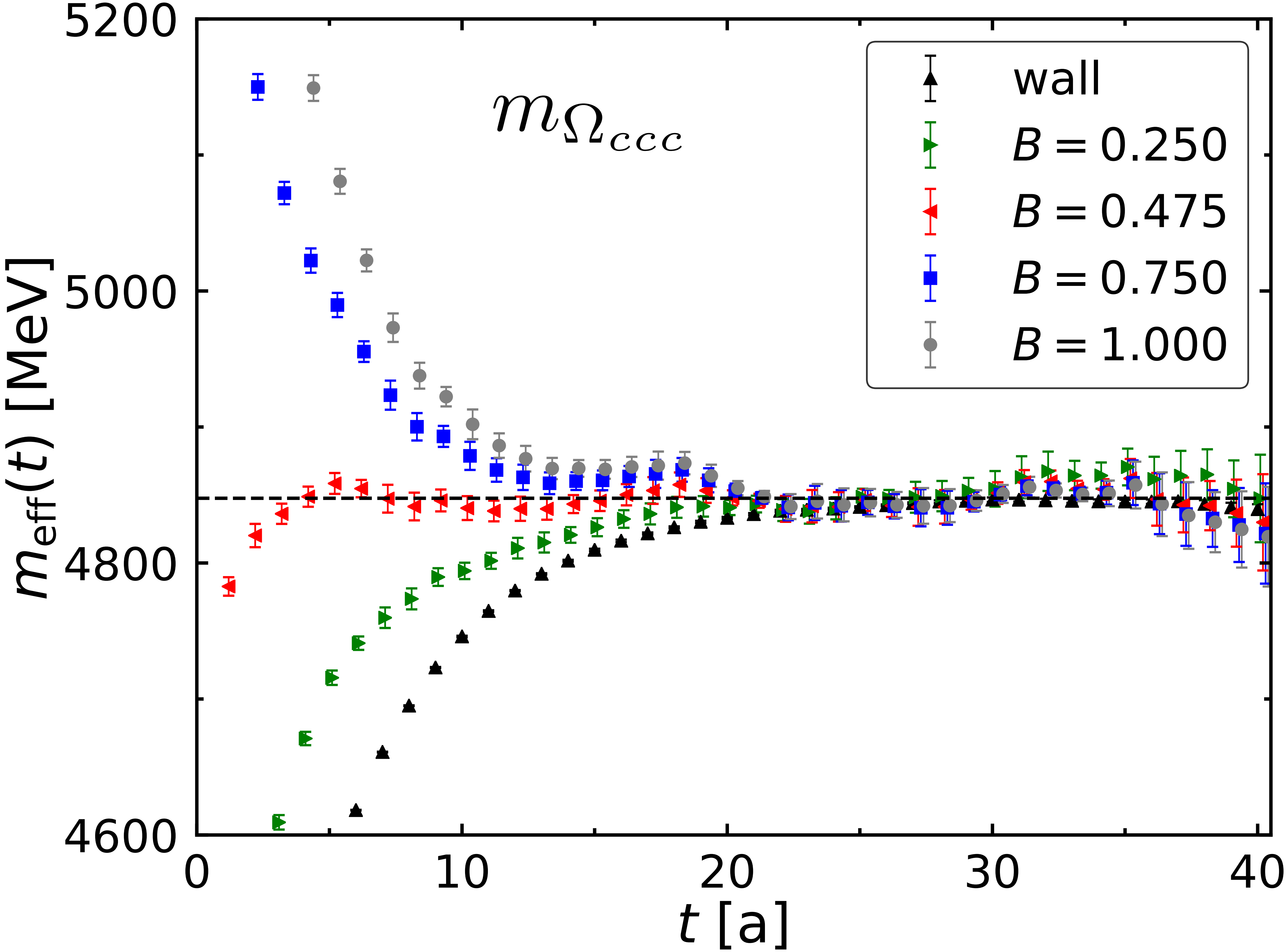
Old methods good for one hadron are not guaranteed to work for two baryons (hadrons). We need to invent new methods as many as possible and combined them with old ones for reliable results on multi-hadrons.

Thank you for listening !

