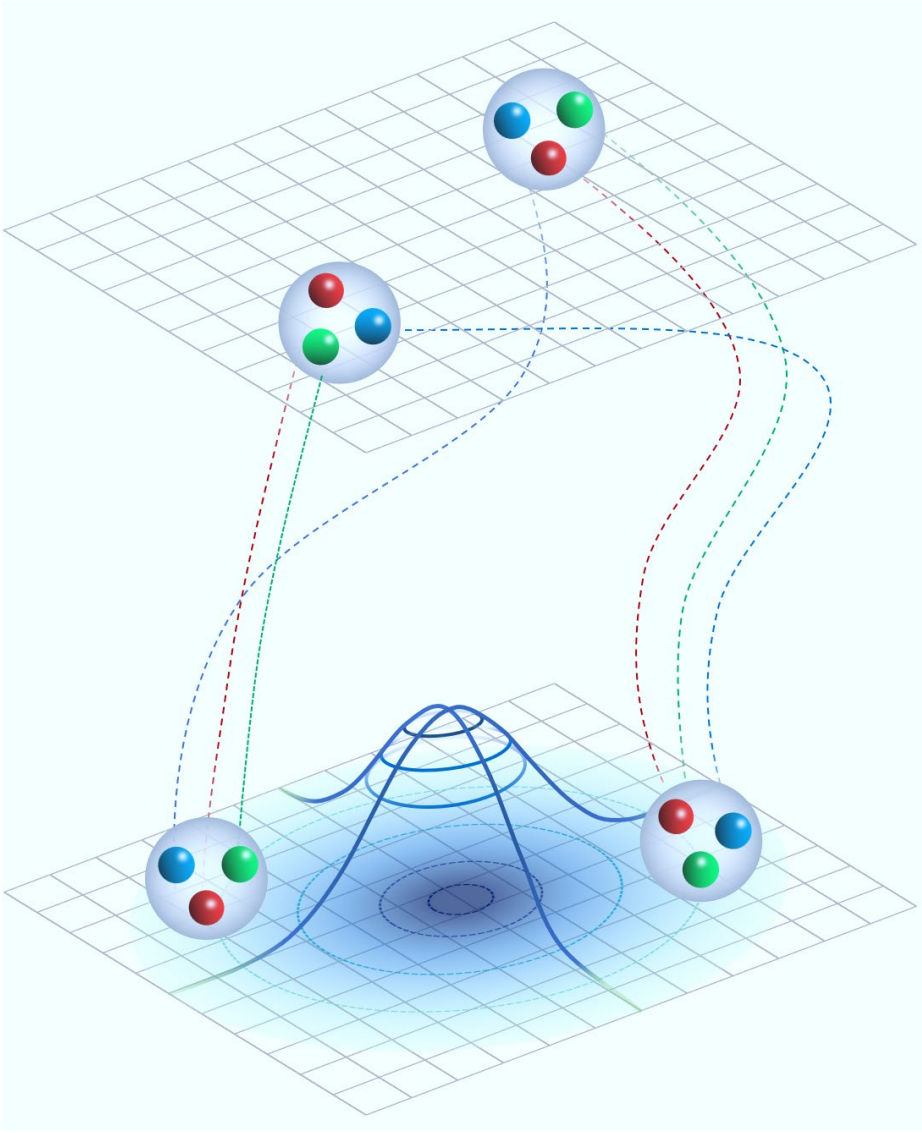
第五届中国格点量子色动力学研讨会
近代物理研究所, 惠州, 10/10-12

Decoding two-hadron states in LQCD with spatial wavefunctions



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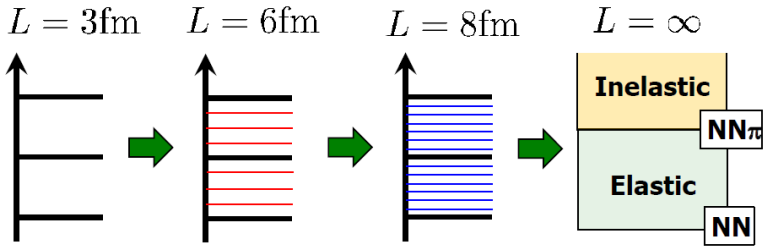
Based on: YL, S. Aoki, T. Doi, T. Hatsuda, K. Murakami, and T. Sugiura, arXiv:2507.09930; 2507.09933

