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Quantization conditions in the finite volume within the plane wave basis expansion

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In this work, we propose an alternative approach of Lüscher's formula to extract the two-body interaction from the finite volume energy levels. We adopt the plane wave expansion rather than the partial wave expansion in calculation. In this framework, the exponential suppressed effect and partial wave mixing effect are embedded naturally. We use the spin singlet NN system and $\pi\pi$ system in ρ channel as examples of non-relativistic and relativistic examples. For spin singlet NN system, the one-pion-exchange interaction at physical pion mass will make the single channel Lüscher's formula unreliable. For S-wave dominant states, Lüscher's formula gives rise to significant deviation for the $L = 3$ fm box. For the ${}^1P_1$ dominant states, the mixing effect from the higher partial wave components is significant even in the box with $L = 8$ fm. We adopt a toy model to illustrate the combination of effective field theory and the plane wave expansion approach can solve the problems. For the ρ channel $\pi\pi$ interaction, we use a phenomenological model to fit the lattice QCD results. The fitting results can depict the $\pi\pi$ scattering phase shift well.

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1. Introduction

The lattice QCD simulations are formulated in the discrete space time in a finite volume (FV). The outputs of lattice QCD for investigating the two-body interaction are in general some energy levels in FV. Three decades ago, Lüscher proposed an approach of extracting the two-particle elastic scattering phase shifts from their energy levels in a finite box with periodic boundary conditions [1–3]. Apart from the original derivation, one can also obtain Lüscher formula by expanding the Lippmann-Schwinger equation (LSE) in FV with partial wave basis [4]. There are two attractive features of Lüscher formula, the model-independence and one-to-one correspondence. If the box size L is much larger than the interaction range R, such that the exponentially suppressed corrections $e^{-L/R}$ are negligible. The Lüscher formula can set up the relation independent of the two-body interaction. However, some interesting interaction for example, one-pion-exchange (OPE) interaction are long-range compared with the box size using in practical lattice QCD simulations. For the second feature, if one keeps only the lowest partial wave component, the Lüscher formula sets up a one-to-one relation between the energy level in FV with the phase shift. However, in the box, the rotational symmetry is broken into symmetries describing by some point groups. The partial wave mixing effect is unavoidable, which could play important roles.

In order to overcome the limits, one can incorporate the partial mixing effect in Lüscher formula by parameterizing the T-matrix with theoretical frameworks, for example, the effective range expansion. In addition, many alternative approaches were proposed, the HAL QCD method [5], unitarized chiral perturbation theory in FV [6], Hamiltonian effective field theory [7].

We propose an another alternative approach of Lüscher formula by combing the plane wave expansion and effective field theory (EFT). Lüscher formula is the quantization conditions in sense of partial wave expansion. However, due to the loss of the rotational symmetry, we choose to expand the LSE in FV with plane wave basis with discrete momenta. The long-range interaction is usually known, e.g. the OPE interaction. We use the EFT to embed the known long-range part and determine the short-range part by lattice QCD inputs.

2. Theoretical formalism

In the plane wave expansion, the LSE becomes an matrix equation,

$$\mathbb{T} = \mathbb{V} + \mathbb{V}\mathbb{G}\mathbb{T}, \quad \text{with } \mathbb{T}_{\boldsymbol{n}',\boldsymbol{n}} = T\left(\frac{2\pi}{L}\boldsymbol{n}', \frac{2\pi}{L}\boldsymbol{n}; E\right), \quad \mathbb{G}_{\boldsymbol{n},\boldsymbol{n}'} = \frac{1}{L^3}\frac{1}{E - \frac{q_{\boldsymbol{n}}^2}{m_N}}\delta_{\boldsymbol{n}',\boldsymbol{n}}, \tag{1}$$

where we adopt the periodic boundary conditions and truncate the momenta at $n^2 < n_{max}^2$. If the interaction is energy-independent, one can transform the LSE into a eigenvalue problem,

