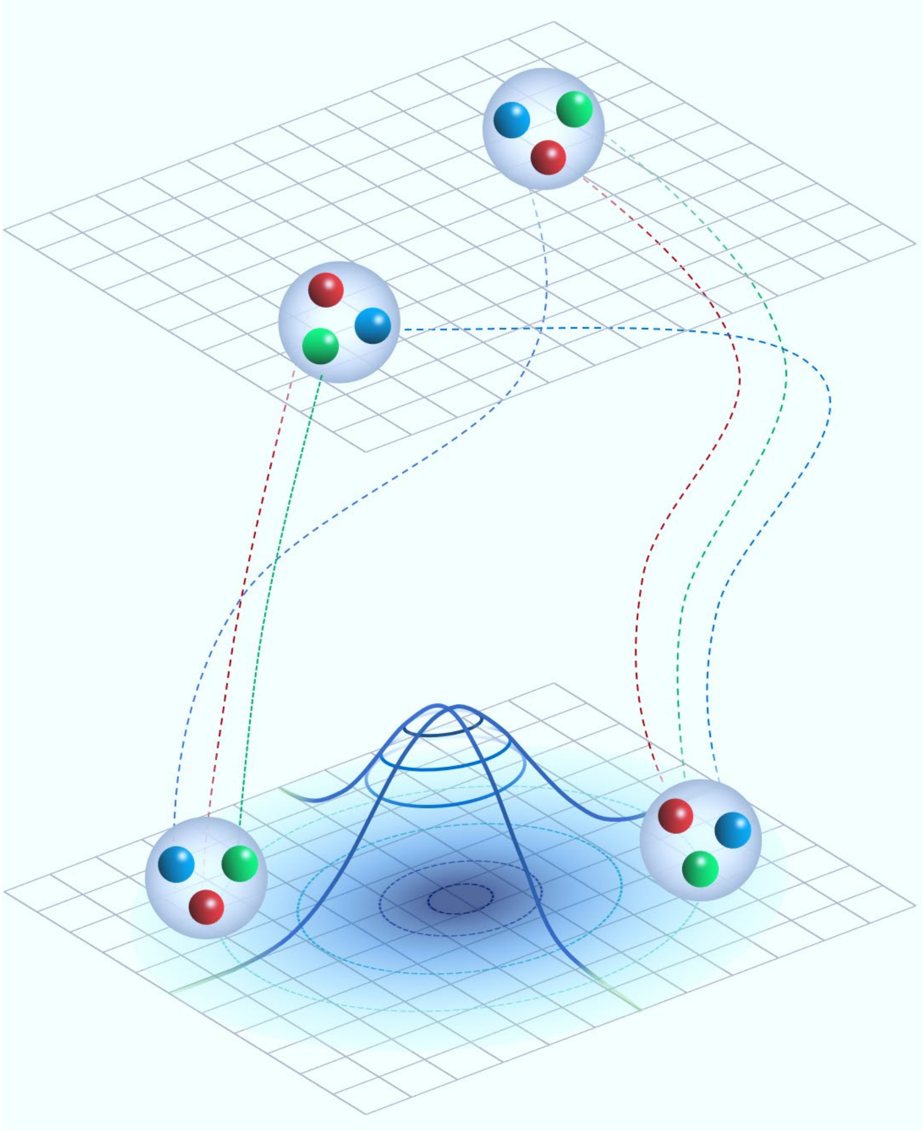
Decoding two-hadron states in LQCD with spatial wavefunctions



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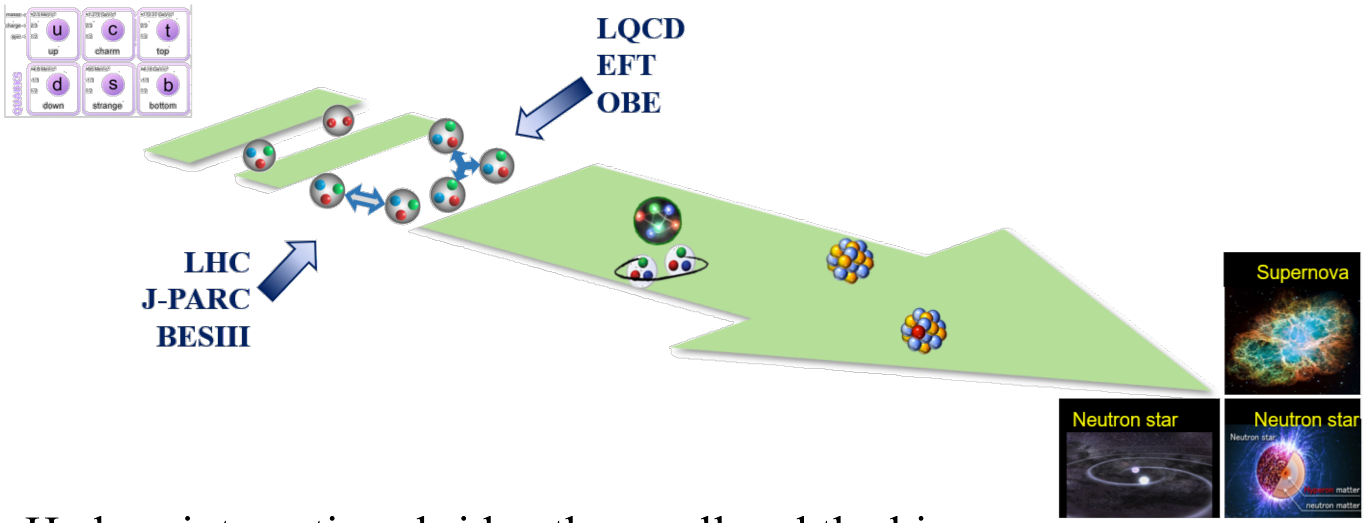
Aug. 21, 2025

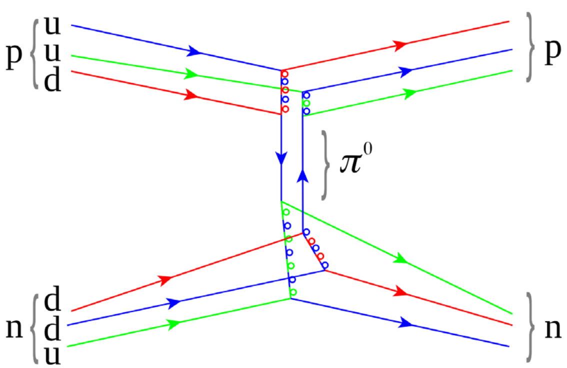
From quarks to the Universe

- Milestones in the path from quarks to the Universe



- Hadron interactions bridge the small and the big

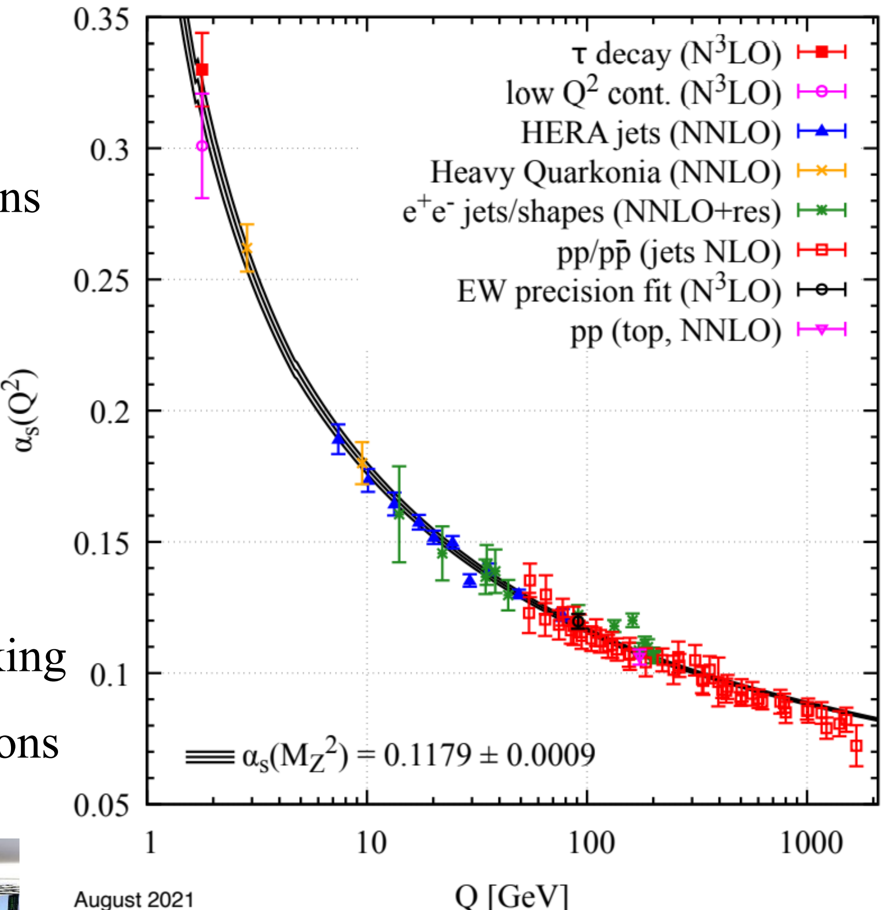
- In theory, QCD governs not only the interaction among quarks and gluons, but also the interaction between color-neutral hadrons



- Strong interaction strength strongly depends on energy scale (Q)