Multi hadrons on lattice QCD

- Multi-hadron states are essential for studying
  - Hadron interactions: nucleon interaction relevant to nuclei and nuclear matter
  - Hadronic matrix elements: nucleon matrix element relevant to $0\nu\beta\beta$ *etc*

- Challenges for muti-hadron systems
  - Dense spectra of scattering states

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



  - Signals deteriorate exponentially for baryonic systems

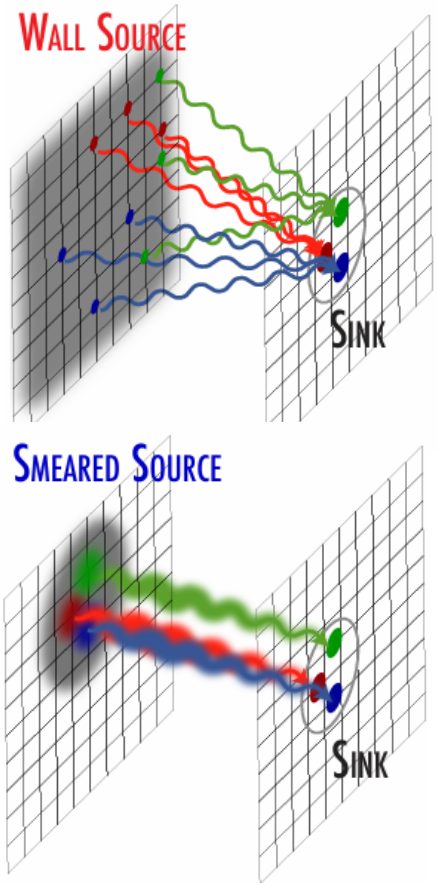
$$\frac{\mathcal{S}}{\mathcal{N}} \sim \frac{e^{-m_N t}}{e^{-3/2 m_\pi t}} = e^{-(m_N - 3/2 m_\pi)t}$$

Optimized multi-hadron operators are highly desired

Lessons from single hadron: the "shape" matters

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

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



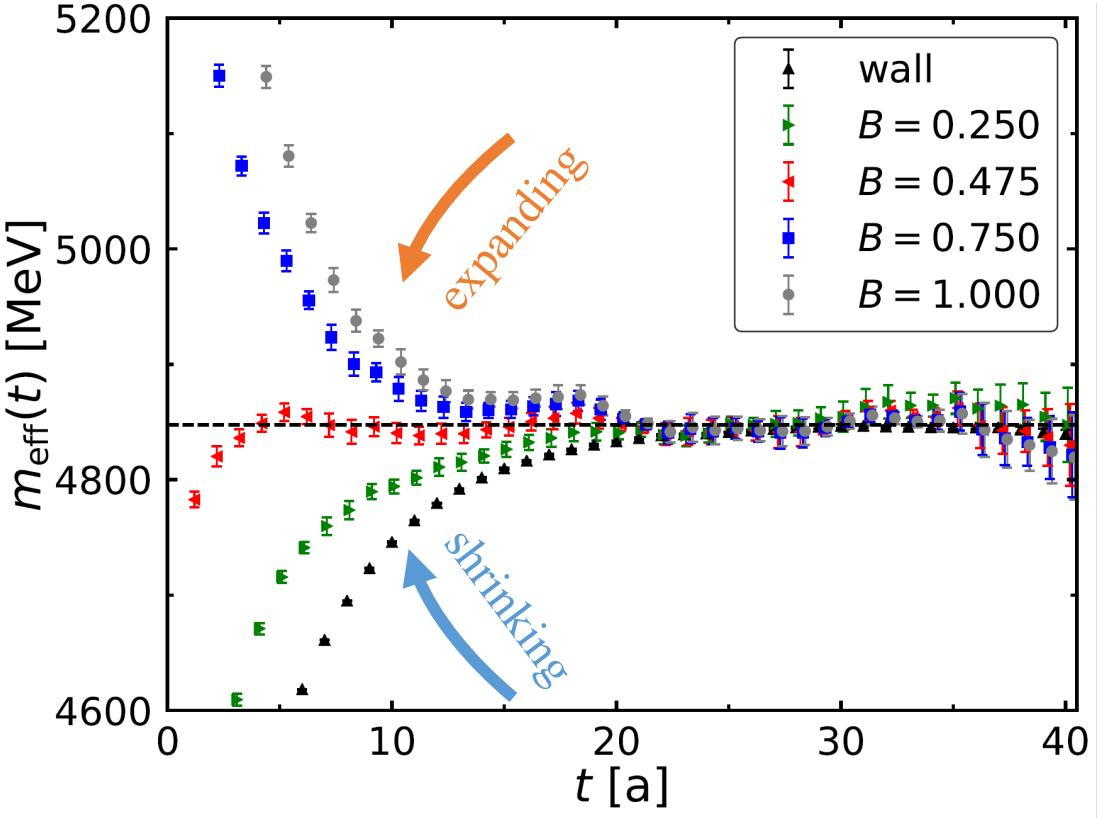
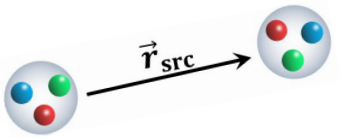


