Padé phenomenology for NN scattering: $^1S_0$ phase shifts

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Recently developed Padé approximant techniques are applied to two sets of $^1S_0$ NN scattering data. In the first, the unconstrained $^1S_0$ np phase shifts of MacGregor *et al.* are used to generate a scattering function, $F(k^2) = k\cot(\delta_0)$, which is fitted with high precision. A six-parameter [3/2] Padé fit gives four terms of the effective range expansion; the resulting Marchenko-type potential is expressible as the sum of a Yukawa one-pion-exchange potential and a shorter range part, the repulsion peaking at the origin at near 4 GeV. In a second application, Padé fits are made to the scattering function of the Reid soft-core potential. The [3/2] approximant which fits $F(k^2)$ through the wave numbers consistent with the Lambert, Corbella, and Thomé criterion, to $k = 2.5$ fm^{-1}, leads to a potential with a core height of 4.6×10^4 GeV. In both [3/2] potentials the volume integrals are large and negative, and cannot be made positive by adjoining more repulsive high energy phase shifts. By application to the Reid soft-core potential the Padé formalism is shown to generate useful $[L/L-1]$ Padé approximants with increasing L. The analytic structure of $F(k^2)$ beyond $k = 224$ fm^{-1} is used in the construction of higher Padé approximants that (a) satisfy the Lambert, Corbella, and Thomé criterion and (b) might lead to saturation.

[NUCLEAR REACTIONS Padé approximants used to solve inverse scattering problem for NN $^1S_0$ phase shifts; effective range expansion and short range repulsion computed.]

I. INTRODUCTION

The NN interaction is currently being intensively investigated, for the purpose of improving both the empirical understanding and the theoretical foundations[1,2] of strong interactions. At the same time, the usefulness of realistic NN interactions in computing nuclear structure is steadily growing as can be inferred, for example, in the unfolding program of nuclear self-consistent field (SCF) calculations.[3] A major effort is still required in the important process of translating between experimental scattering and an NN interaction. For a part of this process a new approach has been developed,[4] based upon new techniques for applying Padé approximants (PA).[5] The approach, referred to as a "physical inverse scattering method," makes use of incompletely known phase shifts to generate the scattering function $F(k^2)=k\cot(\delta_0)$ and a local potential. Details of the testing of this method are given in a previous paper, hereafter referred to as I.[4] In the present application, nonrelativistic local potentials are developed, based on high precision fits of NN $^1S_0$ phase shifts, and effective range expansions are carried out to four terms. A further analysis is made of the nature of the short-range NN repulsion.

We use our approach here to fit the unconstrained $^1S_0$ np phase shifts of MacGregor, Arndt, and Wright (MAW),[6,7] even though newer data and phase shifts have recently become available.[1] The MAW phase shifts have been so extensively used in the decade of their existence that the body of references to them provides some useful standards for evaluation of the techniques presented. We emphasize that we do not present a statistical analysis, but rather we treat the MAW phase shifts as a given function to be approximated. The objective of the present paper is to show how the Padé ansatz provides a simple and useful approach to the determination of NN potentials. A more complete statistical analysis of newer, energy independent phase shifts is also being undertaken, and will lead to a class of potentials rather than one, with similarities to the one we present here.

For a second application of the Padé scheme we use the Reid soft core potential (RSC) (Ref. 8) to generate NN $^1S_0$ (isotriplet) phase shift data. Because the RSC is so strongly repulsive, yet is distinguishable from an infinite hard core, it provides a fertile ground for the study of the short-range repulsion. It is known that momentum contributions of NN potentials as high as $k=6$ fm^{-1} can be important in computing phase shifts at low energies.[9] We find a dramatic kind of converse of this result in having to employ phase shifts beyond $k=224$ fm^{-1} in an attempt to recover an important property related to saturation of the RSC, namely, a positive volume integral.

