Wavefunction-optimized operators for two hadron systems in lattice QCD

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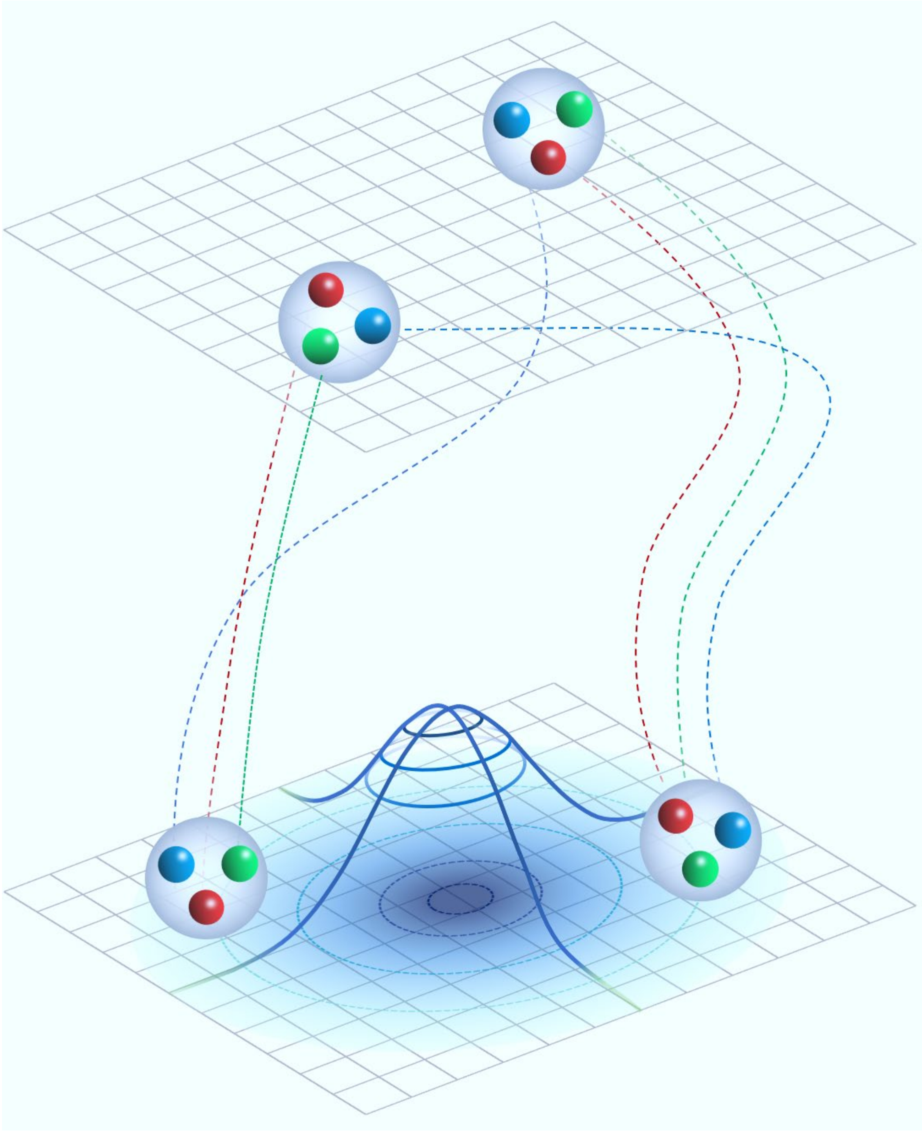
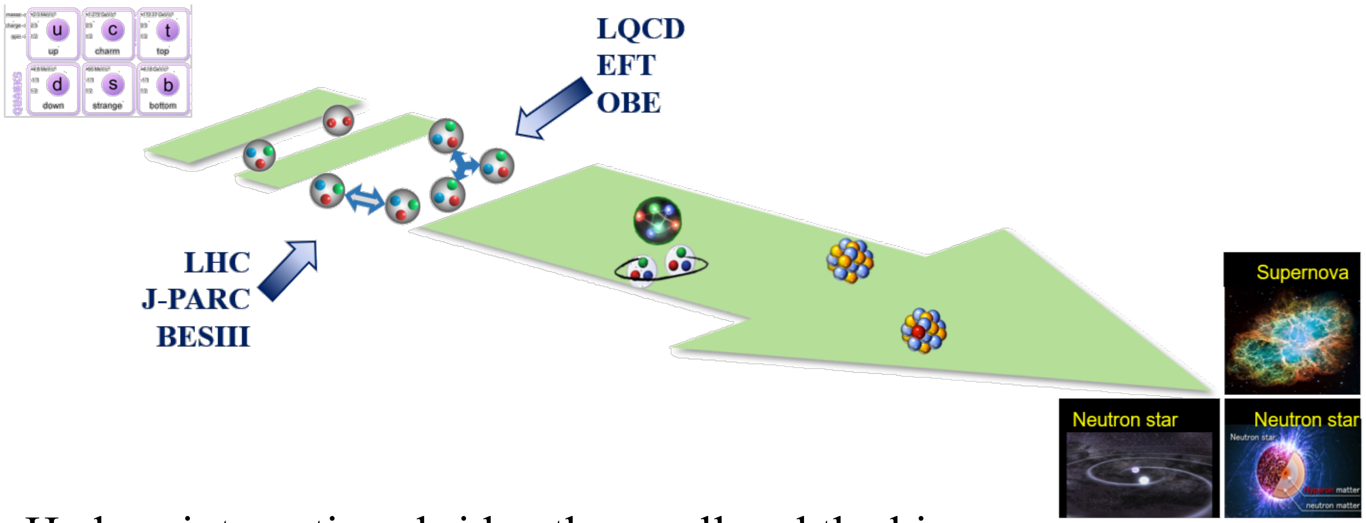


Monsoon Hadrons 2026,
Tata Institute of Fundamental Research, Mumbai

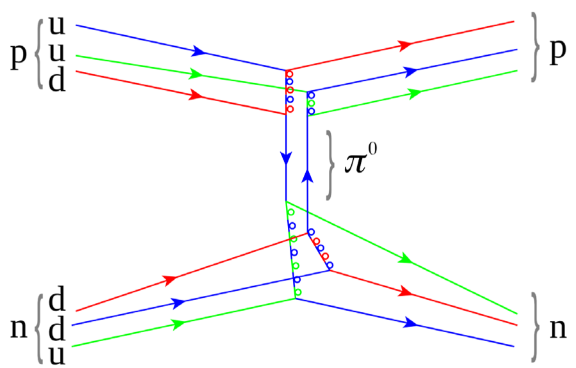
From quarks to the Universe

- Milestones in the path from quarks to the Universe



- Hadron interactions bridge the small and the big

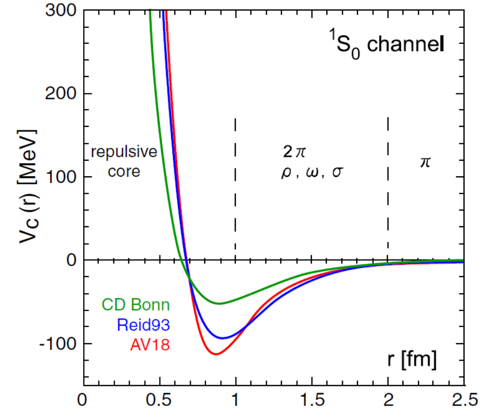
- In theory, QCD governs not only the interaction among quarks and gluons, but also the interaction between color-neutral hadrons



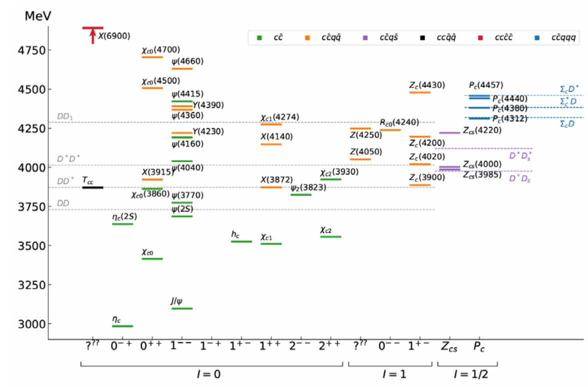
Hadron-hadron interaction

- Phen. models and EFT have been successful in the light quark sector with constraints from rich experimental data
  - NN interaction constrained by thousand of data

	AV18	CD Bonn	EFT	
# parameters	40	38	24 (NR-N3LO)	19(R-N2LO)



- Hadron-hadron interaction in the heavy quark sector
  - Experimental data are limited
  - Yet, exhibits rich dynamics
    - Scale separation between heavy and light flavors
    - Heavy quark spin symmetry
    - Channel coupling



M. Albaladejo et al. (JPAC), Prog. Part. Nucl. Phys. 127 (2022) 103981

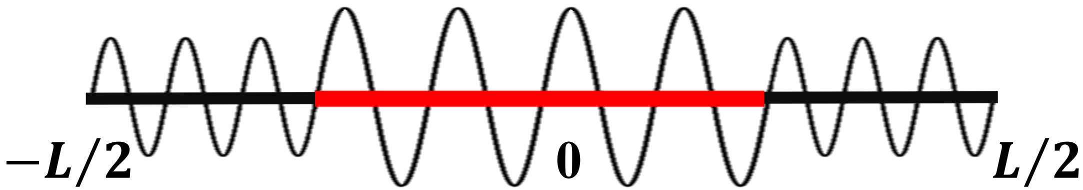
- As a first-principles approach, LQCD is crucial for studying hadron–hadron interactions, especially those difficult in experiments