Fig. from T. Iritani

The "shape" of two-hadron states

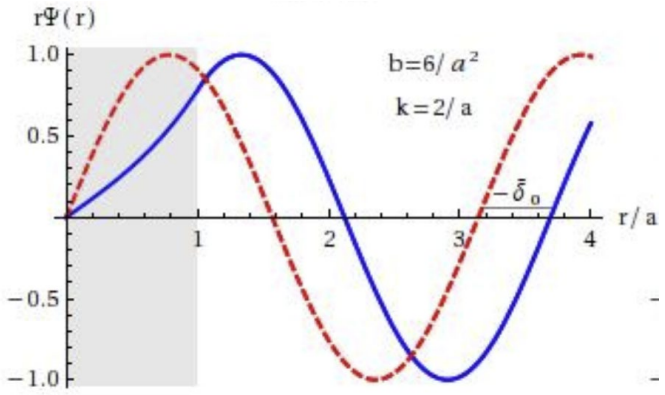
- (Equal-time) Nambu-Bethe-Salpeter (NBS) amplitude ($t_0 = 0$)

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



  - 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

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

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 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

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

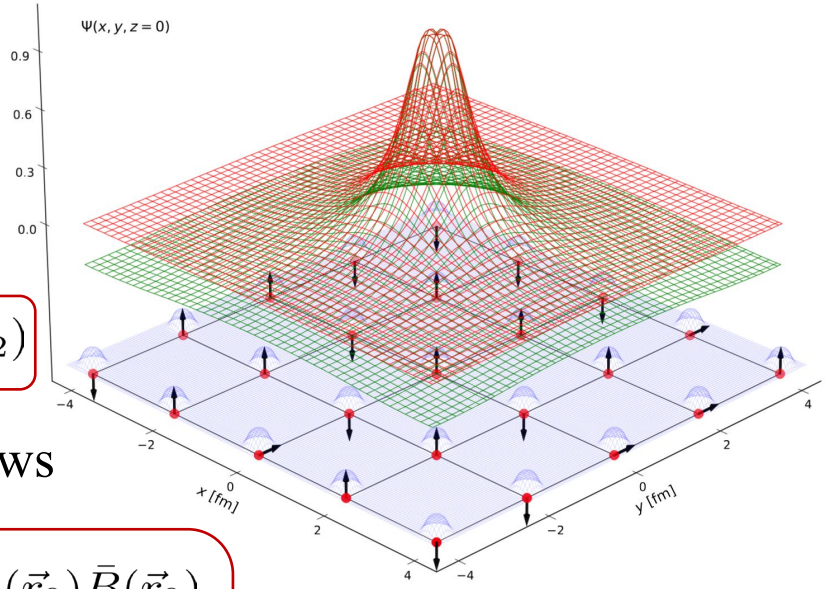
- Novel quark smearing functions at the source

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

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

- $f(\vec{r})$ 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

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

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

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

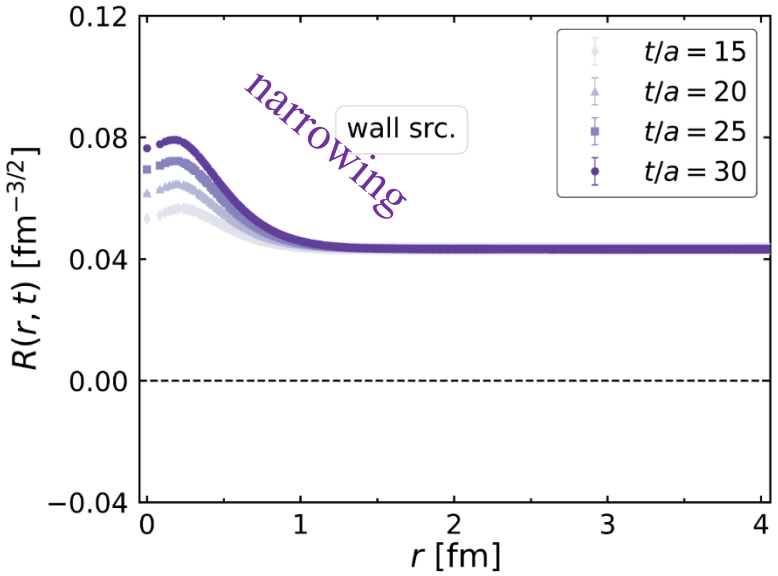
- Why $\Omega_{ccc}\Omega_{ccc}$?
  - extremely dense spectra
  - both bound state and scattering states
  - smaller statistical fluctuations

