A comparative study of two lattice approaches to two-body systems

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Motivation

Study hadron interactions from first principles.

Luescher's finite size formula : spectrum in a box → phase shifts.

Method to extract the spectrum from LQCD?

Compare two methods:

- Variational method : use the time dependence of correlators.
- HAL QCD method : use the spatial information of wave functions.

I adapt the idea of HAL QCD's potential method to compare it more directly to the standard use of variational method + finite size formula.

Finite size formula

Two particles of mass m interacting in a box with periodic b.c.

In the *non-interacting region* (r > R), the wave functions for elastic eigenstates satisfy the Helmoltz equation

$$(\nabla^2 + k^2)\Psi_k(\mathbf{r}) = 0 \qquad E = 2\sqrt{m^2 + k^2}$$

The b.c. restrict the solutions of this equation.

Using the *asymptotic behaviour* of the wave functions, the allowed energies in the box can be related to the infinite volume phase shifts.

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

Variational method

Construct a N x N correlation matrix with elements

$$G_{ij}(t) = \langle 0|\mathcal{O}'_i(t)\mathcal{O}_j|0\rangle$$

O_j (resp. $\mathcal{O}'_i(t)$): arbitrary source (resp. sink) operators coupling to the targeted eigenstates.

Insert a complete set of eigenstates,

$$G_{ij}(t) = \sum_n a_{in} b_{nj} e^{-E_n t} \qquad \text{with} \quad \begin{cases} a_{in} = \langle 0|\mathcal{O}'_i(t_0)|n\rangle e^{E_n t_0} \\ b_{nj} = \langle n|\mathcal{O}_j|0\rangle \end{cases}$$

Assuming only N eigenstates contribute, matrix relation:

$$G(t) = AD(t)B \qquad \text{with} \quad d_{mn}(t) = \delta_{mn} e^{-E_n t}$$

sink | eigenstate — eigenstate | source

Assuming $\{(b_{nj})_n\}_j$ are linearly independent, extract the energies by solving the *generalized eigenvalue problem*

$$\boxed{G(t)V = G(t_{\text{ref}})VD(t - t_{\text{ref}})} \qquad V = B^{-1}$$

HAL QCD method I

The wave functions are computed on the lattice as

$$\Psi_i(\mathbf{r},t) = \langle 0|\mathcal{S}(\mathbf{r},t)\mathcal{O}_i|0\rangle e^{2mt}$$

O_i: arbitrary source operators coupling to the targeted eigenstates.

$\mathcal{S}$: interpolating operator for two particles with definite separation.

Insert a complete set of eigenstates,

$$\Psi_i(\mathbf{r},t) = \sum_n a_n^i(t)\phi_n(\mathbf{r})$$

computed unknown

with

$$\begin{cases} a_n^i(t) = \langle n|\mathcal{O}_i|0\rangle e^{-\Delta E_n t} \\ \phi_n(\mathbf{r}) = \langle 0|\mathcal{S}(\mathbf{r},t)|n\rangle e^{E_n t} \\ \Delta E_n = E_n - 2m \\ E_n = 2\sqrt{m^2+k_n^2} \end{cases}$$

"Combinations of eigenstates' wave functions with (i,t)-dependent coefficients."

HAL QCD method II

For a set C of source and time indices, *find a linear operator U* (constrain the value on a few vectors → many possibilities) s.t.

$$\forall (i,t) \in C, \quad \underbrace{U \cdot \Psi_i(\cdot,t)}_{\sum_n a_n^i(t)\, U\cdot\phi_n \text{ by linearity}} = \underbrace{(\nabla^2 - m\partial_t + \partial_t^2/4)\Psi_i(\cdot,t)}_{\sum_n a_n^i(t)\,(\nabla^2+k_n^2)\phi_n \text{ using the time dependence of } a_n^i}$$

This leads to,

$$\forall (i,t) \in C, \quad \sum_n a_n^i(t) \underbrace{\left[U\cdot\phi_n - (\nabla^2+k_n^2)\phi_n\right]}_{\text{i, t independent}} = 0$$

Assuming only $|C|$ eigenstates contribute and $\{(a_n^i(t))_n\}_{(i,t)\in C}$ are linearly independent, the contributing eigenstates satisfy

$$U\cdot\phi_n = (\nabla^2 + k_n^2)\phi_n$$

"Find a functional relation on enough combinations that it must hold for each eigenstate."