Finite volume method

E_{FV} FV energy	⟷	$\delta(E_{\text{FV}})$ Phase shift

- 1d scattering

PBC: $\psi(x) = \psi(x+L)$

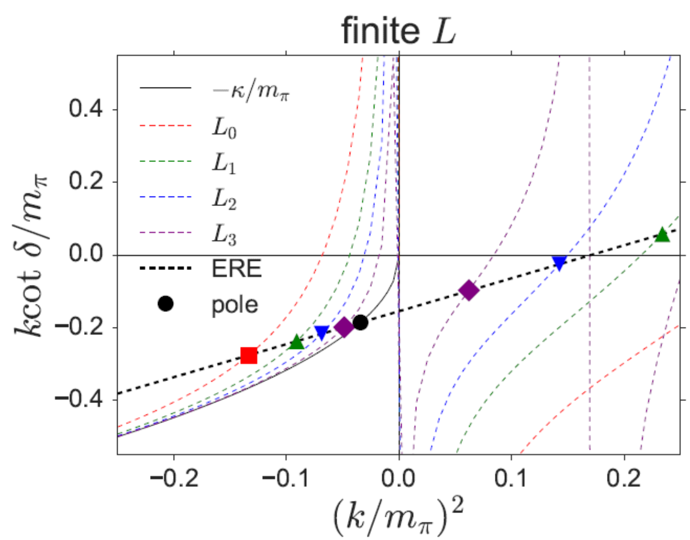


$$\psi(x) \sim \cos(k|x| + \delta(k)), \quad k + \frac{2}{L}\delta(k) = \frac{2n\pi}{L}$$

- 3d scattering

$$k \cot \delta_0(k) = \frac{2}{\sqrt{\pi}L} Z_{00}(1, q^2)$$

$$Z_{00}(s, q^2) = \frac{1}{\sqrt{4\pi}} \sum_{\vec{n}\in\mathbb{Z}^3} \frac{1}{(\vec{n}^2 - q^2)^s}, \quad q = \frac{kL}{2\pi}$$



M. Lüscher, Nucl. Phys. B 354, 531 (1991)

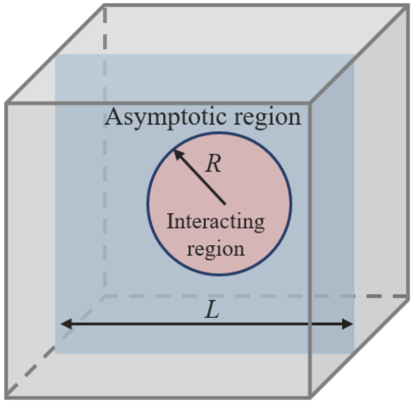
HAL QCD method

- Nambu-Bethe-Salpeter (NBS) amplitude

$$\psi^k(\boldsymbol{r})e^{-Et} = \langle 0|\hat{D}^*(\boldsymbol{r},t)\hat{D}(\boldsymbol{0},t)|D^*(\boldsymbol{k})D(-\boldsymbol{k});E\rangle$$

- Asymptotic region: $\psi_l^k(r) \simeq A\frac{\sin(kr-l\pi/2+\delta(k))}{kr}$
- Interacting region: nonlocal energy-independent potential

$$(\nabla^2+k^2)\psi^k(\boldsymbol{r}) = 2\mu\int d\boldsymbol{r}' U(\boldsymbol{r},\boldsymbol{r}')\psi^k(\boldsymbol{r}')$$



- R correlator (superposition of NBS amplitudes) $R(\boldsymbol{r},t) = \sum_n a_n\psi_n(\boldsymbol{r})e^{-\Delta E_n t}$

$$\left(\frac{1}{8\mu}\frac{\partial^2}{\partial t^2} - \frac{\partial}{\partial t} + \frac{\nabla^2}{2\mu}\right)R(\boldsymbol{r},t) = \int d\boldsymbol{r}' U(\boldsymbol{r},\boldsymbol{r}')R(\boldsymbol{r}',t)$$

- Derivative expansion: $U(\boldsymbol{r},\boldsymbol{r}') = \sum V_i(\boldsymbol{r})\,\nabla^i\delta(\boldsymbol{r}-\boldsymbol{r}')$

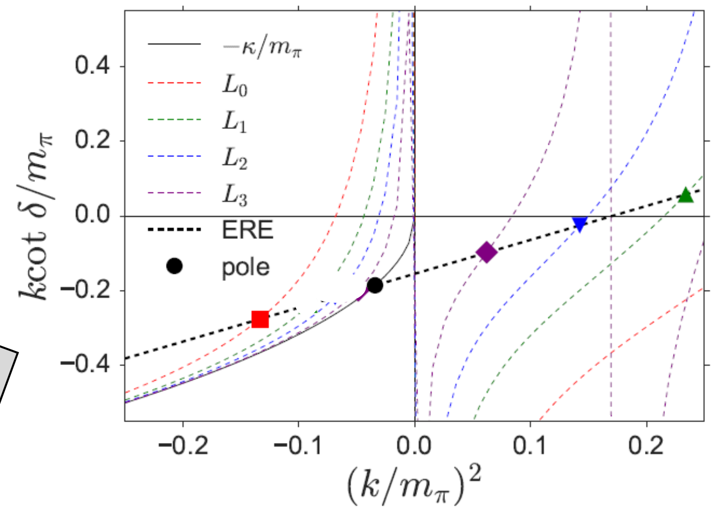
$$V(r) = R(\boldsymbol{r},t)^{-1}\left(\frac{1}{8\mu}\frac{\partial^2}{\partial t^2} - \frac{\partial}{\partial t} + \frac{\nabla^2}{2\mu}\right)R(\boldsymbol{r},t)$$

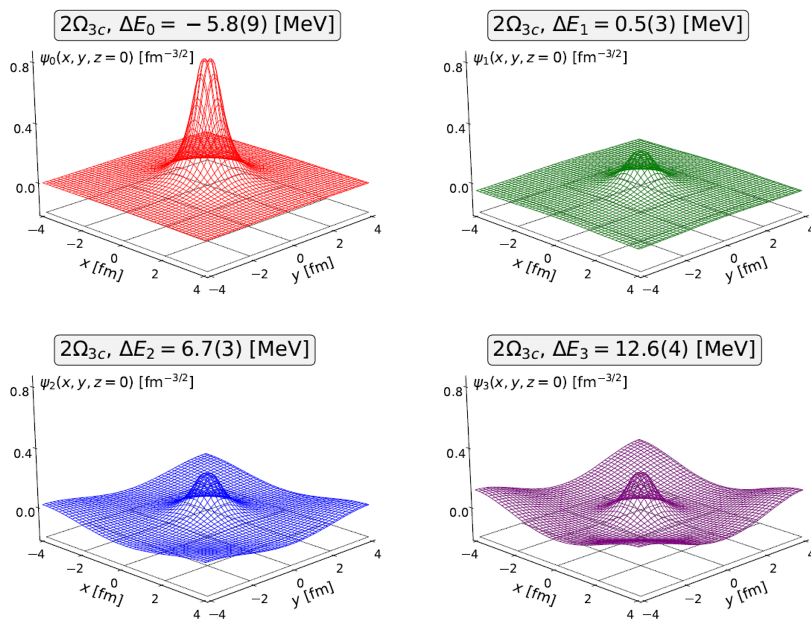
N. Ishii, S. Aoki and T. Hatsuda, Phys. Rev. Lett. 99, 022001 (2007)
N. Ishii, *et al.* [HAL QCD Coll.], Phys. Lett. B 712, 437 (2012)

Finite volume vs HAL QCD

- If two-particle eigenstates are available
  - FV: $\Delta E_{0,1,2,3\ldots} \rightarrow$ phase shifts
  - HAL: $\psi_{0,1,2,3\ldots} \rightarrow$ potential