- Lattice gauge configurations

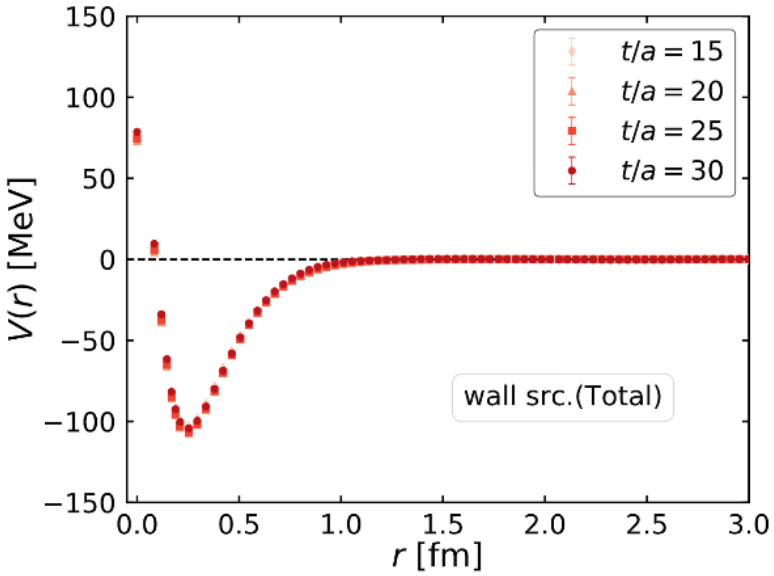
$L^3 \times T$	a [fm]	m_π [MeV]	$m_\pi L$
$96^3 \times 96$	0.0846	137.1(3)	5.63(1)

