Determining values for parameters of Chiral Perturbation Theory using lattice QCD

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***Abstract*— This paper presents values of parameters for Unitarized SU (3) Chiral Perturbation Theory (ChPT) that are found using lattice QCD (LQCD). The phase shifts for Pi-Pi scattering at a range of energies and at an unphysically high quark mass are fitted to the ChPT model using the *Minuit* software package. This was done for a state with isospin and angular momentum of 1. Once values for these parameters are obtained, the model (at the physical quark mass) is compared with experimental data.**

***Index Terms*—Chiral Perturbation Theory, lattice QCD, Unitarized, and Parameters**

I. Introduction

UNITARIZED Chiral Perturbation Theory has only recently started to become a full working theory in Nuclear Physics. This is in part due to the advances in modern computational speeds and capacities. This is one reason for the use of LQCD as a means of finding the phase shifts at specific energies. In the past LQCD wouldn't have been as effective due to the computational needs. ChPT is a great tool for the prediction of π, K, and η meson-meson scatterings. However, it is not yet complete because there are 8 constants whose values have not been found completely.

Finding the values of these constants has been attempted by some, but not with the use of LQCD. It previously has been done using experimental data at different energy levels and was fitted to the model in order to find the values of the parameters. This has been successful to within some accuracy. However, by using experimental data, ChPT will no longer be purely a theoretical prediction of reality. With the use of LQCD, by performing seemingly the same idea of fitting the model to these values of the phase shift at different energies, we will find the values for the parameters. This will maintain a completely theoretical prediction of meson-meson interaction. The type of meson-meson interaction used for the fitting is Pi-Pi scattering at a specific isospin and angular momentum channel of (I,J)=(1,1). This specific type and channel is used due to the simplicity of the model that describes this interaction. However, this could be expanded to other types of meson-meson scatterings.

II. Background Theory

This research is based on the interaction of the Pi mesons (Pions). There are three types of Pions (π^+, π^0, π^-). All three are composed of two quarks that are $u\bar{d}(\pi^+), u\bar{u}\ or\ d\bar{d}(\pi^0)$, and $d\bar{u}(\pi^-)$. Even though these particles were not discovered until 1947, they were theorized in 1935. They are the lightest of mesons with masses of about 140 MeV. The attractive force between these particles is the strong force. [1]

The strong force is one of the four fundamental interactions of nature among electromagnetism, the weak force and gravity. This force is appropriately named since it is the most attractive force in nature being 10^{38} times more attractive than gravity. However, it is rarely seen in everyday life because its affective range is small. The strong force is described in quantum field theory by Quantum Chromodynamics (QCD). In QCD, the electric charge analog is referred to as color. For this reason, the naming of QCD includes "chromo", which is close to the Greek word for color. [1]

The direct use of QCD has proven to be impossible due to the equations not being analytically solvable. This is the reason for the use of LQCD in describing the interactions caused by the strong force. The lattice approach to QCD takes the points of space and time to discrete values. This and the use of a supercomputer allow us to make close approximations of interactions such as the phase shift.

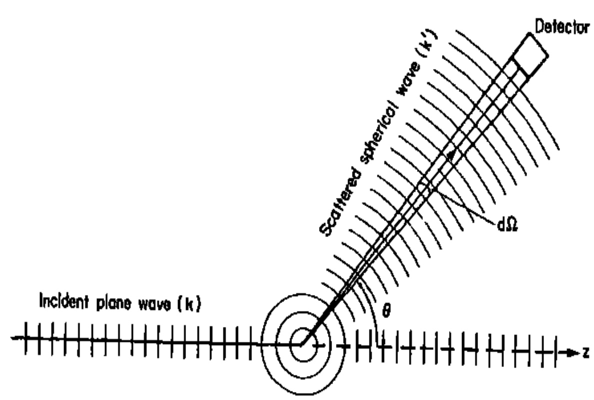

Fig. 1. A sketch of scattering waves taken from [1]

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The phase shift of a meson-meson interaction is the difference in the phase of a wave for a meson as it is entering and leaving a region of interaction. This is described in detailed by LQCD and gives insight into the interaction of the scattering. The phase shift can tell if the interaction was attractive or repulsive as well as being able to find the strength, range, and scattering length. [2] This can be seen through experiments and is used for the data that was fitted for this paper.