There are two specific issues we hope to address

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successfully by future applications of our precision Padé techniques to develop a potential model. On a fundamental level, one issue is the extent to which the current understanding of meson theory explains the NN scattering data. A more phenomenological issue is the detailed structure of the interaction at short range where $r \lesssim 1$ fm and strong repulsions are present. Local short-range repulsions that have been investigated include infinite hard cores,[20] Yukawa cores,[8] and supersoft cores.[10] Several questions of fundamental import may hinge on the strength of the core, such as the size of meson current effects in nuclei.[11]

There is also a question as to the mechanisms by which nuclear saturation occurs in a nonrelativistic framework with a realistic two-body NN interaction. The short-range repulsion is clearly of importance,[12] and could be crucial in satisfying inequalities necessarily required of two-body potentials for saturation, as given by Calogero and Simonov (CS).[13,14] Volume integrals of NN $^1S_0$ potentials are a useful index of the repulsive strength. In some of the CS inequalities satisfied by a saturating local two-body potential[13] the volume integral of the NN singlet even potential occurs additively in expressions that must be positive. The RSC NN $^1S_0$ potential, employed in calculations that show saturation,[12] has a volume integral of 685 MeV fm^3. A possible shortcoming of some of our approximating potentials is that their volume integrals are negative. We discuss and partly implement modifications for obtaining positive volume integrals.

The supersoft core in the $^1S_0$ np interaction (SSC) developed by Sprung and Srivastava[10] has some particularly desirable features. With a repulsive core height near 90 MeV, the SSC can, unlike most of the other local interactions previously derived from NN scattering data, be used in Hartree-Fock calculations of nuclear structure.[3] The SSC was simply constructed starting with the ansatz of a rational S matrix and ending with an analytical form derived using the Marchenko inverse scattering method. The SSC has had high credibility because it is based on an excellent fit of the 40 MAW phase shifts ($\chi^2 = 12.2$ for the $^1S_0$ np state), improved still further (to $\chi^2 = 3.9$ for 20 phase shifts) when an one-pion exchange potential (OPEP) Yukawa tail is grafted on for the purpose of consistency with meson theory.

The SSC volume integral is -864 MeV fm^3, which contributes to the saturation inequalities with the wrong sign.[13] If the SSC is made to be repulsive at the origin by extending the repulsive peak to the origin at constant height, there is only a small change of the volume integral. If a complete NN local potential contained the SSC, a larger burden of the repulsion needed for saturation would be placed on the triplet odd potential than with the Reid potential, for example.[13]

The present results comprise a refinement of previous phenomenological fits of phase shifts by a potential, and in particular, of Sprung and Srivastava's work. We apply the Padé ansatz directly to the scattering function $F(k^2) = k\cot(\delta_0)$ by writing $F(k^2) = P_L(k^2)/Q_M(k^2) \equiv [L/M]$ in the notation of Baker,[5] where the numerator and denominator polynomials are of degrees $L = 3$ and $M = 2$, respectively, for the excellent fits we obtain. A χ^2-minimization algorithm MINIRAT introduced earlier[4] quickly leads, generally in just a few iterations, to an optimal PA. Extensive testing of the entire method has shown that in every example the Padé interpolative accuracy is excellent, and that the effective range expansion, obtained analytically from the PA, gives reliable values through the first four terms. Examples previously tested, all possessing some characteristics of the $^1S_0$ np interaction, include the hard core, square well, hard core square well, and the hard core Yukawa.

Another refinement we present here is an analysis showing that upon solution of the Marchenko equation[15] our resulting local potential, $V_{\rm exp}$, plausibly contains the significant effects of an OPEP Yukawa tail, $V_{\rm OPEP}$. If we write $V_{\rm SR} = V_{\rm exp} - V_{\rm OPEP}$, then $V_{\rm SR}$ has a smaller intrinsic range, which is more characteristic of heavy meson exchange. Also, in view of the excellent fit already achieved, grafting a Yukawa tail onto $V_{\rm exp}$ could not be expected to lead to a significant improvement.

II. MAW np $^1S_0$ PHASE SHIFTS

The 40 phase shifts of the unconstrained MAW solution are at energy points between $E_{\rm lab} = 1$ MeV and $E_{\rm lab} = 460$ MeV. We employ a nonrelativistic potential model which is not strictly consistent, physically, with fitting phase shifts at intermediate energies.[9] The procedure adopted in this paper is to transform relativistically from $E_{\rm lab}$ to $E_{\rm C.M.}$ before doing the nonrelativistic phase shift calculation. This in effect fixes the definition of $E_{\rm lab}$ for our RSC fits at ultrahigh wave numbers.