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

- Correlation functions



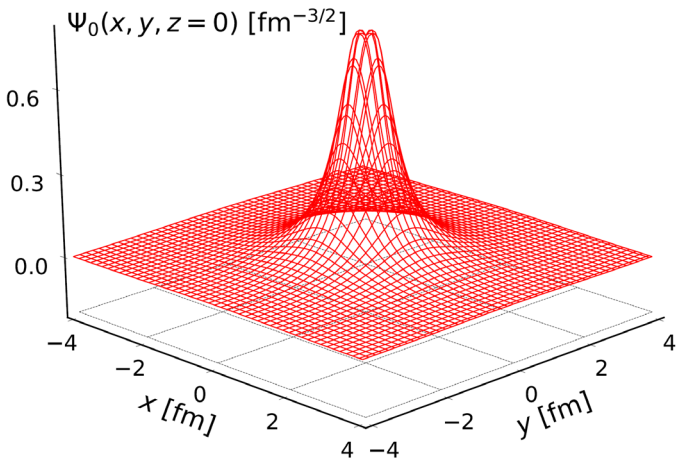
- The potential

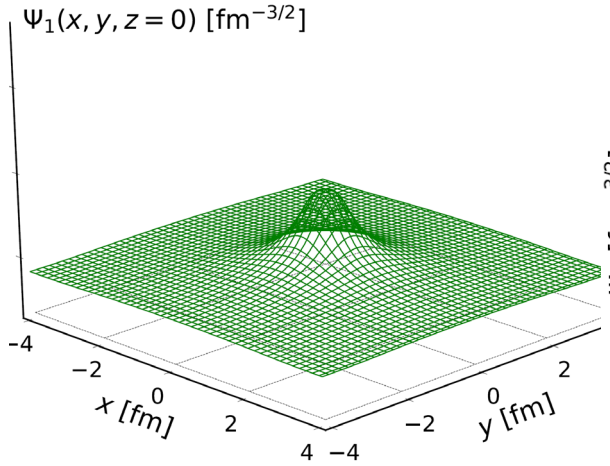


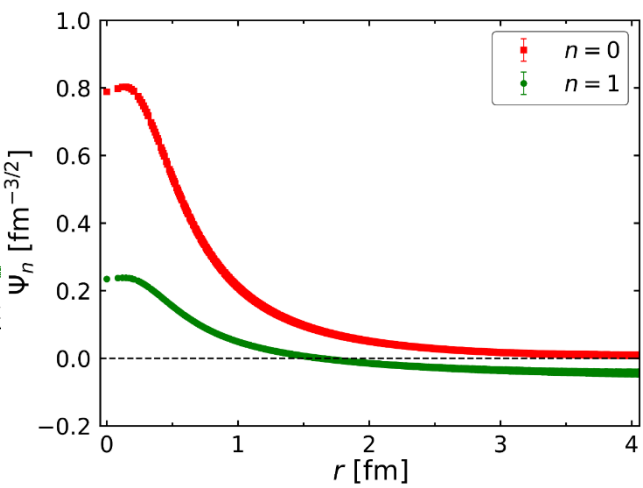
- Clear t-dependence in correlation functions: flat profile → localized profile
- The potential shows mild t-dependence

Eigen functions on a finite box

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





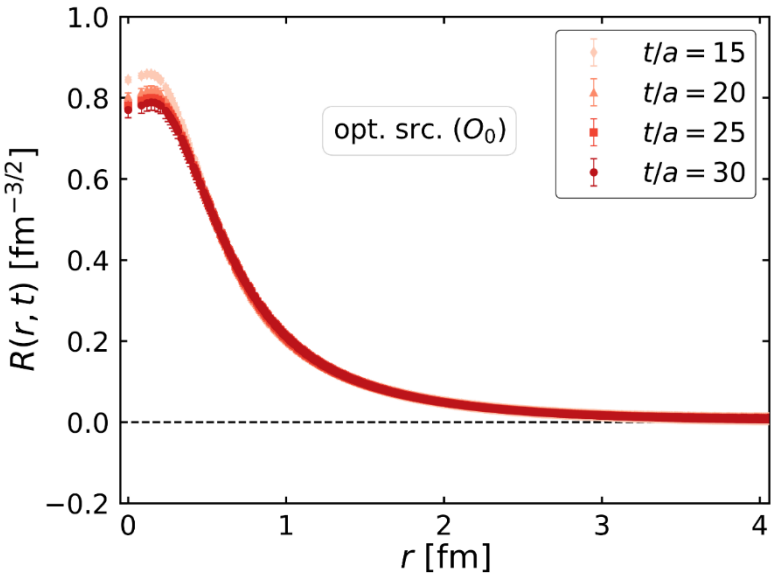


ε_0 [MeV]	ε_1 [MeV]
-4.6(4)	0.6(1)

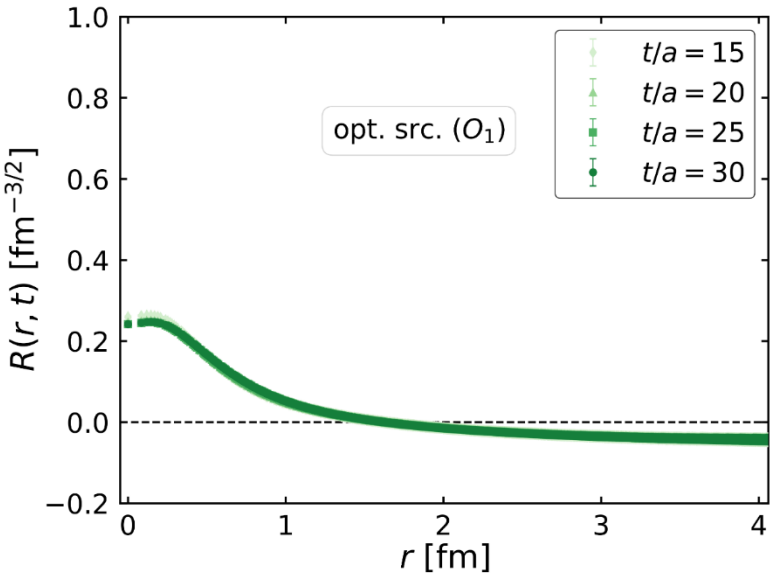
- $\Psi_0(\vec{r})$ is very localized, similar to typical bound state wavefunctions
- $\Psi_1(\vec{r})$ is much more extended, and has one node