LQCD can give values for the phase shift at specific energies. However, since it takes a super computer to find the values, ChPT is faster and thus a more applicable tool for the prediction of interactions. This is another reason to find the values for ChPT considering it gives a model to describe the phase shifts for the lightest meson scattering.

III. Finite Volume Quantization Condition

In freshman quantum the particle in a square well situation is studied extensively. This is because it is one of the simplest cases in which quantized energy levels began to show up. The results of this can be described with a nice analytic formula and the wave function is a solution to the one-dimensional time independent Schrödinger equation. [3]

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V_0\psi(x)=E\psi(x) \qquad (1)$$

The case of two particles in a 3D-square well that interact with each other through the strong force, is just a complicated version of the freshman quantum problem described above. However, this problem will require graduate level quantum to describe, such as this form of the Schrödinger equation. [2]

$$\nabla^2\psi(r,\theta,\phi)+\frac{m}{\hbar^2}\big(E-V(r)\big)\psi(r,\theta,\phi)=0 \qquad (2)$$

Where $\psi(r,\theta,\phi)$ is now a 2-particle wave function, r is the relative coordinate, and $V(r)$ is the potential energy describing the interaction. This is the form for two particles in their center of mass reference frame. The data used for this paper is extended to other reference frames thus showing that this Schrödinger equation will not suffice for all meson- meson interactions. Meson-meson scattering is quantized like the 1D problem, when applied in a finite volume.

In the 1D free case, the quantized energy levels are given by:

$$E_n=\frac{h^2n^2}{8mL^2} \qquad n=1,2,3\ldots \qquad (3)$$

Where this result depends on the box length and has a quantum number of n. In the case of Pi-Pi scattering,

$$\sqrt{EM_\pi}\cot(\delta)=\sqrt{\frac{4}{\pi L^2}}Z\left(E\left(\frac{L^2M_\pi}{2\pi}\right),\vec{d},M_1,M_2,l,m,L\right) \qquad (4)$$

Lusher's equation is the general form of (3) and was derived by the famous paper [4]. The quantum numbers used for this equation are seen as variables for the Z-Function. The Z-Function that is used in Lusher's equation is more use full than the functions used previously. The Z-function is defined in the appendix and can be seen in the work of [5]. The reason why the Z-function is more useful is because it isn't limited by which reference frame is used, it can uses relativistic calculations, and is used for a larger range of interactions.

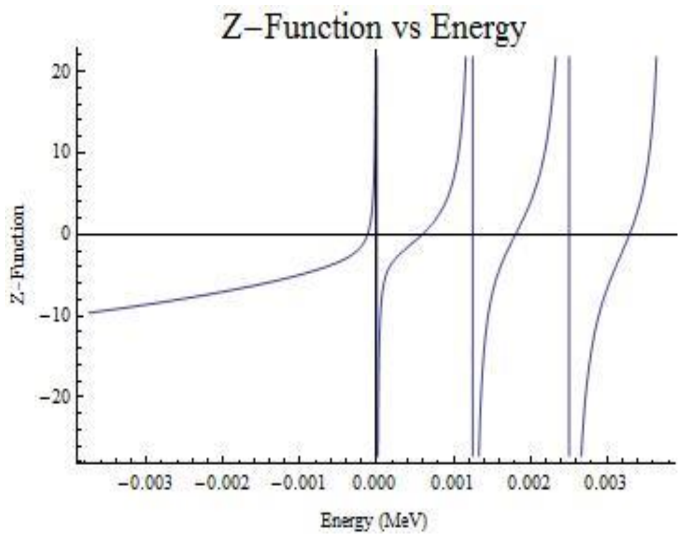

Fig. 2. The Z-Function plotted against energy to see the points that are analogous to quantized states.

This gives the ground work for determining the phase shift at a given energy level, that the LQCD was based on. However, the actual calculations of the energies required path integration of all possible paths that particles can take given the use of a Monte Carlo program. The work done for this project did not go into detailed on this but is only concern with the data that it gives. The LQCD calculations was performed by [6]. This data gives a small set of phase shifts vs energies and we hope to use a larger set of data in the future. The larger set of data has already been calculated by the super computer of Jefferson Laboratory, so we are just waiting on access.

