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Finite volume NN systems using plane wave expansion and eigenvector continuation

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In this talk, I will illustrate an alternative approach to Lüscher's formula for extracting the nuclear force from finite volume energy levels using the plane wave basis and eigenvector continuation. We adopt the formalism of semilocal momentum-space regularized chiral nuclear force to investigate the two-nucleon energy levels in the finite volumes using plane wave basis with no reliance on the partial wave expansion. In the chiral EFT framework, the long-range one-pion-exchange interaction is included nonperturbatively. Thus, this approach works well for the small boxes. We compare our method with Lüscher's formula for scattering states and bound states. We also determine the low energy constants of chiral EFT by fitting lattice QCD data at m_π=450 MeV from NPLQCD Collaboration. In the calculation, the eigenvector continuation is used to accelerate the fitting and uncertainty quantification, which also generates an easy-to-use interface to fit the upcoming lattice QCD results in the future.

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1. Introduction

Lüscher's formula is an approach to extract the two-body scattering amplitudes from the finite volume energy levels [1]. The Lüscher's formula sets up a one-to-one relation between finite volume energy level and the scattering phase shift at this energy if one truncates it at the leading partial wave. However, in the finite volume, the rotation symmetry is broken by the boundary conditions, see periodic condition. The partial wave mixing effect becomes unavoidable. Considering the partial wave mixing effect, the Lüscher's formula becomes a determinant equation, where the one-to-one relation disappears. One has to choose a paramerization scheme of T-matrix which is framework-dependent. Meanwhile, one has to use some root-finding algorithm to solve the determinant equation, which is unstable sometimes. In addition, the Lüscher's formula becomes exact only when the box size is much larger the the interacting range. However, in the realistic system, the long-range interaction could be very important, for example, the one-pion-exchange (OPE) interaction in the nuclear force. Considering the computational cost, the box size in the practical lattice QCD simulation could not be very large. Therefore, n alternative approach of Lüscher's formula could embed the partial mixing effect and consider the long-range interaction in the small box is called for.

In our previous work [2], we proposed a approach based on plane wave expansion and chiral effective field theory (ChEFT). The plane wave expansion renders the natural inclusion of the partial wave mixing effect and explicit OPE interaction in ChEFT make it work well for small box. In this work, we develop this approach by using the eigenvector continuation to accelerate the calculation and make it more practical.

2. Theoretical formalism

The ChEFT is the modern theory to construct nuclear force. As shown in Fig. 1, the one-pion-exchange interaction, two-pion-exchange interaction and contact interaction are included systemically according to the power counting [3]. Meanwhile, the chiral nuclear force was given in momentum space and in then energy-independent formalism, which is easy to use for the plane wave basis Hamiltonian method. In this work, we use the semilocal momentum-space regularized chiral nuclear force [4], which is the state of the art. In the formalism, the OPE interaction reads,

$$V_{1\pi}(\vec{p}', \vec{p}) = -\frac{g_A^2}{4F_\pi^2}\left(\frac{\vec{\sigma}_1 \cdot \vec{q}\vec{\sigma}_2 \cdot \vec{q}}{q^2 + m_\pi^2} + C(m_\pi)\vec{\sigma}_1 \cdot \vec{\sigma}_2\right) e^{-\frac{q^2+m_\pi^2}{\Lambda^2}}, \tag{1}$$

where g_A is known and $C(m_\pi)$ is introduced to subtract the short-range part in the OPE interaction. We will benefit from the known long-range interaction. For the short-range interaction, we will determine the low energy constants (LECs) of contact interactions by fitting the finite volume energy levels. We could use the irreducible representations (irreps) of the corresponding discrete group to re-decompose the contact terms. For the specific irrep, only a few independent LECs have contribution.