- High Q (> few GeV), perturbative
  - ✓ asymptotic freedom
  - ✓ weakly interacting quarks and gluons
  - ✓ "pen and paper"

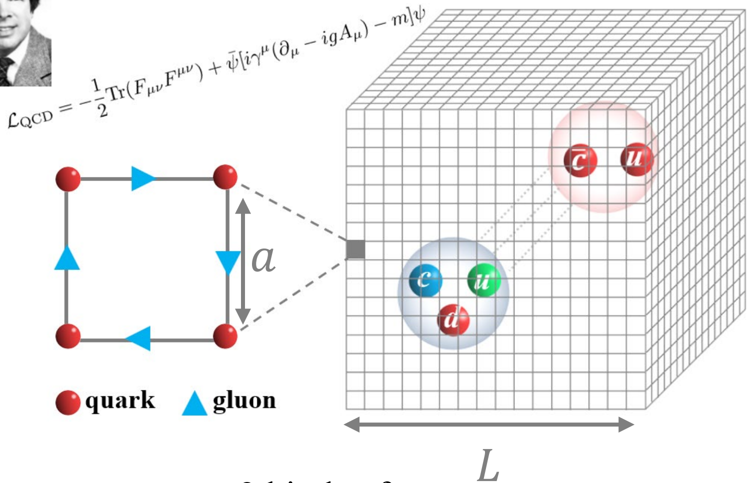
- Low Q (< 1 GeV), non perturbative
  - ✓ chiral symmetry spontaneous breaking
  - ✓ strongly interacting quarks and gluons
  - ✓ LQCD simulations



PDG, https://pdg.lbl.gov/

Lattice QCD

K.G. Wilson, Phys. Rev. D 10, 2445 (1974)



2 kinds of parameters: m_q, g

Lattice regularization

- UV cutoff $\sim \frac{1}{a}$; IR cutoff $\sim \frac{1}{L}$
- Quark field $q(x)$ on lattice sites
- Gauge field $U_\mu(x) = e^{iagA_\mu(x)}$ on links

Path integral

- dof: $\sim 100^4 \times 8 \times 4$

$$\langle \hat{O} \rangle = \frac{1}{Z_E} \int [\mathcal{D}\bar{q}][\mathcal{D}q][\mathcal{D}U] O e^{-S_E}$$

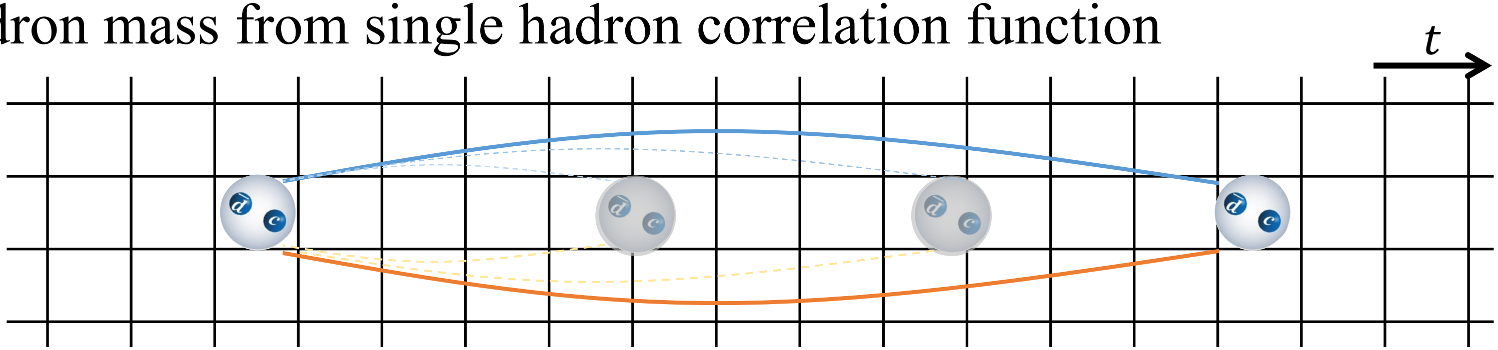
Monte Carlo Simulation

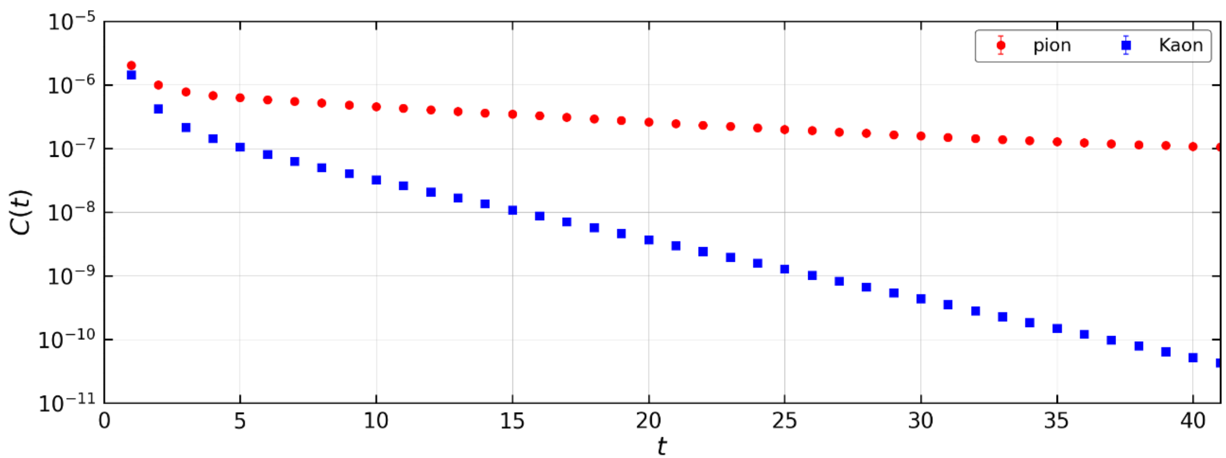
- Importance sampling: a series of QCD configurations with probability e^{-S_E}
- Multiple measurements $O_1, \cdots, O_N$

$$\langle \hat{O} \rangle = \bar{O} \pm \frac{\sigma}{\sqrt{N}}$$

A typical paradigm of lattice calculations

➢ Hadron mass from single hadron correlation function



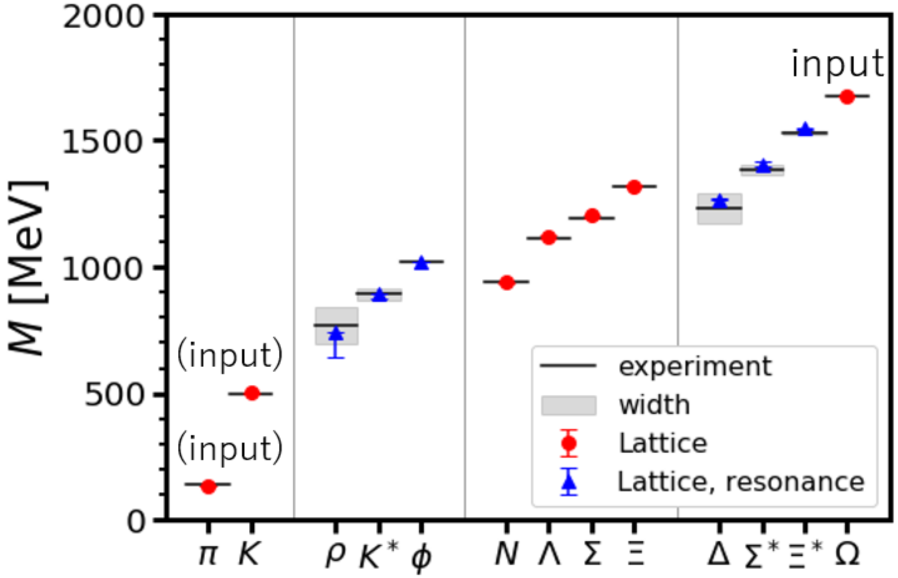


$$C(t) = \langle \hat{O}(t)\hat{O}^\dagger(0)\rangle = \sum_n |\langle 0|\hat{O}|E_n\rangle|^2 e^{-E_n t}$$
$$= |\langle 0|\hat{O}|E_0\rangle|^2 e^{-E_0 t} + O(e^{-E_1^* t})$$

- The mass of hadron can be obtained when the ground state dominates $C(t)$
  - ✓ $t \gg \frac{1}{E_1 - E_0}$, and/or $\langle 0|\hat{O}|E_0\rangle \gg \langle 0|\hat{O}|E_{n\neq 0}\rangle$

Singal hadron from LQCD

- LQCD has been successful in describing single hadron systems



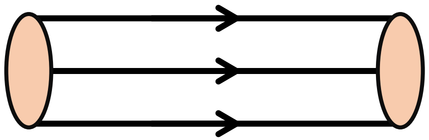
T. Aoyama *et al.* [HAL QCD Coll.], Phys. Rev. D 110, 094502 (2024)

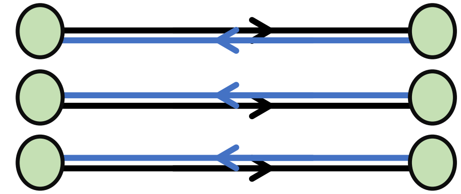
- One of frontiers in LQCD lies in two-hadron systems
  - nucleon interaction relevant to nuclei and nuclear matter
  - nucleon matrix element relevant to $0\nu\beta\beta$ *etc*