HAL QCD method III

The contributing eigenstates' wave functions can be recovered by solving the *eigenvalue problem*

$$(-\nabla^2 + U)\phi_n = k_n^2 \phi_n$$

For contributing *elastic eigenstates*, the wave function satisfies the Helmoltz equation outside the interacting region

$$\forall r > R, \quad (\nabla^2 + k_n^2)\phi_n(\mathbf{r}) = U \cdot \phi_n(\mathbf{r}) = 0$$

Their associated eigenvalues k_n^2 can thus be related to the phase shifts of the system through the *finite size formula*.

Workflow

Lattice simulations

Correlation matrices

$$G_{ij}(t) = \langle 0|\mathcal{O}'_i(t)\mathcal{O}_j|0\rangle$$

Wave functions

$$\Psi_{i,t} = \langle 0|\mathcal{S}(r,t)\mathcal{O}_i|0\rangle e^{2mt}$$

Workflow

Eigenstate wave functions

$\phi_n \propto \sum_i V_{in} \Psi_{i,t}$

Variational method

Solve the generalized eigenvalue problem

$G(t)V = G(t_{\mathrm{ref}})VD(t - t_{\mathrm{ref}})$

Eigenstate energies

$D_{nn}(t) = e^{-E_n t}$

Lattice simulations

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HAL QCD method

Find an operator U s.t.

$$U \cdot \Psi_{i,t} = (\nabla^2 - m\partial_t + \partial_t^2/4)\Psi_{i,t}$$

Solve the eigenvalue problem

$$(-\nabla^2 + U)\phi_n = k_n^2\phi_n$$

Eigenstate wave functions

$$\phi_n(r)$$

Eigenstate energies

$$E_n = 2\sqrt{m^2 + k_n^2}$$

Workflow

Variational method

Solve the generalized eigenvalue problem

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Lattice simulations

Correlation matrices

$$G_{ij}(t) = \langle 0|\mathcal{O}'_i(t)\mathcal{O}_j|0\rangle$$

Wave functions

$$\Psi_{i,t} = \langle 0|\mathcal{S}(r,t)\mathcal{O}_i|0\rangle e^{2mt}$$

Phase shifts

$$\delta_0(k_n) = f(k_n, L)$$

HAL QCD method

Find an operator U s.t.

$$U \cdot \Psi_{i,t} = (\nabla^2 - m\partial_t + \partial_t^2/4)\Psi_{i,t}$$

Solve the eigenvalue problem

$$(-\nabla^2 + U)\phi_n = k_n^2\phi_n$$

Eigenstate wave functions

$$\phi_n(r)$$

Eigenstate energies

$$E_n = 2\sqrt{m^2 + k_n^2}$$

Numerical application

Isospin 2 pion-pion system

- Simple system which allows a thorough comparison.
- Compute the wave functions for 5 momentum wall sources

$$\mathcal{O}_i = \pi^+(\tfrac{2\pi}{L}\mathbf{q}_i)\pi^+(-\tfrac{2\pi}{L}\mathbf{q}_i), \quad \mathbf{q}_i \in \{(0,0,0),(1,0,0),(1,1,0),(1,1,1),(2,0,0)\}$$

Spin singlet nucleon-nucleon system in the SU(3) limit

- More complex system where the variational method is limited.
- Compute the wave function for the wall source.

For a first comparison, we take the simple operator $[U \cdot \phi](\mathbf{r}) = V(\mathbf{r})\phi(\mathbf{r})$.