Our best χ^2 (for 40 phase shifts), $\chi^2 = 0.0786$, produces errors on the order of 0.01° at low energies and 0.1° at higher energies. Only two iterations were required to achieve this fit, by which the first four parameters in the effective range expansion are reliably determined. If we write

$$k\cot(\delta_0) = -\frac{1}{a} + \tfrac{1}{2}r_0k^2 - Pr_0^{\,3}k^4 + Qr_0^{\,5}k^6$$

then we find

$a = -23.664 \pm 0.002$ fm,

$r_0 = 2.5048 \pm 0.0006$ fm,

$P = 0.0178 \pm 0.0004$,

$Q = 0.0109 \pm 0.0003$,

where the errors quoted are the maximum variations resulting from varying χ^2 by 20%. Since an $[L/M]$ Padé approximant reproduces the first $L+M+1$ terms of a Taylor series,[5] our [3/2] approximant can be expected to contain information about $F(x)$ through terms of order k^{10}. However, as the errors above show, even an excellent determination of [3/2] by minimizing χ^2 produces uncertainties in lower orders of k^2.

Now we present our final numerical results.[16] In terms of $x = k^2$, we write $P_3 = a_0 + a_1x + a_2x^2 + a_3x^3$ and $Q_2 = 1 + b_1x + b_2x^2$. Then for our best fit, $a_0 = 0.042\,258\,4$ fm^{-1}, $a_1 = 1.307\,42$ fm, $a_2 = 1.330\,51$ fm^3, $a_3 = 0.102\,903$ fm^5, $b_1 = 1.301\,65$ fm^2, and $b_2 = 0.485\,844$ fm^4. The kernel of the Marchenko equation depends upon the S matrix S through the three poles of S-1 in the upper half k plane. These poles and their residues are easily computed from $F(x)$, and are listed in Table I with those found by Sprung and Srivastava and those for the Marchenko-Padé potential for the RSC discussed in the next section. The poles in the lower half plane, which are not shown in Table I, vary considerably among potentials. These variations are largely responsible for the differences, including signs, between the residues of Ref. 10 and those of the present Marchenko-MAW potential. The potentials of the present work bear the greatest similarity to each other, even though they fit different data. The Marchenko potential V_{exp} which results from our best fit is shown in Fig. 1, together with V_{SR}, where, following Sprung and Srivastava, we use $V_{OPEP}(r) = -10.463(e^{-0.7r})/(0.7r)$ for the OPEP tail. The Reid soft core potential is also shown together with a Padé-Marchenko approximant which is discussed in the next section. Figure 2 shows the phase shifts given by our Marchenko potential

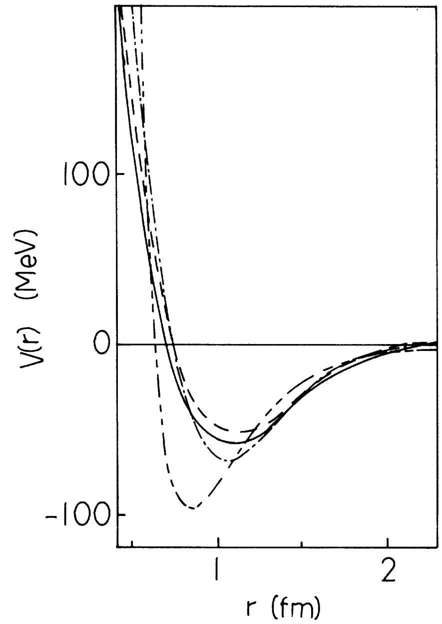

FIG. 1. V_{exp}(————), V_{SR}(— — —), RSC(— - - -), Marchenko approximant to the RSC (— - — - —).

through intermediate energies. These, of course, are exactly what is given by our [3/2] Padé fit of $F(x)$, and reflect the strong short-range repulsion we find. As seen in Fig. 2, our phase shifts at $E_{lab} \geq 400$ are intermediate between those of the SSC and the RSC.

The core height is $V_{exp}(0) = 3.889$ GeV for our best fit. Within a 20 percent variation of χ^2, we find a 5 percent variation of $V_{exp}(0)$. Another interesting characteristic of V_{exp} is its intrinsic range, which is 2.35 fm, as compared with 3.01 fm for V_{OPEP} and 1.93 fm for V_{SR}. Comparison of these numbers illustrates what is more difficult to see graphically, namely, that subtracting off an OPEP tail from V_{exp} removes much of the long range effect. The relatively larger tail of V_{exp} and the harder core of V_{SR} mainly account for the difference in the intrinsic ranges.