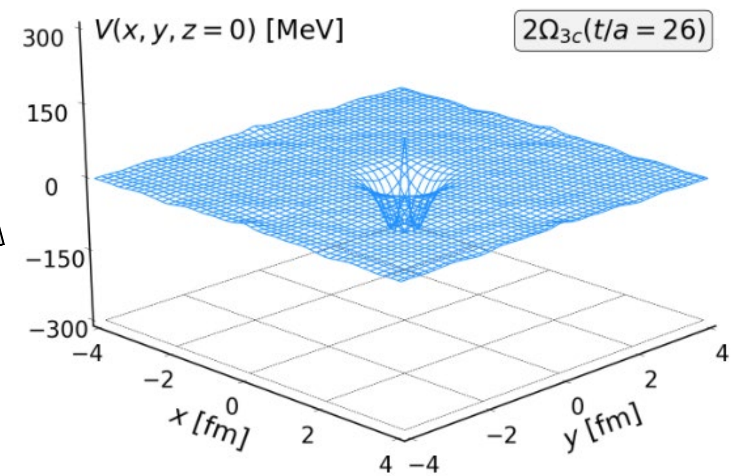
phase shift





FV

HAL

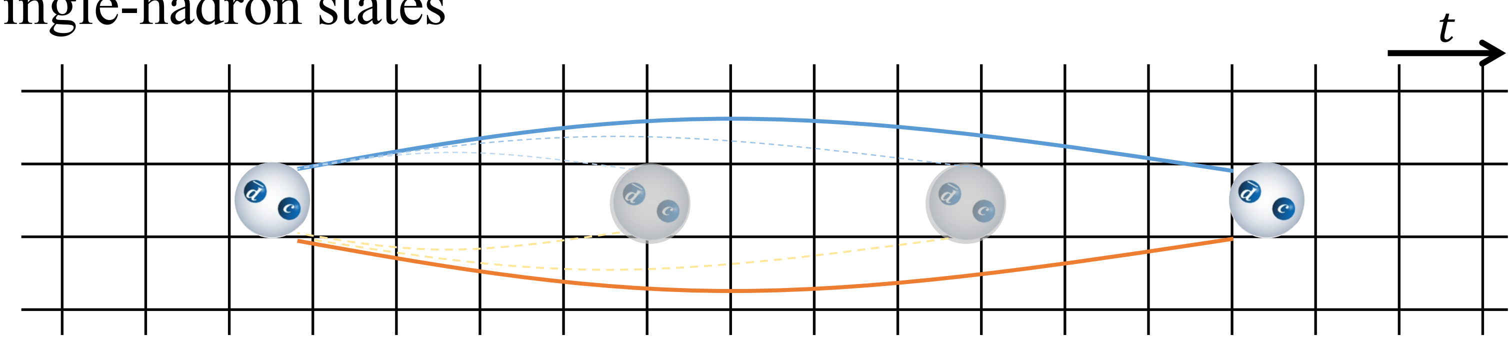


eigenstates

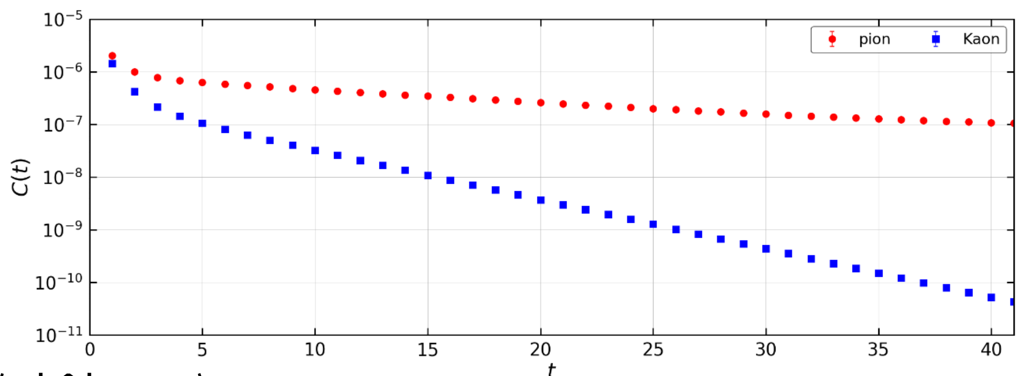
potential

QCD eigenstates from lattice calculations

- Single-hadron states



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



✓ $t \gg \frac{1}{E_1 - E_0}$, and/or $\langle 0|\hat{O}|E_0\rangle \gg \langle 0|\hat{O}|E_{n\neq 0}\rangle$

- Two-hadron states

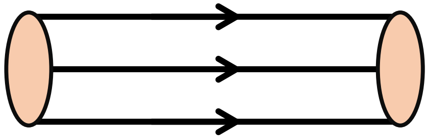
$$F(\boldsymbol{r},t) = \langle \hat{O}(\boldsymbol{r},t)\hat{O}^\dagger(0)\rangle = \sum_n \langle 0|\hat{O}(\boldsymbol{r},t)|n\rangle \langle n|\hat{O}^\dagger(0)|0\rangle$$

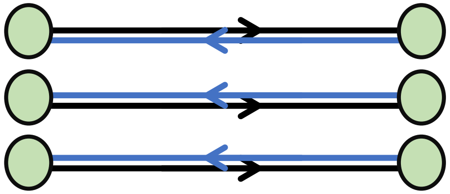
$$= \sum_n a_n \psi_n(\boldsymbol{r}) e^{-E_n t} \xrightarrow{t \gg \frac{1}{E_1 - E_0}} a_0 \psi_0(\boldsymbol{r}) e^{-E_0 t}$$

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

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

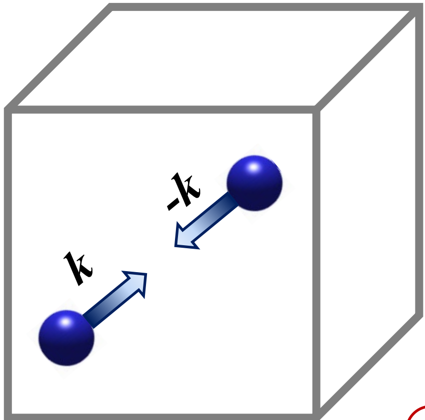
  - t can not be sufficiently larger than $t_{ns} = \frac{1}{m_N - 3/2 m_\pi}$

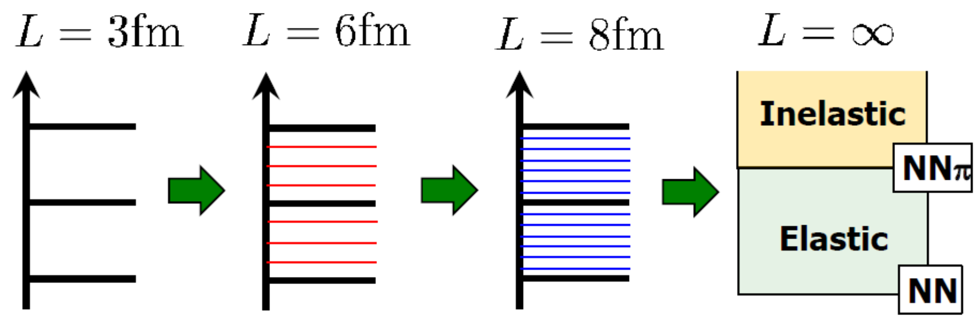
- More severe for two-nucleon systems

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

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

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, to appear in PRD

Lessons from single hadron: the "shape" matters

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

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

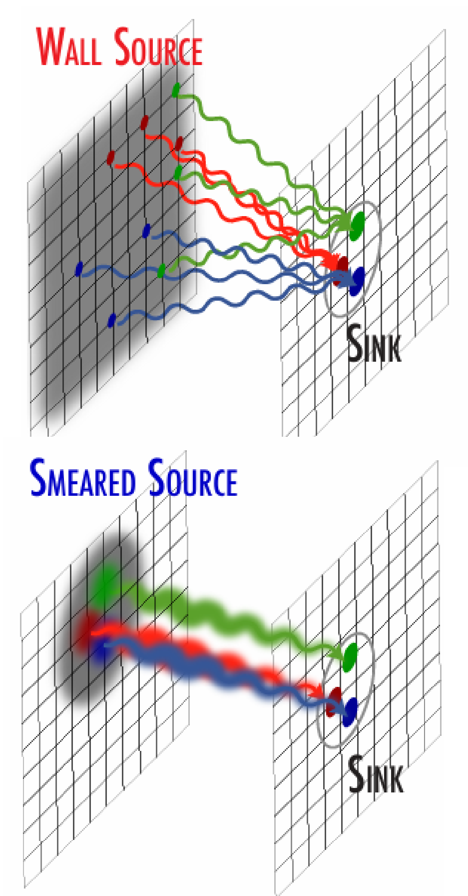
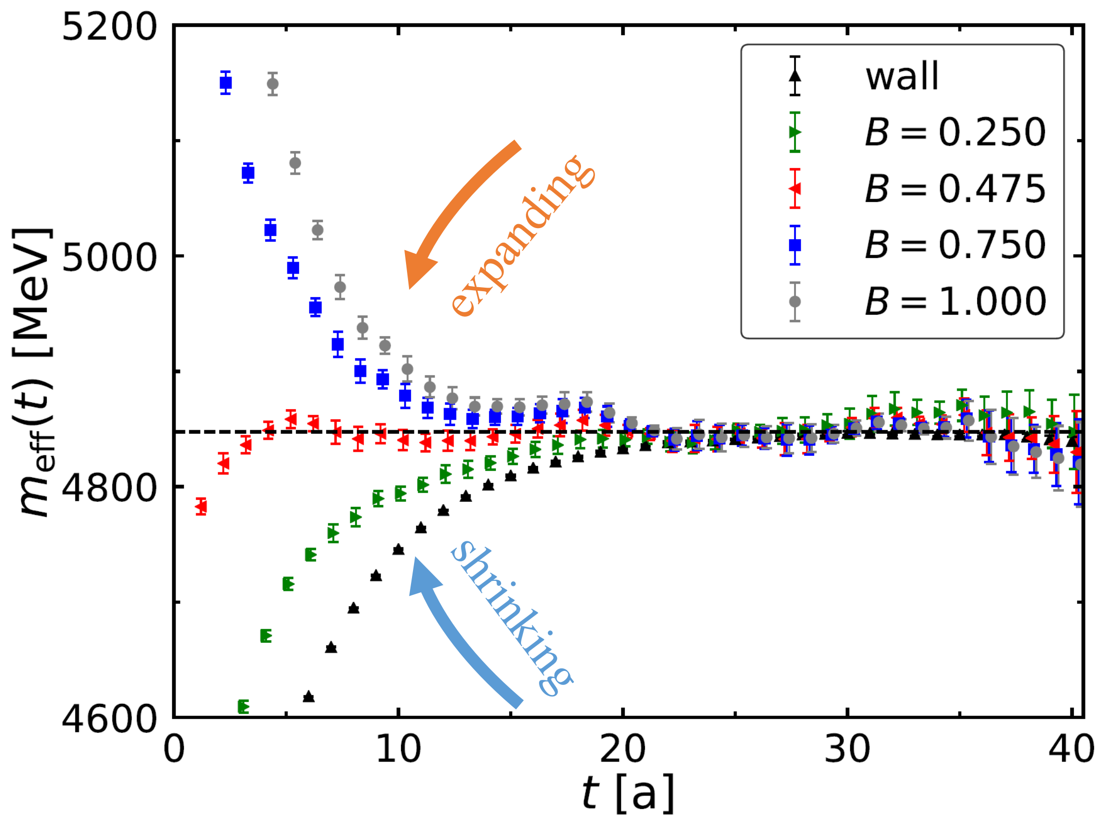
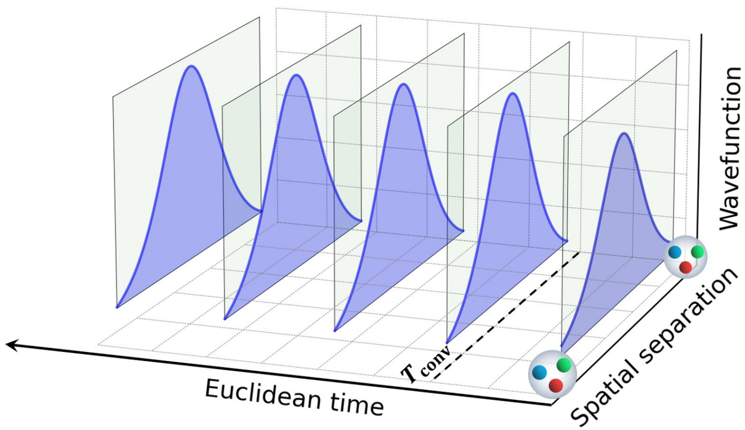


