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The phase-shift of isospin-2 $\pi\pi$ scattering from lattice QCD

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Finite-volume lattice QCD calculations offer the possibility of extracting resonance parameters from the energy-dependent elastic phase-shift computed using the Lüscher technique. In this letter, as a trial of the method, we report on the extraction of the non-resonant phase-shift for S and D-wave $\pi\pi$ isospin-2 scattering from dynamical lattice QCD computations. We define a variational basis of operators resembling pairs of pions of definite relative momentum and extract a spectrum of excited states that maps to phase-shifts at a set of discrete scattering momenta. Computations are performed with pion masses between 400 and 520 MeV on multiple spatial volumes. We observe no significant quark mass dependence in the phase-shifts extracted which are in reasonable agreement with the available experimental data at low momentum.

a. Introduction: The hadron spectrum and interactions of QCD can be studied from first principles using numerical simulation of the quark and gluon fields on a finite lattice. While significant progress has been made in studying isolated excited meson states with $q\bar{q}$-like operators [1, 2], it remains challenging to extract properties of resonances that appear in the scattering of stable hadrons. One procedure, due to Lüscher [3], maps the discrete spectrum of eigenstates of QCD in a finite cubic volume to the phase shift for elastic scattering. By extracting multiple excited eigenstates within a given quantum number sector, one can map out the phase shift as a function of scattering momentum and, if present in that channel, observe resonant behaviour.

In this letter, we demonstrate the feasibility of the technique in a simple sector, that of $\pi\pi$ scattering in isospin-2 ($I = 2$), where the interaction is not strong enough to form a resonance, but rather is weak and repulsive. For the first time using this method, we extract the S- and D-wave phase shifts as a function of scattering momentum. This procedure is carried out independently on multiple volumes to validate the finite-volume method. We find through computations at a range of quark masses that at the level of precision attained the phase shift is largely quark mass independent.

Previous lattice QCD calculations of $\pi\pi$ scattering have limited themselves to extracting the phase shift at near-zero energy, more conveniently expressed via the scattering length [4, 5], or by performing the same calculation in a moving frame, a single phase shift point at non-zero energy [6].

In contrast, we use the "distillation" method [7] to construct both creation and annihilation operators of definite $\pi\pi$ relative momentum, and employ them to form a variational basis of composite QCD operators that resemble pairs of pions. This enables us to extract a spectrum of multiple states with $I = 2$, $\ell^P = 0^+, 2^+$ (ℓ is the partial wave and P the parity) and, using the Lüscher technique, we find the phase shift as a discrete function of the scattering momentum. This sets the groundwork for investigating resonances in other meson-meson scattering channels.

Experimentally, $\pi\pi$ $I = 2$ phase shifts have been extracted from $\pi N \to \pi\pi N'$ charge-exchange scattering reactions, treating the dominantly-exchanged pion as approximately on-shell owing to the proximity of the t-channel pole to the physical small-t region. The extant data [8–11] for $\delta_{\ell=0}$ and $\delta_{\ell=2}$ are broadly consistent in the low-energy region measured and there is little statistically significant evidence for inelasticity.

b. Finite volume analysis: Lüscher's method relates the discrete spectrum of energy levels in a finite volume to phase shifts evaluated at the scattering momenta corresponding to the extracted energy values. Complications arise from the cubic symmetry of the lattice boundary which reduces the irreducible symmetry channels from the set of all integer spins to a finite set of irreducible representations. The relevant *irreps*, Γ, for $\pi\pi$ isospin-2 scattering at low momentum are A_1^+ which contains continuum spins $\ell = 0, 4\ldots$, $T_2^+(\ell = 2, 4\ldots)$, $E^+(\ell = 2, 4\ldots)$ and $T_1^+(\ell = 4\ldots)$. Odd ℓ do not contribute due to Bose symmetry.