Lattice details

Clover fermions + Iwasaki gauge action

I=2 ππ

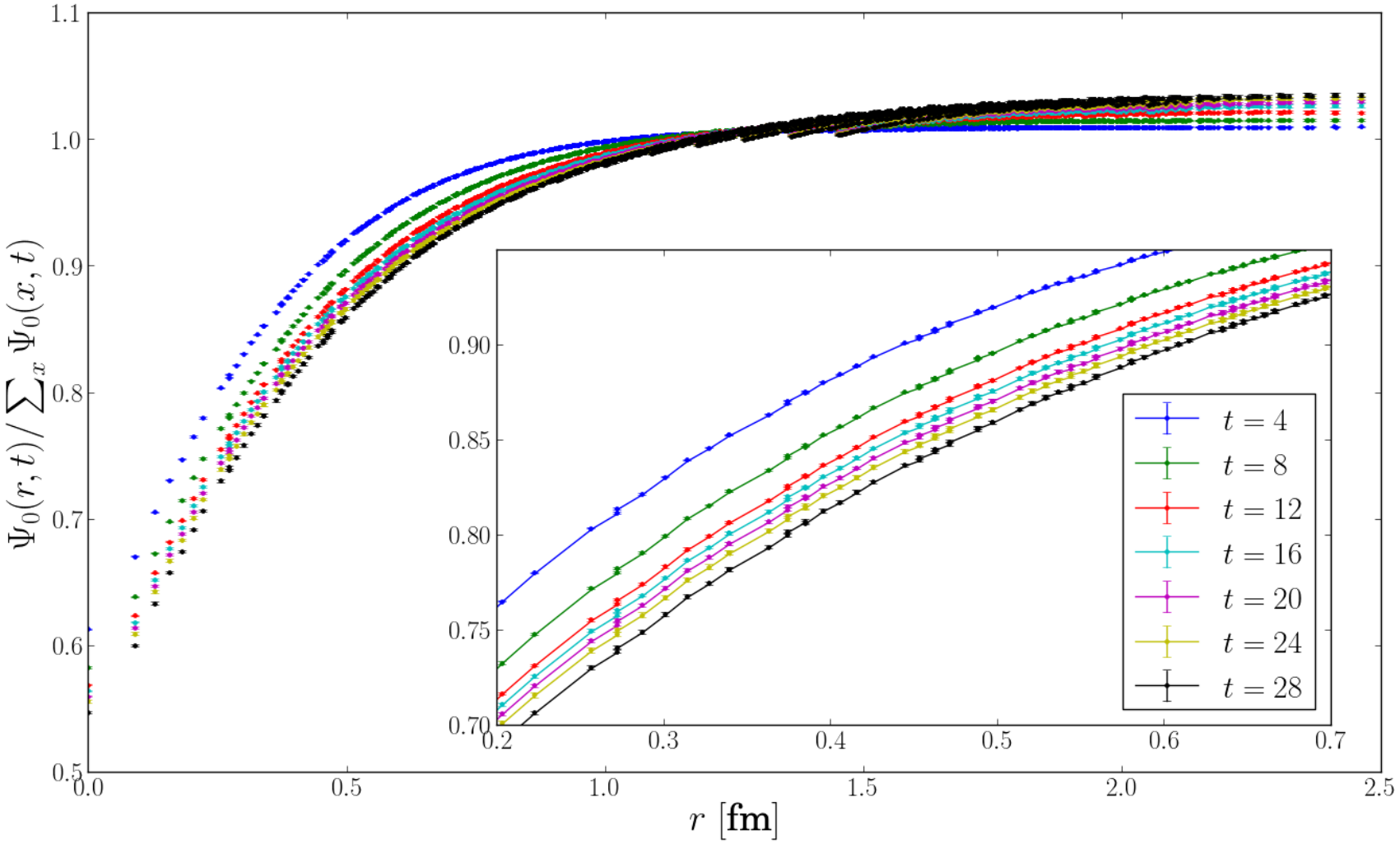
- Configurations generated by the PACS-CS collaboration.
- 32^3 x 64 lattice, κ_{ud} = 0.1370, κ_s = 0.1364, a = 0.09 fm, β=1.9
- m_π = 0.7 GeV

SU(3) NN

- 24^3 x 32 lattice, κ_{uds} = 0.1376, a = 0.12 fm, β=1.83
- $m_{p.s.}$ = 0.8 GeV, $m_{oct.\ bar.}$ = 1.7 GeV

I=2 ππ: wave functions

Time dependence of the wave function for the first source.
Wave functions normalized by their means to compare the shape.