IV. Model from ChPT

The model used for our specific case of Pi-Pi scattering on the (I,J)=(1,1) channel was derived in [7] where they gave a full description of ChPT for different types of scattering at a number of channels. The model that we want is a function that gives the phase shift and only depends on the energy and parameters that we are looking for. This is because the data from LQCD will be given in terms of energy and phase shifts. The first thing to do is to define the T-matrix since it can be related to the phase shift. For this case, the T-matrix simplifies down to a single equation.

We will need the amplitude function for our scattering case in order to arrive at the T-matrix. Looking at [7] we find that, for our case, the amplitude function is:

$$T_a(s,t,u) = T_{lo}(s) + T_{nlo}(s,t,u) \quad (5)$$
$$= T_{lo}(s) + A + B\alpha_1 + C\alpha_2 + D\alpha_3 + E\alpha_4$$

In this function, s, t, u, A, B, C, D, E, T_{lo} and the parameters $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ are defined in the appendix. The parameters have been combined in order to make this process easier, but they will only give a linear combination of the actual parameters that ChPT is needing. Also, it is important to realize that this function is broken up into two parts where T_{lo} and T_{nlo} refer to the leading order and the next to leading order. Since the T-matrix is defined in terms of these two, this is important to break the amplitude up into these separate parts. This is the general amplitude function for Pi-Pi scattering and we will need the amplitude for the specific channel that we are working at.

$$T^1(s,t,u) = T_a(t,s,u) - T_a(u,t,s) \quad (6)$$
$$= \left(T_{lo}(t) - T_{lo}(u)\right) + \left(T_{nlo}(t,s,u) - T_{nlo}(u,t,s)\right)$$
$$= T_{lo}^1 + T_{nlo}^1$$

This is now the amplitude that will need to be integrated over all possible scattering angles in order to find the total projection of this channel on the amplitude. It is easier to integrate the amplitude for the leading order and the next to leading order separately for reasons that will become apparent when the T-matrix if finally defined. These total projections of the amplitudes will be defined the same way that [7] defined them in order to distinguish the integrated leading order terms and next to leading order terms from the ones that are not integrated.

$$T_2 = \frac{1}{64\pi}\int_{-1}^{1} x\, T_{lo}^1\, dx \quad (7)$$

$$T_4 = \frac{1}{64\pi}\int_{-1}^{1} x\, T_{nlo}^1 dx \quad (8)$$

Now we have the appropriate amplitude for our specific meson-meson scattering and we are now ready to define the T-matrix in order to relate it to the phase shift. The T-matrix for our case is defined as the following.

$$T = \frac{(T_2)^2}{T_2 - Re(T_4) - i\sigma(T_2)^2} \quad (9)$$

The σ is defined in the appendix.

Now that we have the T-matrix, we can finally relate it to the S-matrix which, because of its unitarity and the simplicity of our interaction, is defined as the following,

$$S = 1 + 2i\sigma T \quad (10)$$
$$= e^{2i\delta} \quad (11)$$

where δ is the phase shift. After some simplification we can relate δ to the T-matrix as such.

$$\delta(E,\alpha_1,\alpha_2) = \frac{90}{\pi}\tan^{-1}\left[\frac{2\sigma(T_2)^2(T_2 - A - B\alpha_1 - C\alpha_2)}{(T_2 - A - B\alpha_1 - C\alpha_2)^2 - \sigma^2(T_2)^4}\right] \quad (12)$$

This function gives us the model that we will use to perform the least squared fit in order to find the values of the parameters. For the channel (I,J)=(1,1), only two of the parameters are used in the phase shift function because the other two cancel out. However, for the (I,J)=(2,0) channel, the last two parameters do not cancel out. It should also be noted that 180/π had to be multiplied in order for the output to be in degrees. Also, due to the definition of the output for inverse tangent, all negative angles had to have 180 degrees added to them in order for the appropriate angle to be achieved.