Once the finite volume energy levels, $E_{\pi\pi}$ are obtained from an explicit Monte-Carlo calculation on a fixed volume (L^3) lattice, the scattering momenta follow assuming a continuum-like dispersion relation, $k = \sqrt{(E_{\pi\pi}/2)^2 - m_\pi^2}$. The desired phase-shifts are embedded in an equation

$$\det\left[e^{2i\boldsymbol{\delta}(k)} - \mathbf{U}_\Gamma\left(k\tfrac{L}{2\pi}\right)\right] = 0, \qquad (1)$$

where $\mathbf{U}_\Gamma\left(k\frac{L}{2\pi}\right)$ is a matrix in the space of partial waves, ℓ, of known functions particular to this irrep, Γ, evaluated at the scattering momentum, k. $e^{2i\boldsymbol{\delta}(k)}$ is a diagonal matrix featuring phase-shifts, $\delta_\ell(k)$, for all partial waves

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contributing to the irrep Γ. The dimension of these matrices is formally infinite, since there are an infinite number of possible partial waves contributing to each irrep Γ. However, one can argue that, since higher waves typically contribute less at low momentum, one can cut-off the dimension at some low-spin and, provided the results are reasonably insensitive to this cutoff, reliably extract the phase shift for low partial waves. This is the core of the Lüscher method [3].

The aim then is to solve for some set of phase-shifts $\{\delta_\ell(k)\}$, but since Equation 1 is one equation (per energy level) in several unknowns, this will not be possible. Instead we will attempt to bound the size of all $\delta_\ell(k)$ for ℓ higher than the lowest in each irrep using other information. In practice we will assume that, in the energy region accessible to us, $\delta_{\ell>4} \approx 0$ and consider only the effect of a non-zero $\delta_4(k)$.

c. Correlator construction and variational analysis: In order to obtain the finite-volume energy spectrum, we form a matrix of correlators using a basis of $\pi\pi$ operators that is then diagonalised using the variational method [2, 12, 13]. The operators are constructed to resemble a pair of pions with total momentum zero and definite relative momentum:

$$\mathcal{O}^{\Gamma,\gamma}_{\pi\pi}(|\vec{p}|) = \sum_m \mathcal{S}^{\ell,m}_{\Gamma,\gamma} \sum_{\hat{p}} Y^m_\ell(\hat{p})\, \mathcal{O}_\pi(\vec{p})\mathcal{O}_\pi(-\vec{p}).$$

The *subduction* coefficients, $\mathcal{S}^{\ell,m}_{\Gamma,\gamma}$, project operators of definite ℓ into definite *irreps*, Γ - their explicit forms can be found in Appendix A of [2]. The sum over directions of momentum, $\hat{p}$, at a fixed magnitude is limited to those allowed by the periodic cubic boundary conditions. On a lattice with spatial extent L these are $\vec{p} = \frac{2\pi}{L}\vec{n}$ for a vector of integers $\vec{n}$.

In this first study we utilise only a simple operator capable of interpolating a pion at momentum $\vec{p}$ from the vacuum,

$$\mathcal{O}_\pi(\vec{p}) = \sum_{\vec{x}} e^{i\vec{p}\cdot\vec{x}} \left[\bar{\psi}\Box_\sigma\gamma^5\Box_\sigma\psi\right](\vec{x}),$$

where the quark fields are acted upon by a distillation smearing operator that emphasises the low momentum quark and gluon modes that dominate low mass hadrons. In this study we use $\Box_\sigma = \sum_{n=1}^{N_{\text{vecs}}} e^{\sigma^2\lambda_n/4}\xi_n\xi_n^\dagger$ where λ_n, ξ_n are the eigenvalues and eigenvectors of the gauge-covariant three-dimensional Laplacian operator (see [2, 7] for details; $\sigma = 0$ was used in [1, 2]). It is distillation that factorises the construction of correlators in such a way as to make possible the projection onto definite inter-pion momentum at both source and sink, something that is not possible in the traditional "point-all" method. Details of the distillation correlator construction can be found in [7].