$$\det\left(\mathbb{G}^{-1} - \mathbb{V}\right) = 0 \rightarrow \det\left(\mathbb{H} - E\mathbb{I}\right) = 0, \quad \text{with} \quad \mathbb{H}_{\boldsymbol{m},\boldsymbol{n}} = \frac{1}{L^3}\mathbb{V}_{\boldsymbol{m},\boldsymbol{n}} + \frac{q_{\boldsymbol{n}}^2}{m_N}\delta_{\boldsymbol{m},\boldsymbol{n}}, \tag{2}$$

where $\mathbb{H}$ is the Hamiltonian matrix. The $\mathbb{H}$ matrix can be reduced to block-diagonal ones according to the reducible representations (irreps) of the relevant point group,

$$\mathbb{H} \xrightarrow{\text{reduction}} \begin{pmatrix} \mathbb{H}_{\Gamma_i} & & \\ & \mathbb{H}_{\Gamma_j} & \\ & & \ddots \end{pmatrix}_{\text{block-diagnal}}, \quad \det\left(\mathbb{H}_\Gamma - E_\Gamma \mathbb{I}\right) = 0. \tag{3}$$

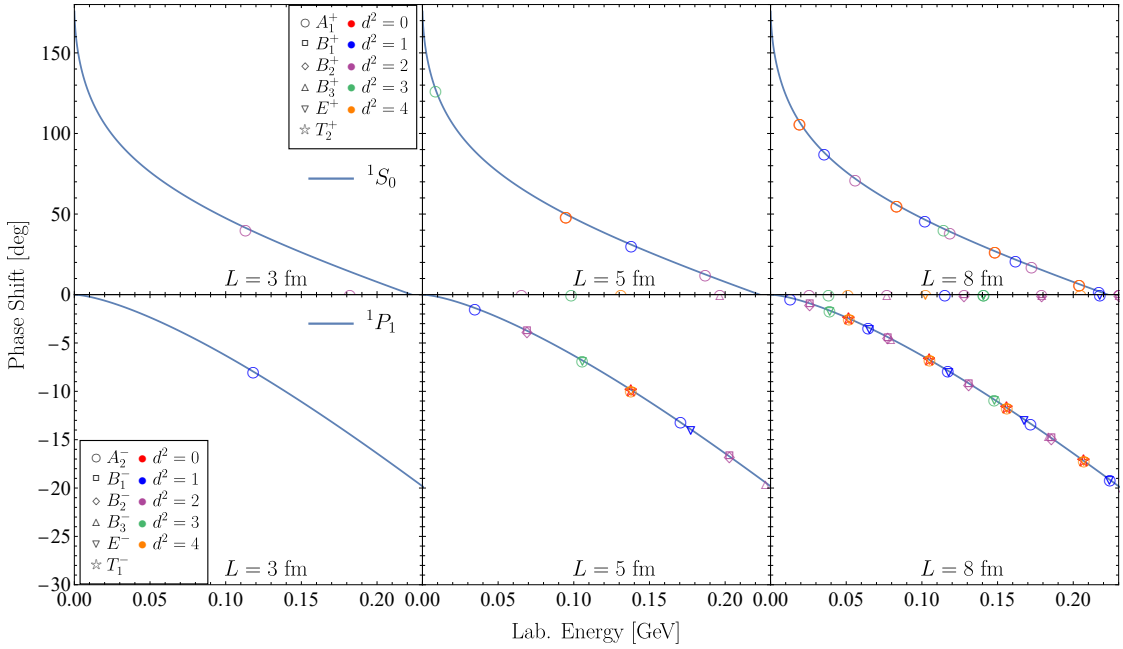

Figure 1: Upper (lower) row: Various symbols show the ^{1}S$_0$ (^{1}P$_1$) phase shifts calculated from the FV energy spectra using the single-channel Lüscher formula for the case of pionless EFT at NLO.