Challenge: exponential degradation of S/N

- The nucleon two-point function

G. Parisi, Phys. Rept. 103, 203 (1984)
G. P. Lepage, From actions to answers: Proceedings of the tasi (1989)





$$\mathcal{S} = \langle \hat{N}(t)\hat{N}^\dagger(0)\rangle \simeq \langle G_q^3(t)\rangle \sim e^{-m_N t}$$

$$\mathcal{N}^2 = \langle |\hat{N}(t)\hat{N}^\dagger(0)|^2\rangle - |\langle \hat{N}(t)\hat{N}^\dagger(0)\rangle|^2 \simeq \langle |G_q^*(t)G_q(t)|^3\rangle \sim e^{-3m_\pi t}$$

- Signal-to-noise ratio

$$\frac{\mathcal{S}}{\mathcal{N}} \sim \frac{e^{-m_N t}}{e^{-3/2 m_\pi t}} = e^{-(m_N - 3/2 m_\pi)t}$$

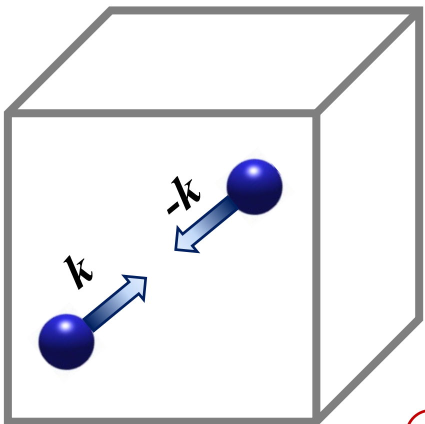
  - t can not be sufficient larger than $t_{ns} = \frac{1}{m_N - 3/2 m_\pi}$

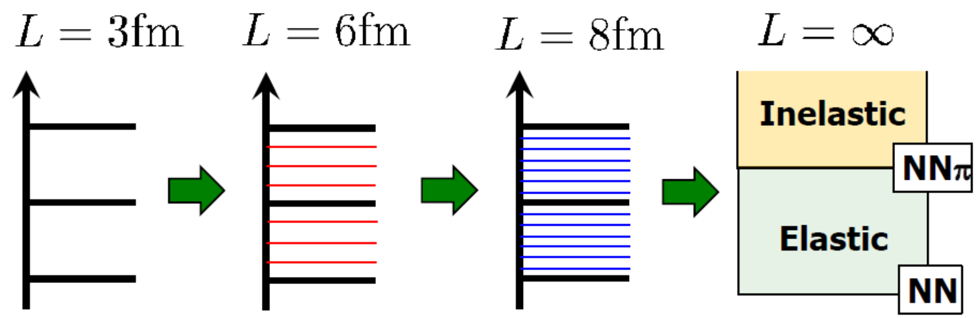
- More severe for two-nucleon systems

$$\left.\frac{\mathcal{S}}{\mathcal{N}}\right|_{2B} \sim e^{-(2m_N - 3m_\pi)t}$$

Challenge: dense two-hadron spectra

➢ Elastic two-hadron states





$$\Delta E \simeq \frac{p^2}{m} = \frac{(2\pi/L)^2}{m} = \frac{4\pi^2}{mL^2}$$

- Denser spectra with larger volume L/ heavier mass m
- To suppress elastic contaminations $t \gg \frac{1}{\Delta E} \sim 10$ fm, without opt operators

Optimized two-hadron operators are highly desired

Contents

Based on: YL, S. Aoki, T. Doi, T. Hatsuda, K. Murakami, and T. Sugiura, arXiv:2507.09930; 2507.09933

Lessons from single hadron: the "shape" matters

➢ Smearing: mimic realistic spatial profile ("shape") of single hadron

$$q(\vec{x}) \longrightarrow q_f = \sum_{\vec{y}\in\Lambda} f(|\vec{x}-\vec{y}|)q(\vec{y})$$

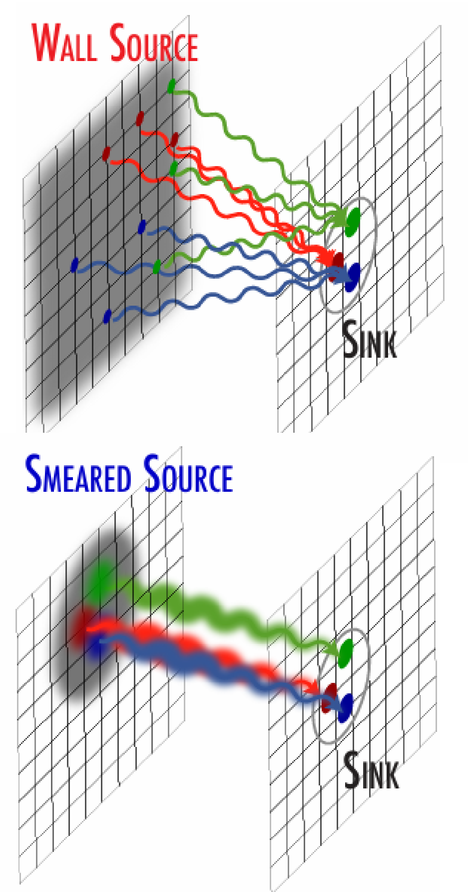
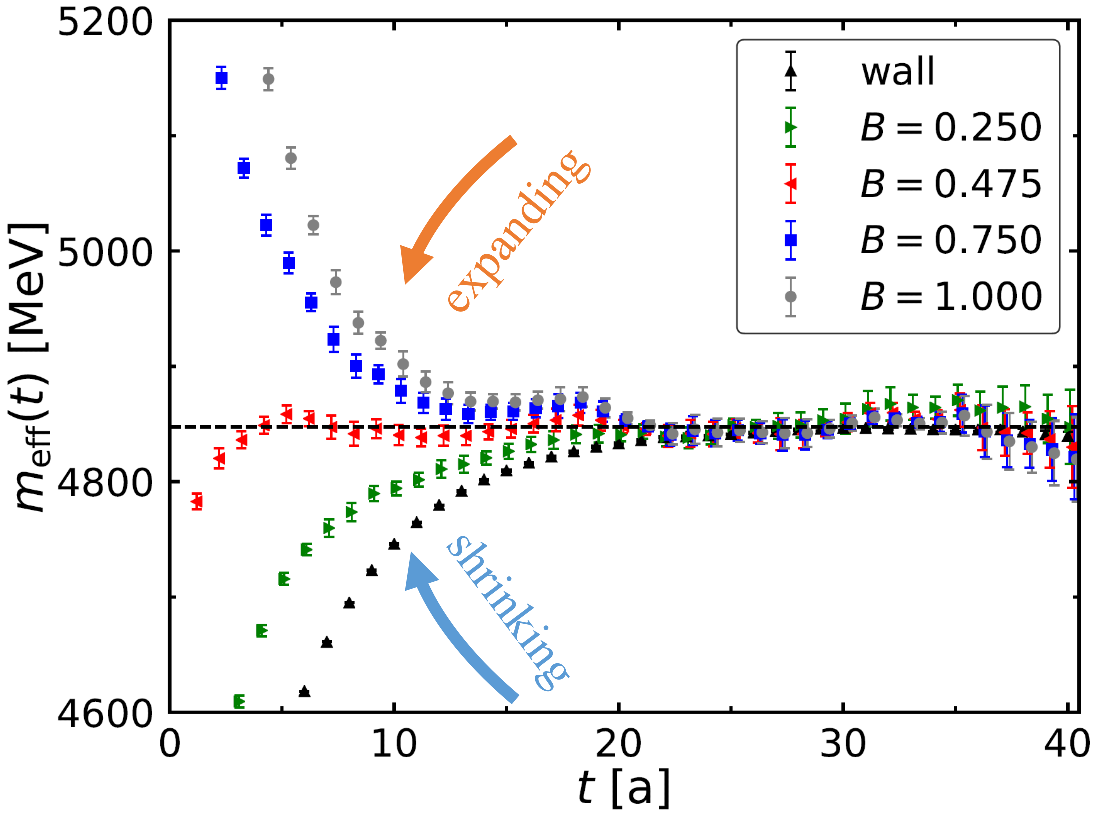


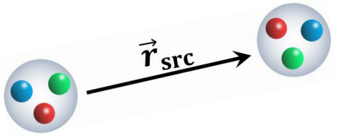
Fig. from T. Iritani



The "shape" of two-hadron states

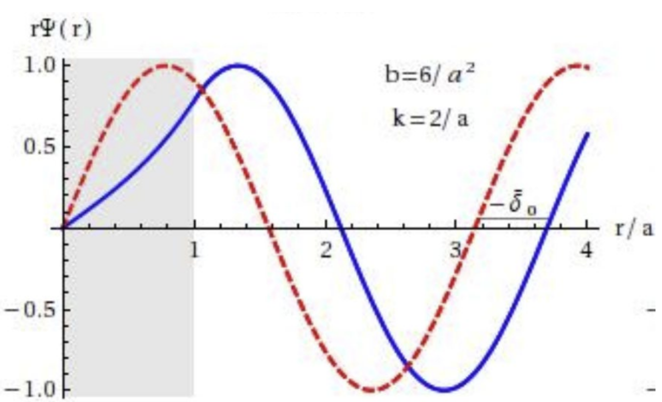
- (Equal-time) Nambu-Bethe-Salpeter (NBS) amplitude ($t_0 = 0$)

$$\psi_n(\vec{r}) = \frac{1}{V}\sum_{\vec{x}\in\Lambda}\langle 0|\hat{B}(\vec{x}+\vec{r},t_0)\hat{B}(\vec{x},t_0)|2B, E_n\rangle$$