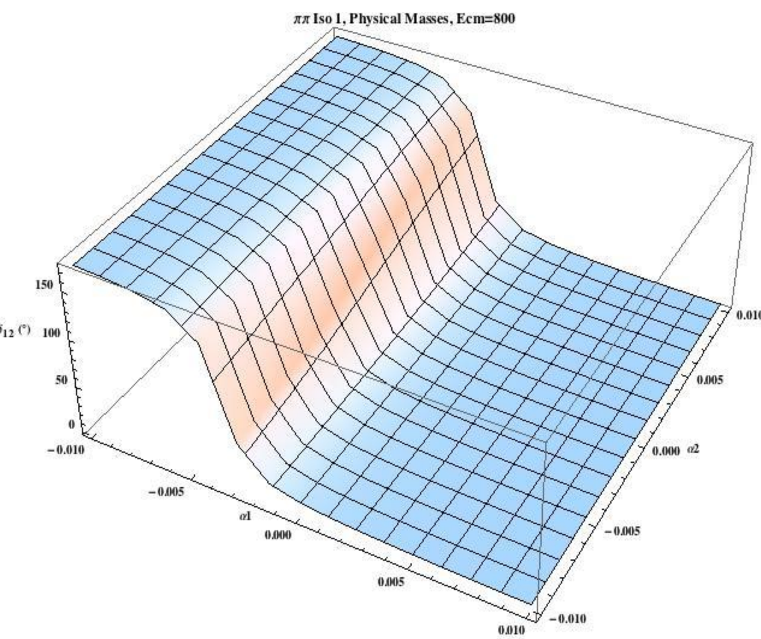

Fig. 3. Phase shifts at 800 MeV, with the parameters as variables.

When looking at the figure above in comparison for the expected values of the phase shift at this specific energy, there seems to be a region in which there is a set of parameters that will give the appropriate answer. This is curious since it implies that the set of parameters that will work is larger than expected. With this in mind perhaps the fitting will give better results than looking at this plot.

V. Fitting

After defining how the model and LQCD can be related by the phase shift and the energy, the next step is to use the points from the LQCD calculations to fit the model. This process was done with the use of *Minuit* which is a computer program that has been used for years as one of the most reliable fitting programs and was developed by CERN. The exact technique that was used is called a least squared fit and is well defined. With the use of the manual [8], the coding for this part of the project proves to be the fastest part after learning the language for *Minuit*. This allows for the coding of equation (12) to be used as the fit function for *Minuit*.

Once the fit function is defined then the chi squared function is defined. The chi squared function gives a value for how well the model and the data "fit" together. It is always a matter of finding the lowest value for chi squared, since this means a good fit was achieved. For our project chi squared was on the order of about 10 which is not great but gives decent results. The chi squared function is defined as follows.

$$\chi^2 = \sum_i \frac{\left(\delta_{i_{data}} - \delta_{i_{fit\,function}}\right)^2}{\sigma^2_{i_{\delta_{data}}} + \sigma^2_{i_{\delta_{fit\,function}}}} \tag{13}$$

The first data set has only 31 data points in it. Because of this, using the error on the energy as a range, the one data set was turned into 100 different sets of data points. The sets all had 31 points in them and were all within one sigma of the original data set. After running all 100 data sets, the values for the parameters and chi squared function were all averaged. The average values are what are reported as the values for the parameters. The error is the standard deviation of all 100 parameter values.

The second data set has less data points in it because the higher energy points are omitted. This is done in hopes of finding better parameter values because once the energy gets to a point, then ChPT no longer is a good model for the interactions of mesons. This data set has about 23 data points and just like the first set, we are using the error on the energy to create another 100 data sets. The values for the parameters, chi squared function, and errors are all found the same as before. Below are the results of the project compared to previously published results where they used experimental data to perform a fit. [7]

	$\alpha_1(10^{-3})$	$\alpha_2(10^{-3})$	χ^2	$\sigma_{\alpha_1}(10^{-4})$	$\sigma_{\alpha_2}(10^{-4})$
Data1	−3.74866	−1.62508	11.1412	3.68337	9.18696
Data2	−1.99217	2.66938	6.22726	3.83385	9.39679
Pub. values	-2.88	0.68	Not pub.	2.4	4.8

Fig. 4. Values for the two parameters, chi squared, and the errors for each of the data sets/previously published [7].