In the calculation, we choose the plane wave basis $|\boldsymbol{p_n}, \boldsymbol{\eta}\rangle$ in the direct product representation to deal with the spin space, where $\boldsymbol{p_n}$ is discrete momentum constrained by the periodic condition

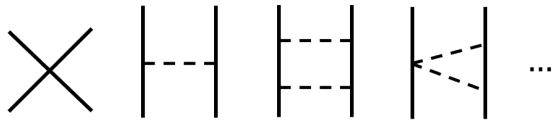

Figure 1: Feynman diagrams in calculating chiral nucleon force. For the pow counting in details, see Ref. [3].

and $\boldsymbol{\eta}$ is polarization vector for spin-triplet system. Apparently, under the space rotation $\hat{D}(g)$ and space inversion $\hat{P}$, the basis transforms as,

$$\hat{D}(g)|\boldsymbol{p},\boldsymbol{\eta}\rangle = |g\boldsymbol{p}, g\boldsymbol{\eta}\rangle, \hat{P}|\boldsymbol{p},\boldsymbol{\eta}\rangle = |-\boldsymbol{p},\boldsymbol{\eta}\rangle. \tag{2}$$

Thus, the space spanned by $|\boldsymbol{p_n},\boldsymbol{\eta}\rangle$ forms a representation space of the discrete group for either static or moving two-body system in the cubic box. In this basis, the finite volume energy level can be obtained by solving a eigenvalue problem,

$$\det(\mathbb{H} - E\mathbb{I}) = 0 \quad \text{or} \quad \mathbb{H}\boldsymbol{v} = E\boldsymbol{v}, \tag{3}$$

where $\mathbb{H}$ is the Hamiltonian matrix. If we treat Lüscher's formula as the quantization conditions (QCs) in partial wave basis, the above relation is the QCs in plane wave basis. We use the projection operator technique (see Ref. [2] for details) to reduce the above equation into different irreps,

$$\mathbb{H} \xrightarrow{\text{reduction}} \text{diag}\{\mathbb{H}_{\Gamma_i},\mathbb{H}_{\Gamma_j},...\}, \quad \mathbb{H}_\Gamma\boldsymbol{v} = E_\Gamma\boldsymbol{v}, \tag{4}$$

therefore, we get the Hamiltonian equation for the specific irrep, which makes it easy to fit the lattice QCD data classified by irreps and reduce the dimension of matrix.

The remaining problem is the dimension of the $\mathbb{H}_\Gamma$ is still very large. A typical estimation is

$$\dim \sim \left(\frac{\Lambda_{\text{UV}}}{2\pi/L}\right)^3 \times \frac{1}{10} \sim O(1000), \tag{5}$$

where L is the box size and Λ_{UV} is the UV cutoff. We has assumed the $\mathbb{H}$ is decomposed into ten irreps (it is exact for the cubic group with parity for the equal-mass system) and each of them has the same dimension. Basically, we are dealing with the following eigenvalue problem,

$$|\psi\rangle = a_m|\phi_m\rangle, \quad \langle\phi_m|H(c_i)|\phi_n\rangle a_n = \mathcal{E}\langle\phi_m|\phi_n\rangle a_n, \tag{6}$$

where c_i are the unknown LECs in the Hamiltonian. $|\phi_i\rangle$ is the basis and a_i is the coefficient. In our calculation, it is probably not hard to solve a single eigenvalue problem with thousands of dimension, however, the repeating calculations in the fitting and uncertainty quantifying procedure make it a large cost. To accelerate the calculation, we adopt the eigenvector continuation (EC) to perform the subspace learning [5]. As shown in the left panel of Fig. 2, we could choose a small number of possible parameter sets (training points) to solve the eigenvalue problem exactly. This process is called subspace learning. We suppose the subspace spanned by the eigenvectors of the training points is a good approximation of the whole space. We can solve the remaining eigenvector problems with different parameter sets using the vectors in the subspace as basis,