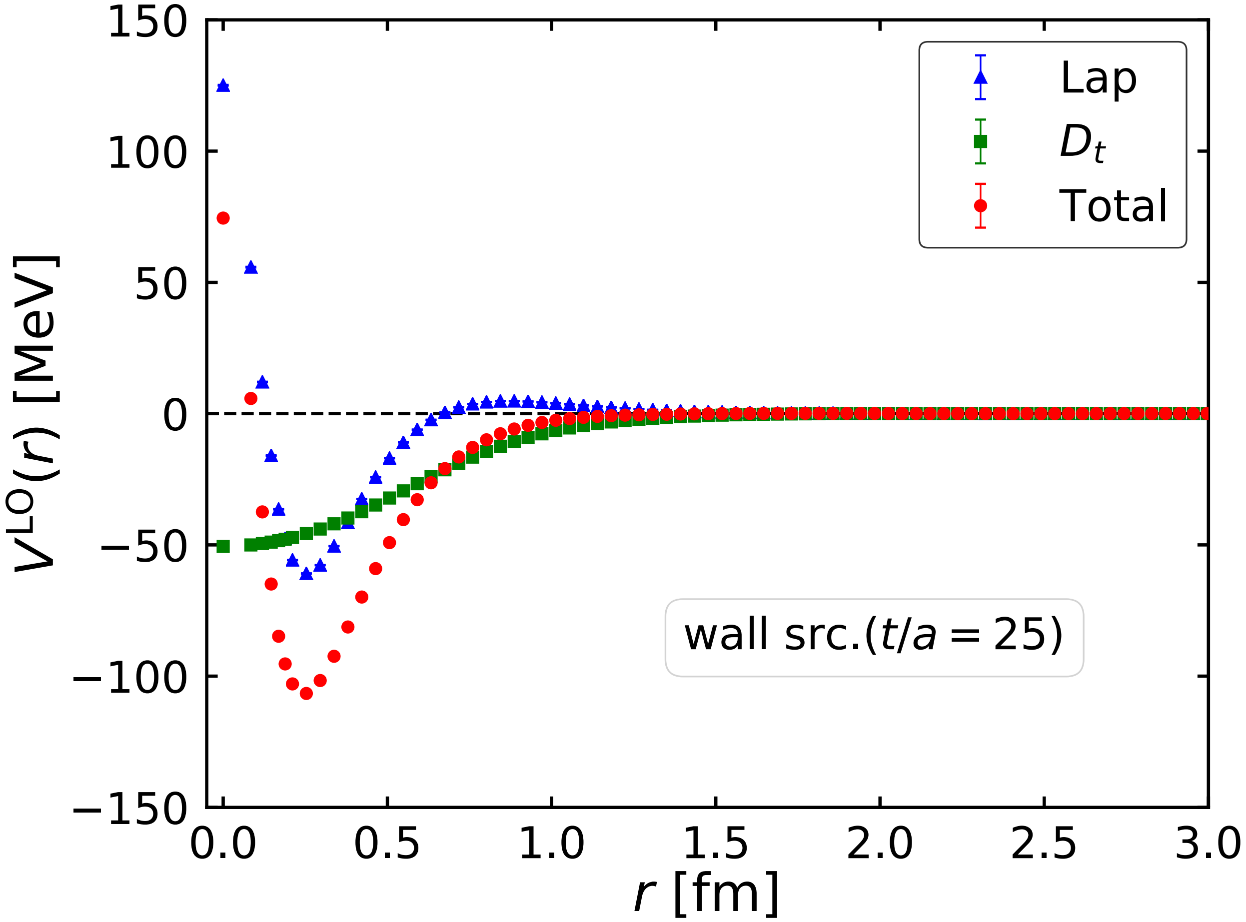
Back-up slides

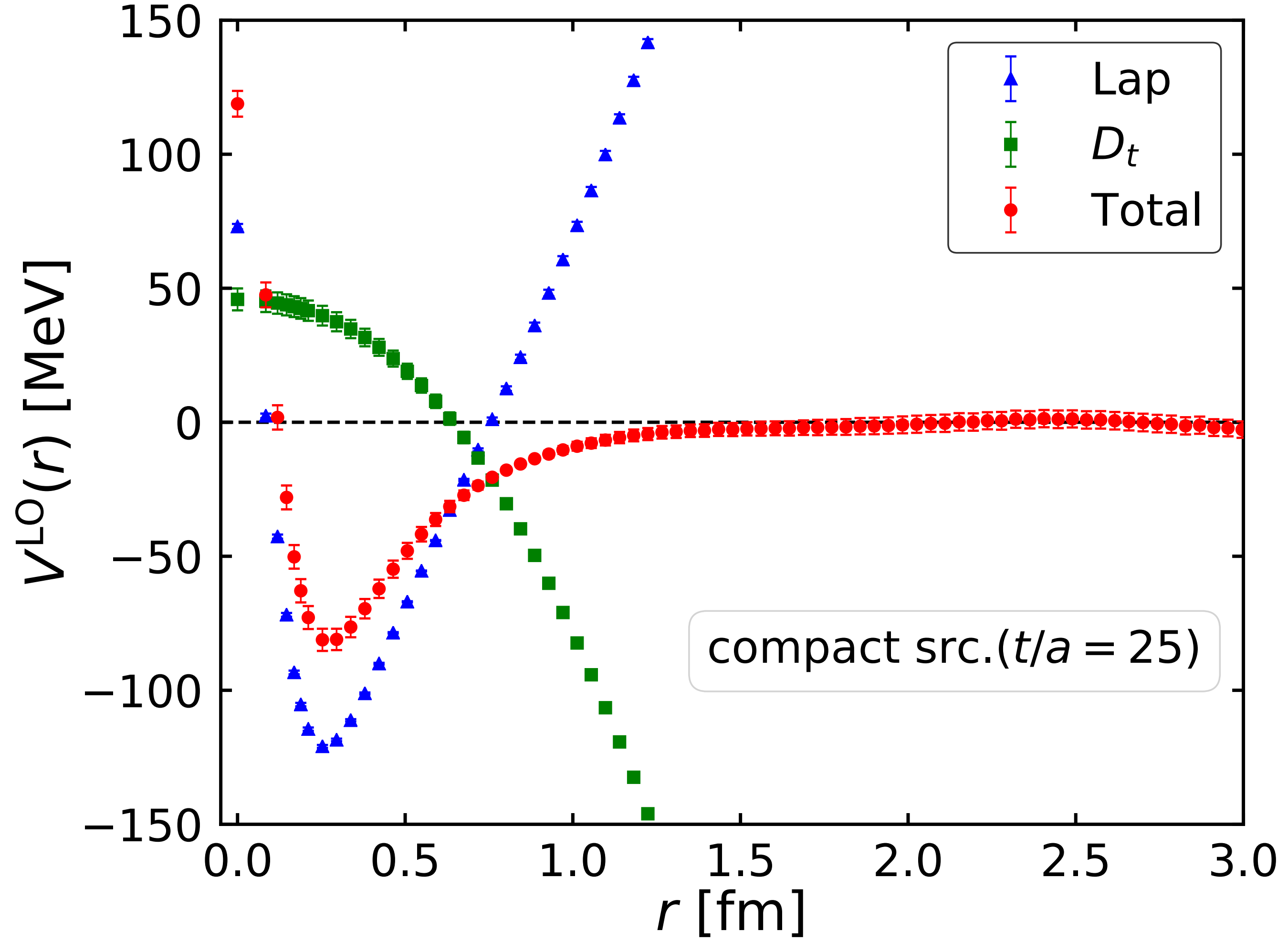
Quark smearing parameter for one Ω_{ccc}

smearing function $f^{\mathrm{expo}}(\vec{r}) = e^{-B|\vec{r}|}$ $\longrightarrow$ $B = 0.475/a$



