Padé Approximants in Three-Body Calculations*

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The Faddeev equations are solved by means of Padé approximants. As an application of the method, the doublet and quartet scattering lengths of neutron-deuteron scattering are calculated for the case that the nucleon-nucleon interactions are described by central local Yukawa potentials.

I. INTRODUCTION

In recent years there has been considerable interest in the study of the three-nucleon problem in the framework of the Faddeev theory.[1] In most of these calculations, however, separable interactions have been used to describe the two-particle forces.[2] The main advantage for using this type of interaction in the three-body problem is the tremendous simplification it leads to for the equations one has to study. On the other hand, one has certain beliefs that a local-potential description for the nucleon-nucleon interaction might be valid at low energies at least. Therefore, it is of some interest to find suitable methods to study the Faddeev equations for local interactions. Several attempts have been made in this direction.[3–6] One particular line of approach has been followed recently by Malfliet and the present author[6] in the study of some properties of the ground state of the three-nucleon system. The method is based essentially on the idea that one can obtain certain informations from the perturbation series solution. In this paper we show that by using Padé techniques on the perturbation series one can in principle also determine the scattering matrix elements. As a specific example we study the case of three identical particles interacting through local Yukawa potentials.

In Sec. II we describe the relevant expressions for the case of scattering of three identical bosons. Furthermore, it is shown here how the Padé technique is applied to the calculation of the S matrix describing the scattering of a particle from a bound state of the other two particles.

Section III is devoted to the determination of the scattering lengths of neutron-deuteron scattering. In this calculation the two-particle forces are described by central local interactions of the Yukawa type. The results obtained are discussed in the last section.

II. SCATTERING OF THREE IDENTICAL BOSONS

For definiteness, let us consider a system of three spinless particles of mass m in which any two of the particles can form a bound state. Furthermore, let us assume that the particles interact only through two-body forces; i.e., the total Hamiltonian of the three-particle system will be given by

$$H=H_0+\sum_i V_i, \tag{1}$$

where V_i is the potential between the particles j and k $(\neq i)$. H_0 is the total kinetic energy of the system which can be expressed in terms of the relative momenta $\mathbf{p}_1$ and $\mathbf{q}_1$ in the over-all c.m. system

$$H_0=p_1^2+q_1^2, \tag{2}$$

with

$$\mathbf{p}_1=\frac{1}{2\sqrt{m}}(\mathbf{k}_2-\mathbf{k}_3), \quad \mathbf{q}_1=-\frac{\sqrt{3}}{2\sqrt{m}}\mathbf{k}_1.$$

Here $\mathbf{k}_i$ is the momentum of the ith particle. We shall denote the corresponding normalized plane-wave state by $|\mathbf{p}_1,\mathbf{q}_1\rangle_1$.

The scattering amplitude for the process in which particle i with relative momentum $\mathbf{q}_i$ is scattered from a bound state of the other two particles to a final state in which particle j is free with momentum $\mathbf{q}_f$ while the other two particles form a bound state, may be defined by

$$M_{ji}={}_j\langle \mathbf{q}_f\alpha_f|\, U_{ji}(s+i\epsilon)\,|\mathbf{q}_i\alpha_i\rangle_i, \tag{3}$$

with

$$U_{ji}(z)=\sum_{k\neq j} V_k-\sum_{k\neq j} V_k G(z)\sum_{l\neq i} V_l. \tag{4}$$

Here s is the total energy of the three-particle system, $G(z)=(H-z)^{-1}$, and $|\mathbf{q}\alpha\rangle_i$ is an eigenstate of the Hamiltonian $H_i=H_0+V_i$, describing a free particle i with momentum $\mathbf{q}$ and a bound state of the other two particles characterized by the quantum numbers α. Let us now restrict ourselves to the case of identical bosons. Then, instead of Eq. (3), we only have to consider one

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[1] L. D. Faddeev, Zh. Eksperim. i Teor. Fiz. **39**, 1459 (1960) [Soviet Phys. JETP **12**, 1014 (1961)].

[2] References can be found in H. P. Noyes and H. Fieldeldey, in *Proceedings of the Texas A&M Conference on Three-Particle Scattering in Quantum Mechanics*, edited by J. Gillespie and J. Nuttall (Benjamin, New York, 1968); see also L. M. Delves and A. C. Phillips, Rev. Mod. Phys. **41**, 497 (1969).