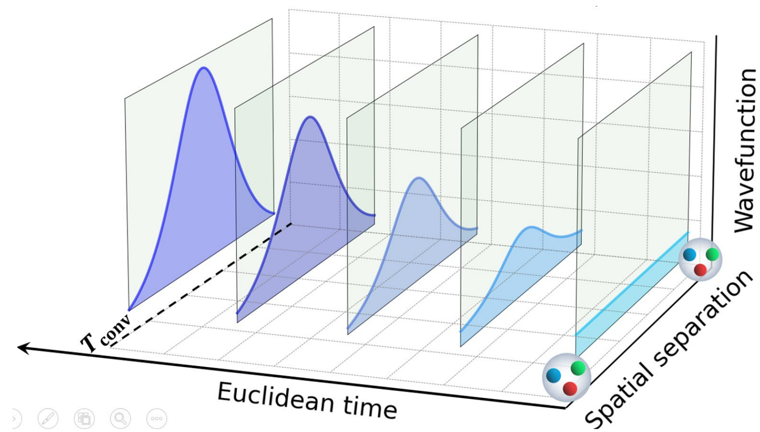
Fig. from T. Iritani



The "shape" of two-hadron states

- Euclidean time evolution in QM, $e^{-Ht}|\psi\rangle$
  - Optimized initial shape
  - Flat initial shape





- Rigorous definition in QFT: (equal-time) NBS amplitude

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

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

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)

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

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

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

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

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

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

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

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

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

- The NBS amplitude $\psi_n(\vec{r})$ can be well-approximated, allowing to construct Ψ_n

  - Models, EFTs …
  - Overlapping factors from a variation method
  - HAL QCD potential

- These initial Ψ_n can be updated based on their generated lattice data if necessary

Implementation of optimized operators

- In lattice QCD, quark propagators are calculated using source smear function f

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

  - 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

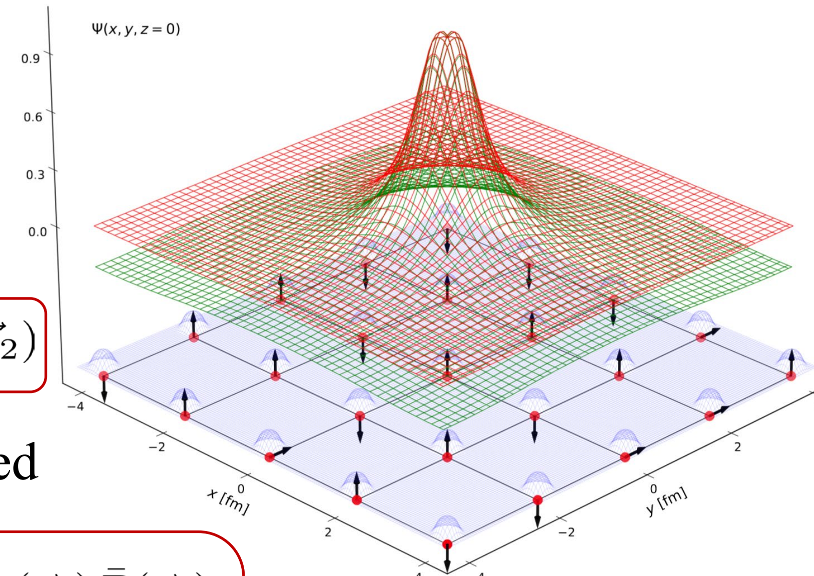
- Novel quark smearing functions at the source

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

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

- $f(\vec{r})$ 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 at source are realized as follows

$$\begin{aligned}(\bar{q}_G)^3(\bar{q}_{F_n})^3 &= \frac{1}{V_{\mathrm{sub}}}\bar{B}(\vec{0}) \sum_{\vec{r}_0\in\Lambda_{\mathrm{sub}}} \Psi_n(\vec{r}_0)\bar{B}(\vec{r}_0)\\ &\simeq \frac{1}{V}\bar{B}(\vec{0}) \sum_{\vec{r}_0\in\Lambda} \Psi_n(\vec{r}_0)\bar{B}(\vec{r}_0)\end{aligned}$$

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

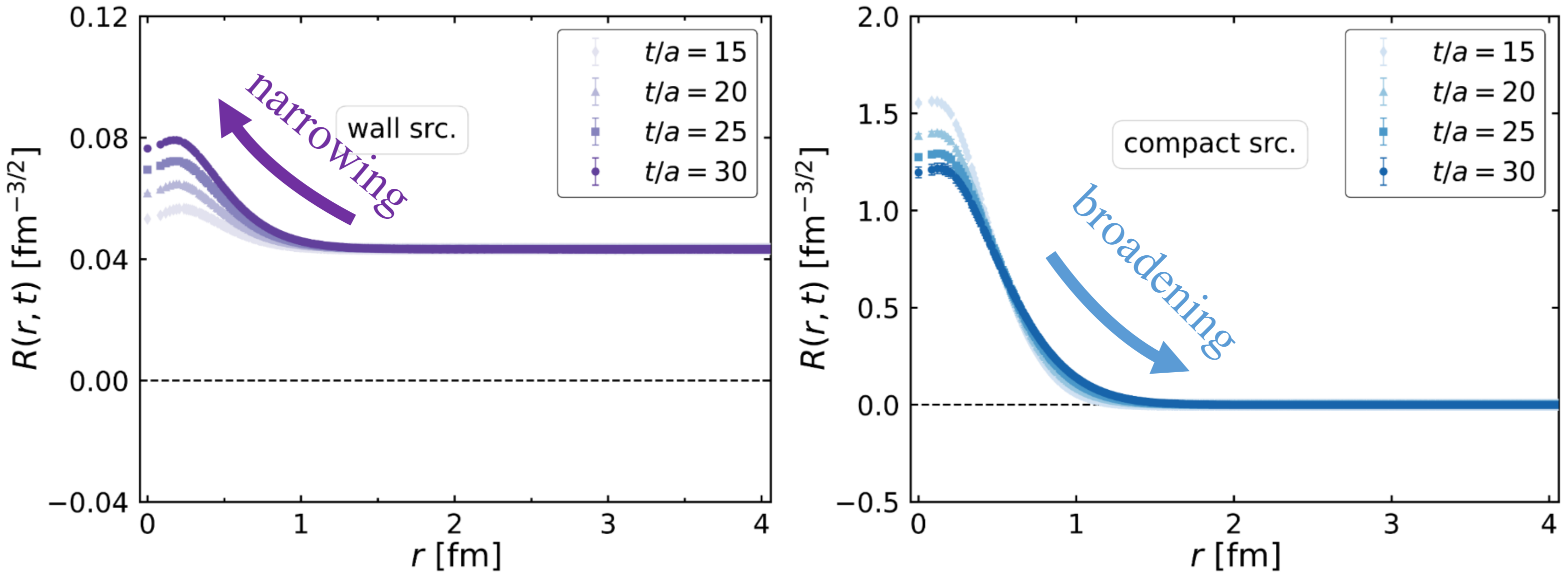
- Why $\Omega_{ccc}\Omega_{ccc}$?
  - State identification is challenging, as spectra extremely dense
  - Allowing to test the method on both bound state and scattering states
  - Smaller statistical fluctuations