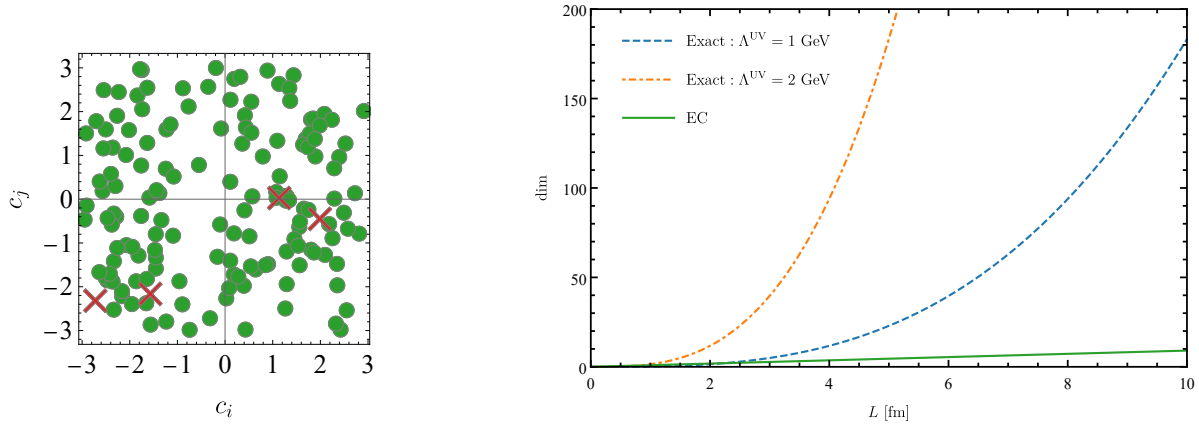

Figure 2: Choosing training points (left) and comparisons of Hamiltonian matrix dimensions of the exact calculation and eigenvector continuations with the box sizes (right).

namely, substituting $|\phi_i\rangle$ with the eigenvectors of training points. In this way, we accelerate the calculation by optimize the choice of the basis functions. The typical dimension of the subspace reads

$$\dim^{EC} = \frac{2\pi p}{L} \times n_{\rm training} \sim O(10), \tag{7}$$

where p is the scale to control the valid range of the subspace learning usually smaller than the $\Lambda_{\rm UV}$ in Eq. (5). $n_{\rm training}$ is the number of the training points. One can see we decrease the cubic relation of $1/L$ in Eq. (5) to the linear relation. As shown in right panel of Fig. 2, the typical dimension of the subspace is at $O(10)$. For the EFT, the naturalness of the LECs would make EC more reliable.

In Fig. 3, we present an example with known $V_{1\pi}$ and unknown $V_{\rm contact}$ with two LECs $\{c_1, c_2\}$ in the $L = \{2.70, 3.73, 5.60\}$ fm boxes. We choose two training points, $\{c_1^{\rm phy}, 0\}$ and $\{0, c_2^{\rm phy}\}$ to keep first four energy levels for each points to span the subspace. From Fig. 3, we can see the $\mathbb{H}^{EC}$ with dim = 8 gives very precise results below the highest energy inputs. The p in Eq. (7) is just the highest energy inputs. If we aim to obtain higher energy level, we could input more energy levels. Therefore, we could solve the Hamiltonian problem in the finite volume fast and accurate with the help of EC. We do need some computational cost for the subspace learning, but it is one-time cost. What is more important, after subspace learning, we can provide a easy-to-use interface, namely $\mathbb{H}_0^{EC}$ and $\mathbb{V}_i^{EC}$ to the lattice community. The users could solve the eigenvalue problem of the Hamiltonian matrix with dim $\sim O(10)$,

$$\mathbb{H}^{EC} = \mathbb{H}_0^{EC} + c_i \mathbb{V}_i^{EC}, \quad \mathbb{H}^{EC} \boldsymbol{v} = E \boldsymbol{v}. \tag{8}$$

There is no need for the users to know the details of ChEFT.