The present analysis relies heavily upon our

TABLE I. S-matrix poles in the upper half plane and their residues for three potentials.

Poles and Residues (fm^{-1})	Ref. 10	Present Marchenko-MAW	Marchenko-Reid
pole	$0.878\,8i$	$0.611\,66i$	$0.624\,365i$
residue	$1.591i$	$0.427\,2i$	$0.477\,601i$
pole	$1.565\,9 + 0.8i$	$1.1529 + 1.2054i$	$1.152\,14 + 1.521\,98i$
residue	$-0.097\,39 - 0.5736i$	$1.5374 - 1.2910i$	$2.575\,60 - 3.043\,88i$
pole	$-1.565\,9 + 0.8i$	$-1.1529 + 1.2054i$	$-1.152\,14 + 1.521\,98i$
residue	$0.097\,39 - 0.5736i$	$-1.5374 - 1.2910i$	$-2.575\,60 - 3.073\,88i$

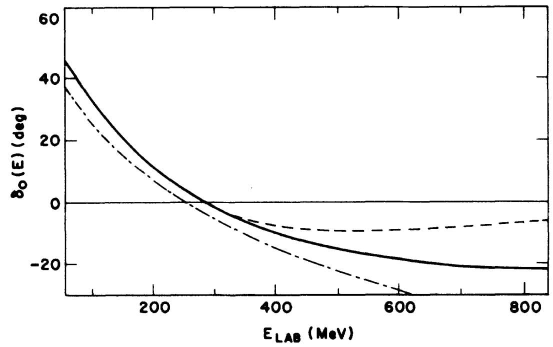

FIG. 2. Phase shifts to intermediate energies predicted by V_{exp} (————). For V_{exp}, $\delta_0(E)$ reaches a shallow minimum of −30° beyond 2 GeV. Also shown are the SSC (— — —) and the RSC (— - —).

ability to calculate phase shifts, Padé approximants, poles, and residue with precision.
An important self-consistency check is to use V_{exp} to recompute the experimental phase shifts. We use the Noumerov algorithm for integrating the Schrödinger equation, which tests to a precision of better than 10^{-8} for phase shifts. Using the MAW standard errors, we obtain a χ^2 of 10^{-6} when we compare the phase shifts of V_{exp} with those produced by the Padé fit to the experimental data.

V_{exp} has heavily damped tail oscillations occuring for $r > 2$ fm, which is also true to a lesser extent of V_{SR}. These are artifacts of our specific Padé fit. We do not consider them a serious problem, even though such oscillations are not predicted by meson theory, for three reasons. First, the effects upon the phase shifts of cutting off the tail are small for V_{SR}. Second, long range effects of a one pion exchange potential appear to be well approximated in our phase shift fits and hence in V_{exp}. Table II compares phase shifts at various low energies (E_{lab}) for different cutoffs which set

TABLE II. Phase shifts of V_{exp}, V_{SR}, and V_{OPEP} showing effect of a cutoff setting the potential to 0 for $r \geq R$.

		Phase shifts in degrees		
		1 MeV	10 MeV	30 MeV
Experimental (Ref. 6)		62.43	61.23	50.73
Potential	R (fm)			
V_{exp}		62.430	61.223	50.704
	5	61.546	61.203	50.583
	2.3	53.064	59.946	50.577
V_{SR}		19.061	37.332	36.865
	5	19.380	37.337	36.915
	2.3	21.066	39.389	37.974
V_{OPEP}		5.908	12.300	13.191
	5	5.268	12.071	13.101
	2.3	2.895	8.131	11.182

the potentials V_{exp}, V_{SR}, and our V_{OPEP} to zero $r \geq R$. There is a clear distinction, especially at the lower energies, between the longer range behavior of V_{exp} and of V_{SR}, from which the long range effects of one pion exchange have been subtracted. Finally, we note that tail oscillations are not an inevitable consequence of the method, and a statistical analysis along the lines mentioned in the Introduction might result in some excellent fits without these oscillations. Although oscillating terms in the potential are always associated with poles of S off the imaginary k axis, such poles do not necessarily cause oscillations that extend into the tail region, as seen in our next example, which is the RSC.

Regarding saturation, the volume integral is -825 MeV fm^3, only 5 percent closer to a positive value than given by the SSC.

