Off-shell momentum as a variational parameter in calculations of matrix Padé approximants in potential scattering

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In calculations using matrix Padé approximants, an off-shell momentum (or several off-shell momenta) is introduced. In previous work, this momentum was chosen arbitrarily and not varied. However, it is a variational parameter and may be varied to find points where the phase shift has an extreme value. At such points, the matrix Padé approximants are extraordinarily accurate, even for potentials with strong repulsive cores.

I. THE METHOD

For potential scattering, the Schrödinger equation in momentum space is[1]

$$(k'|K|k) = (k'|V|k) + \frac{2}{\pi}\mathrm{P}\int dk''(k'|V|k'')\frac{1}{k''^2 - k_0^2}(k''|K|k), \tag{1}$$

where k_0 is the on-shell momentum, and

$$(k_0|K|k_0) = \tan\delta/k_0. \tag{2}$$

Equation (1) can be solved by iteration,

$$\begin{aligned}(k'|K|k) &= (k'|V|k) + \frac{2}{\pi}\mathrm{P}\int dk''(k'|V|k'')\frac{1}{k''^2 - k_0^2}(k''|V|k_0) + \cdots, \\ &\equiv (k'|V_1|k) + (k'|V_2|k) + \cdots .\end{aligned} \tag{3}$$

The elements of K required by Eq. (2) are

$$(k_0|K|k_0) = (k_0|V_1|k_0) + (k_0|V_2|k_0) + \cdots , \tag{4}$$

and from the first two terms of this expansion one forms the ordinary (1/1) Padé approximants,[2]

$$(k_0|K|k_0) = (k_0|V_1|k_0)\frac{1}{(k_0|V_1|k_0) - (k_0|V_2|k_0)} \times (k_0|V_1|k_0). \tag{5}$$

For potentials with strong repulsive square-well cores, this (1/1) ordinary Padé approximant is not accurate; it becomes worse as the strength of the repulsion increases, approaching the phase shift for a hard repulsive core no matter what attraction lies outside the core. (Numerical evidence for these facts is presented in Tables I–IV; see Sec. II below.)

This difficulty is overcome by the following scheme. Choose one off-shell momentum k, and calculate the following elements of K:

$$\begin{pmatrix}(k_0|K|k_0) & (k_0|K|k)\\ (k|K|k_0) & (k|K|k)\end{pmatrix} = \begin{pmatrix}(k_0|V_1|k_0) & (k_0|V_1|k)\\ (k|V_1|k_0) & (k|V_1|k)\end{pmatrix} + \begin{pmatrix}(k_0|V_2|k_0) & (k_0|V_2|k)\\ (k|V_2|k_0) & (k|V_2|k)\end{pmatrix} + \cdots . \tag{6}$$

Equation (3) may be used in this way because it is valid for any of the elements of K, in particular the above four elements of K. With the understanding that everything is now a 2×2 matrix,

$$K = V_1 + V_2 , \tag{7}$$

from which one forms a (1/1) matrix Padé approximant,[3]

$$K = V_1\frac{1}{V_1 - V_2}V_1. \tag{8}$$

The (1/1) matrix Padé approximant to $\tan\delta/k_0$ is gotten from the k_0, k_0 element of this last matrix.

As a practical matter, it is somewhat easier to calculate the terms in the Born series, not by iterating Eq. (1), but by iterating

$$U_k(r) = \frac{\sin kr}{k} + \int_0^\infty G_0(r, r')V(r')U_k(r')dr', \tag{9}$$

where G_0 is the on-shell Green's function,

$$G_0(r, r') = \frac{\sin k_0 r_< \cos k_0 r_>}{k_0}, \tag{10}$$

and substituting the result into

$$(k'|K|k) = -\int dr\,\frac{\sin k'r}{k'}V(r)U_k(r). \tag{11}$$

TABLE I. Phase shifts and scattering length given by the ordinary and matrix Padé approximants compared to the exact results for the potential of Eq. (12) with $c_1=0.68\ F$, $c_2=1.92\ F$, $V_1=-170.05$ MeV, $V_2=34.01$ MeV. The units are MeV, fermi, or (fermi)$^{-1}$, as appropriate.