The fits for the data could change depending on the step size used in Minuit, but after running multiple times at different step sizes, the values started to converge to the numbers presented above. It does seem that there are a set of parameters that could minimize chi squared implying some sort of linear relationship between the two parameters.

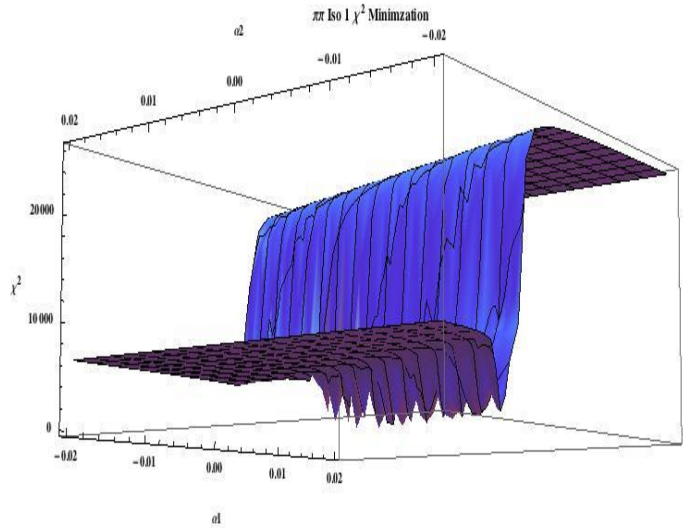

Fig. 5. The chi square function ploted at different values for the parameters in order to see the lowest point.

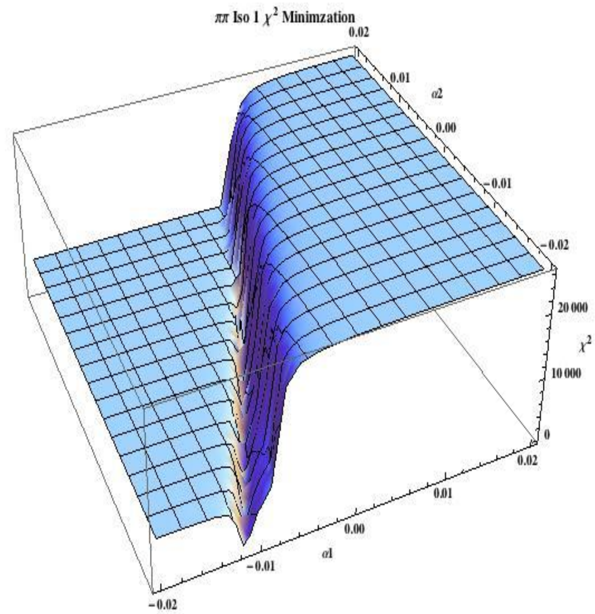

Fig. 6. The same plot as the fig above but at a differnet angle to see the length of the vally.

It can be seen in the 3D plots above that there seems to be this vally where the lowest point for chi squard doesn't change much for differnet parameter values. This is problimatic because this techinic for finding the best parameter values depends on finding the lowest value for chi squard. This could be one reason why our values for the parameters differ from the ones published in the past, and again reach the same conclusion as the one mention when looking at Fig. 3.

VI. Experiment Comparison

After finding values for the parameters the next thing to do was to graph the final model against experimental data in order to see how well it fits to reality. The experimental values for the phase shift at these energies had been done before by [9]. The first thing to do was to take the unphysical masses for the Pions and replace them with the actual values for our universe. The values for the parameters should be the same due to the fact that the parameters are independent of the mass size. They are just values consistent with the type of scattering caused by the strong force.

The first graph of the model using the parameters as variables showed promise in that the model could accurately predict values for the phase shift. This showed that the values for the parameters when found will yield a prediction that is within one or two sigmas away of experimental results. When using the values from the first data set and graphing the model against experimental data this is the result.