[3] J. W. Humberston, R. L. Hall, and T. A. Osborn, Phys. Letters **27B**, 195 (1968).

[4] J. S. Ball and D. Y. Wong, Phys. Rev. **169**, 1362 (1968).

[5] D. D. Brayshaw, Phys. Rev. **182**, 1658 (1969).

[6] R. A. Malfliet and J. A. Tjon, Nucl. Phys. **A127**, 161 (1969); Phys. Letters **29B**, 391 (1969); **30B**, 293 (1969).

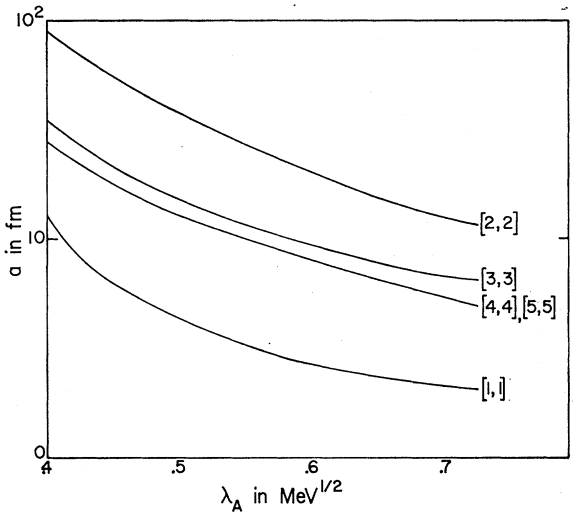

FIG. 1. Dependence of the scattering length a as a function of the coupling constant λ_A for various Padé approximants.

amplitude for bound-state scattering. It is given by

$$M=\sum_{i=1}^{3} M_{ji}. \tag{5}$$

Here we assume that the states $|\mathbf{q}\alpha\rangle_i$ are symmetric with respect to interchange of particles j and k ($\neq i$). It should be noted that Eq. (5) does not depend any more on the index j due to the symmetrization of the initial state. By certain rearrangements of the terms in Eq. (5), we may also write instead of it

$$M={}_1\langle \mathbf{q}_f\alpha_f|\sum_{k=2}^{3} V_k|\mathbf{q}_i\alpha_i\rangle_k+{}_1\langle \mathbf{q}_f\alpha_f| \times \sum_{\substack{k,l,m;\\ l\neq 1;\ k\neq m}} T_k{}^l(s+i\epsilon)|\mathbf{q}_i\alpha_i\rangle_m. \tag{6}$$

In Eq. (6) the operators $T_k{}^l$ are defined by

$$T_k{}^l(z)=V_k\delta_{kl}-V_lG(z)V_k. \tag{7}$$

Using the Faddeev technique, we may write formally the following coupled set of integral equations for the operators $T_k{}^l$:

$$\begin{pmatrix} T_k{}^1(z)\\ T_k{}^2(z)\\ T_k{}^3(z)\end{pmatrix}=\begin{pmatrix} T_1(z)\delta_{k1}\\ T_2(z)\delta_{k2}\\ T_3(z)\delta_{k3}\end{pmatrix} -\begin{pmatrix} 0 & T_1(z) & T_1(z)\\ T_2(z) & 0 & T_2(z)\\ T_3(z) & T_3(z) & 0\end{pmatrix}G_0(z)\begin{pmatrix} T_k{}^1(z)\\ T_k{}^2(z)\\ T_k{}^3(z)\end{pmatrix}, \tag{8}$$

where $G_0(z)=(H_0-z)^{-1}$ and $T_i(z)$ are the two-body T matrices in the three-particle Hilbert space. They satisfy the Lippmann-Schwinger equation

$$T_i(z)=V_i-V_iG_0(z)T_i(z).$$

Although the Padé method can be applied to any angular momentum state of the three-particle system, we consider here as an illustrative example the case that the system is in a $J=0$ state while the two-body T matrices can be approximated by only their $l=0$ part. Equation (8) can then be simplified by making an angular momentum decomposition.[7] In doing so, an integral equation in two continuous variables is obtained for the matrix elements

$$U(p,q)=\sum_{\substack{k,l,m;\\ k\neq m;\ l\neq 1}} {}_l\langle p,q|T_k{}^l(s+i\epsilon)|q_i\alpha_i\rangle_m,$$