- 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

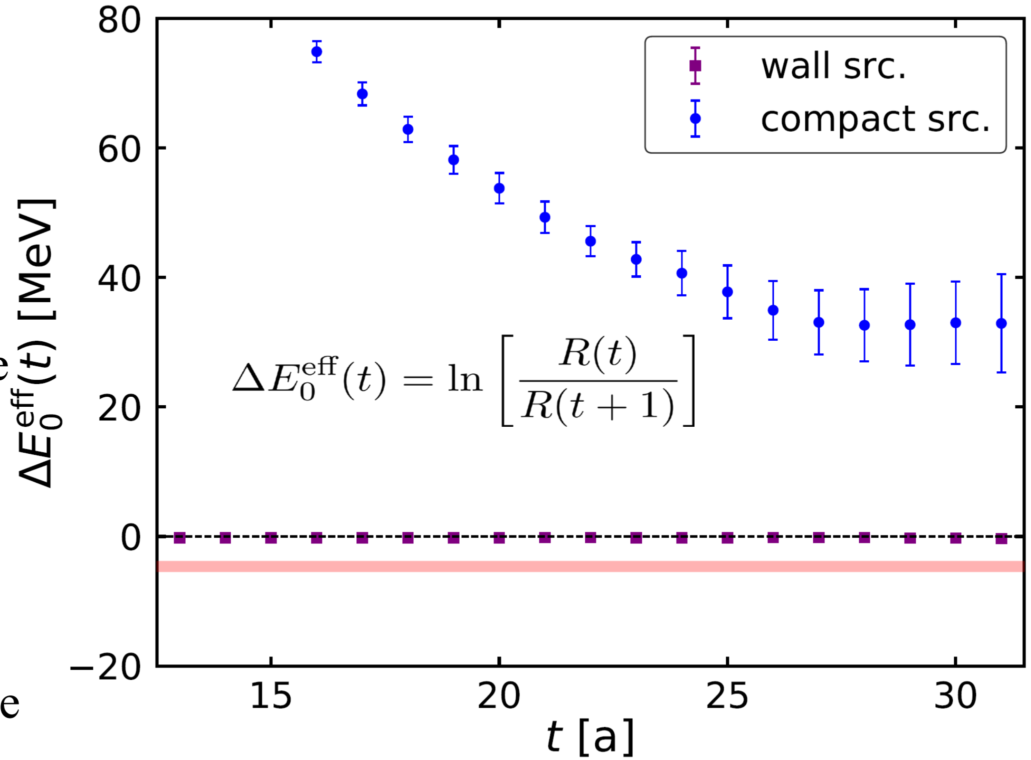
The ground-state energy

➢ Ground-state energy derived from the temporal correlation functions

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

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

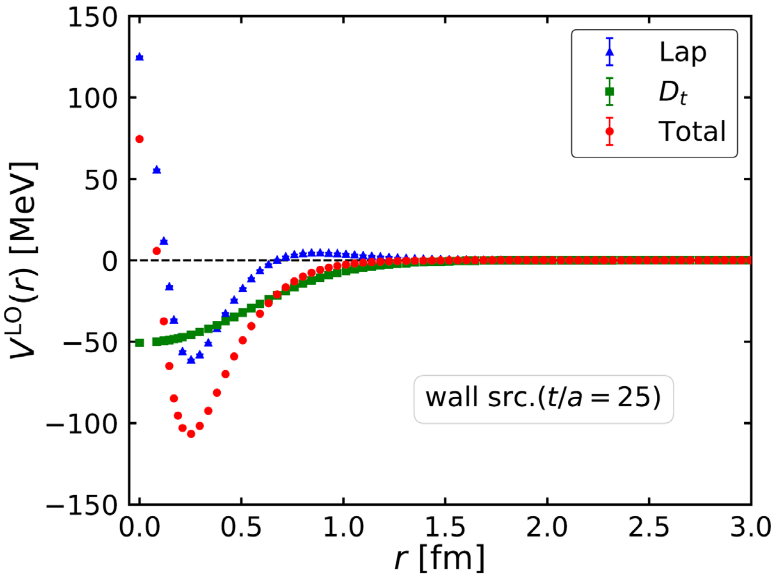
- To make sink operators resemble the source operators
  - ✓ Wall: equally weight summation over entire box
  - ✓ Compact: summation is restricted by the size of single hadron

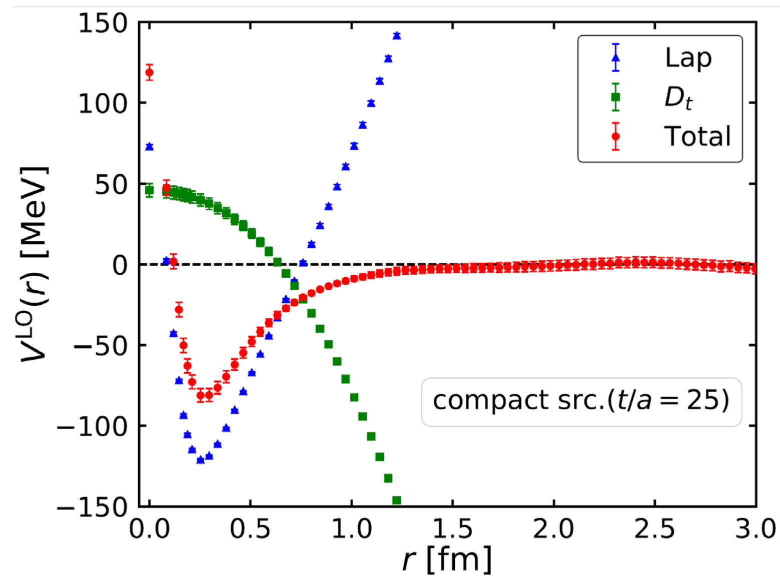


- Fake plateaux appear due to contaminations from nearby states, resulting in two different energies both deviating from the correct ground state energy (the band)

HAL QCD potentials

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

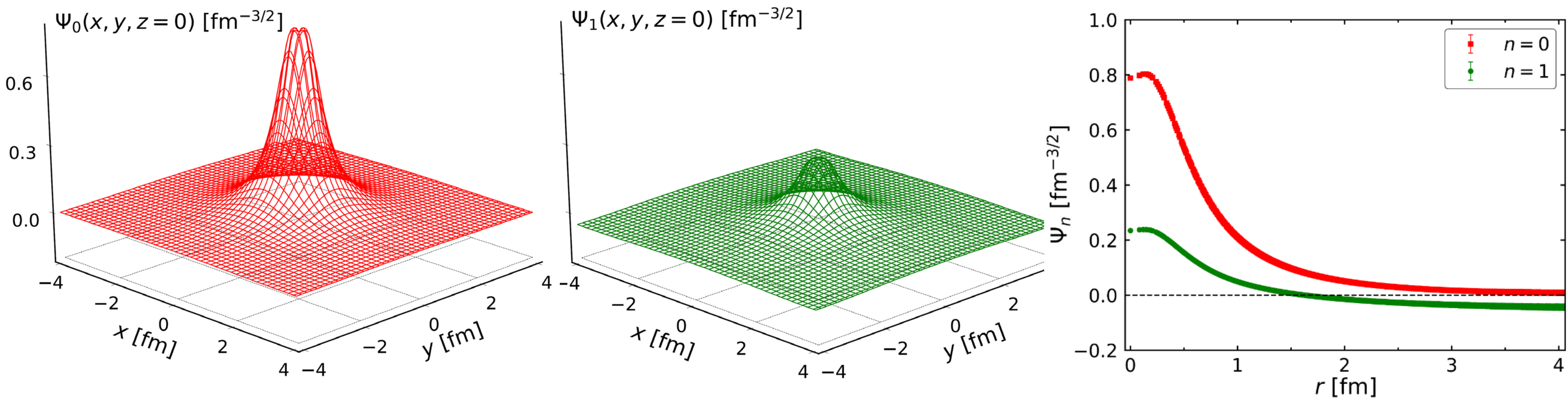




- Total potentials are quite similar, although each component is radically different
  - Different combinations of elastic scattering states lead to a nearly identical potential
  - Leveraging both temporal and spatial information is crucial to obtain the underlying potential

Eigen functions on a finite box

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

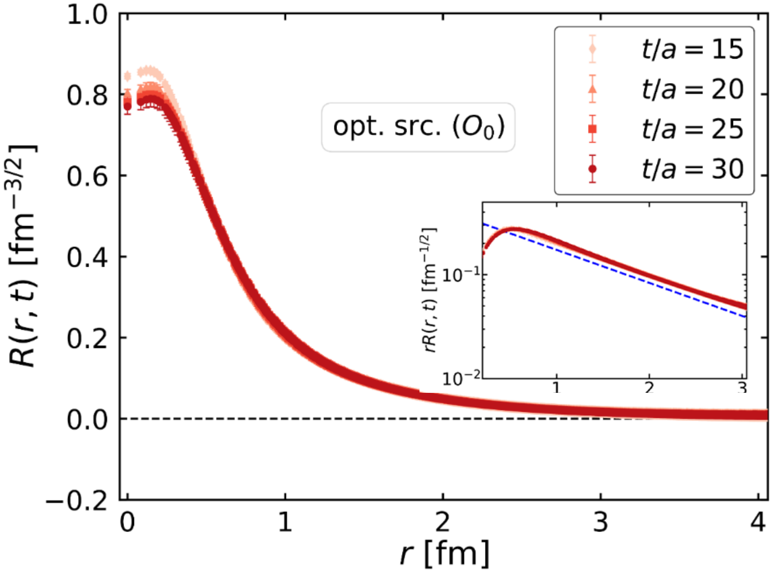


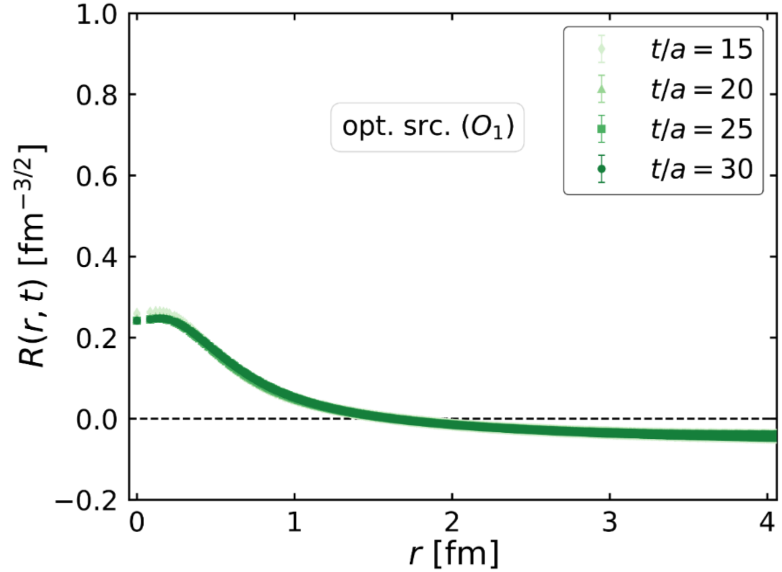
$\boldsymbol{\varepsilon_0}$ [MeV]	$\boldsymbol{\varepsilon_1}$ [MeV]
-4.6(4)	0.6(1)