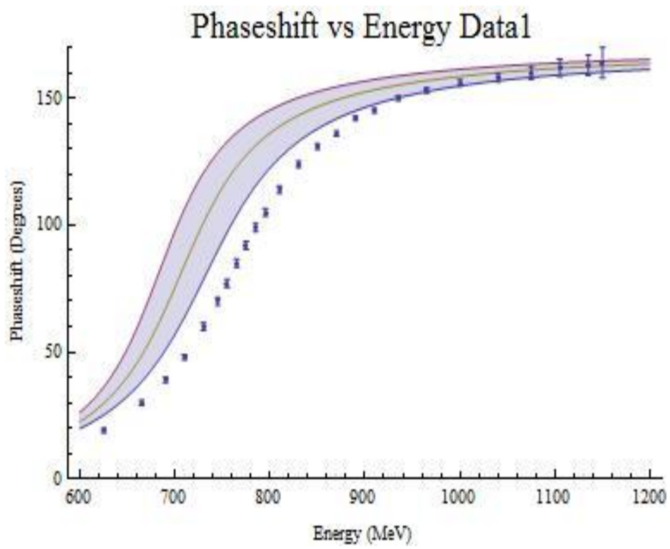

Fig. 7. Plot of the phase shift using the parameters found by the first data set and the experimental data set [9].

The middle line is the actual model at these parameters and the band is due to the uncertainty in the parameter values. The points are the experimental values for the phase shift at the given energies with the appropriate error bars. It can be seen that the model is an over prediction of the experimental data. However, the experimental values are within two sigma of the prediction which shows promise for this approach to find the parameter values. It might be that the code for the Minuit program needs to be set at different step sizes or use less of the higher energy values.

When taking into account for the higher energy values, the second data set is more truncated toward the lower energies in hopes that it would fit better with energies ranging from 600-1000 MeV. The second data set was done with a let's see what would happen type of approach since the first data set was a good fit to the higher energy values rather than the lower ones. The results of this idea are plotted in the next graph.

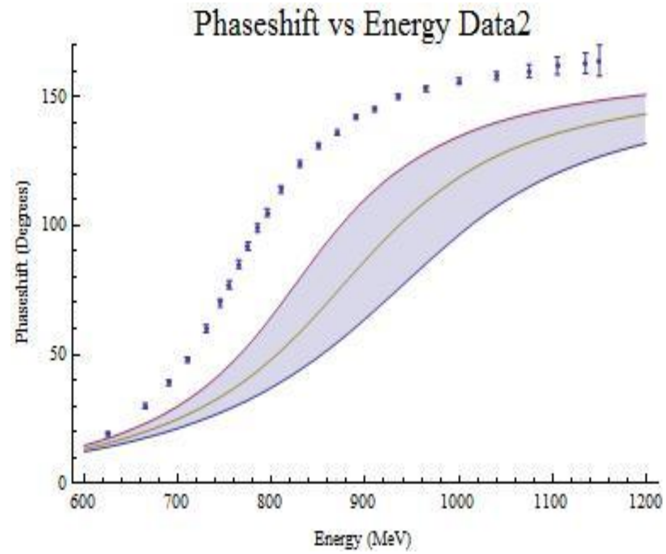

Fig. 8. Plot of the phase shift using the parameters found by the second data set and the experimental data set [9].

Unlike the first data set this data set was a under prediction of the experimental data. This result is somewhat unexpected due to that fact that the error band is larger. The experimental values are within two sigmas of the prediction still but the reason why this isn't a good fit to the lower energies is still a mystery. If given more time to evaluate this data set the next logical step would be to add back some of the higher energy values in hopes that there will be a middle ground of the over/under predictions of the two fits.

VII. Conclusion

After looking at the values for the parameters that are found one things remains certain, that there is a set of parameters that will fit the data at this channel. If given more time with this data set better values for the parameters would have been found, or at the least the range of parameters that minimize chi squared would have been mapped out. Perhaps trying to find the fit with just the (1,1) channel is too broad of a task, but running the fit at multiple channels could narrow down the parameters needed. The isospin 2 or (2,0) channel is also another easily defined function for ChPT and could prove to be what is needed. The LQCD calculations for this channel have already been done and would have been added to this paper given more time.

This gives hope that in the future with more time devoted to manipulated *Minuit* or perhaps the larger data set, values for the parameter will be found completely theoretically. Currently the other co-authors are working with the other channel and data. However, they are still waiting on the larger data set from J. Lab. With the use of this work we are one step closer to finding the parameters values, and one step closer to completing Unitarized Chiral Predication Theory.