3. Scattering states

To compare our approach with the Lüscher's formula, we present static, spin-singlet, even-parity example and moving, spin-triplet, odd-parity example in Figs. 4 and 5 respectively. We first solve the NNLO chiral nuclear force with plane wave basis in the finite boxes to get the energy levels as shown in the dashed lines. Then, we use the Lüscher's quantization conditions truncated

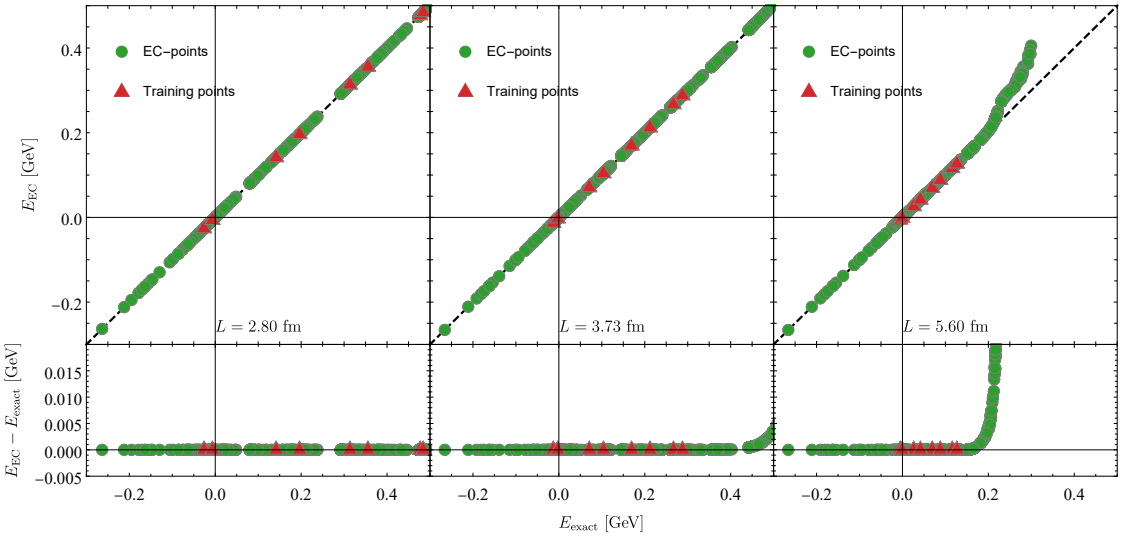

Figure 3: Comparisons of the exact results and EC results.

at different $J_{\rm max}$ to get the discrete points, where the phase shifts of the same interactions are used as inputs. We can see the Lüscher's quantization conditions will finally converge to plane wave expansion results, for both cases, which shows that our approach is consistent with the Lüscher's quantization conditions considering the higher partial wave mixing effect. Meanwhile, we can see the discrepancies appears for the small box with low $J_{\rm max}$ truncation, which means the uncertainties of Lüscher's quantization conditions for there cases could be large. It should be stressed that the visually small uncertainties in the finite volume energy levels could correspond to large uncertainties for the phase shift, because the energy levels often appear in the proximity of the singularity of Lüscher's Zeta functions.

4. Bound states

In addition to the scattering states, we also compare Lüscher's formula for bound states with the plane wave expansion results. In Lüscher's formula, the differences of binding momentum (or energy) between finite volume and infinite volume is described by the exponential relation [6–9],

$$\kappa = \kappa_0 + \frac{Z^2}{L} F(L, \kappa_0) + O(e^{-2\kappa L}), \tag{9}$$