- $\Psi_0(\vec{r})$ 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





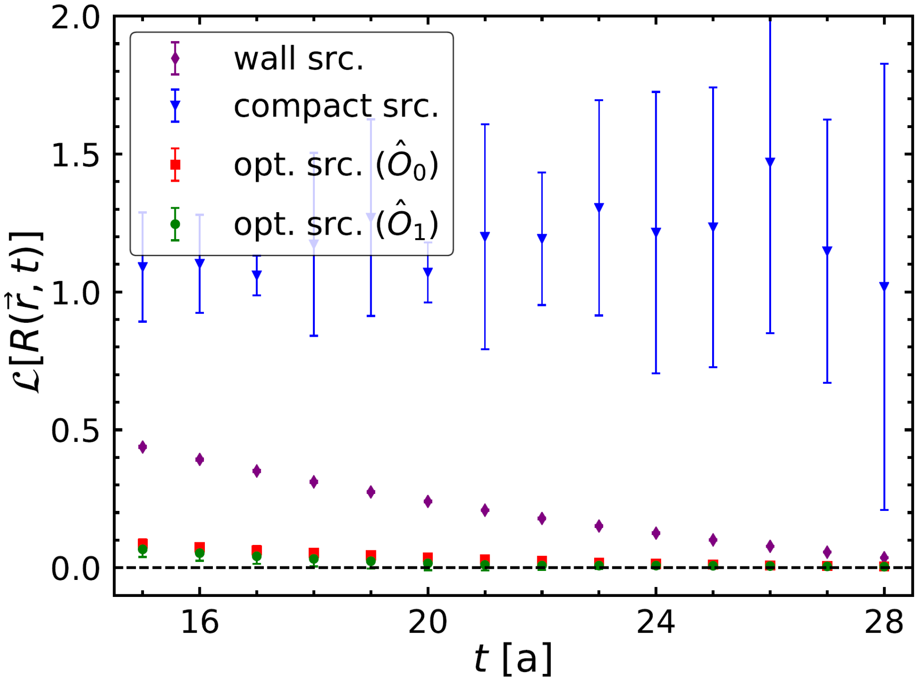
- Both exhibit very stable spatial profiles against a long period of Euclidean time $t/a = 15 \sim 30$
- $R_0(r)$ exhibits characteristic bound-state wf, $rR_0(r) \sim e^{-kr}$
- The operators have been optimized enough to strongly couple to respective low-energy states

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 $R(\vec{r}, t_f = 30)$

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

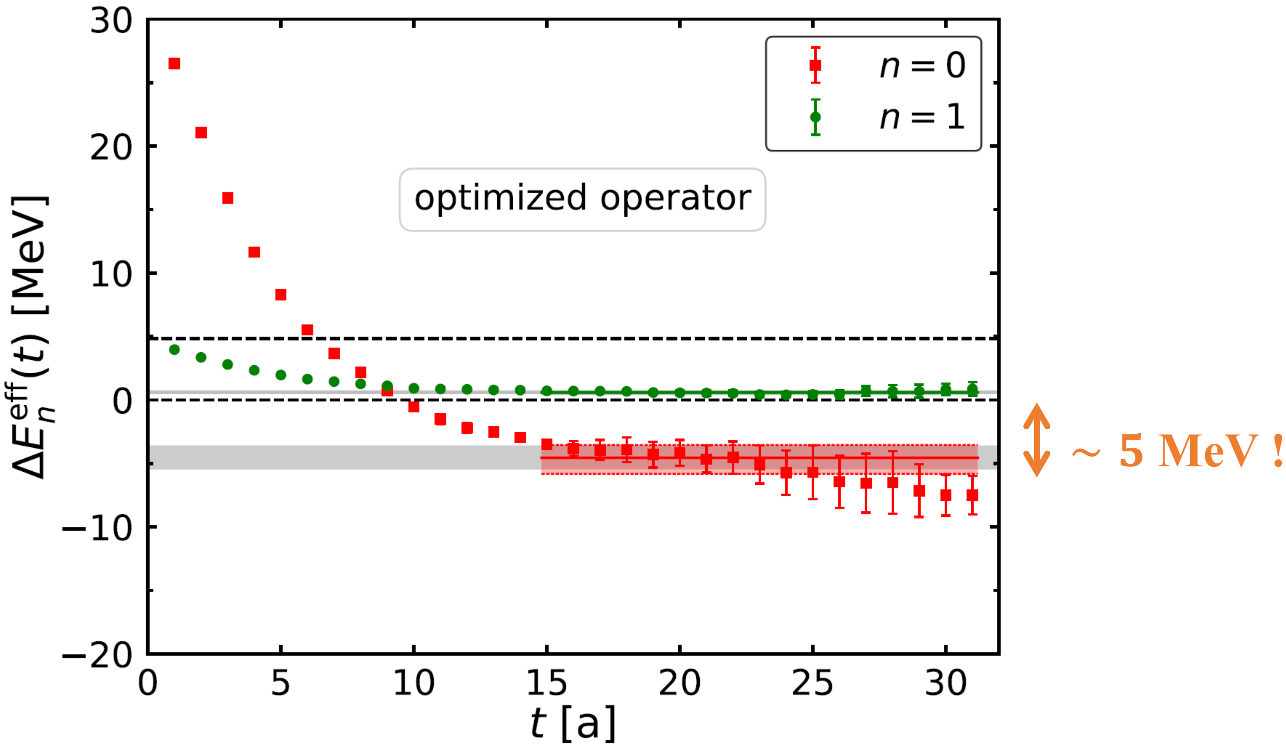
  - The residue factor vanishes if $R(\vec{r}, t)$ is dominated by single state



Effective energies

- The ground/first excited state energy derived from

$$R_{0,1}(t) = \langle \hat{O}_{0,1}(t)\hat{O}^\dagger_{0,1}(0)\rangle = \sum_{\vec{r}\in\Lambda} \Psi^*_{0,1}(\vec{r}) R_{0,1}(\vec{r},t)$$

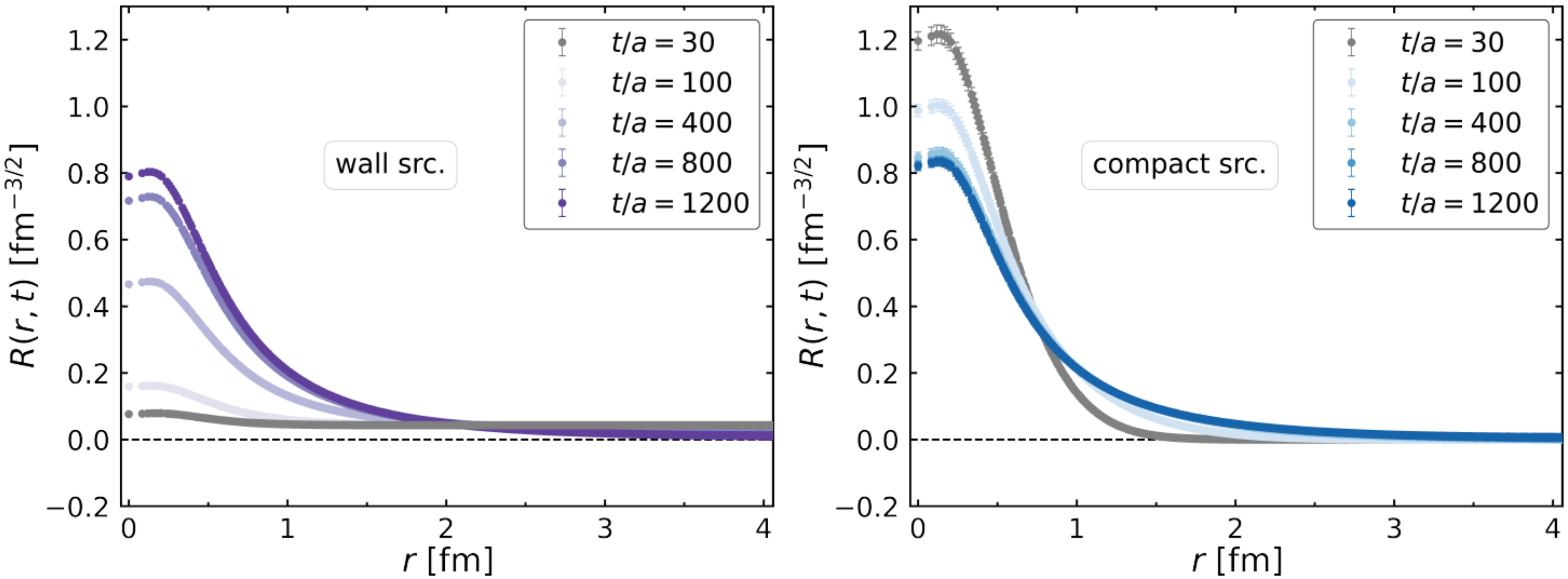


- Spectra identification is achieved around $t/a \sim 15$ for states with energy gap ~5 MeV
- Spectra are consistent with the engine values (gray bands) from the potential

How large t is required for wall/compact source ?