  - The probability amplitude of finding two Bs with a separation $\vec{r}$
  - Encoding scattering phase shift at asymptotic region
    - ✓ Scattering phase shifts $\psi_n^l(r) \simeq A\frac{\sin(kr+\delta(k_n)-l/2\pi)}{kr}$

- A quantum mechanics analogy: stationary scattering wavefunctions



Optimized two-hadron operators

- General hadronic correlation functions for two-hadron systems

$$\mathcal{R}(\vec{r}_{\rm snk}, t; \vec{r}_{\rm src}) = \frac{e^{2m_B t}}{V^2} \sum_{\vec{x},\vec{y}\in\Lambda} \langle \hat{B}(\vec{x}+\vec{r}_{\rm snk}, t)\hat{B}(\vec{x}, t)\bar{\hat{B}}(\vec{y}+\vec{r}_{\rm src}, 0)\bar{\hat{B}}(\vec{y}, 0)\rangle$$
$$= \sum_{n=0}^{N} \psi_n(\vec{r}_{\rm snk})\psi_n^*(\vec{r}_{\rm src})e^{-\Delta E_n t} + O(e^{-\Delta E^* t})$$

- Optimizing two-hadron operators by incorporating inter-hadron w.f. $\Psi_n(\vec{r})$

$$\hat{O}_n(t) = \frac{1}{V^2} \sum_{\vec{x},\vec{r}\in\Lambda} \hat{B}(\vec{x}+\vec{r}, t)\hat{B}(\vec{x}, t)\Psi_n^*(\vec{r})$$

$$\frac{1}{V} \sum_{\vec{r}\in\Lambda} \Psi_n^*(\vec{r})\psi_m(\vec{r}) = \delta_{nm}$$

- Applying $\hat{O}_n$ as the source operator

$$R(\vec{r}_{\rm snk}, t) = \frac{e^{2m_B t}}{V} \sum_{\vec{x}\in\Lambda} \langle \hat{B}(\vec{x}+\vec{r}_{\rm snk}, t)\hat{B}(\vec{x}, t)\hat{O}_n^\dagger(0)\rangle \simeq \psi_n(\vec{r}_{\rm snk})e^{-\Delta E_n t}$$

Optimized vs Conventional operators

- Optimized operators incorporate realistic spatial information $\Psi_n(\vec{r})$

- Conventional operators can be interpreted as certain approximations to $\Psi_n(\vec{r})$
  - The compact operator (place two hadron operators at the same position)

$$\Psi_n(\vec{r}) \sim \delta(\vec{r})$$

  - The wall operator (not localized operator, but conceptionally spatial points are equally weighted)

$$\Psi_n(\vec{r}) \sim 1$$

  - Operators from the variational method using plane-wave basis $\{B(\vec{p})B(-\vec{p})\}$

$$\Psi_n(\vec{r}) \sim \tilde{\Psi}_n(\vec{p}_0)\tilde{\Psi}_n(-\vec{p}_0)e^{i\vec{p}_0\cdot\vec{r}} + \tilde{\Psi}_n(\vec{p}_1)\tilde{\Psi}_n(-\vec{p}_1)e^{i\vec{p}_1\cdot\vec{r}} + \cdots$$

Construction of dual functions $\Psi_n(\vec{r})$

- $\Psi_n(\vec{r})$ can be constructed with the NBS kernel $\mathcal{K}$

$$\Psi_n(\vec{r}) = \sum_{m=0}^{N} \mathcal{K}_{nm}^{-1} \psi_m(\vec{r}), \quad \mathcal{K}_{nm} = \langle \psi_n | \psi_m \rangle$$

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

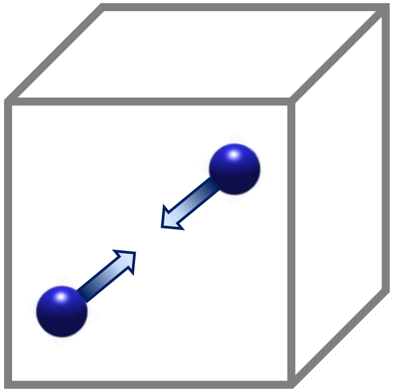
  - All NBS amplitudes below inelastic threshold $\psi_{n<N}(\vec{r})$ are needed

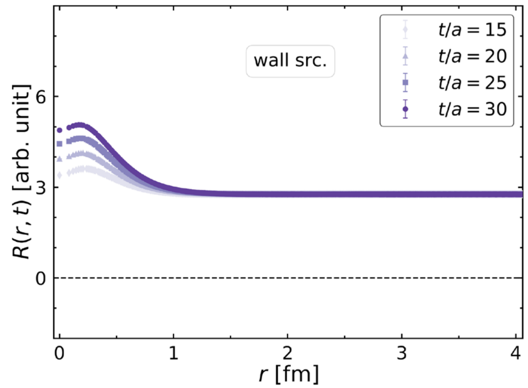
- The NBS amplitude $\psi_n(\vec{r})$ can be obtained through an iterative procedure

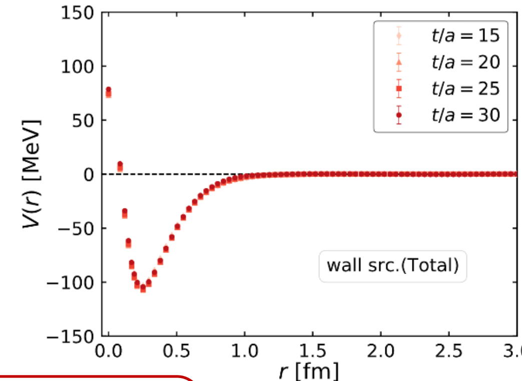
  - Initial guess $\psi_n^{(0)}(\vec{r})$
    - Models, EFTs …
    - Overlapping factors from a variation method
    - HAL QCD potential
  - Using $\Psi_n^{(0)}(\vec{r})$ at the source to calculate correlation function $R_n^{(1)}(\vec{r}, t)$
  - Verifying if $R_n^{(1)}(\vec{r}, t)$ is stable against t, if not, extracting $\psi_n^{(1)}(\vec{r})$ from it and iterate this process until convergence

Initial w.f.s from the HAL QCD potential

➢ HAL QCD method: extract an effective potential from a spatiotemporal correlation function without requiring ground-state dominance







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

N. Ishii, S. Aoki and T. Hatsuda, Phys. Rev. Lett. 99, 022001 (2007)
N. Ishii, *et al.* [HAL QCD Coll.], Phys. Lett. B 712, 437 (2012)

➢ Eigen equations on a finite box

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

- Periodic boundary condition is applied

T. Iritani, *et al.* [HAL QCD Coll.], JHEP 03, 007 (2019)
YL *et al.*, Phys. Rev. D 105, 074512 (2022)

- Eigenfunctions provide good approximation to underlying NBS amplitudes

Implementation of optimized operators

- In lattice QCD, quark propagators are calculated using the smeared quark field

$$\langle q(\vec{x},t)\bar{q}_f(\vec{y},0)\rangle = \sum_{\vec{r}\in\Lambda}\langle q(\vec{x},t)\bar{q}(\vec{r},0)\rangle f(\vec{r}-\vec{y})$$

  - Spatial index at source is contracted with the smearing function
  - Spatial index at sink is open

- A direct way to implement the optimized operators needs to compute the quark propagator for all spatial points at the source (all-to-all propagator)
  - Prohibitive computational cost

- Our proposal: one can design appropriate source functions
  - Embedding the wavefunction $\Psi_n(\vec{r})$ directly
  - Optimized operators are realized automatically

Novel smearing functions

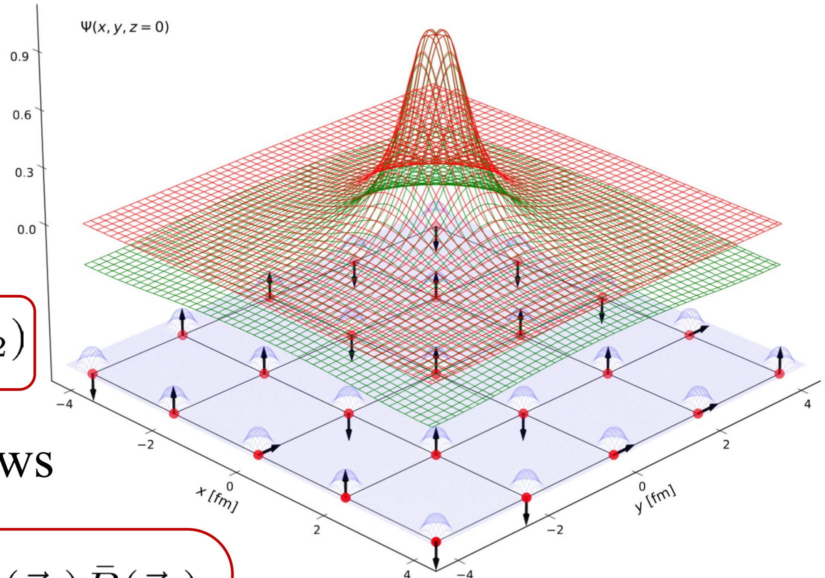
- Novel quark smearing functions at the source

$$G(\vec{r}) = f(\vec{r}), \to \bar{q}_G = \sum_{\vec{r}\in\Lambda} \bar{q}(\vec{r})G(\vec{r})$$

$$F_n(\vec{r}) = \frac{1}{V_{\rm sub}^{1/3}} \sum_{\vec{r}_0\in\Lambda_{\rm sub}} Z_3(\vec{r}_0)\Psi_n^{1/3}(\vec{r}_0)f(\vec{r}-\vec{r}_0), \to \bar{q}_{F_n} = \sum_{\vec{r}\in\Lambda} \bar{q}(\vec{r})F_n(\vec{r})$$