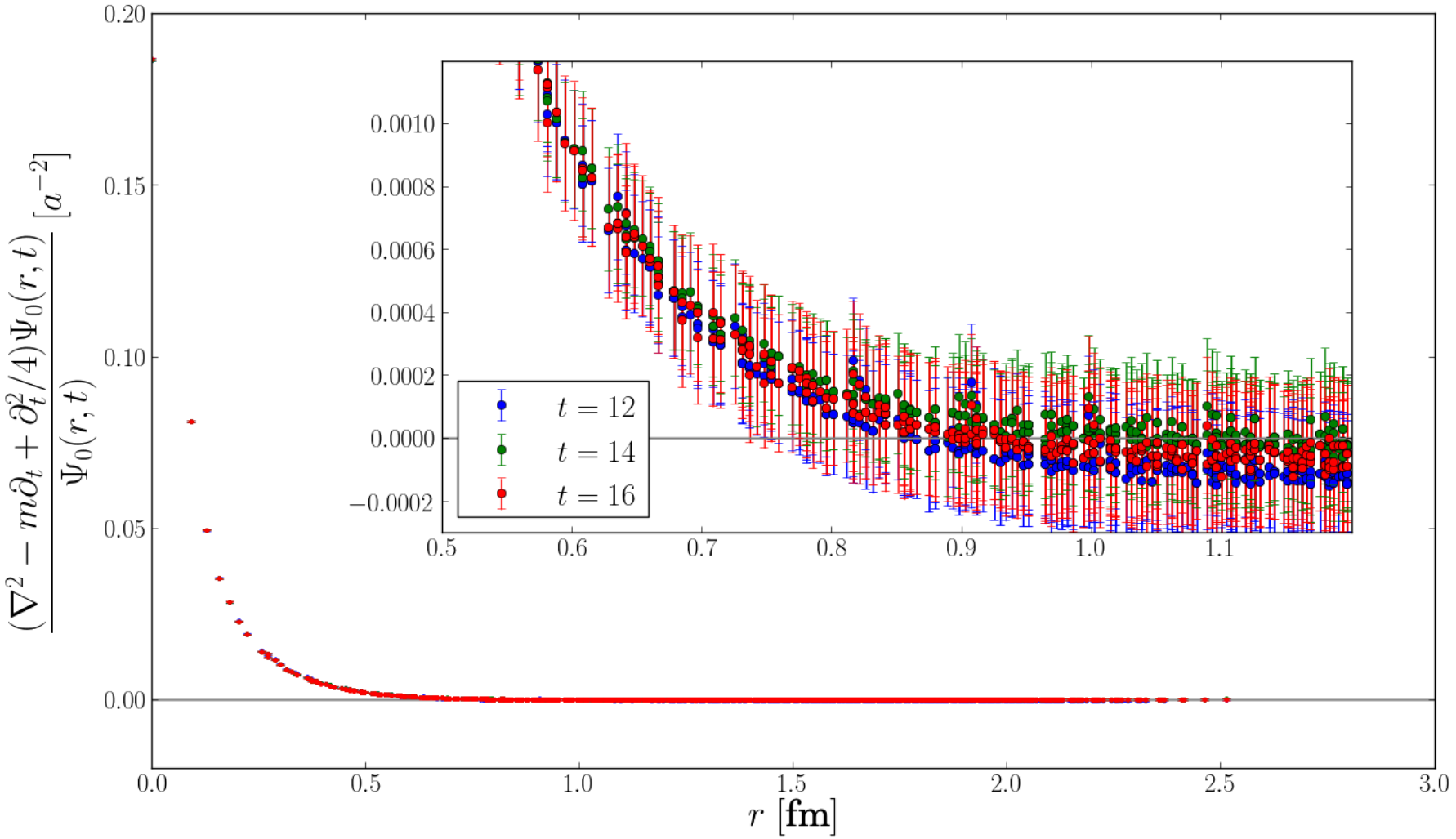


No ground state saturation, even at large t.

I=2 ππ: operator