We final get the determinant equation with specific irrep. In the reductions, projection operator techniques [8] are used. For example, the representation space of cubic group O_h is constructed as

$$\{n_1, n_2, n_3\} \equiv \{|n_1, n_2, n_3\rangle + \text{perm. } n_1, n_2, n_3 + \text{change signs}\}. \tag{4}$$

Under such a plane wave basis, the representations is $\langle \boldsymbol{n}'|\hat{D}(g)|\boldsymbol{n}\rangle = \delta_{\boldsymbol{n}',g\boldsymbol{n}}$. We totally get seven patterns of representation space,

$$\{0,0,0\}_1, \{0,0,a\}_6, \{0,a,a\}_{12}, \{0,a,b\}_{24}, \{a,a,a\}_8, \{a,a,b\}_{24}, \{a,b,c\}_{48}, \tag{5}$$

where the subscription is the dimension of the space. We can reduce each representation space into the direct sum of the irreps of O_h group, for example, $\{0,0,a\}_6 = A_1^+ \oplus E^+ \oplus T_1^-$. For the general case with elongated box, moving systems, arbitrary spin systems, the general process is

$$\text{Symmetric group (character table)} \xrightarrow{\hat{P}^\Gamma} \text{unitary irrep matrices} \xrightarrow{\hat{P}^\Gamma_{\alpha\beta}} \text{rep. space } |p_n\rangle \to \text{irreps.}, \tag{6}$$

where $\hat{P}^\Gamma$ and $\hat{P}^\Gamma_{\alpha\beta}$ are character projection operator and projection operator, respectively.

3. Application I: spin-singlet NN scattering

The first application is nonrelativistic NN scattering. We focus on the spin-singlet systems. We first adopt contact interaction as a benchmark,

$$V^{(0)}_{\text{cont}}(\boldsymbol{p},\boldsymbol{p}') = C_S, \quad V^{(2)}_{\text{cont}}(\boldsymbol{p},\boldsymbol{p}') = C_1\boldsymbol{q}^2 + C_2\boldsymbol{k}^2, \tag{7}$$

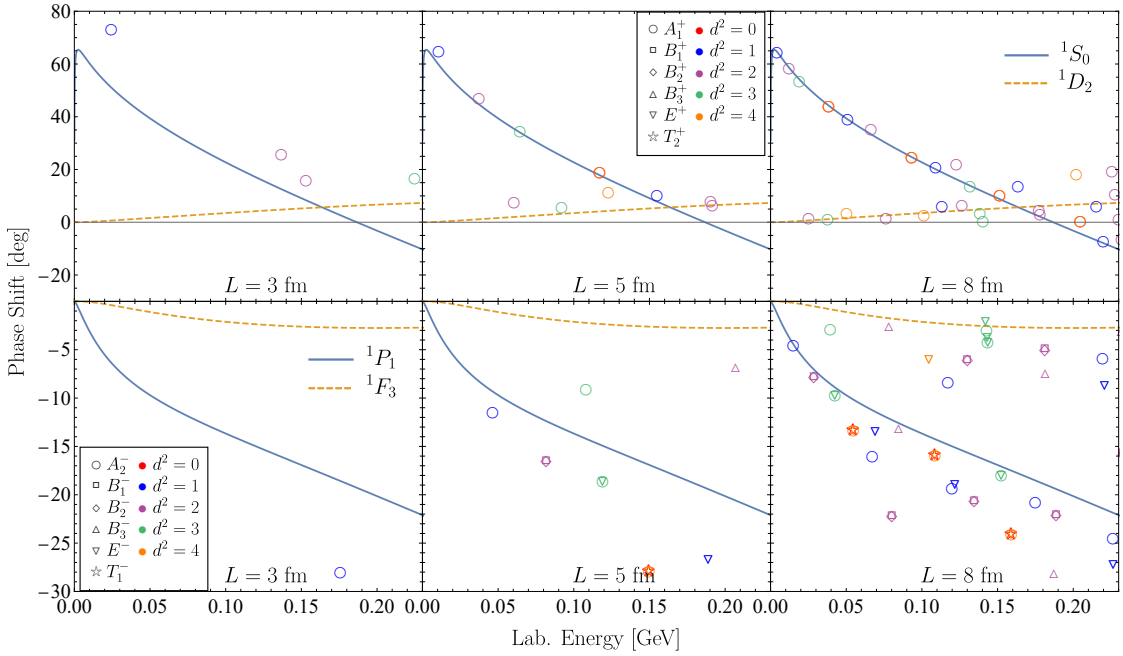

Figure 2: Upper (lower) row: Various symbols show positive-parity (negative-parity) phase shifts calculated from the FV energy spectra using the S-wave (P-wave) Lüscher formula for the chiral EFT potential at NNLO. For remaining notations see figure 1.