Our variational basis in the irrep A_1^+ consists of operators with $|\vec{p}|^2 = \left(\frac{2\pi}{L}\right)^2 (0, 1, \ldots 4)$ each with two smearing radii $\sigma = 0.0, 4.0$, giving a ten dimensional basis. For E^+ we have $|\vec{p}|^2 = \left(\frac{2\pi}{L}\right)^2 (1, 2, 4)$ and two smearings and T_2^+ with $|\vec{p}|^2 = \left(\frac{2\pi}{L}\right)^2 (2, 3)$ and two smearings. The T_1^+ irrep has lowest spin $\ell = 4$ for two pions. However the lowest momentum from which a T_1^+ operator can be constructed is $|\vec{p}|^2 = 5\left(\frac{2\pi}{L}\right)^2$ and this is the only one we used. With these operators at source and sink, we form all correlators using Wick contractions relevant for $I = 2$.

m_π/MeV	$(L/a_s)^3 \times (T/a_t)$	N_{cfgs}	$N_{\text{t}_{\text{srcs}}}$	N_{vecs}
524	$16^3 \times 128$	496	4	64
	$20^3 \times 128$	377	4	96
444	$16^3 \times 128$	605	5	64
	$20^3 \times 128$	321	3	128
396	$16^3 \times 128$	439	16	64
	$20^3 \times 128$	535	3	128
	$24^3 \times 128$	548	4	162

TABLE I: Lattices used in this study. N_{vecs} indicates the number of eigenvectors of the laplacian used in the distillation method.

Computations are performed on anisotropic lattices with three dynamical flavors of Clover fermions with spatial lattice spacing $a_s \sim 0.12\,\text{fm}$ and finer temporal spacing, $a_t^{-1} \sim 5.6\,\text{GeV}$, see Table I and [14]. A precise measure of the anisotropy, $\xi = a_s/a_t$, is required to determine the spatial length of the lattice in temporal lattice units, $L/a_t = \xi L/a_s$. Fitting single-pion correlators at finite momentum, $a_s\vec{p} = \frac{2\pi}{L/a_s}\vec{n}$, determines $a_t E_\pi(|\vec{n}|)$ and ξ follows from fitting the dispersion relation

$$\left(a_t E_\pi(|\vec{n}|)\right)^2 = (a_t m_\pi)^2 + \tfrac{1}{\xi^2}\left(\tfrac{2\pi}{L/a_s}\right)^2 |\vec{n}|^2,$$

for multiple values of $|\vec{n}|$ and L/a_s. Explicitly we find $\xi = 3.459(4), 3.454(5), 3.459(3)$ on respectively the $m_\pi = 396, 444, 524$ MeV lattices, showing the lack of quark mass dependence observed previously and utilised in the dynamical tuning of the lattice action[15]. Mass-dimension quantities multiplied by the temporal lattice spacing, a_t, are scale-set using the procedure outlined in [2], using the Ω-baryon mass determined on the same lattice, $m = \frac{a_t m}{a_t m_\Omega} \cdot m_\Omega^{\text{phys.}}$. The continuum scaling of the results is not investigated in this calculation at a single lattice spacing.

In Figure 1 we show the finite-volume spectra obtained with $m_\pi = 396\,\text{MeV}$ and $L/a_s = 16, 20, 24$. We clearly observe shifts relative to the energy of two non-interacting pions with back-to-back momentum of $\vec{p} = \frac{2\pi}{L}\vec{n}$, $E_{\pi\pi} = 2\sqrt{m_\pi^2 + |\vec{p}|^2}$. It is this energy shift that Lüscher's method relates to the scattering phase shift through Equation 1. It is the fact that we are able to resolve excited energy levels with a statistical precision below 1% that makes possible an extraction of the scattering phase shift as a function of scattering momentum.