where $kappa$ and κ_0 are binding momentum in the finite box and infinite volume. For $\boldsymbol{d} = (0,0,0)$, one has $F(L,\kappa) = 6e^{-\kappa L} + 6\sqrt{2}e^{-\sqrt{2}\kappa L} + \frac{8}{\sqrt{3}}e^{-\sqrt{3}\kappa L}$. The relations can be derived from expanding the Lüscher's quantization conditions at the κ_0 in the analytical continuation sense. We use the LO chiral nuclear force at $m_\pi = 138, 300, 450$ MeV. We tune $theV_{\rm contact}$ to permit bound states $B_d = 2, 10, 20$ MeV. We put the interaction into boxes with $L = 2.80$, 3.3, 3.73, 4.0, 4.5, 5.0, 5.60, 6.0, 6.5, 7.0, 7.5, 8.0 fm and obtain the finite volume energy levels from the plane wave expansion method. Finally, we try to fit these energy levels with exponential relations to check their consistence. We illustrate the spin-singlet results in Fig. 6 to show the fitting results. We assign constant uncertainties for every energy levels, thus the best fits will not depend on the uncertainties.

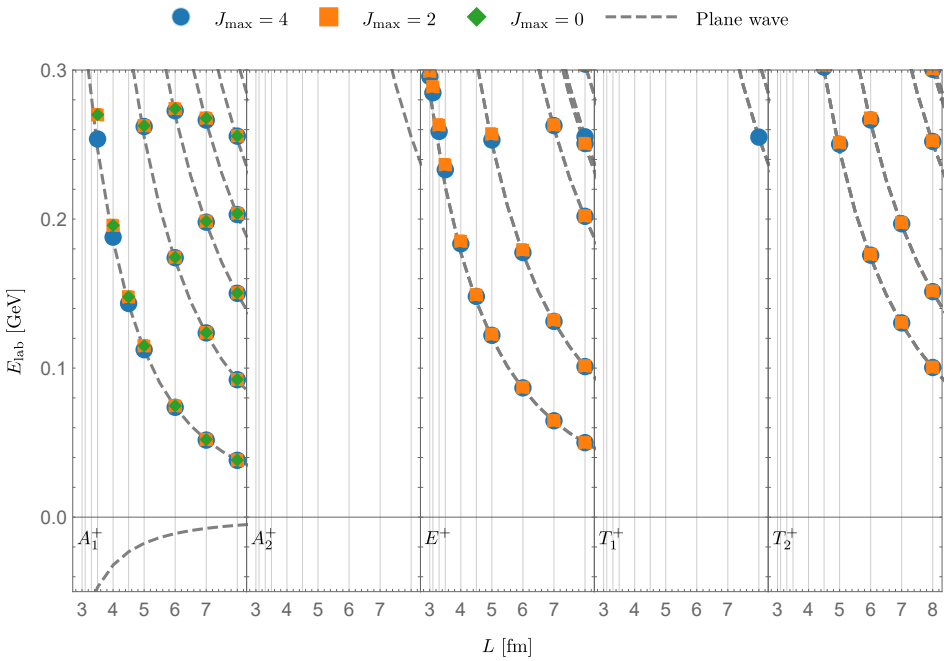

Figure 4: Comparisions of the Lüscher's quantization conditions truncated at different $J_{\max}$ and plane wave wave expansion method for the spin-singlet, even-parity NN systems with $d = 0$.