where the interaction only contribute to S-wave and P-wave in the infinite volume. The phase shifts are presented in the solid line in Fig. 1. We put the interaction into boxes with L =3,5,8 fm and then obtain the FV energy levels via plane wave expansion. The phase shifts corresponding to these energy levels are extracted from the Lüscher formula with the lowest partial wave. The phase shifts from one-channel Lüscher formula agree with the accurate one very well. One can notice many energy levels with vanishing phase shifts which are non-interacting D-, F- and higher partial wave states. In the plane wave expansion scheme, the high partial wave states are included naturally.

Next, we adopt a realistic NN interaction from the NNLO chiral effective field theory [9],

$$V = V_{\text{cont}}^{(0)} + V_{1\pi}^{(0)} + V_{\text{cont}}^{(2)} + V_{2\pi}^{(2)} + V_{1\pi}^{(2)} + V_{2\pi}^{(3)}. \tag{8}$$

The comparisons between plane wave expansion and Lüscher formula for parity-even and parity-odd states are presented in Figs. 2. One can see the Lüscher formula can extract the S-wave phase shift in the larger box with $L = 5$ fm well. However, the deviations of Lüscher formula for the small box $L = 3$ fm is significant. For the odd-parity states, however, increasing the box do not improve the single-channel Lüscher formula.

In order to understand the deviations, we adopt a more simple interaction, OPE interaction. Apart from the full OPE interaction, we can decompose the interaction in the partial wave basis,

$$V(\boldsymbol{p}, \boldsymbol{p}') = \sum_l \frac{2l+1}{4\pi} V_l(p, p') P_l(z), \quad V_{\text{S-wave}}(\boldsymbol{p}, \boldsymbol{p}') = (4\pi)^{-1} V_0(p, p') P_0(z), \tag{9}$$

One can choose to switch off some partial wave contributions. In above equation, we give the interaction switch off all partial wave except the S-wave part. The results for these interactions are