d. Phase shift: For each $\pi\pi$ energy level in each irrep in Figure 1 we can set up an Equation 1 to be solved

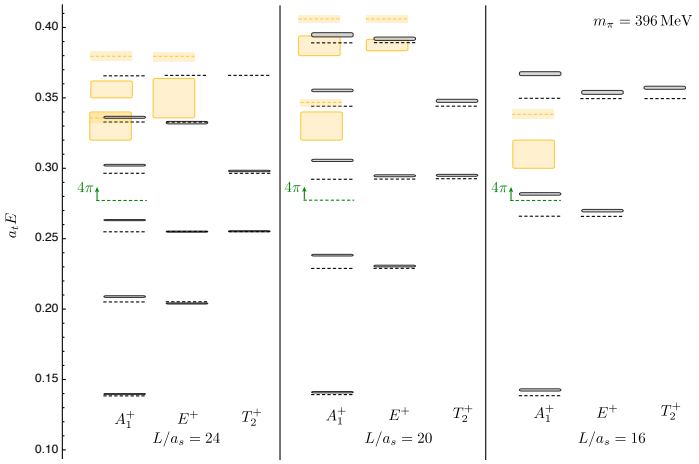

FIG. 1: Low-lying spectrum, in units of the temporal lattice spacing, of finite volume states in irreps A_1^+, E^+, T_2^+ at $m_\pi = 396\,\mathrm{MeV}$ for $L/a_s = 16, 20, 24$. The box height indicates the statistical uncertainty on the energy. Orange boxes correspond to states suspected of being $\pi\pi^\star$ scattering states. Dashed lines indicate the non-interacting energy of pion pairs with the allowed lattice momenta between them.

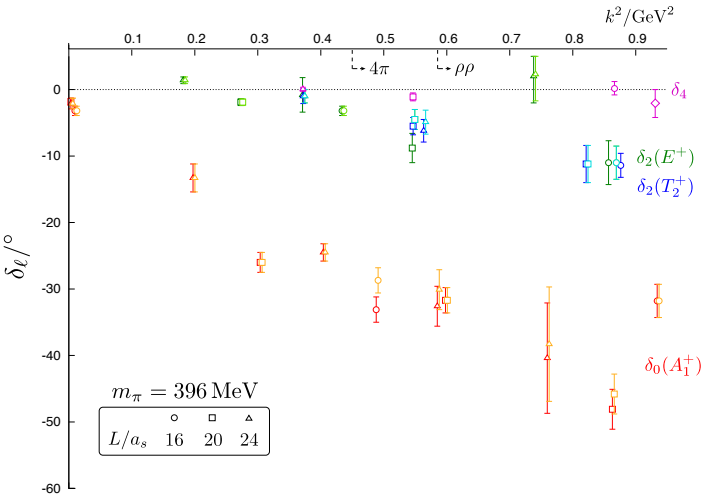

FIG. 2: Phase-shifts extracted from spectra with $m_\pi = 396\,\mathrm{MeV}$. Red (A_1^+), green (E^+), blue (T_2^+) colored points assume $\delta_4 = 0$; orange (A_1^+), light green (E^+), cyan (T_2^+) colored points (shifted slightly to the right) used estimated δ_4 as described in the text: note that the corrected δ_2 values from E^+, T_2^+ coincide by construction at momenta near $|\vec{p}|^2 = 2 \cdot \left(\frac{2\pi}{L}\right)^2$. Estimated δ_4 shown by pink points. Also indicated are the positions of inelastic thresholds into 4π and $\rho\rho$.

for the phase shifts, δ_ℓ. The simplest way to solve these equations is to neglect the contribution of $\ell \geq 4$ to obtain δ_0 from A_1^+ and δ_2 from T_2^+ or E^+. Doing so gives the red, green and blue colored points in Figure 2. The small discrepancies between E^+ and T_2^+ extractions of δ_2 at $k^2 \sim 0.35, 0.55, 0.85\,\mathrm{GeV}^2$ (corresponding to the levels at $a_t E \sim 0.25, 0.29, 0.36$ in Figure 1), have a possible origin in the neglect of a non-negligible value of δ_4. We can estimate the size of this δ_4 by solving the coupled system of Equations 1 for T_2^+ and E^+ at the relevant energy for the two unknowns, δ_2, δ_4. The values of δ_4 so extracted are shown by the pink points in Figure 2.