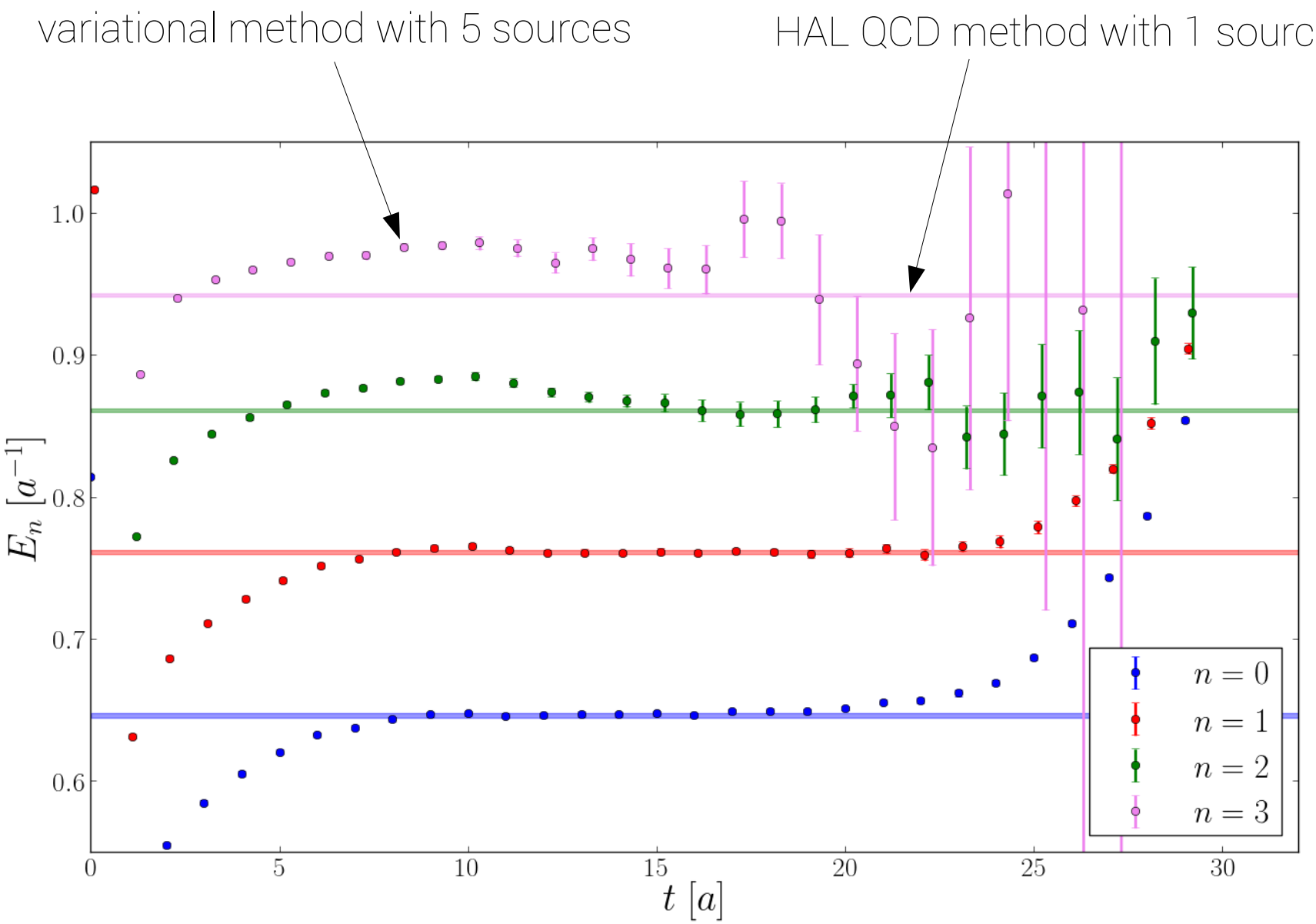
Diagonal operator $[U \cdot \phi](\mathbf{r}) = V(\mathbf{r})\phi(\mathbf{r})$