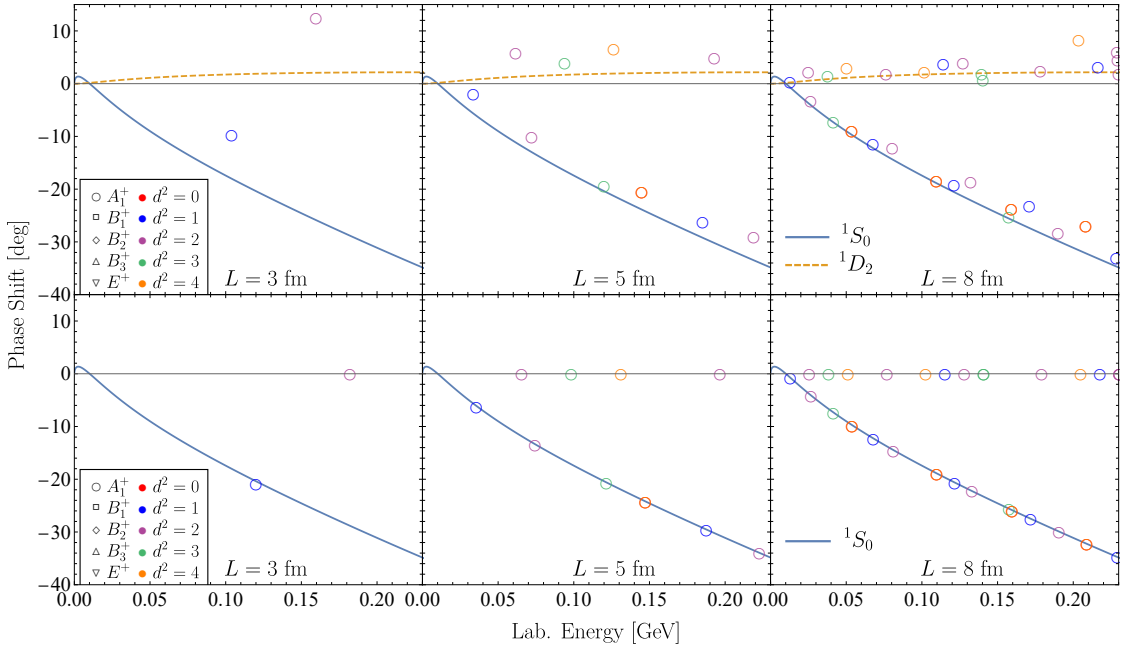

Figure 3: Phase shifts in the positive-parity channels extracted from the FV energy spectra using the S-wave Lüscher formula (various symbols) in comparison with the infinite-volume results for the OPE potential (upper row) and the S-wave projected OPE potential (lower row).

given in Figs. 3 and 4. One can see that for the full OPE interaction the deviations of Lüscher formula are qualitatively similar to the NNLO chiral interaction. Meanwhile, when the high partial wave interactions are turned off, the derivations disappear except in the smallest box. For the odd-parity state, when the P-wave and F-wave interaction are both included, the pattern in the lower sibfigure of Fig. 4 return to mess. Therefore, we can conclude that the partial wave mixing effect in FV results in the derivations of the single-channel Lüscher formula. The results are sensitive to the second lowest partial wave components, which was indicated in Ref. [10] as well.

In order to overcome the limits of Lüscher formula, we adopt an EFT-inspired approach. We first generate “synthesis" lattice QCD data through a toy model,

$$V_{\rm toy} = V_{1\pi} + V_{1h} = -\left(\frac{g_A}{2F_\pi}\right)^2 \frac{M_\pi^2}{\boldsymbol{q}^2 + M_\pi^2} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + (c_{h1} + c_{h2} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) \frac{1}{\boldsymbol{q}^2 + m_h^2}, \tag{10}$$

where $V_{1\pi}$ and V_{1h} are OPE interaction and heavy-meson exchange interaction. The mass of the heavy meson is $m_h = 0.5$ GeV. We fit the FV energy levels generate from the above interaction with an EFT interaction

$$V_{\rm EFT} = V_{\rm OPE}^{(0)} + V_{\rm cont}^{(0)} + V_{\rm cont}^{(2)} + V_{\rm cont}^{(4)} + \ldots \tag{11}$$

where $V_{\rm OPE}$ is the OPE interaction and $V_{\rm cont}^{(\alpha)}$ is the short-range interaction order by order. In the fitting, we use the determinant residual method [11] and only the ground state of each irreps as the inputs. The results are presented in Fig. 5. One can see that the fitting is improved with orders. We present the phase shift in Fig. 6. Compared with the real phase shifts, the fitting phase shifts are also improved order by order. One can see the fitting do uncover the underlying theory even in a