➢ Time evolution from an effective Hamiltonian constructed using potential

$$R(\vec{r},t) = e^{-H(t-t_i)}R(\vec{r},t_i), \quad H = -\frac{\nabla^2}{m_B} + V(\vec{r})$$



- Ground-state dominance requires $t/a > 1000(400)$ for the wall (compact) source
- As the energy gap is very narrow, $\epsilon = E_1 - E_0 \simeq 5$ MeV, to achieve less-than 10% contimanation, $e^{-\Delta E t} < 10\%$ requires $t/a \simeq 1000$

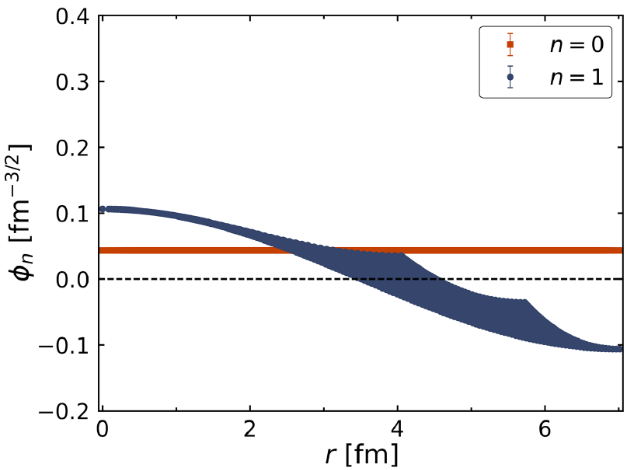
In comparison w/ plane-wave operators

- Plane wave operators are just trivial case of our wf-optimized operators where the realistic wavefunction is replaced by a plane wave

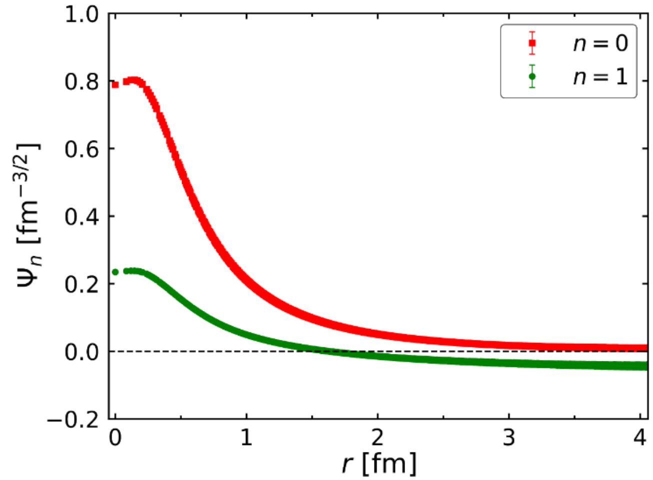
$$\tilde{O}(\vec{p},t) = \tilde{B}(\vec{p},t)\tilde{B}(-\vec{p},t) = \frac{1}{V^2}\sum_{\vec{x},\vec{r}\in\Lambda} B(\vec{x}+\vec{r},t)B(\vec{x},t)\phi^*_{\vec{p}}(\vec{r})$$

$$H_0\phi_{\vec{p}}(\vec{r}) = \frac{\vec{p}^2}{m_B}\phi_{\vec{p}}(\vec{r})$$

- Plane waves



- Realistic wfs

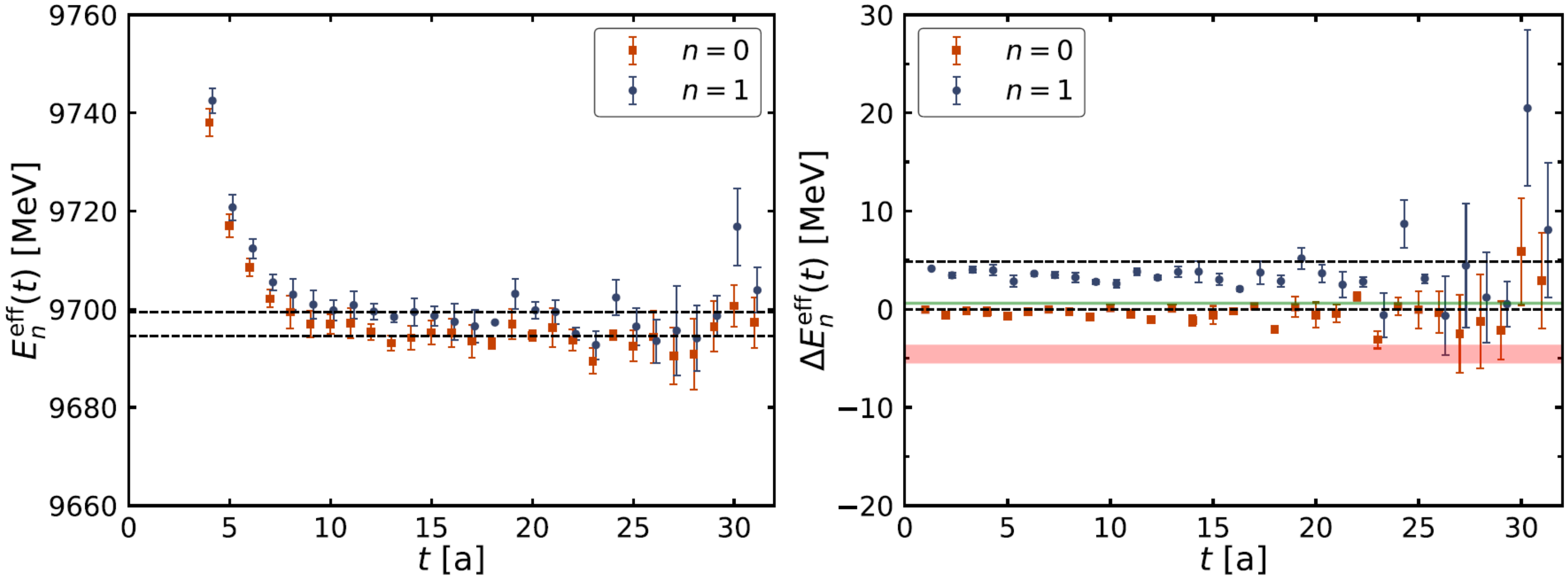


- $\phi(\vec{r})$ is a good approximation of realistic wf only for weakly interacting cases
- In general case, $\phi(\vec{r})$ is expected to deviate from the realistic wf

Energies from GEVP using plane-wave operators

$$C_{mn}(t) = \langle \tilde{O}_m(t)\tilde{O}_n^\dagger(0)\rangle, \quad C(\tau_D)v_n = \lambda_n C(\tau_0)v_n$$

- Energies from first two plane-wave operators



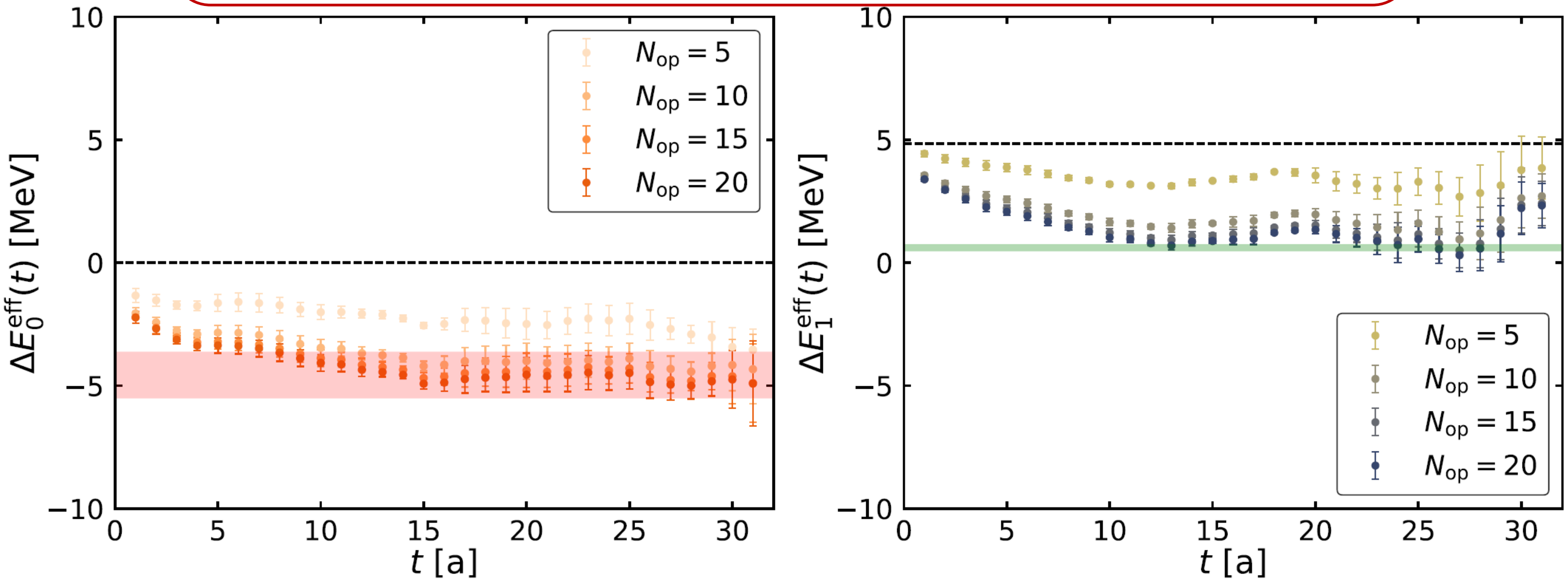
- $E_{0,1}^{\rm eff}$ rapidly fall toward the noninteracting energy levels
- $\Delta E_{0,1}^{\rm eff}$ further reveal clear discrepancies from the genuine energy levels
- Two plane-wave operators are insufficient to strongly couple to eigenstates

How many plane-wave operators are needed in GEVP?