- $f(\vec{r})$ fined tuned for single hadron
- Each point is weighted by $\Psi_n^{-1/3}(\vec{r}_0)$
- Z_3 ensures no mixing terms in $(\bar{q}_{F_n})^3$

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



- The optimized operators are realized as follows

$$(\bar{q}_G)^3(\bar{q}_{F_n})^3 = \frac{1}{V_{\rm sub}} \bar{B}(\vec{0}) \sum_{\vec{r}_0\in\Lambda_{\rm sub}} \Psi_n(\vec{r}_0)\bar{B}(\vec{r}_0)$$

$$\simeq \frac{1}{V} \bar{B}(\vec{0}) \sum_{\vec{r}_0\in\Lambda} \Psi_n(\vec{r}_0)\bar{B}(\vec{r}_0)$$

Application to $\Omega_{ccc}\Omega_{ccc}$

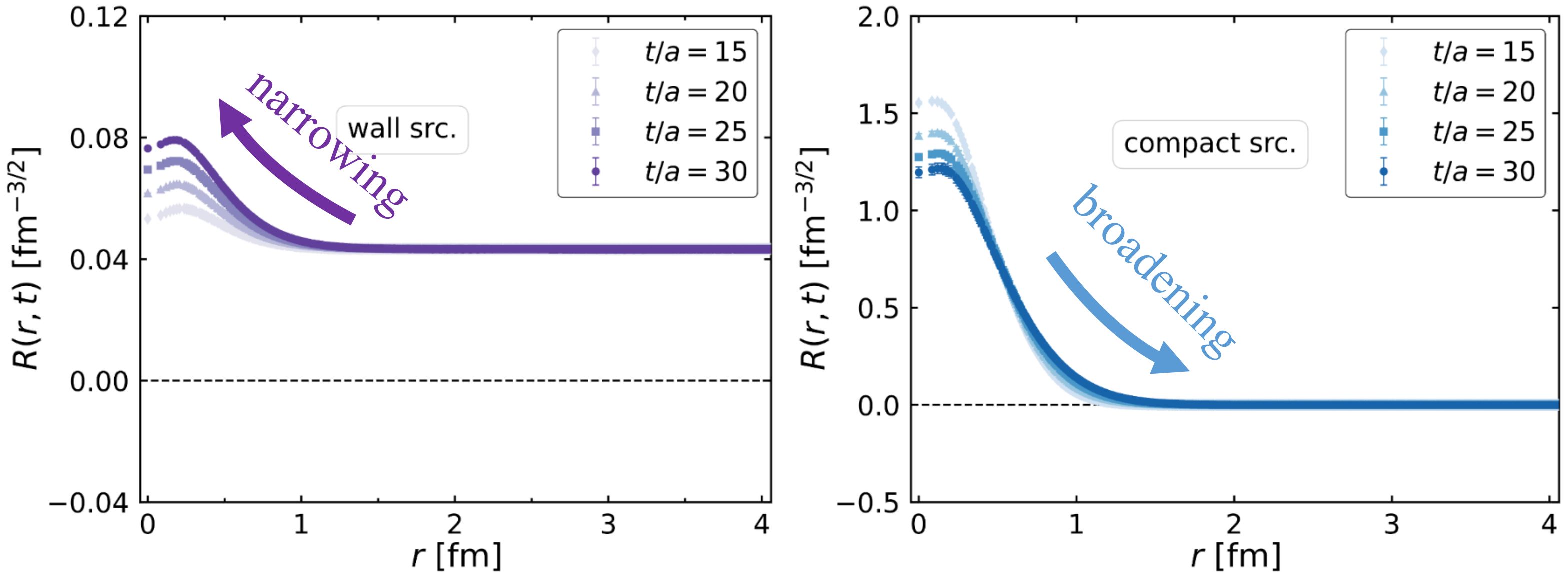
- Why $\Omega_{ccc}\Omega_{ccc}$?
  - State identification is challenging, as spectra extremely dense
  - Allowing to test the method on both bound state and scattering states
  - Smaller statistical fluctuations

- Lattice gauge configurations at physical point (HAL-conf-2023)
  - Iwasaki gauge action
  - $O(a)$-improved Wilson quark action for uds quark
  - Relativistic heavy quark action for c quark

$L^3 \times T$	a [fm]	La [fm]	m_π [MeV]	m_K [MeV]	$m_\pi L$
$96^3 \times 96$	0.0846	8.1	137.1(3)	501.8(3)	5.63(1)

T. Aoyama *et al.* [HAL QCD Coll.], Phys. Rev. D 110, 094502 (2024)
Y. Namekawa *et al.* [PACS Coll.], *Proc. Sci.*, LATTICE2016 125 (2017)

Correlation functions from wall/compact sources



- Clear t dependence is observed for each source
  - For wall source: flat profile → localized profile
  - For compact source: delta-like profile→ extended profile

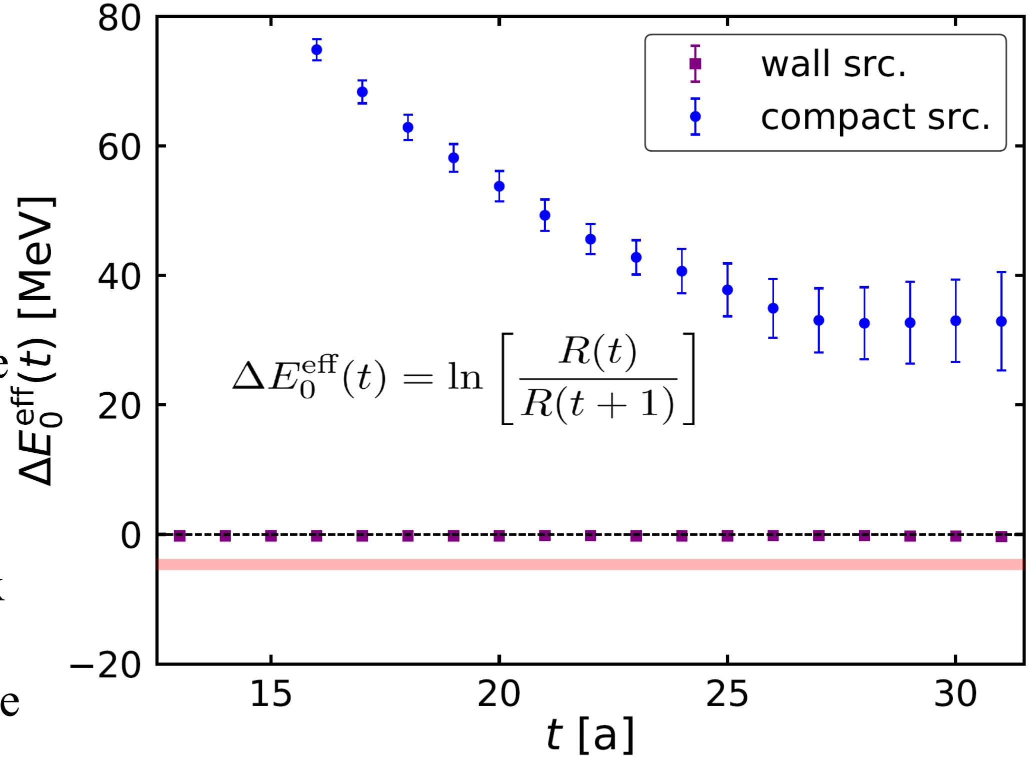
- The flat and delta profiles are two extremes, while realistic profiles should lie somewhere in between

The ground-state energy

- Ground-state energy derived from the temporal correlation functions

$$R_{\mathrm{wall}}(t) = \sum_{\vec{r}\in\Lambda} R_{\mathrm{wall}}(\vec{r}, t)$$

$$R_{\mathrm{compact}}(t) = \sum_{|\vec{r}|<r_B} R_{\mathrm{compact}}(\vec{r}, t)$$