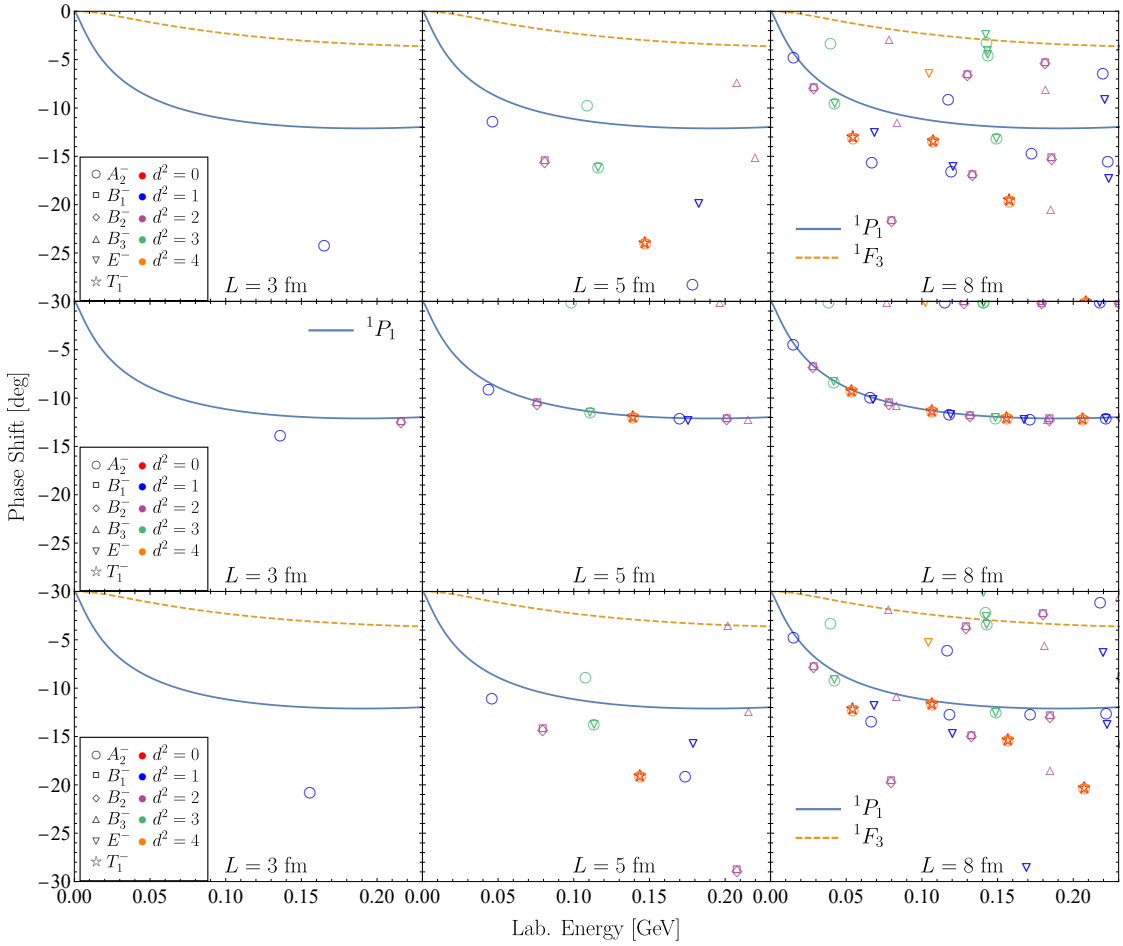

Figure 4: Phase shifts in the negative-parity channels extracted from the FV energy spectra using the P-wave Lüscher formula (various symbols) in comparison with the infinite-volume results for the OPE potential (upper row), the P-wave projected OPE potential (middle row) and the P- and F-wave projected OPE potential.

small box $L = 3$ fm. What is more important, we include some energy levels of which phase shifts from Lüscher formula derive significantly from the real ones. However, these energy levels do not prevent us from good fitting. Because we include all partial wave components.

4. Application II: ρ-channel $\pi\pi$ scattering

For the relativistic system, ρ-channel $\pi\pi$ scattering, we adopt an phenomenological interaction

$$V(\boldsymbol{p}, \boldsymbol{p}'; E) = -\frac{2\boldsymbol{p}\cdot\boldsymbol{p}'}{f^2}\left(1 + \frac{2G_V^2}{f^2}\frac{E^2}{M_0^2 - E^2}\right), \tag{12}$$

where three parameters f, G_V and M_0 can be determined by fitting experimental phase shift [12, 13] as shown in left subfigure in Fig. 7. We put the interaction into the finite box and obtain the energy levels. The phase shifts extracted from the energy levels via the Lüscher formula are given in the middle subfigure of Fig. 7. One can see Lüscher formula works very well, because the interaction in