			Phase shifts (degrees)		
Energy	k_0	k	Matrix Padé	Ordinary Padé	Exact solution
20	0.49	4.2	54.88	55.28	54.94
100	1.10	3.9	24.20	25.59	24.20
140	1.30	3.8	14.93	18.13	14.93
210	1.59	3.7	3.453	−0.312	3.459
220	1.63	3.6	2.190	−0.966	2.198
230	1.67	3.5	1.007	−1.749	1.017
240	1.70	3.5	−0.099	−2.576	−0.088
300	1.90	3.4	−5.320	−7.05	−5.298

	Scattering length (fermis)		
k	Matrix Padé	Ordinary Padé	Exact solution
4.20	−20.37	−21.44	−20.75

The principal point of this paper is this: Since the matrix Padé approximant can be derived from a variational principle,[4] k is a variational parameter and one should look for those places where the phase shift δ is stationary when k is varied (maximum or minimum). The calculations reported in the next section show that the phase shift calculated in this way is extraordinarily accurate.

TABLE II. Phase shifts and scattering lengths, for $c_1=0.53\ F$, $c_2=1.92\ F$, $V_1=-364.3$ MeV, $V_2=33.12$ MeV. See caption of Table I.

			Phase shifts (degrees)		
Energy	k_0	k	Matrix Padé	Ordinary Padé	Exact solution
20	0.49	4	55.05	57.88	55.10
100	1.10	3.8	24.59	31.59	24.60
140	1.30	3.8	15.37	−59.28	15.38
210	1.59	3.6	3.847	− 1.441	3.882
220	1.63	3.6	2.568	− 2.336	2.605
230	1.67	3.6	1.365	− 3.065	1.405
240	1.70	3.6	0.234	− 3.89	0.277
300	1.90	3.4	−5.226	− 8.38	−5.146

	Scattering length (fermis)		
k	Matrix Padé	Ordinary Padé	Exact solution
4.0	−20.33	−33.53	−20.59

TABLE III. Phase shifts and scattering lengths, for $c_1=0.45\ F$, $c_2=1.95\ F$, $V_1=-666.7$ MeV, $V_2=31.75$ MeV. See caption of Table I.

			Phase shifts (degrees)		
Energy	k_0	k	Matrix Padé	Ordinary Padé	Exact solution
20	0.49	4	54.75	64.73	54.77
100	1.10	3.8	23.34	−79.64	23.96
140	1.30	3.8	14.67	− 1.20	14.71
210	1.59	3.6	3.174	− 3.37	3.252
220	1.63	3.6	1.90	− 4.23	1.98
230	1.67	3.6	0.706	− 5.09	0.797
240	1.70	3.6	−4.16	− 5.92	−0.319
300	1.90	3.4	−5.838	−10.27	−5.676

	Scattering length (fermis)		
k	Matrix Padé	Ordinary Padé	Exact solution
4.0	−20.54	−67.04	−20.71

II. CALCULATIONS

We have done calculations for the $^1S_0$ state of nucleon-nucleon scattering using a two-square-well potential

$$V(r)=V_1\theta(c_1-r)+V_2\theta(c_2-r), \tag{12}$$

with $c_2\geq c_1$, V_1 positive (repulsive), and V_2 negative (attractive). Adjusting three of these parameters to fit the nucleon $^1S_0$ scattering length and

TABLE IV. Phase shifts and scattering lengths, for $c_1=0.4\ F$, $c_2=1.95\ F$, $V_1=1323$ MeV, $V_2=32.27$ MeV. See caption of Table I.

			Phase shifts (degrees)		
Energy	k_0	k	Matrix Padé	Ordinary Padé	Exact solution
20	0.49	3.9	54.67	−60.10	54.49
100	1.10	3.7	23.36	− 9.26	23.29
140	1.30	3.7	13.83	− 0.86	13.93
210	1.59	3.6	1.96	− 7.09	2.115
220	1.63	3.6	0.63	− 8.00	0.79
230	1.67	3.6	−0.61	− 8.89	−0.45
240	1.70	3.5	−1.80	− 9.74	−1.62
300	1.90	3.5	−7.57	−14.16	−7.32