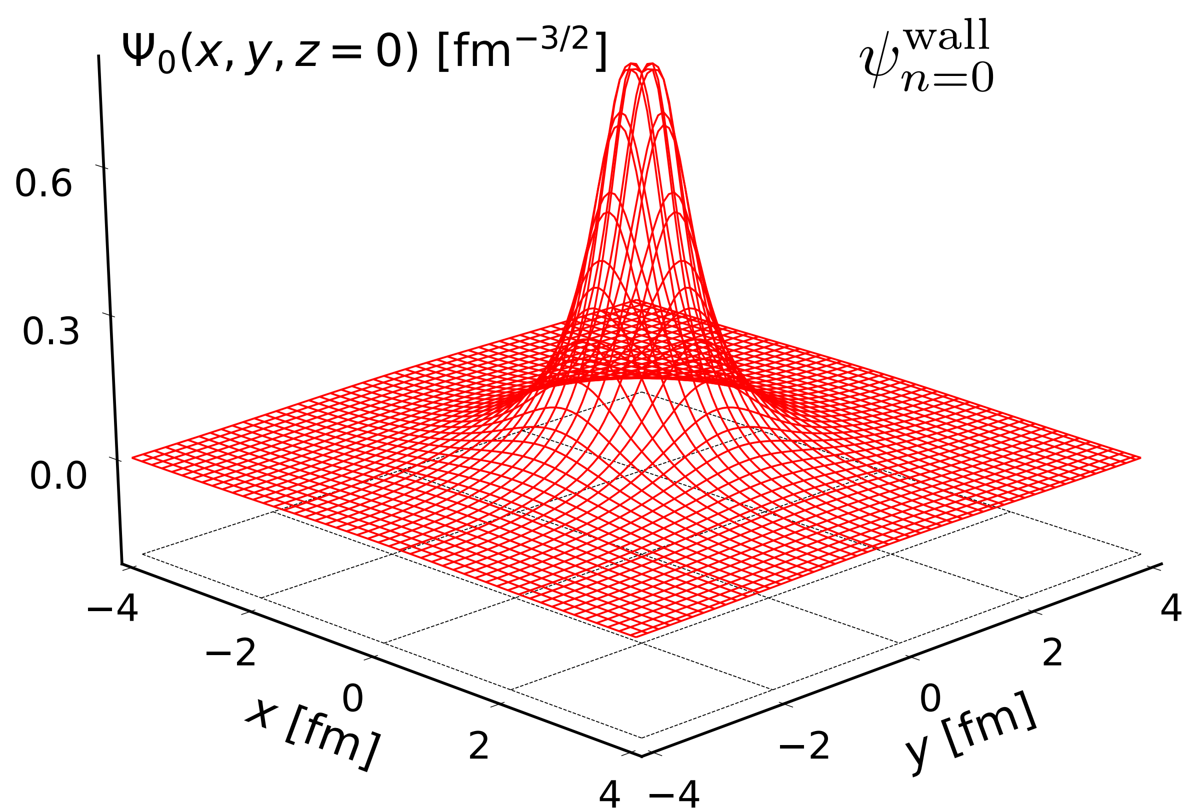
LO potentials

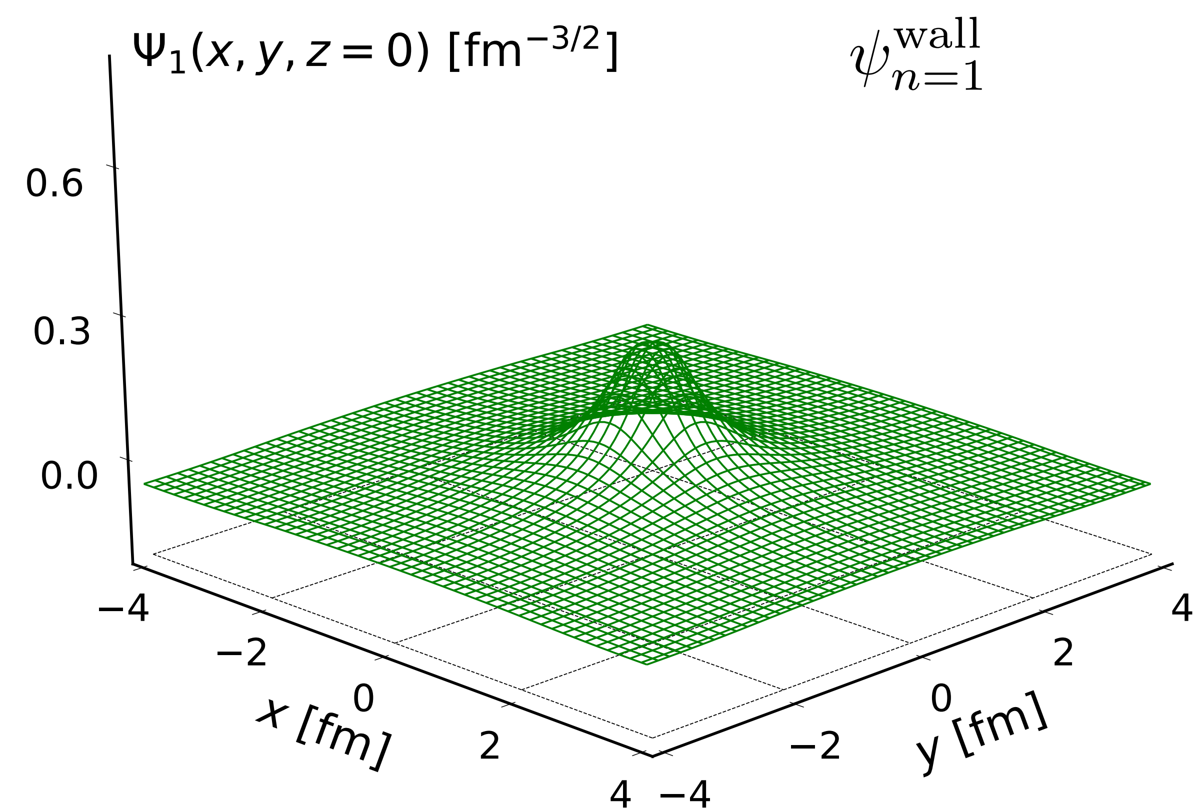


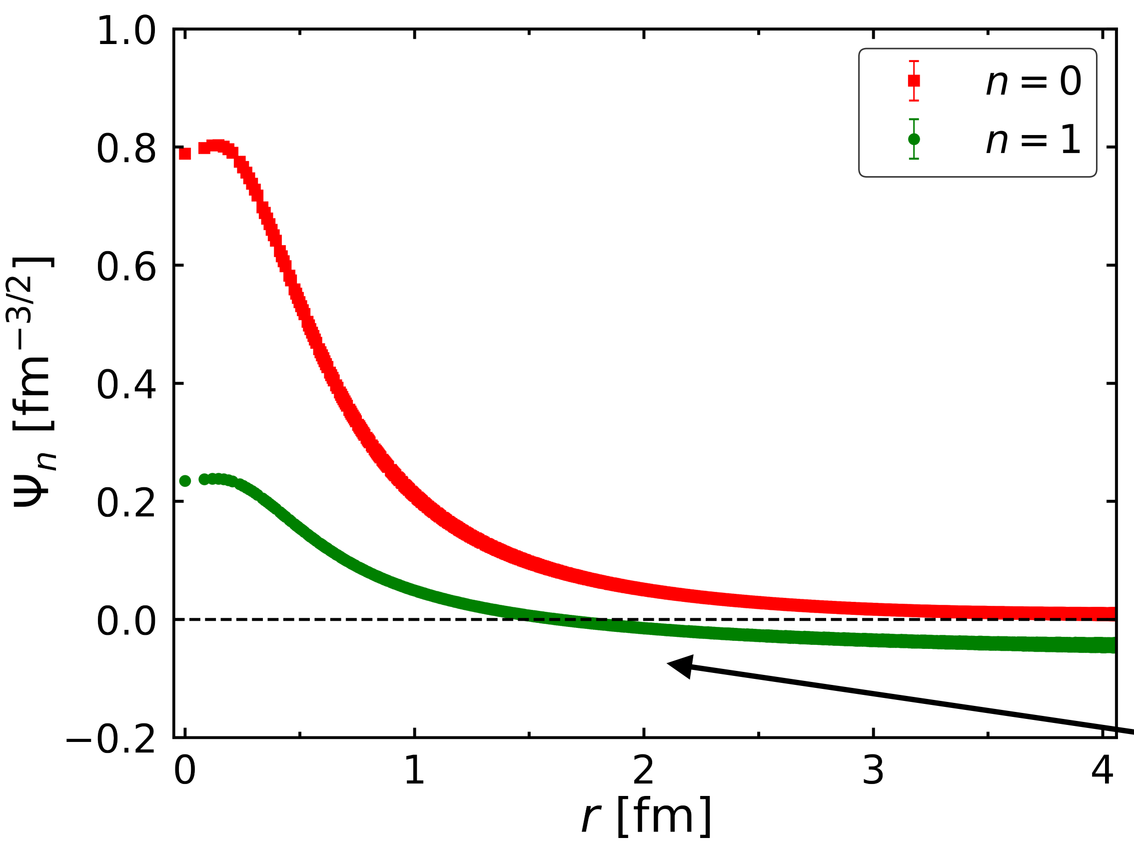


The total potentials look similar between wall and compact sources, while individual contributions are very different between them, in particular, at long distances.