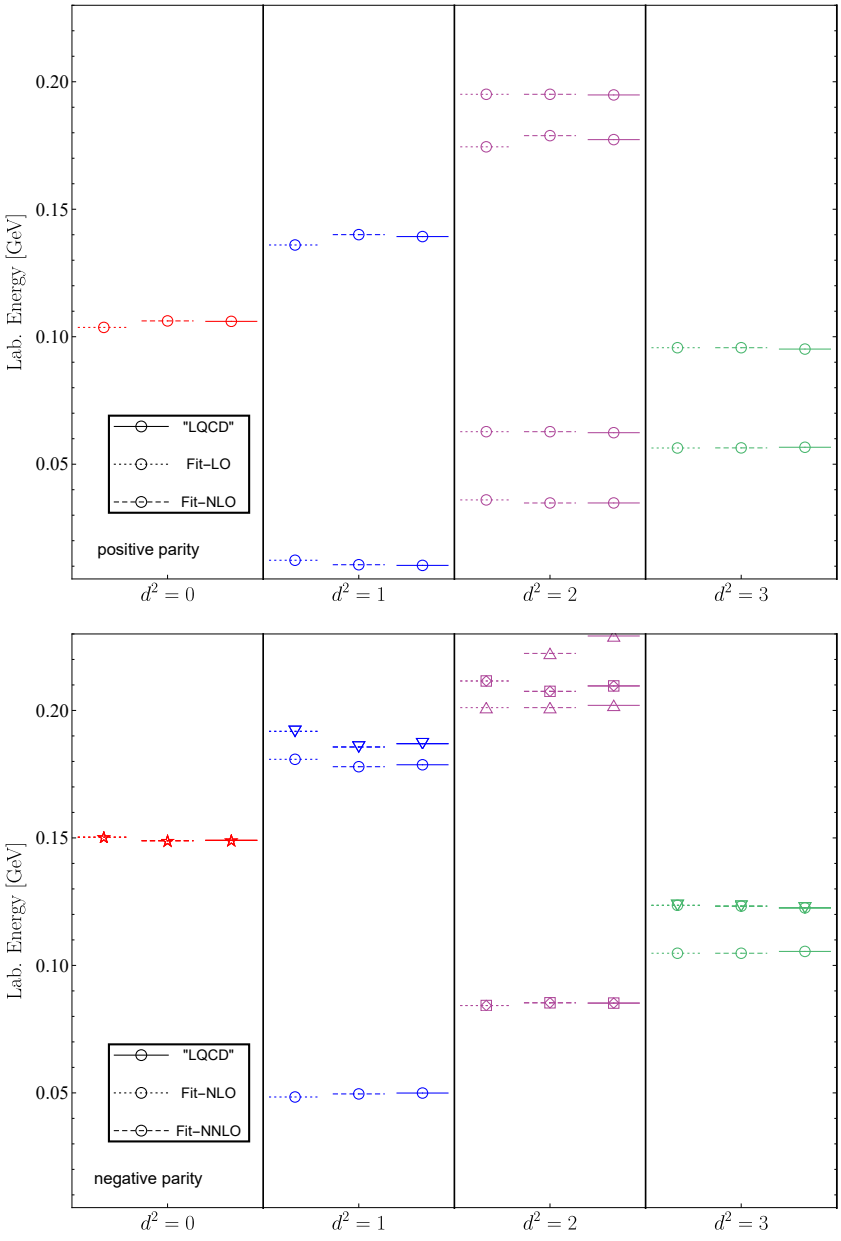

Figure 5: Comparisons of the synthetic lattice energy levels with positive (upper) and negative (lower) parity in the box with $L = 5$ fm and those from the EFT determined by fitting (see figure 1 for marker meaning).

(12) only contributes to the P-wave. Meanwhile, the lattice QCD energy levels in this channel were obtained in Ref. [14]. Thus, we use our plane wave expansion approach to determined the three parameters by lattice QCD energy levels below the $4m_\pi$ threshold. The results are presented in right subfigure of Fig. 7. One can see we could obtain the phase shift roughly. The large uncertainties can be reduced by adopting more rigorous $\pi\pi$ scattering framework.