III. REID NN $^1S_0$ POTENTIAL (RSC)

We solve the Schrödinger equation with the RSC to generate phase shifts and $F(k^2)$. Data are evaluated at the energies used by MAW, and also at higher energies. Higher energy data are used to determine whether the strongly repulsive RSC can lead to a [3/2] or a higher order Padé-Marchenko potential with a volume integral of the same positive sign as for the RSC. We continue to use χ^2 minimization, which gives essentially the same Padé approximants at least-squares fitting,[4] and we set the standard errors at 4 degrees at the higher energies.

There is a constraint upon our fits to $F(k^2)$ if we use them to derive finite potentials. Lambert, Corbella, and Thomé (LCT) have shown[17] that if no two-body bound states occur, the condition $\delta(0)-\delta(\infty)=0$ is both necessary and sufficient for the solubility of the Marchenko equation. The highest energy for which a [3/2] approximant which minimizes χ^2 is soluble is $E_{lab} = 540$ MeV. Fitting higher energy data forces the [3/2] scattering function $F(k^2)$ to become more repulsive and to give $\delta(0)-\delta(\infty)=\pi$.

As seen in Table III, the volume integral of the resulting [3/2] Padé-Marchenko potential is still negative, contrasted with the positive value for

TABLE III. Volume integrals and core heights of various NN $^1S_0$ potentials.

Potential	Volume integral (MeV fm^3)	Core height (MeV)
RSC	685	∞
Ref. 10	−864	91
[3/2] Marchenko-MAW	−825	3.89×10^3
[3/2] Marchenko-Reid	−615	4.6×10^7

the RSC. This is clear evidence that finite NN $^1S_0$ [3/2] potentials can not be constructed with positive volume integrals. Our potential is shown in Fig. 1. We have determined that it has no tail oscillations, unlike our Marchenko-MAW potential.

Baker has conjectured that the positive sign of the volume integral might be used as a constraint on Padé fits to $F(k^2)$.[18] To accomplish this there are two options. One possible procedure, which has been tested in other problems,[19] is to obtain a more strongly repulsive [3/2] fit by going to higher energies and to introduce an infinite hard core via the hard core inverse scattering method presented in Ref. 4. Another option, as yet not fully tested, is to seek $[L/L\text{-}1]$ fits with $L>3$ that are soluble and to obtain $V(r)$ from the Marchenko equation. We have carried out the first part of this second procedure, starting with a numerical computation of $F(k^2)$. The needed sectors of the RSC scattering function are shown in Fig. 3 on a logarithmic plot, and examples of [3/2], [4/3], and [5/4] fits are plotted as phase shifts in Fig. 4. The sector structure in Fig. 3 suggests a simple pole behavior that would be well approximated by a rational function. All four sectors shown are needed to obtain $\delta(0)-\delta(\infty)=0$ for solubility of the Marchenko equation. So closely is $F(k^2)$ reproduced by the [5/4] fit that their curves in Fig. 4 are indistinguishable through 10 fm^{-1}.

Although reasonable [4/3] fits can be made to data at higher wave numbers than shown on Fig. 4, all our [4/3] fits yield $\delta(0)-\delta(\infty)=\pi$ and hence do not give a soluble Marchenko equation. In practice it is not possible to go into the fourth sector in Fig. 3 and obtain a good [4/3]. Even attempts at [4/3] fits in the third sector cause large increases of χ^2.

Table IV compares the various fits in terms of χ^2 per data point and the first four effective range

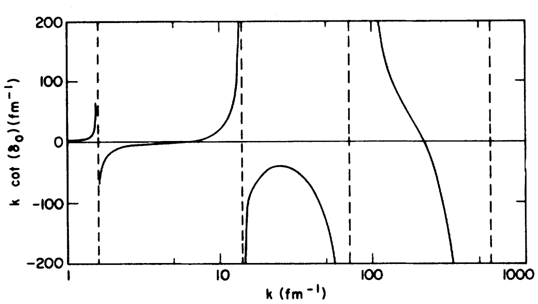

FIG. 3. The RSC scattering function $F(k^2)$ versus k, on a logarithmic plot. Zeros are at $k=5.3$ and 224 fm^{-1}. Vertical asymptotes delineating the four sectors are at $k=1.6$, 14.0, 71, and 580 fm^{-1}. Estimated numerical precision of phase shifts at highest energies is better than 1 degree.