LO eigenfunctions







$$E^{(0)}_{n=0} = -4.6(4)\ \mathrm{MeV} \qquad E^{(0)}_{n=1} = 0.6(1)\ \mathrm{MeV}$$

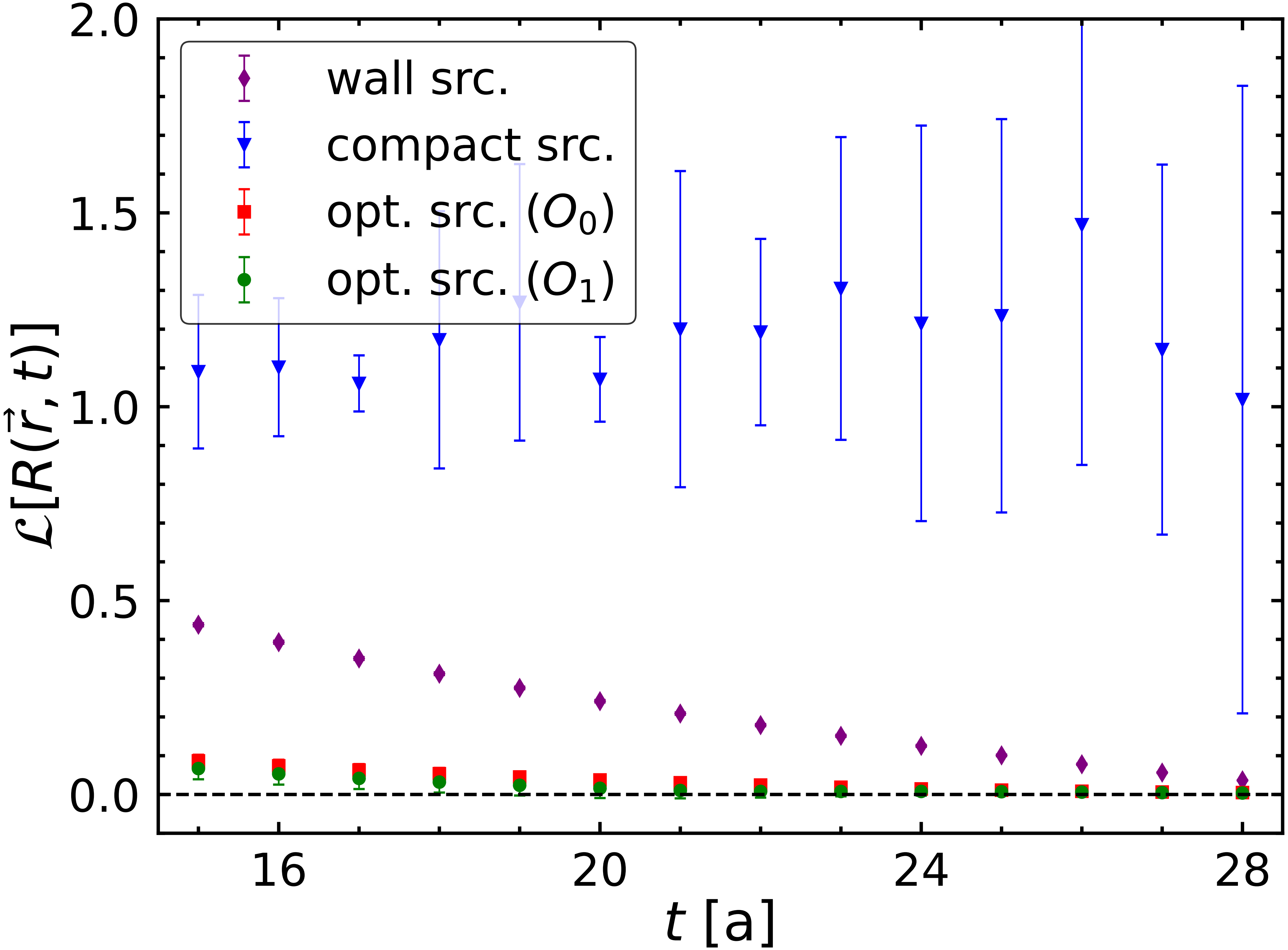
$$\Delta E := E^{(0)}_1 - E^{(0)}_0 = 5.2(4)\ \mathrm{MeV}$$