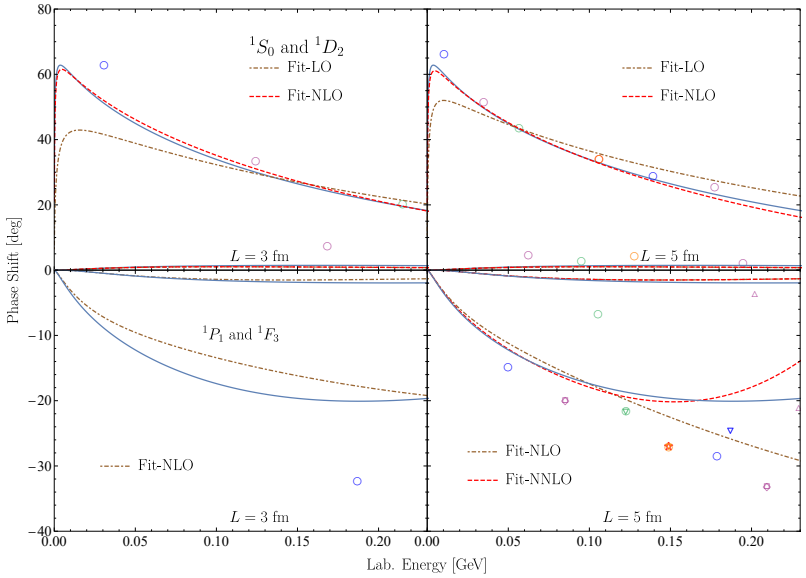

Figure 6: ^{1}S$_0$ (upper row) and ^{1}P$_1$ (lower row) phase shifts extracted by matching the EFT to the finite-volume spectra for the toy-model example in comparison with the underlying phase shifts shown by the solid blue lines.

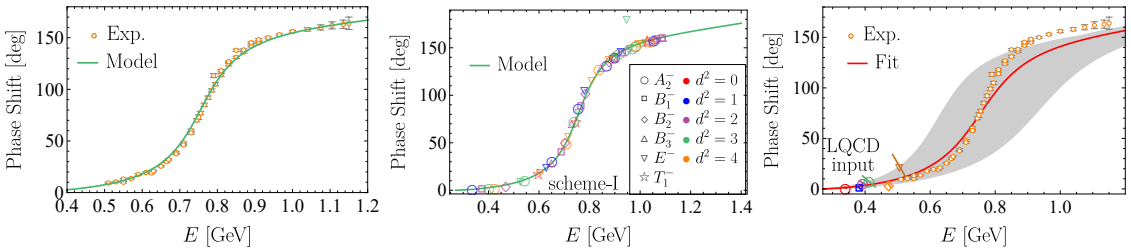

Figure 7: P-wave $\pi\pi$ phase shifts from phenomenological model [Eq. (12)] (left), Lüscher formula (middle) and fitting lattice QCD data (right).

5. Summary

In this work, we propose an alternative approache of Lüscher's formula to extract the information of the two-body interaction from the FV energy levels. We adopt the plane wave expansion rather than the partial wave expansion. Within the projection operator technique, we reduce the discrete plane wave basis into the direct sum of several irrep spaces of the corresponding discrete groups. LSE can be represented in matrix equations with fixed irreps. The FV energy levels are obtained by finding the poles of these LSEsin the FV. For the non-relativistic systems, we use the spin singlet NN systems as an example. Our results show that one can not extract reliable NN interactions by the single-channel Lüscher's formula from the lattice simulation in a small box ($L \lesssim 3$ fm) or when the partial wave mixing effect is significant ($^1P_1$ channel). We adopt a toy model to illustrate that the plane wave expansion approach can solve above problems. In this approach, we do not introduce the partial wave expansion and thus the partial wave mixing effect due to the breaking of rotational symmetry in the FV is embed naturally. Meanwhile, we do not presume the

relation of the box size and the interaction range. In fact, we include the exponential suppressed effect. Thus, such an approach could be used to the investigate the FV effect in the small box. For the relativistic system, we use the $\pi\pi$ scattering in the ρ channel as an example. We demonstrate that our approach can be used to extract the infinite interaction from the FV energy levels.

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