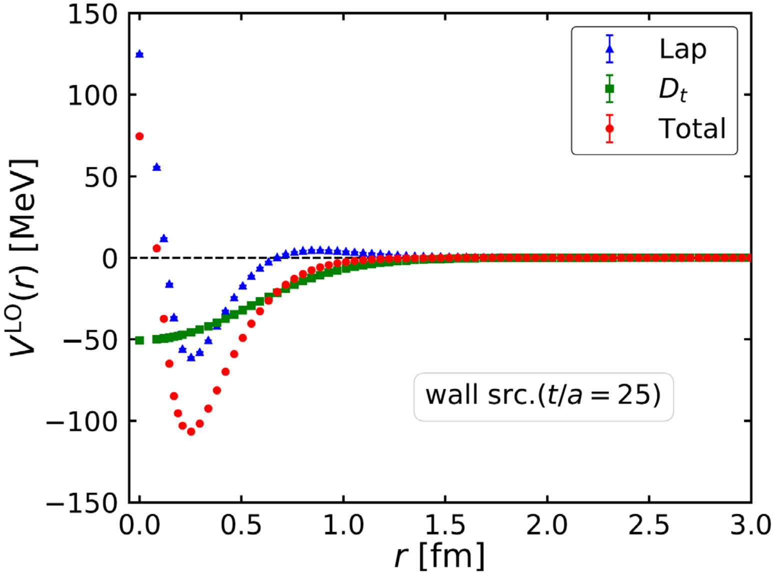


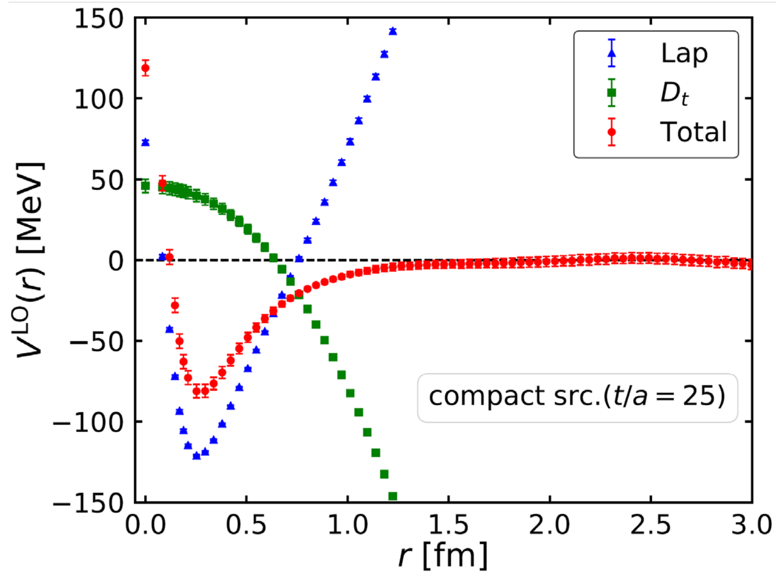
- To make sink operators resemble the source operators
  - ✓ Wall: equally weight summation is over entire box
  - ✓ Compact: summation is restricted by the size of single hadron

- Fake plateaux appear due to contaminations from nearby states, resulting in two different energies both deviating from the correct ground state energy (the band)

HAL QCD potentials

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

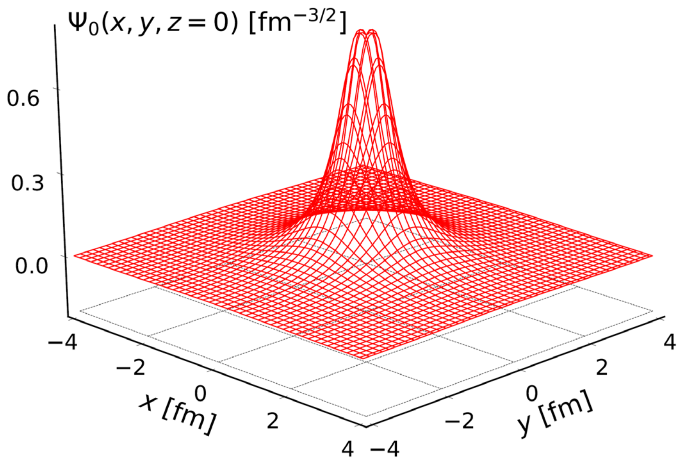


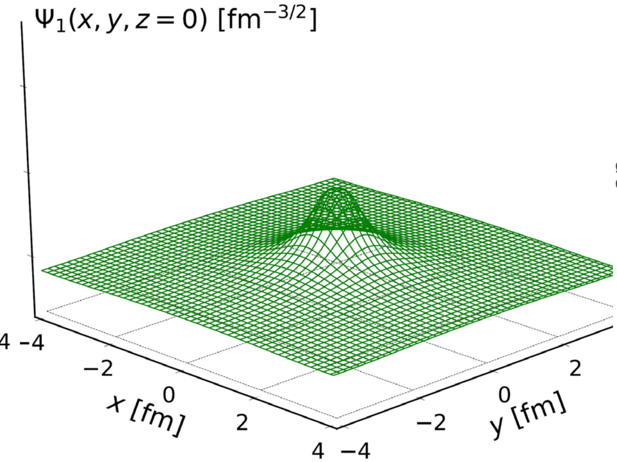


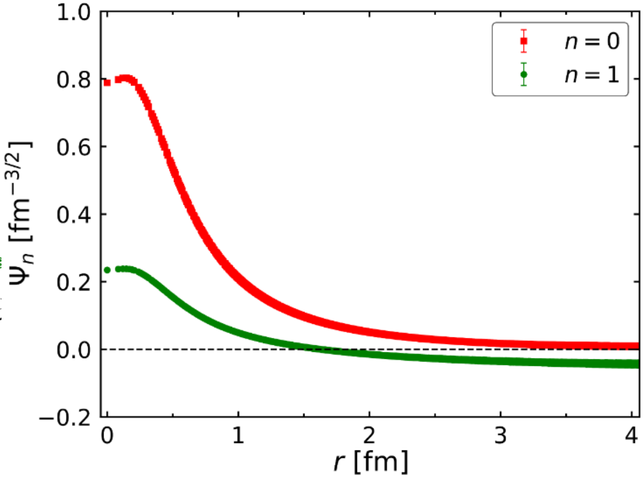
- Total potentials are quite similar, although each component is radically different
  - Different combinations of elastic scattering states lead to a nearly identical potential
  - Leveraging both temporal and spatial information is crucial to obtain the underlying potential

Eigen functions on a finite box

- Solving the eigen equation with the HAL QCD potential under a discrete periodic three-dimensional box





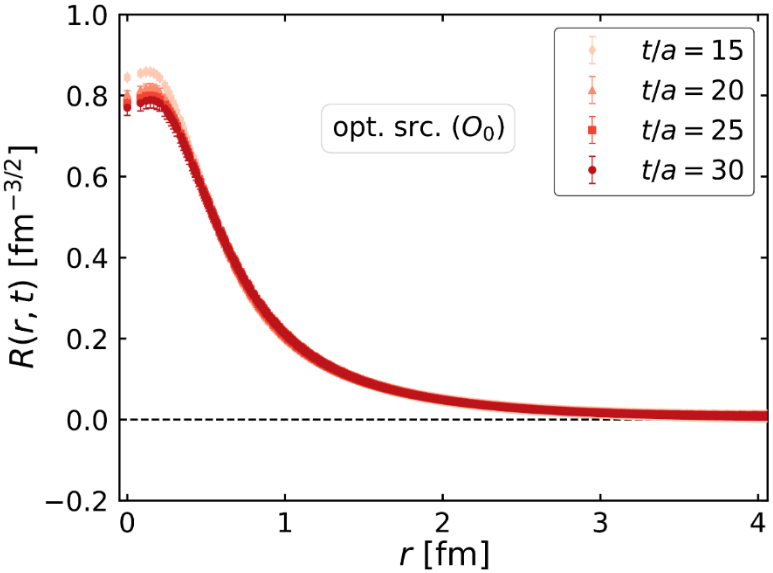


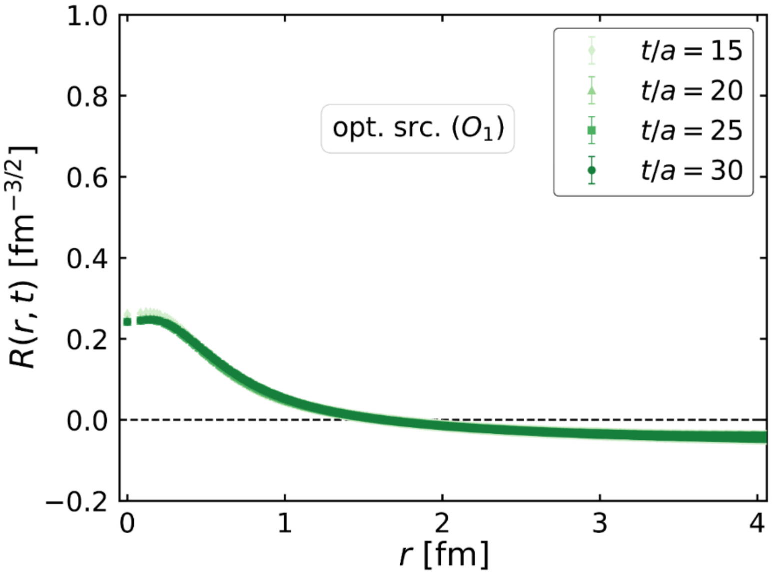
ε_0 [MeV]	ε_1 [MeV]
-4.6(4)	0.6(1)

- $\Psi_0(\vec{r})$ is very localized, similar to typical bound state wavefunctions
- $\Psi_1(\vec{r})$ is much more extended, and has one node