as expected

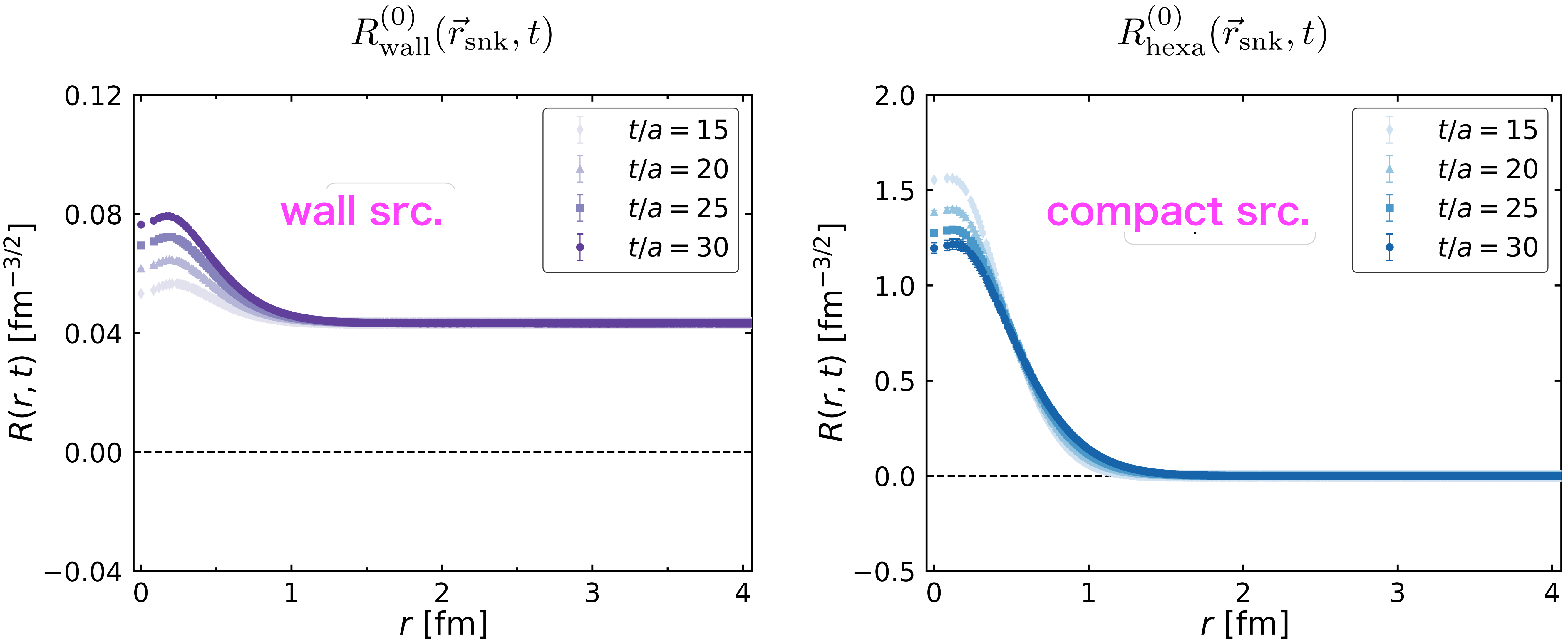
node

Residual factor

$$\mathcal{L}[R(\vec{r},t)] := \frac{1}{V}\sum_{\vec{r}\in\Lambda}\left|\frac{R(\vec{r},t)/R(\vec{0},t)}{R(\vec{r},t_f)/R(\vec{0},t_f)} - 1\right| \qquad t_f = 30$$



Standard sources



1. Significant time dependences are observed.

2. Profiles are different between two sources.

→ A ground state saturation is not achieved in this time range.

consistency $$-\frac{\nabla^2}{m_B}\psi_n(\vec{r}) \to \frac{p_n^2}{m_B}\psi_n(\vec{r}), \quad r \to \infty$$