For a direct estimate of δ_4 from T_1^+, only the $L/a_s = 24$ lattice has a point within our plotted range of scattering momentum. The extracted point is shown by the pink diamond in Figure 2, and is in good agreement with the other estimates, showing that $|\delta_4|$ is less than 2° over the whole of the explored momentum range.

With an estimated magnitude of $\delta_4(k)$ in hand (from interpolation between the determined points), we can solve Equation 1 including the effect of the $\ell = 4$ wave. This gives rise to the orange, light green and cyan colored points in Figure 2 which are seen to differ relatively little from the points with δ_4 assumed to be zero. For final presentation we enlarge the errorbar to include the effect of the estimated δ_4 giving rise to asymmetric errorbars in Figure 3.

As indicated in Figure 2, the 4π threshold opens within the energy range of our extracted phase-shifts and technically for energies above this the formalism leading to Equation 1 is not rigorously correct. On the other hand, there is relatively little evidence experimentally for considerable inelasticity in the $\pi\pi$ isospin-2 channel in the energy range so-far probed - what little data there is does not show statistically significant deviation from an elastic approximation [9, 10]. As an initial approximation, we shall assume that the inelasticity is negligible and continue to use Equation 1 above the inelastic threshold. The $\ell = 2$ phase-shift extracted from E^+, T_2^+ irreps should be less sensitive to any inelasticity since the effective threshold in finite-volume is higher as it requires at least one unit of relative momentum in the 4π system. Future calculations should test the elasticity assumption by computing correlators using operators that resemble four pions projected into isospin-2 in the appropriate partial waves.

e. Results: In Figure 3 we show our results for S and D-wave phase shifts, at a range of pion masses, along with experimental data taken from [8–11]. We observe reasonable agreement with the experimental data at lower scattering momenta, where the scattering is purely elastic, for all the pion masses computed. This suggests that it is possible that the phase-shift is only mildly dependent upon pion mass. Of course, one requires lattice computations at smaller pion masses to verify that the agreement with experiment continues.

Using only $\pi\pi$ and π correlators at zero momentum we can perform the extraction of the scattering length using the methodology of [4, 5]. The scattering lengths so obtained are shown in Figure 4, where they are seen to be in reasonable agreement with the precision data of [4], computed on a lattice of similar spatial lattice spacing.

We can also obtain estimates for the scattering length and effective range by fitting the k dependence of $\delta_0(k)$, where we find that scattering lengths largely agree with