Correlation functions from optimized sources

- The ground state
- The first excited state





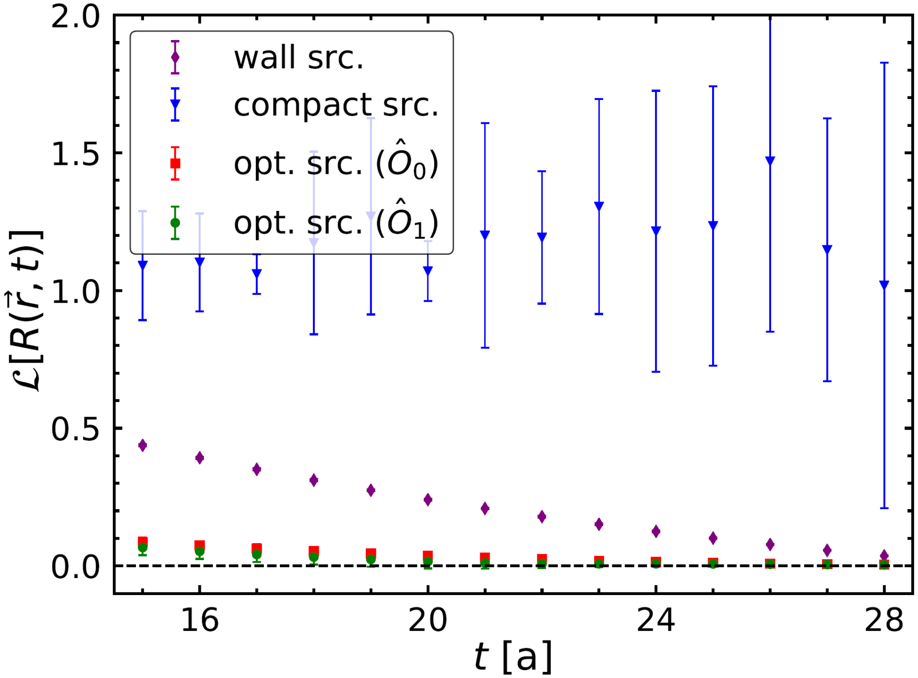
- Both exhibit very stable spatial profiles against a long period of Euclidean time $t/a = 15 \sim 30$
- The convergence is achieved in the iterative process of operator optimization at this step

Correlation functions: wall/compact vs optimized

- Define a residue factor to quantify spatial variation of $R(\vec{r},t)$ against t with respect to a $R(\vec{r},t_f = 30)$

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

  - The residue factor vanishes if $R(\vec{r},t)$ is dominated by single state

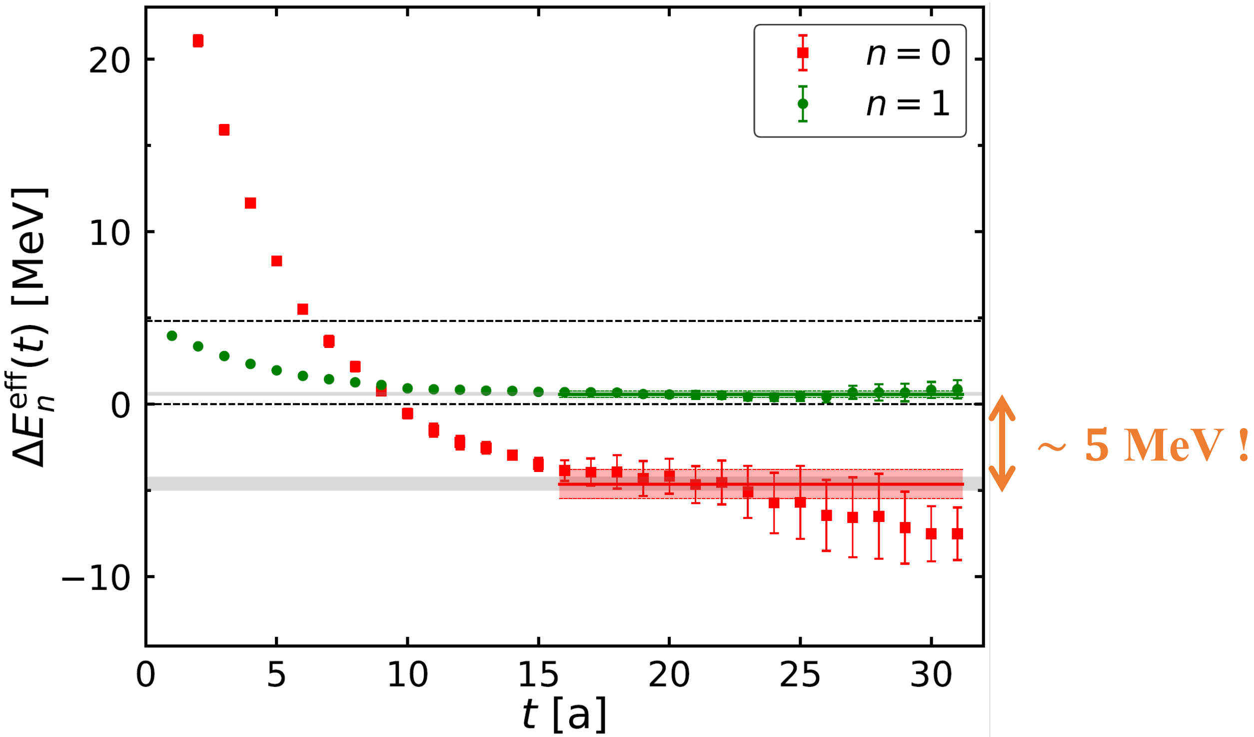


Effective energies

- The ground/first excited state energy derived from

$$R_0(t) = \langle \hat{O}_0(t)\hat{O}_0^\dagger(0)\rangle = \sum_{\vec{r}\in\Lambda} \Psi_0(\vec{r})R_0(\vec{r},t)$$

$$R_1(t) = \langle \hat{O}_1(t)\hat{O}_1^\dagger(0)\rangle = \sum_{\vec{r}\in\Lambda} \Psi_1(\vec{r})R_1(\vec{r},t)$$



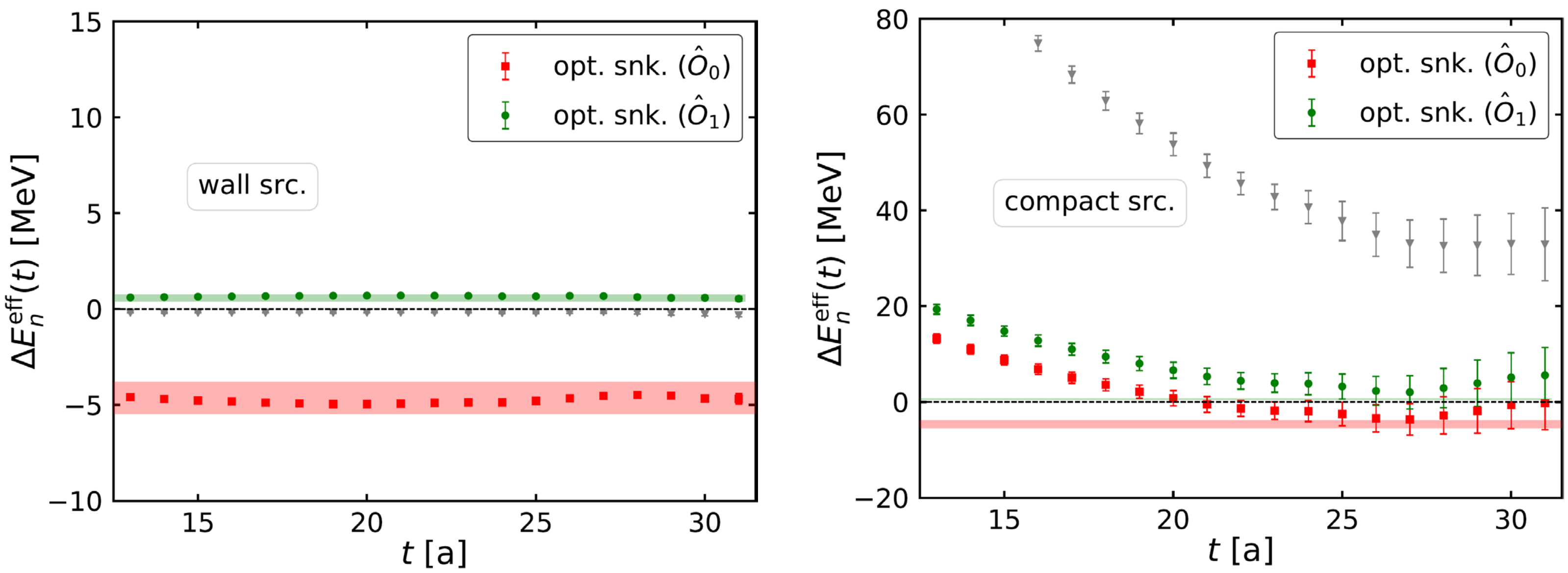
- Spectra identification is achieved for states with energy gap ~5 MeV
- Spectra are consistent with the engine values (gray bands) from the potential
- Without $\hat{O}_{0,1}$, it would require $t > 1000\ [a]$(90 fm) to archive $e^{-\Delta E t} < 10\%$

Applying optimized operators at the sink

- The ground/first excited state energy derived from

$$R_{0,1}(t) = \langle \hat{O}_{0,1}(t)\hat{J}^\dagger(0)\rangle = \sum_{\vec{r}\in\Lambda} \Psi_{0,1}(\vec{r})R_J(\vec{r},t)$$