Correlation functions from optimized sources

- The ground state



- The first excited state



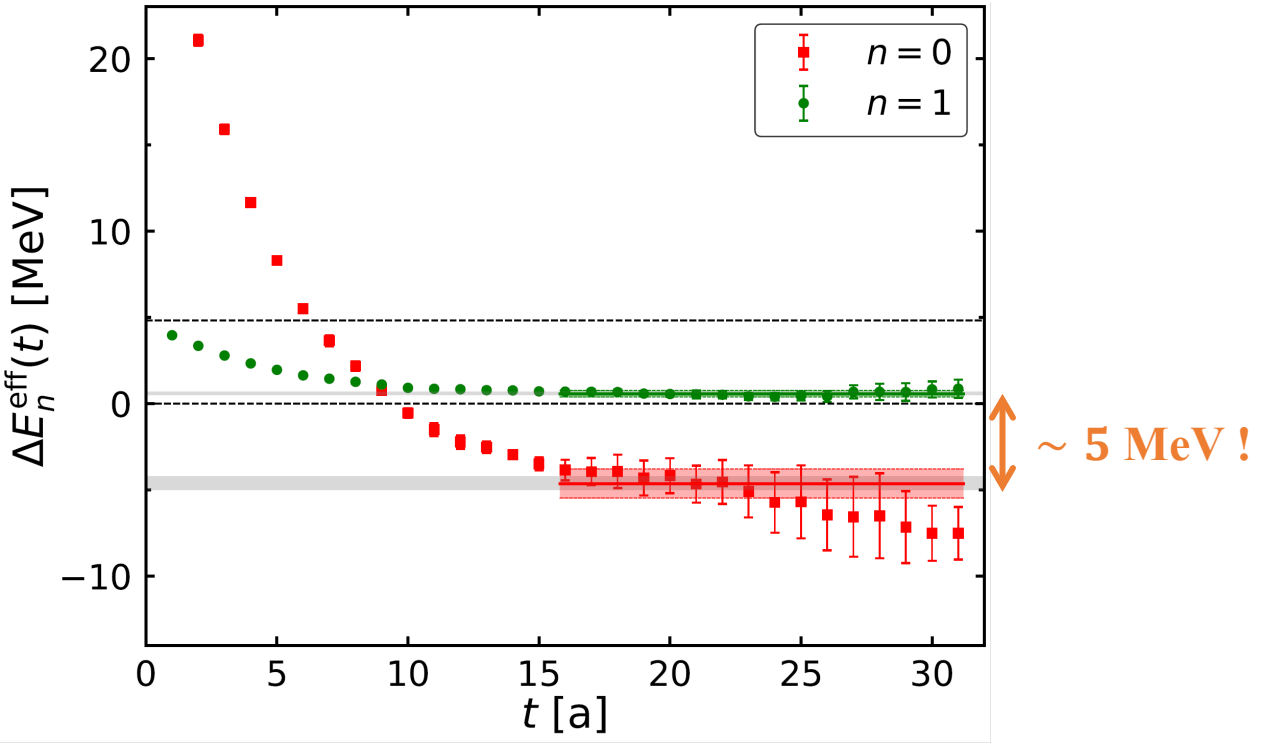
- Both exhibit very stable spatial profiles against a long period of Euclidean time $t/a = 15 \sim 30$
- The convergence is achieved in the iterative process of operator optimization at this step