	Scattering length (fermis)		
k	Matrix Padé	Ordinary Padé	Exact solution
4.0	−20.46	−3.618	−20.74

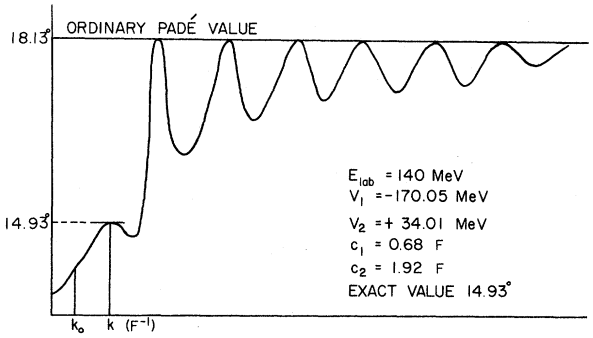

FIG. 1. $^1S_0$ phase shift versus the off-shell momentum k. The calculation is done for $E_{lab} = 140$ MeV, $V_1/V_2 = -5.0$.

effective range and the $^1S_0$ phase shift at $E_{lab} = 240$ MeV leaves one free parameter which we take to be V_1/V_2. For the four potentials for which results are reported in Tables I–IV, $-V_1/V_2 = 5$, 11, 21, and 41 respectively, and all parameters have the values given in the tables.

The result of varying k in one particular calculation is shown in Fig. 1. The phase shift at the first maximum is extraordinarily accurate, not only at this particular energy or for this particular potential, but for all energies and all potentials, as the tables show.

Why the first maximum? We do not know. All maxima other than the first yield the ordinary Padé approximant given by Eq. (5). But the ordinary Padé approximant is derivable from a variational calculation with fewer parameters (that is, without the parameter k) so that a more accurate answer ought to be obtained when k is included, and presumably this more accurate answer is obtained at the first maximum. The minima would not yield a unique answer. In any case, the most accurate extremum is also the one corresponding to a value of k closest to the on-shell momentum k_0, which is not surprising since off-shell momenta close to k_0 contribute more than others. While interesting, these facts are hardly in themselves a rigorous mathematical proof that the first maximum should be used.

Alabiso, Prosperi, and Butera,[4] in their work on the connection of Padé approximants and variational principles for potential scattering, have given methods which, at least for the case of potentials which do not change sign, should make it possible to decide rigorously which extremum should be taken.

We have also done the calculation for the Reid[5]

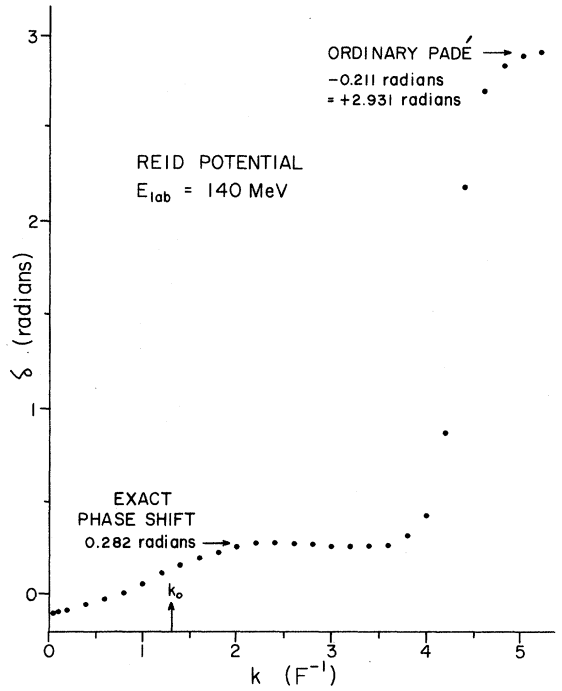

FIG. 2. $^1S_0$ phase shift versus the off-shell momentum k. The calculation is done for the Reid (Ref. 5) potential for $E_{lab} = 140$ MeV.

potential. In this case we calculated $(k'|V_2|k)$ from the momentum-space integral shown in Eq. (3). As shown in Fig. 2, we found that there is only one maximum and one minimum. Again, the value of the phase shift at the maximum is extraordinarily accurate.