where ${}_l\langle p,q|$ are the corresponding partial-wave states of ${}_l\langle \mathbf{p},\mathbf{q}|$. The equation has the form

$$U(p,q)=\phi(p,q)-\frac{4\pi}{q\sqrt{3}}\int_0^\infty dq'^2 \times\int_{A(q,q')}^{B(q,q')} dp'^2\frac{t_0(p,\bar{p};s-q^2+i\epsilon)}{p'^2+q'^2-s-i\epsilon}U(p',q'), \tag{9}$$

with

$$\bar{p}^2=p'^2+q'^2-q^2,$$
$$A(q,q')=\tfrac{1}{3}(2q+q')^2,$$
$$B(q,q')=\tfrac{1}{3}(2q-q')^2,$$

and

$$\phi(p,q)=\frac{16\pi}{\sqrt{3}q_iq}\int_{A(q,q_i)}^{B(q,q_i)} dp'^2 \times t_0(p,(p'^2+q_i{}^2-q^2)^{1/2};s-q^2+i\epsilon)\psi_b(p'). \tag{10}$$

In Eq. (10), ψ_b is the two-particle bound-state wave function. It is normalized as

$$\int_0^\infty |\psi_b(p)|^2p^2dp=1.$$

The numerical solution of the above equations with conventional methods, such as reducing the problem to a finite set of linear equations, is in general far from trivial. On the other hand, the calculation of the Neumann series solution of Eq. (9) is rather feasible with present-day computers. For this reason, we have examined the applicability of the Padé method.[8] Let us for convenience introduce a parameter λ by replacing in Eqs. (9) and (10) the two-body T matrix t_0 by λt_0. This parameter should, of course, be set equal to 1 in the actual calculation. We now assume that we have been able to compute the coefficients M_k of the scattering amplitude M resulting from the Neumann series solution of Eq. (9). The expression

$$M=\sum_{n=0}^{\infty}\lambda^nM_n$$

[7] A. Ahmadzadeh and J. A. Tjon, Phys. Rev. 139, B1085 (1965).
[8] For a review of the theory of Padé approximants, see G. H. Baker, Jr., Advan. Theoret. Phys. 1 (1965).

can then be approximated by the so-called diagonal $[N,N]$ approximant in λ, given by

$$M_{[N,N]}=P_N(\lambda)/Q_N(\lambda),$$

where P_N and Q_N are Nth-order polynomials, the coefficients of which can be determined from M_n. We now know that[9]

$$\lim_{N\to\infty} M_{[N,N]}=M.$$

The main question which arises is whether it converges fast enough. As an example we have studied the case where the potential $V(r)$ is given by

$$V(r)=-\lambda_A e^{-\mu r}/r.$$

The results for the various approximants are shown in Figs. 1 and 2. We have here taken the mass m to be the nucleon mass while $\mu=4.07$ MeV$^{1/2}$. In Fig. 1 is exhibited the rate of convergence of the Padé approximants for the scattering length a as a function of the coupling constant λ_A. Figure 2 shows the dependence of the quantity $q\cot\delta$ as a function of the energy q^2 of the incoming particle for $\lambda_A=0.513$ MeV$^{1/2}$ for the various approximants. For this value of λ_A, the two-body system has a bound state at -2.225 MeV. From Fig. 2 we see that the [1,1] and [2,2] approximants behave quite pathologically. They have a pole at $q^2=0.4$ and 0.5 MeV, respectively. In spite of this peculiar behavior, the rate of convergence as a function of N is rapid enough for practical purposes.

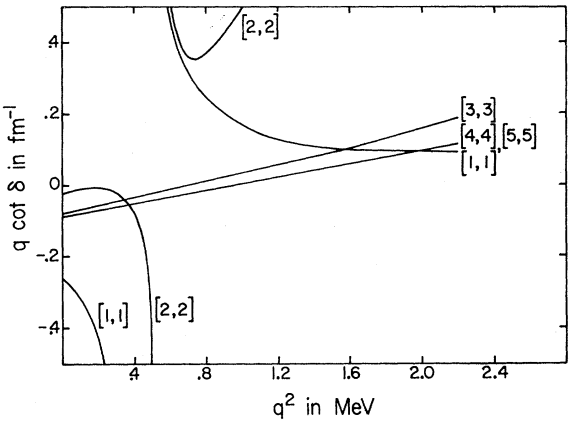

FIG. 2. Dependence of $q\cot\delta$ as a function of the energy q^2 for various Padé approximants.