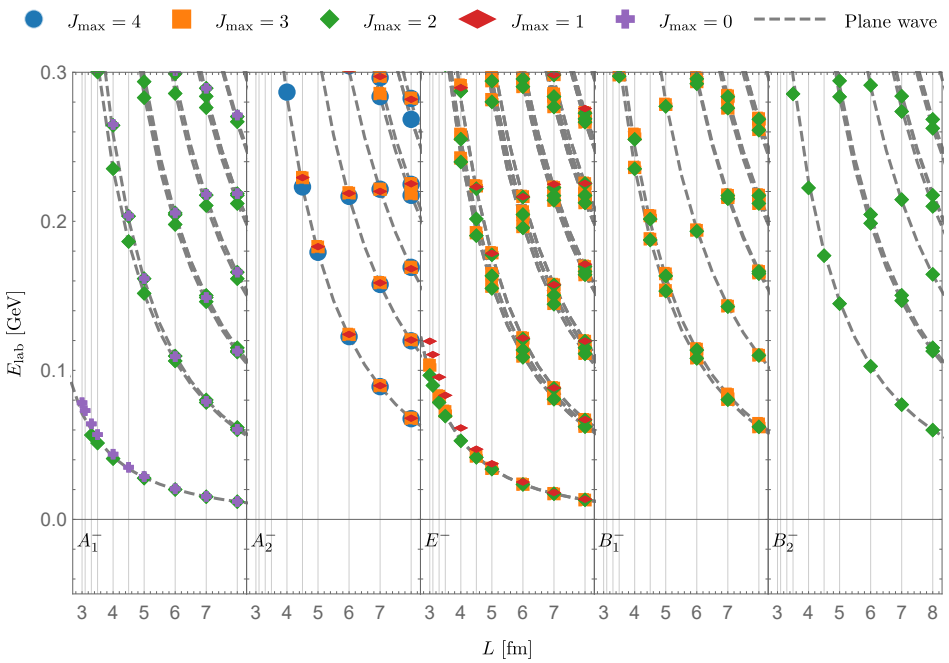

Figure 5: Comparisions of the Lüscher's quantization conditions truncated at different $J_{\max}$ and plane wave wave expansion method for the spin-triplet, odd-parity NN systems with $d = 1$

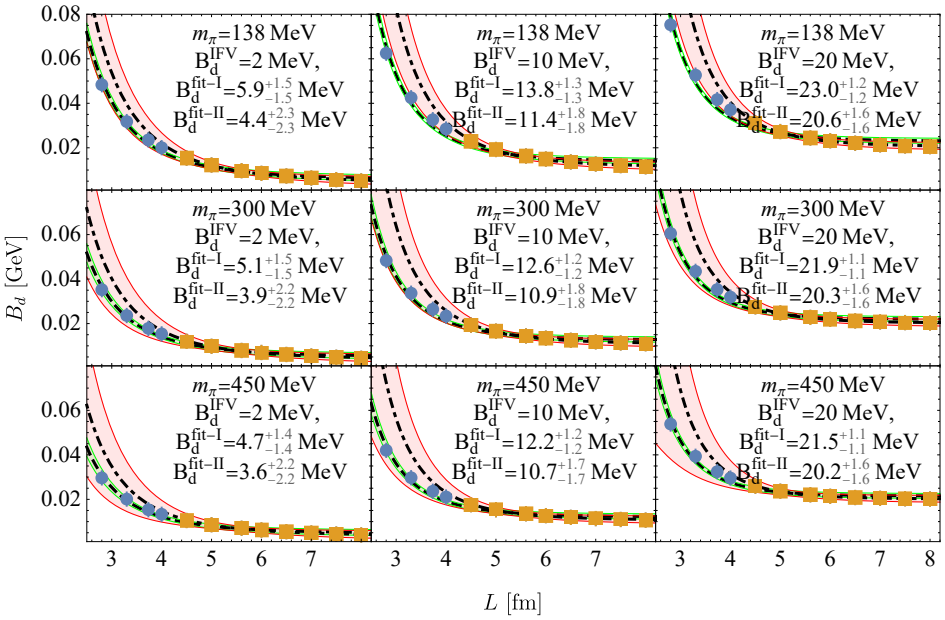

Figure 6: Fitting the finite volume energy levels from plane wave expansions with the Lüscher's formula in Eq. (9) for the bound states. Dashed line and dot-dashed line are for fit-I and fit-II respectively.

We perform two fits, fit-I including all inputs and fit-II only including larger boxes results (the orange ones for $L > 4.0$ fm).

By comparing the best fit results with the exact infinite volume binding energies, one can see the best results with exponential relations are biased, which are larger than the exact results. Meanwhile, one can see the smaller pion mass, the larger bias. If we drop some energy levels from small boxes, we could decrease the bias. Therefore, the bias arise from the small boxes and long-range interaction, where is the chance of the pane wave expansion methods.