Constraints: $U \cdot \Psi_0(\cdot, t) \;=\; (\nabla^2 - m\partial_t + \partial_t^2/4)\Psi_0(\cdot, t)$



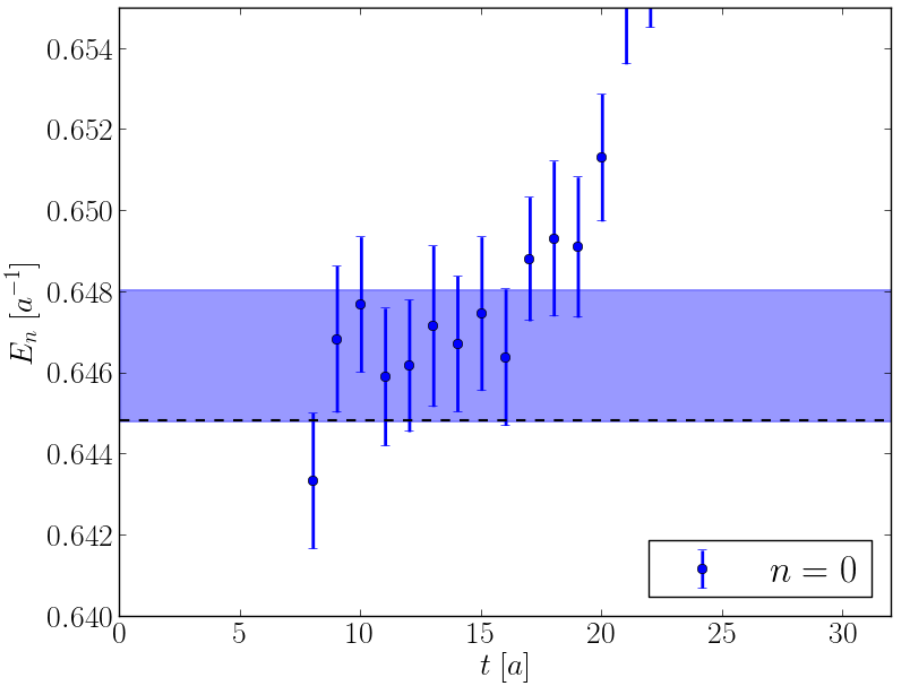
Functional equation with this U is valid for t = 12 ~ 16