Effective energies

- The ground/first excited state energy derived from

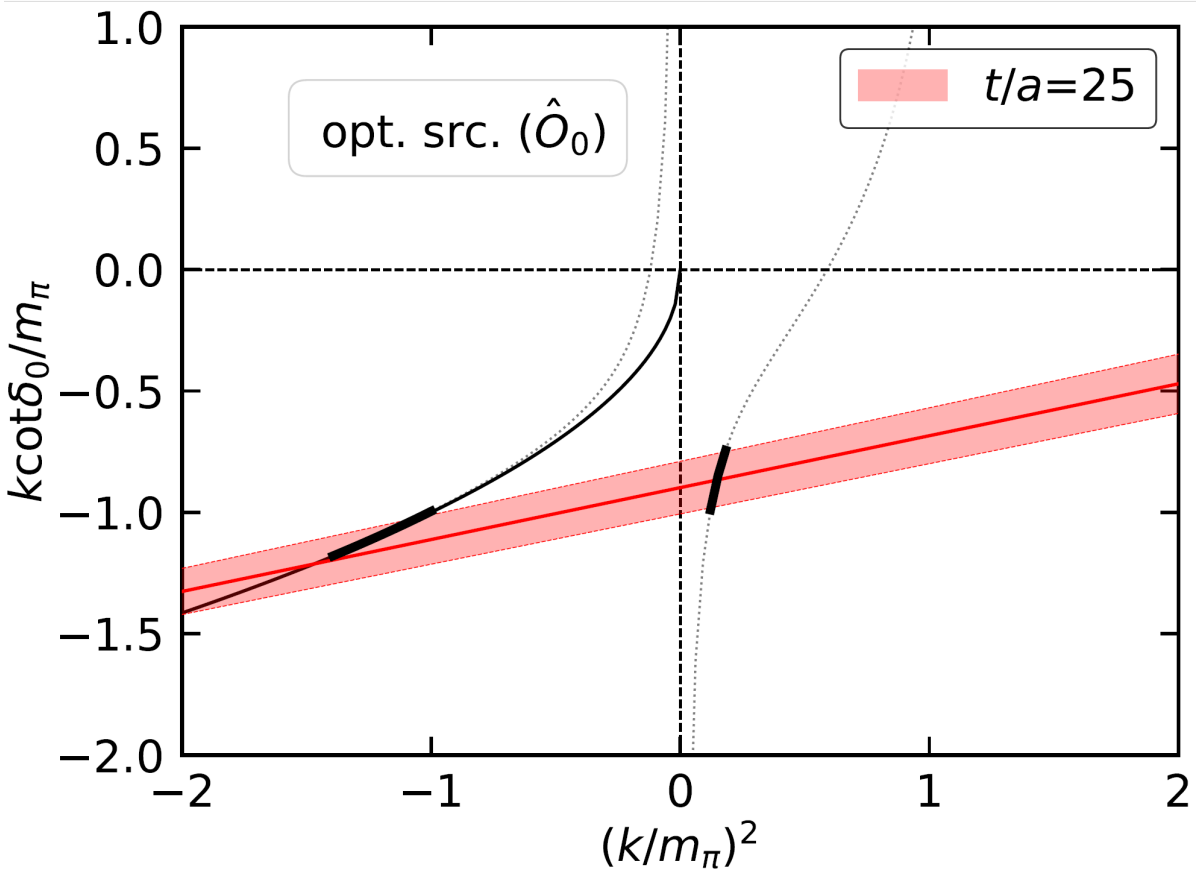
$$R_0(t) = \langle \hat{O}_0(t)\hat{O}_0^\dagger(0)\rangle = \sum_{\vec{r}\in\Lambda} \Psi_0(\vec{r})R_0(\vec{r},t)$$

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



- 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 $t > 1000\ [a](90\ \mathrm{fm})$ to archive $e^{-\Delta E t} < 10\%$

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!

Backup

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 $\{B(\vec{p})B(-\vec{p})\}$