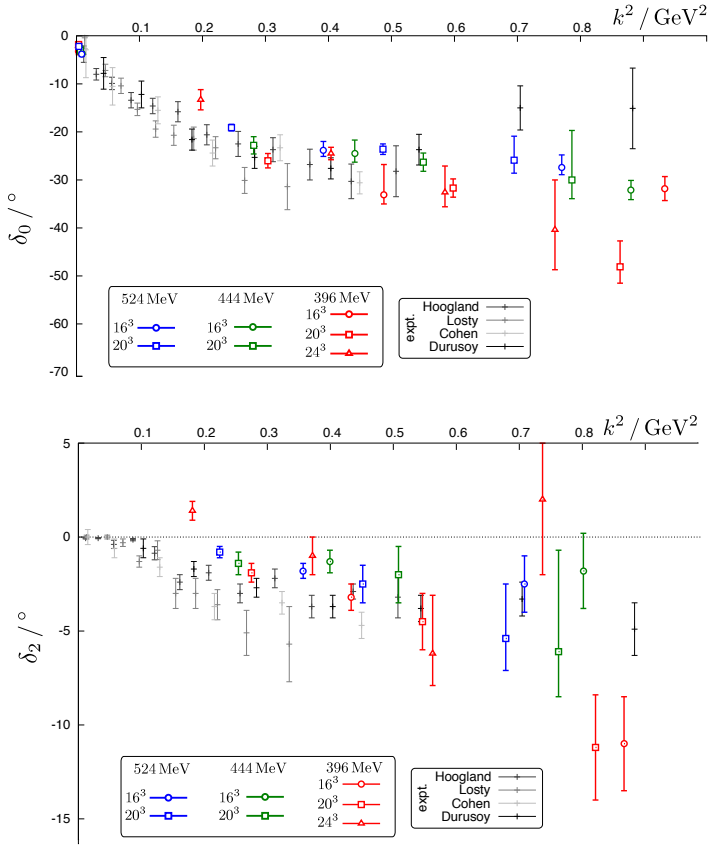

FIG. 3: Phase-shift in degrees for $\pi\pi$ $I = 2$ scattering with $\ell = 0(\delta_0)$ and $\ell = 2(\delta_2)$. Lattice results at various pion masses and volumes. Experimental data from [8–11].

the estimates from the simple method above, while the effective range is small but only poorly determined.

f. Summary and prospects: We have demonstrated the feasibility of an explicit application of the Lüscher finite-volume framework in dynamical lattice QCD. Using multiple excited state energy levels extracted in a single volume, we have determined the S- and D-wave $\pi\pi$ isospin-2 phase shifts as a function of scattering momentum. Multiple volumes are then used for validation and estimation of the effect of neglected higher partial waves. We estimate that $|\delta_4| \lesssim 2°$ for $k < 1\,\mathrm{GeV}$.

We observe no significant pion mass dependence in the phase shift below $k \sim 1\,\mathrm{GeV}$, with results for $m_\pi \gtrsim 400\,\mathrm{MeV}$ being in reasonable agreement with experimental data at low scattering momentum. For *precision* coverage of experimentally relevant kinematics, we would require still larger volumes to sample points at smaller scattering momentum in the elastic region.

This calculation sets the groundwork for an investigation of the resonances in meson-meson scattering that arise from the strong interaction. Inclusion of quark annihilation diagrams in the calculation of correlators [17] will enable the $I = 1$ $\pi\pi$ sector to be studied, where one expects to see the ρ resonance appearing as a rapidly rising phase shift. Some attempts in this direction have been made [18–20], but using only a small basis of operators and subsequently extracting a very limited number of phase-shift points. *Distillation* and stochastic variants [7, 21, 22] will allow us to efficiently construct a large basis and thus map out many points on the phase-shift curve. In future work, we will explore a range of different scattering hadrons in various partial-waves.

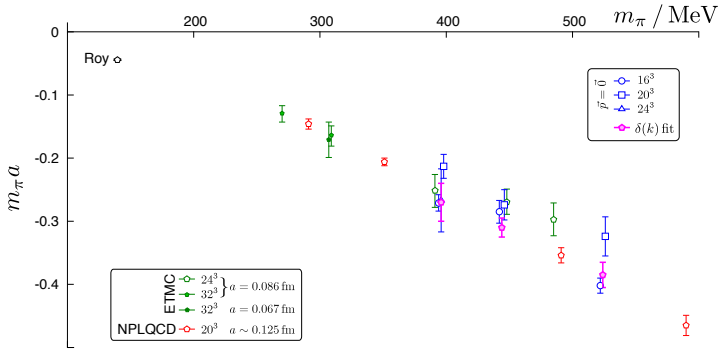

FIG. 4: S-wave scattering length. Blue points from $\vec{p} = \vec{0}$ correlators, pink points from effective range fits to $\delta(k)$. Comparison to lattice results of [4, 5] and Roy equations analysis of experimental data [16].

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