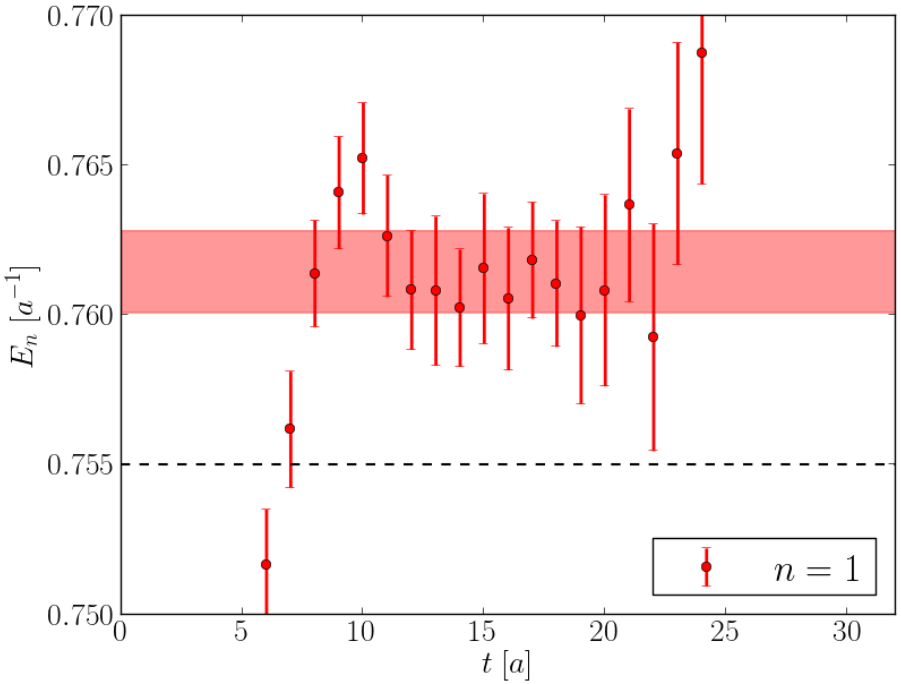
I=2 ππ: spectrum

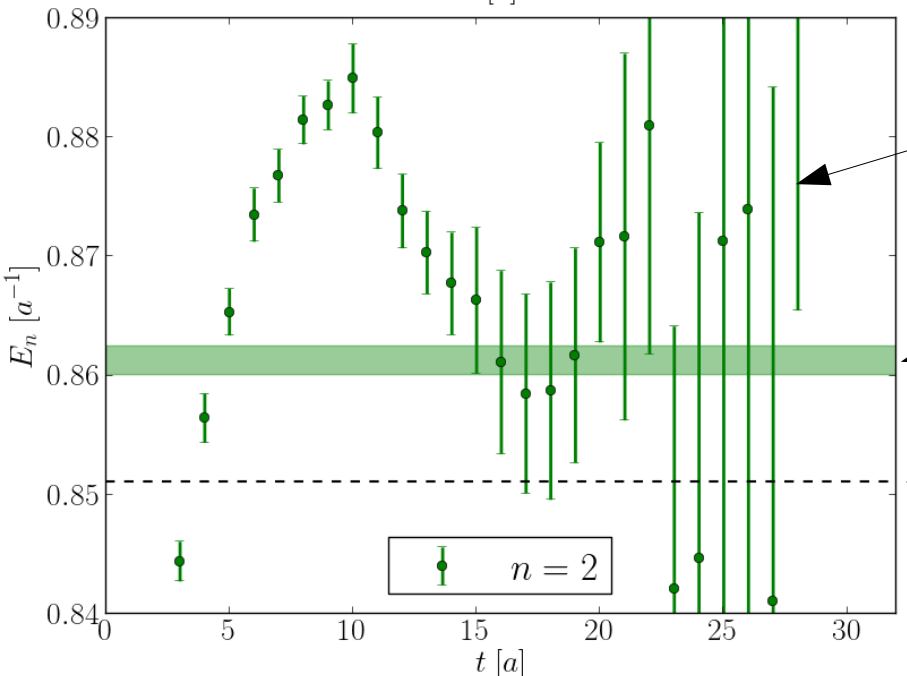


$t_{\mathrm{ref}} = 8$

I=2 ππ: spectrum







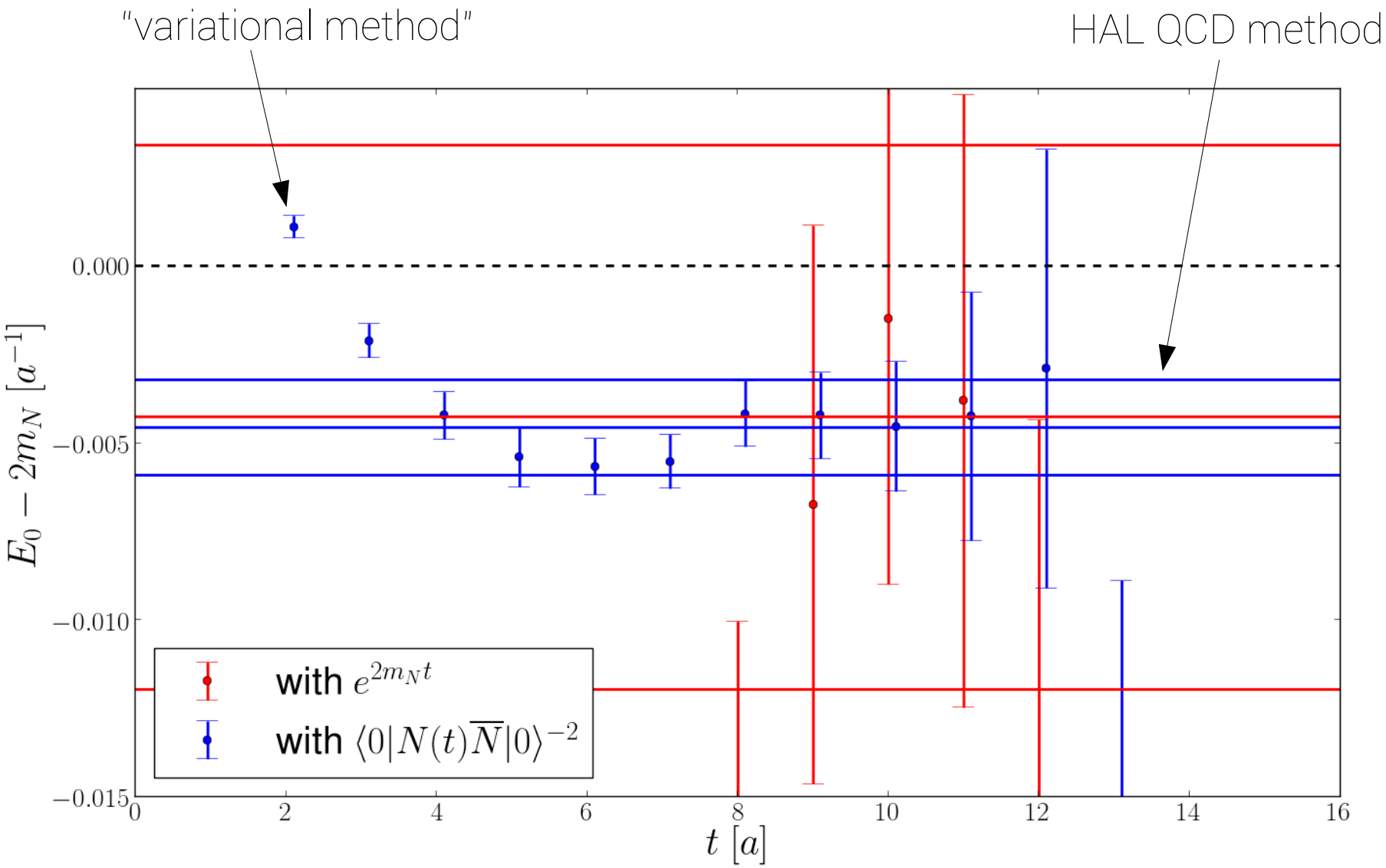
variational method with 5 sources

HAL QCD method with 1 source

free energy

Errors may be underestimated.

NN: energy shift



Normalization by 2-pt function: better signal but no control on time dependence.

Summary

Adapting the idea of HAL QCD's potential method, I presented a method to get the spectrum in a finite box from wave functions computed in LQCD.

I compared it numerically to the variational method for two systems.

Consistent results from two very different methods (time dependence vs spatial dependence).

Several eigenstates energies from one source in $\pi\pi$.

Future:

- Use more general operators U to account for more eigenstates.
- Check systematic error by changing U.
- Apply to other two-particle systems.