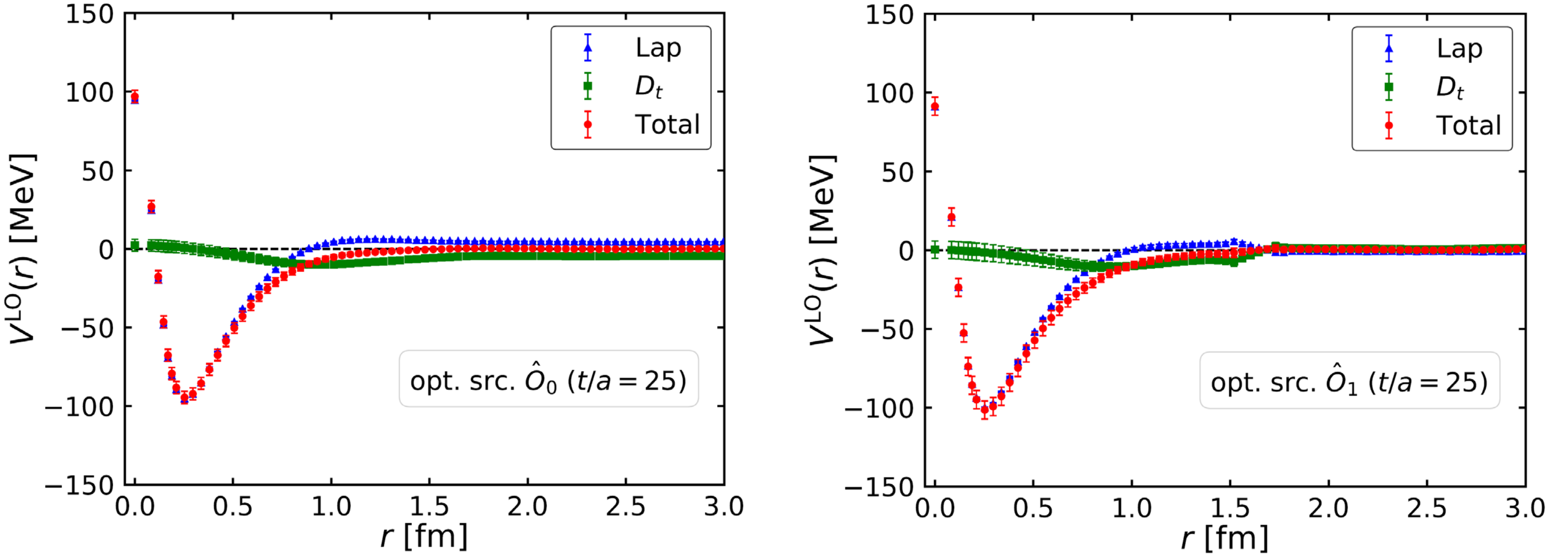
- $\hat{J}^\dagger(0)$ represents the wall/compact source



- The obtained plateaux are consistent with the genuine energies of the ground/ first excited state for each source

HAL QCD potentials

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

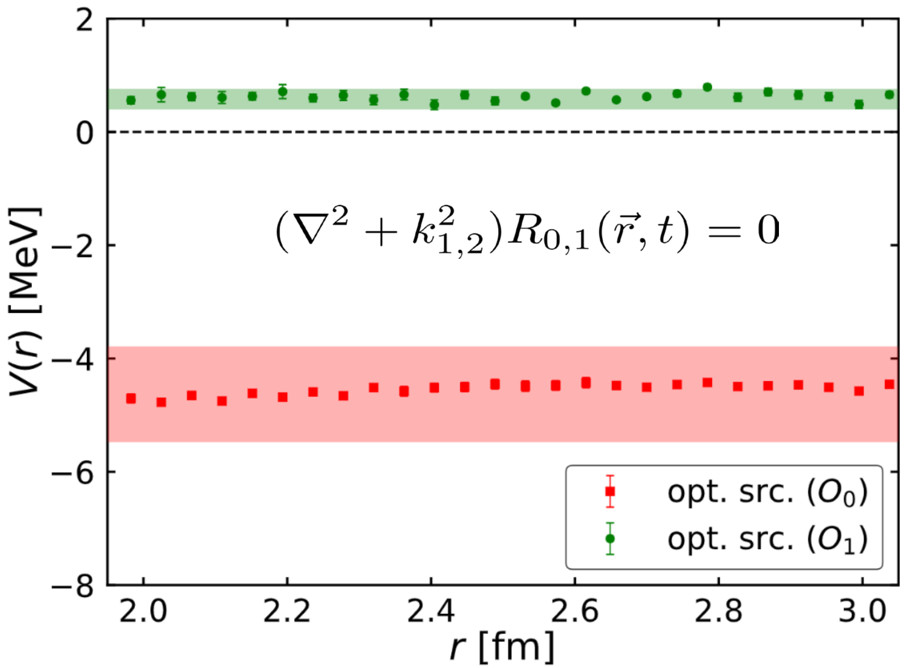


- Total potentials are almost identical
  - Laplacian term provides dominated contribution
  - D_t terms contribute a nearly constant shift

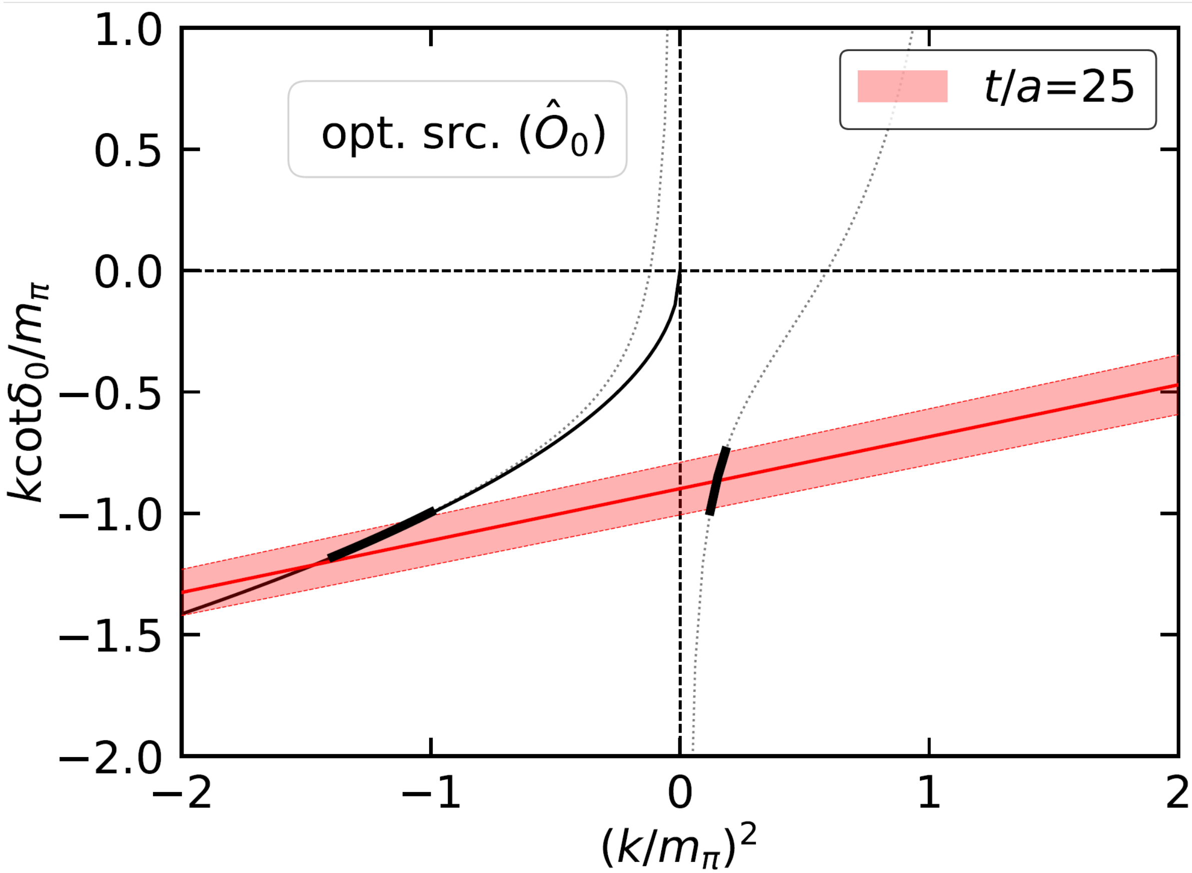
Finite volume effect on the two-particle spectra

- How to confirm the correctness of finite volume spectrum
  - Simple estimation based on dimensionless parameter $m_\pi L$

- Direct confirmation
  - Single-state dominance is achieved in $R_{0,1}(\vec{r}, t)$
  - The lattice volume is large enough to have the asymptotic region



Scattering phase shifts



- Excellent agreement between scattering phase shits from finite volume spectra and those from the potential

Summary

- Operator optimization plays an important role in lattice QCD

  - Developed a systematic way to construct optimized two-hadron operators based on inter-hadron spatial wavefunctions

  - Proposed a novel quark smearing technique using Z_3 noise to effectively implement optimized operators at the source

  - Applied the method to the $\Omega_{ccc}\Omega_{ccc}$ system, and successfully identify two states with energy gap ~ 5 MeV

Discussions

- The proposed method can be used to determine
  - Finite volume spectra for various two-hadron systems
  - Two-hadron matrix element, such as those for $0\nu\beta\beta$ decay

- Further remarks
  - To initiate the iterative process with w.f.s from EFT/models
  - Our operators provide better variational basis than simple plane wave
  - The framework enables an independent treatment of the single hadron and two-hadron systems
    - ✓ Adapt various local smearing for single hadron
    - ✓ Accommodate different inter-hadron w.f.s for two-hadron systems

Thanks for your attention!