III. DISCUSSION

Graves-Morris and Samwell[6] have treated the problem of a two-square-well potential using two variable Padé approximants (the so-called Canterbury approximants). Their (1/1) approximant (more accurately their (1, 1/1, 1) approximant) requires the coefficients of V_1, V_2, V_1^2, V_1V_2, V_2^2, $V_1^2V_2$, and $V_1V_2^2$ in the Born series. We require only the *total* first-order term (not the coefficient of V_1 and V_2 separately) and the *total* second-order term (*not* the coefficients of V_1^2, V_1V_2, and V_2^2 separately). We require off-shell matrix elements and they do not.

The main point in comparing our method with theirs is that we do not require any third-order terms. Consider the following symbolic form of the iterative solution of Eq. (1):

$$(k'|K|k) = (k'|V|k) + \sum_{k''} (k'|V|k'')S_0(k'')(k''|V|k) + \sum_{k'''}\sum_{k''} (k'|V|k'')S(k'')(k''|V|k''')S(k''')(k'''|V|k) + \cdots . \quad (13)$$

While k' and k in our scheme have a limited range of values (actually only two), k'' and k''' have a finite but very large number of possible values corresponding to a discretization of the continuum carried out in order to evaluate the integrals in Eq. (3) numerically. Since $(k'|V|k) = (k|V|k')$ for all k, k', our scheme, which requires only the first- and second-order Born terms, requires the calculation and storage in a computer of $(k|V|k'')$ only, where k takes a few (two) values and k'' takes a finite but large number of values, whereas the Graves-Morris–Samwell scheme, which requires third-order Born terms, requires the calculation and storage in a computer of $(k''|V|k''')$, where both k'' and k''' take a finite but large number of values. If N is the large but finite number, our scheme requires the calculation and storage of $2N$ V-matrix elements, whereas theirs requires $N^2/2$. In short, their scheme requires much more computing and storing than ours.

The Bethe-Salpeter equation for nucleon-nucleon scattering is not so different from Eq. (1). Complications are introduced by relativity and spin, and by positive- and negative-energy states. The number of spin and energy states of two spin-$\frac{1}{2}$ particles is at most 16, and in any state of definite angular momentum the number is at most eight. Let a Greek index, such as α, number the spin and energy states. Let k_4 be the fourth component of the relative momentum of the two particles. Then a state is

$$\text{not } |k), \text{ but } |k_4,\ k,\ \alpha).$$

On-shell, $k_4 = (k^2 + m^2)^{1/2}$, where m is the mass of the nucleon, $k = k_0$, and α would correspond to some positive-energy state. Our scheme would go the same, except that the off-shell values of k_4, k, and α would be chosen independently of each other and varied independently of each other.

Alabiso, Butera, and Prosperi,[4] have discussed the variational principle for the Bethe-Salpeter equation. This work would form the basis for a rigorous mathematical discussion of our method as applied to the Bethe-Salpeter equation.

Tjon and Fleischer[7] solve the Bethe-Salpeter equation by iterating and forming ordinary Padé approximants. They have to compute and store "$N^2/2$" (times factors and still more powers of N due to the spin and energy and the fourth component) matrix elements of V. Their "potential" V, the kernel in the Bethe-Salpeter equation, is composed of one-boson exchange contributions. There are several coupling constants corresponding to coupling of the several bosons with the nucleons. They have not used the Graves-Morris–Samwell scheme because they would have to compute and store "$N^2/2$" matrix elements for each kind of exchange; that is, they would have to compute more, not fewer. The fact that fewer iterations might be required because of the greater accuracy of the Graves-Morris–Samwell scheme is of no consequence because the iterations do not take much time once the necessary elements of V have been computed and stored. Tjon and Fleischer could have used matrix Padé approximants just as Gammel and Menzel[8] did in the case of pion exchange only in the Bethe-Salpeter equation. However, judging from the work of Gammel and Menzel, the (1/1) matrix Padé approximant with several off-shell momenta chosen arbitrarily and not varied is not accurate enough, and any higher order will require the "$N^2/2$" elements. It remains to be seen how our scheme will shorten the time required in the Tjon-Fleischer sort of calculation.

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