5. Fitting NPLQCD results

We also use the plane wave expansion method to fit NPLQCD data for $m_\pi = 450$ MeV [10, 11]. For such a large pion mass, the validity of the ChEFT is questionable. Here, we only perform a proof-of-principle. We first obtained the m_π-dependent g_A, f_π and m_N by fitting the lattice QCD results using the quadratic function of m_π^2 [12]. We use the ChEFT to NLO with the pion-mass-dependent contact interaction,

$$C_i^{phy} \to C_i^{phy}\left[1 + a_i\left(1 - \frac{m^2}{m_{\rm phy}^2}\right)\right], \tag{10}$$

where C_i is the LECs for the contact interactions. This interaction will reduce to physical chiral nuclear force when we take $m = m_{\rm phy}$. We try to fit the NPLQCD results to determined the a_i, where three a_is for spin triplet and two a_is for spin singlet. We only use the ground states of NPLQCD data in different boxes including both moving system and static system,

$$L = \{2.801, 3.734, 5.602\}\ \text{fm} \otimes d^2 = \{0, 4\}. \tag{11}$$

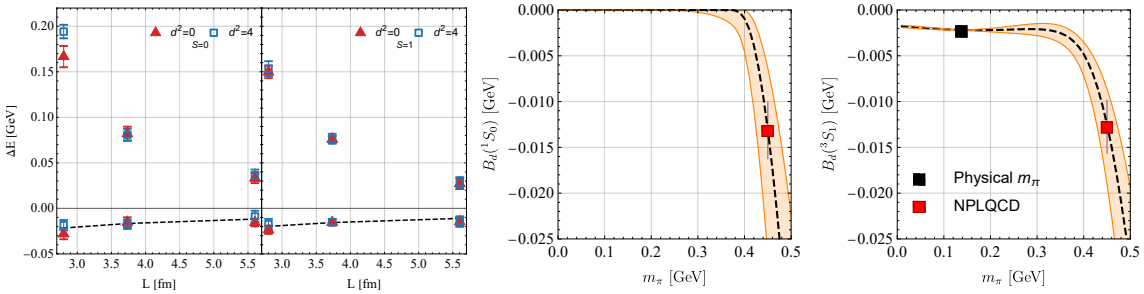

Figure 7: The inputs from the NPLQCD data and the fitting results.

The χ^2 for different systems read,

$$S = 1: \ \chi^2/\text{d.o.f} = 0.87, \quad S = 0: \ \chi^2/\text{d.o.f} = 0.92. \tag{12}$$

We present the m_π-dependent binding energies for the $^1S_0$ and $^3S_1$ systems in Fig. 7. One can see our results are consistent with the binding energies from the Lüscher's formula at $m_\pi = 450$ MeV from NPLQCD group. Meanwhile, our results will go across the physics ones.

6. Conclusion and outlook

In this work, we illustrate an alternative approach of Lüscher's formula to investigate NN systems in the box. The three ingredients and corresponding advantages are list as follows,

- Plane wave expansions: includes the partial wave mixing effect;
- ChEFT: benefits from the known long-range interaction $V_{1\pi}$ and works well for small boxes;
- Eigenvector continuation: accurate and fast, provides an easy-to-use interfaces (Hamitonion matrix with dimension about $O(10)$) to lattice community,

We compare our approach with the Lüscher's formula for the scattering states and showthat the high partial wave effect in Lüscher quantization conditions is important, especially in small boxes. We also show the Lüscher's exponential relation for binding momentum (energy) differences in finite volume and infinite volume could be biased in the small boxes and small m_π. Finally, we use the real lattice QCD data from NPLQCD at $m_\pi = 450$ MeV to further give a proof-of-principle.

Apparently, the advantages of our approach would be more obvious for physical m_π. In the future, we will refine the analysis of pion mass dependence. Meanwhile, we will use the plane wave expansion method for the D^*D and $D^*\bar{D}$ systems to investigate T_{cc} and $X(3872)$ states, where the typical bound state size is unnatural large even larger than the box size of the common lattice QCD simulations, see [13].

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