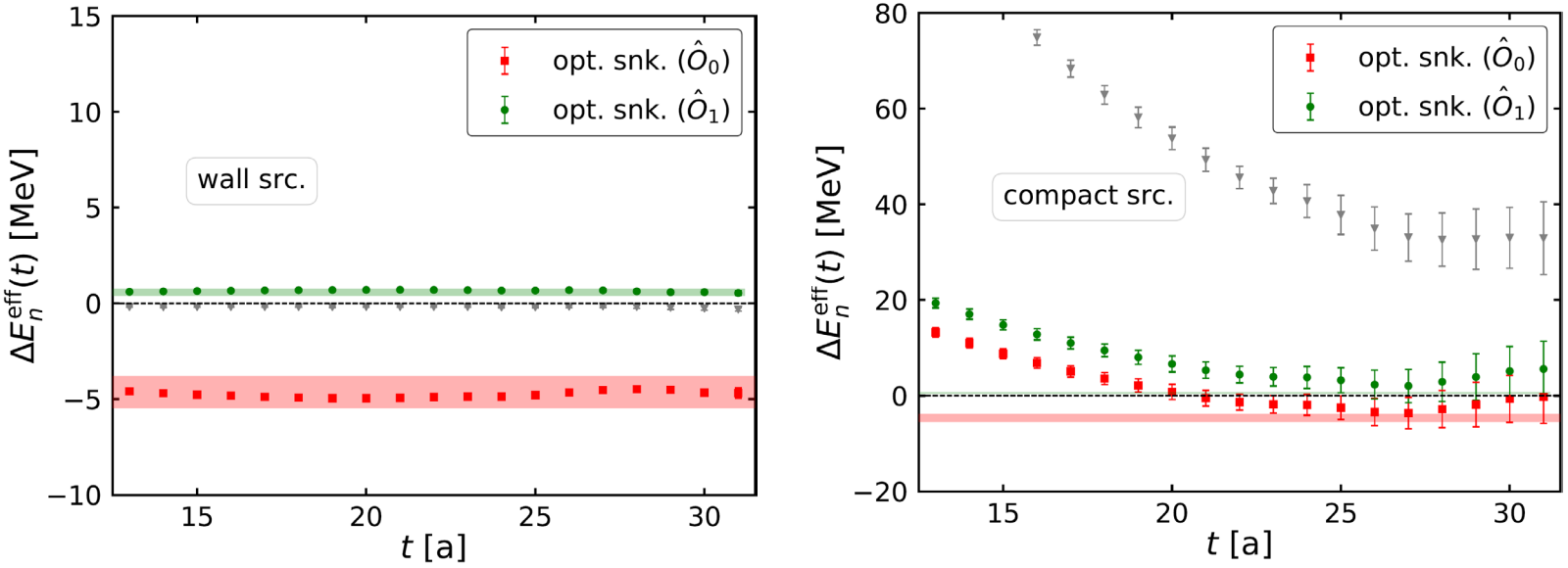
$$\Psi_n(\vec{r}) \sim \tilde{\Psi}_n(\vec{p}_0)\tilde{\Psi}_n(-\vec{p}_0)e^{i\vec{p}_0\cdot\vec{r}} + \tilde{\Psi}_n(\vec{p}_1)\tilde{\Psi}_n(-\vec{p}_1)e^{i\vec{p}_1\cdot\vec{r}} + \cdots$$

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



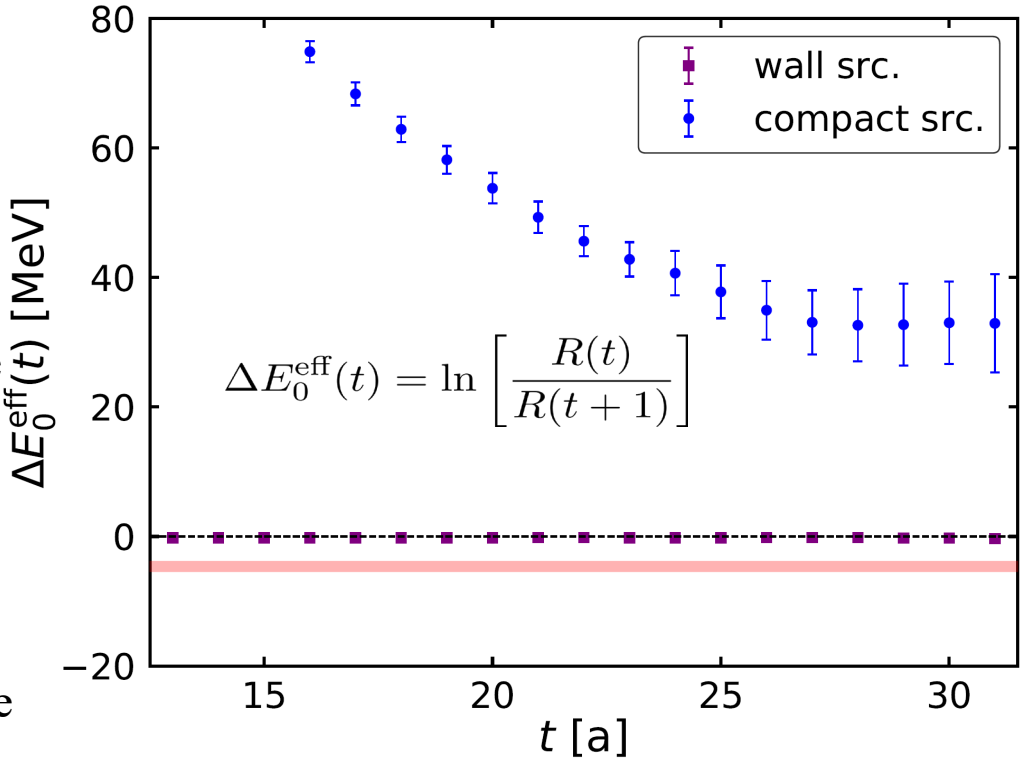
  - The obtained plateaux are consistent with the genuine energies of the ground/ first excited state for each source

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 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)