APPENDIX

Here are all of the equations referenced in the paper.

For the quantization conditions from [5]:

$$Z(\eta, \vec{d}, m_1, m_2, l, m, L)$$
$$= \gamma \int_0^1 e^{t\eta} \sum_{\vec{n} \in Z^3, \vec{n} \neq \vec{0}} (-1)^{A(\vec{n}\cdot\vec{d})} (-i)^l \, y_{l,m}\left(-\frac{\pi \hat{\gamma} \vec{n}}{t}\right) \left(\frac{\pi}{t}\right)^{3/2} e^{-(\pi\hat{\gamma}\vec{n})^2/t}$$
$$+ \gamma \int_0^1 (e^{t\eta} - 1) \left(\frac{\pi}{t}\right)^{3/2} \frac{1}{\sqrt{4\pi}} \delta_{l,0}\delta_{m,0} dt - \gamma\pi\delta_{l,0}\delta_{m,0}$$
$$+ \sum_{\vec{r} \in P_d} y_{l,m}(\vec{r}) \frac{e^{-(r^2-\eta)}}{r^2 - \eta}$$

For the model from [7]:

$$\sigma(E) = \sqrt{1 + \frac{4M_\pi^2}{E^2}}$$
$$s(E) = E^2$$
$$t(E, x) = -2\left(\frac{E^2}{4} - M_\pi^2\right)(1 - x)$$
$$u(E, x) = -2\left(\frac{E^2}{4} - M_\pi^2\right)(1 + x)$$
$$T_{lo}(s) = \frac{s - {M_\pi}^2}{{f_\pi}^2}$$
$$A(s, t, u)$$
$$= -\frac{\mu_\pi}{3{f_\pi}^2 {M_\pi}^2}\left\{4s^2 - 4tu - 4s{M_\pi}^2 + 9{M_\pi}^4\right\}$$
$$- \frac{\mu_K}{6{f_\pi}^2 {M_K}^2}\left\{s^2 - tu + 2s{M_\pi}^2\right\} - \frac{\mu_\eta {M_\pi}^4}{9{f_\pi}^2 {M_\eta}^2}$$
$$+ \frac{4}{{f_\pi}^4}\left(u - 2{M_\pi}^2\right)^2$$
$$+ \frac{1}{576\pi^2 {f_\pi}^4}\left\{30s\left({M_\pi}^2 - s\right) + 21tu - 56{M_\pi}^4\right\}$$
$$+ \frac{1}{2{f_\pi}^4}\left\{\frac{s^2 \bar{J}_{KK}(s)}{4} + \frac{{M_K}^4 \bar{J}_{\eta\eta}(s)}{9} + \left(s^2 - {M_\pi}^4\right)\bar{J}_{\pi\pi}(s)\right\}$$
$$+ \frac{1}{6{f_\pi}^4}\left\{\frac{\left(t - 4{M_K}^2\right)\left(2s + t - 4{M_\pi}^2\right)\bar{J}_{KK}(t)}{4}\right.$$
$$\left. + \left[t(t - u) - 2{M_\pi}^2\left(t - 2u + {M_\pi}^2\right)\right]\bar{J}_{\pi\pi}(t)\right\}$$
$$+ \frac{1}{6{f_\pi}^4}\left\{\frac{\left(t - 4{M_K}^2\right)\left(2s + t - 4{M_\pi}^2\right)\bar{J}_{KK}(t)}{4}\right.$$
$$\left. + \left[u(u - t) - 2{M_\pi}^2\left(u - 2t + {M_\pi}^2\right)\right]\bar{J}_{\pi\pi}(u)\right\}$$

$$B(t) = -\frac{4}{{f_\pi}^4}\left(t - 2{M_\pi}^2\right)^2$$
$$C(s) = \frac{\left(8{M_\pi}^2 s - 16{M_\pi}^4\right)}{{f_\pi}^4}$$
$$\alpha_1 = 2L_1 + L_3 - L_2$$
$$\alpha_2 = 2L_4 + L_5$$
$$\alpha_3 = 2L_1 + L_3$$
$$\alpha_4 = 2L_6 + L_8$$

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