- Effective operators constructed using the first n plane-wave operators

$$\mathcal{O}^{\mathrm{eff}}_{0,1}(t;n) = \sum_{|\vec{p}|\le p_n} \tilde{O}(\vec{p},t)\tilde{\Psi}^*_{0,1}(\vec{p})$$

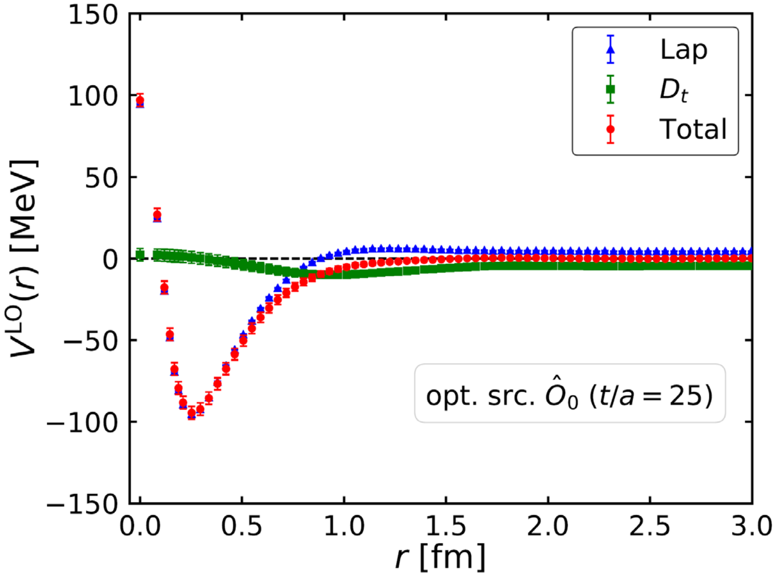
$$\mathcal{C}_0(t;n) = \langle \mathcal{O}^{\mathrm{eff}}_0(t;n)\tilde{O}^\dagger_0(0)\rangle, \quad \mathcal{C}_1(t;n) = \langle \mathcal{O}^{\mathrm{eff}}_1(t;n)\tilde{O}^\dagger_0(1)\rangle$$

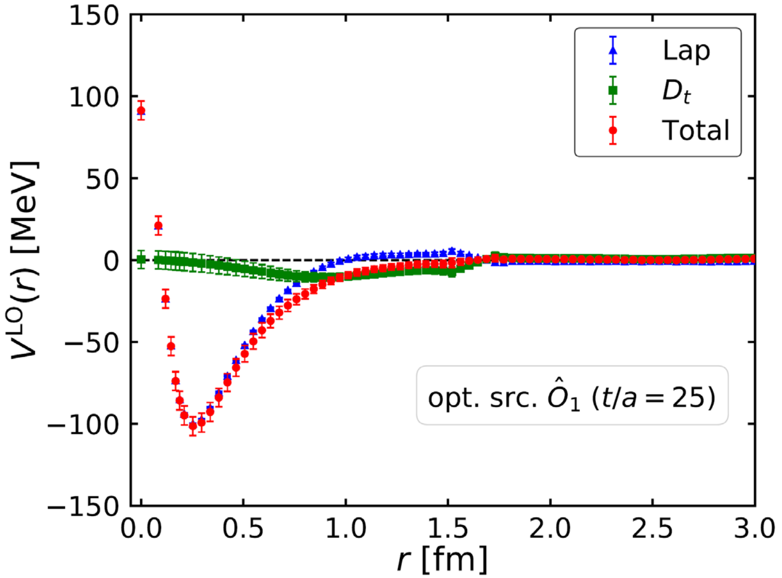


- $\Delta E^{\mathrm{eff}}_{0,1}$ converge to respective true energies at earlier t as the number of operator (N_{op}) used at sink
- To match the performance of our wf-optimized operators, $N_{\mathrm{op}} \ge 10$ (corresponding to 147 momentum modes or more)

HAL QCD potentials from optimized operators

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

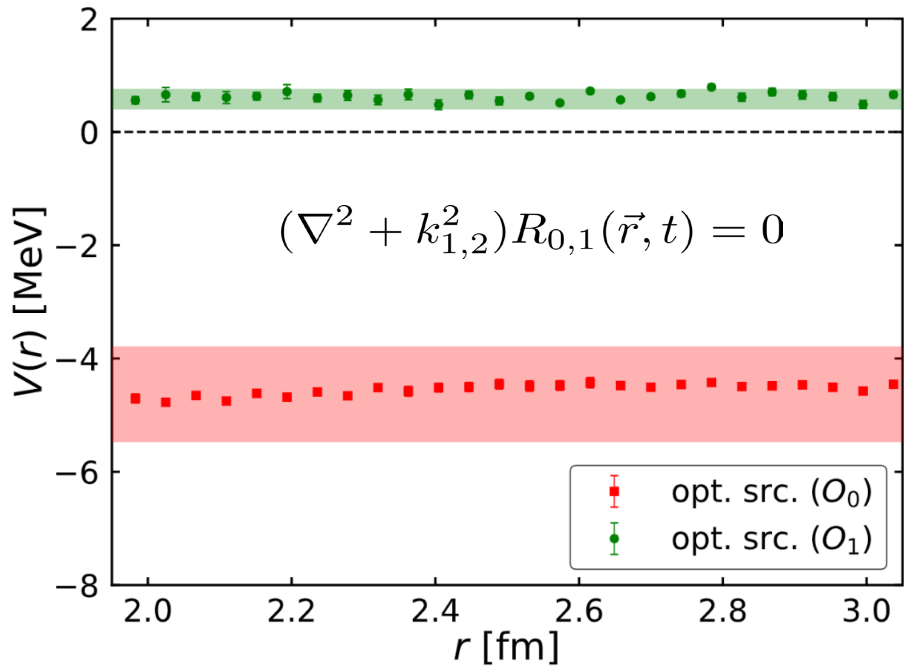




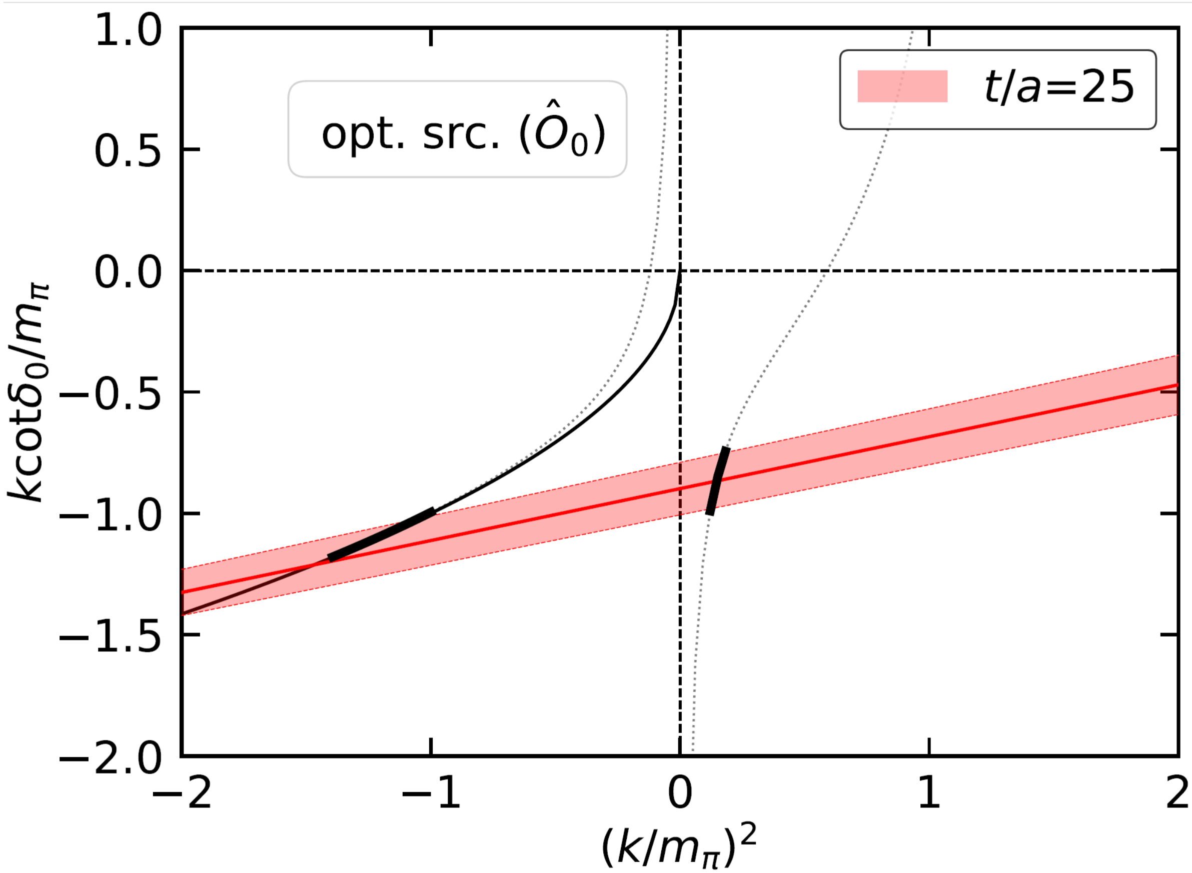
- Total potentials are almost identical
  - Laplacian term provides dominated contribution
  - D_t terms contribute a nearly constant shift

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 FV method and those from the HAL QCD method

Summary

- Operator optimization plays an important role in lattice QCD

  - Developed a systematic way to construct optimized two-hadron operators by incorporating inter-hadron spatial wavefunctions

  - Proposed a novel quark smearing technique using Z_3 vector to effectively implement optimized operators at the source w/o using all-to-all prop.

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

  - Compared w/ conventional variational analysis, and found opt operators outperform combinations of limited plane wave operators in GEVP

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
  - Construct optimized operators using 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!

Backup

N2LO potentials