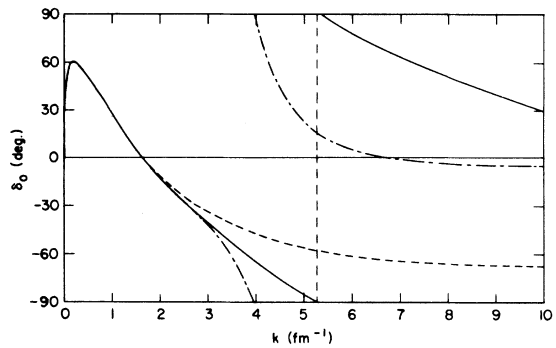

FIG. 4. Phase shifts of the RSC (———), and its approximants [5/4] (———), [4/3] (— - —), and [3/2] (— — —).

parameters. Our standard values of effective range parameters are obtained by minimizing χ^2 for just a few low energy points and then checking interpolational accuracy.[4] We judge the 6-point [3/2] fit to be best, with quoted errors marking the spread of these parameters when various fits, using 4 to 10 points, are made.

Our [5/4] clearly is far more repulsive than the [3/2]. Besides being a candidate for a Marchenko potential with a positive volume integral, the [5/4] fits the entire range of 100 points, approximating singularities and zeros well, and also the scattering length, effective range, and shape parameter.

IV. DISCUSSION

We find the Padé ansatz provides a facile description of NN $^1S_0$ scattering. Both the MAW and the RSC scattering functions are well fitted by [3/2] Padé approximants over the experimentally accessible energy range, while there appears to be good convergence of [5/4] approximants to the RSC beyond $k=224$ fm^{-1}.

An analysis of the RSC has led us to conclude that it is not possible to construct a finite [3/2] Padé-Marchenko potential with a positive volume integral that accurately describes the $^1S_0$ state. However, if the [3/2] approximant is constrained to be so repulsive that $\delta(0)-\delta(\infty)=\pi$, a hard core inverse scattering theory[4,19] can be applied, leading to a saturation-supporting hard core. Also, within the class of fits to the RSC that satisfy $\delta(0)-\delta(\infty)=0$, excellent $[L/L\text{-}1]$ approximants are found, such as our [5/4] fit, that are far more strongly repulsive than any [3/2] fits.

As for the hard core repulsion,[4] so for the RSC: Both scattering functions have an alternating structure of singularities (known to be simple poles for the hard core) and zeros in k^2 that is ideally suited for Padé approximants valid over a

TABLE IV. Comparison of various Padé approximants to RSC scattering function.

Approximant	Highest k fitted (fm^{-1})	No. of phase shifts fitted	χ^2 per data point	Value of $\delta(o)-\delta(\infty)$	a (fm)	r_0 (fm)	P	Q
Ref. 8				0	−17.1	2.80	0.020	
$[3/2]_{st}$ [a]	0.269	6	2.7×10^{-6}		−17.145 ± 0.003	2.803 ± 0.003	0.026 ± 0.002	0.019 ± 0.003
[3/2]	2.47	44	0.097	0	−17.090	2.763	0.0064	0.0057
[4/3]	2.71	50	0.033	π	−17.102	2.771	0.0095	0.0067
[5/4]	457.0	100	0.19	0	−17.073	2.751	0.0025	0.0047

[a] Our $[3/2]_{st}$ is the standard fit for the purpose of obtaining the effective range parameters.

finite range of wave numbers, the precise asymptotic behavior being relatively unimportant.

Within the range of statistically acceptable $^1S_0$ scattering functions for experimentally derived phase shifts there may well be solutions with hard core repulsions. But the imprint of the hard core in the energy range $E_{lab} \leq 460$ MeV is unmistakable. Hard core [3/2] fits satisfy $\delta(0)-\delta(\infty)=\pi$,[4] while our lowest χ^2 fits to MAW lead unequivocally to a strong but finite repulsion and a negative volume integral.

In a larger range of energies up to $E_{lab} \gtrsim 560$ MeV, the [3/2] approximant no longer distinguishes between a Yukawa core and an infinite hard core. Our analysis of the RSC shows how it might be possible, through insertion of poles and zeros of $F(k^2)$ above the experimentally accessible region, to construct stronger finite repulsions using $[L/L\text{-}1]$ fits to the data with $L>3$.

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