III. NEUTRON-DEUTERON SCATTERING

In order to see whether the method is also applicable in an actual calculation, we have considered the problem of determining the scattering length of n-d scattering under the assumption that the interactions in the singlet and triplet channels of the two-nucleon system are dominated only by s waves. The potentials used for these channels are of a local central type and have the form

$$V(r)=-\lambda_A\frac{e^{-\mu_A r}}{r}+\lambda_R\frac{e^{-\mu_R r}}{r}.$$

Since the deuteron has spin 1, there are two possibilities for the total spin of the n-d system: $s=\frac{1}{2}$ and $\frac{3}{2}$. With the above assumptions, the Faddeev equations for the total $J=0$ state reduce to a coupled set of two integral equations for $s=\frac{1}{2}$, while for $s=\frac{3}{2}$ we are left only with one equation.

In a similar way, as described in the previous section for the case of identical bosons, the scattering lengths of n-d scattering are calculated with the aid of the Padé method. Already the [2,2] approximant was sufficient to determine the values for the quartet scattering length a_4, while we needed the [5,5] for the doublet scattering length a_2. Furthermore, the numerical accuracy in the computed values of the scattering lengths was estimated to be better than 0.1 fm. The results for a_2 are summarized in Table I for various choices of the singlet and triplet potentials. The corresponding three-particle bound-state energies are also included in the table. We have for convenience characterized the potentials by their property of possibly having a core (i.e., $\lambda_R\neq 0$), and by their effective range. The values of the potential parameters can be found in Ref. 6. In the calculation of a_4, the only two-particle channel which contributes is the triplet channel. For the triplet potential with repulsion the value of a_4 was found to be 6.35 fm, while the purely attractive potential gave a value of 6.45 fm.

IV. DISCUSSION

We have seen in the previous sections that the Padé approximation can be a very useful tool in determining the solutions of the three-body problem for local interactions. The main practical problem one is faced with is to calculate the coefficients of the series. In doing this one encounters integrations over singularities which one has to take properly into account. For example, in the calculation of $q\cot\delta$ in the scattering region below the breakup threshold, there is a singularity at the two-particle bound-state energy in the two-particle t matrix. This singularity is simply removed by making a sub-

TABLE I. Triton binding energy E_t and doublet scattering length a_2 for various combinations of singlet and triplet potentials.

Singlet	Triplet	E_t (MeV)	a_2 (fm)
no core	no core	−12.1	−5.3
$r_s=2.6$ fm	no core	− 9.1	−0.4
$r_s=2.8$ fm	no core	− 8.4	0.3
no core	with core	−10.0	−1.3
$r_s=2.6$ fm	with core	− 8.8	0.4
$r_s=2.8$ fm	with core	− 8.3	0.9

[9] R. Chisholm, J. Math. Phys. 4, 12 (1963).

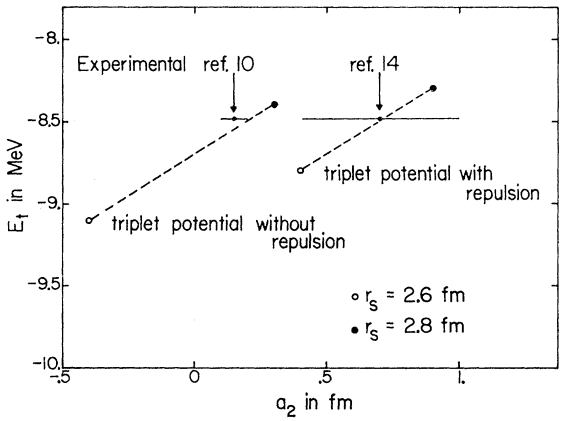

FIG. 3. Relation between the doublet scattering length a_2 and the triton binding energy E_t.

traction in the integrals. For above the inelastic threshold we do not expect drastic differences with respect to the rate of convergence of the Padé approximants. Only the integrals one has to evaluate become somewhat more complicated since one then has, in addition to the above-mentioned singularity, also to treat appropriately the singularity of the Green's function Q_0.

We now turn to the discussion of the results we have obtained for n-d scattering. The quartet scattering length $a_4=6.4$ fm is in reasonable agreement with the latest experimental value of 6.13 ± 0.04 fm.[10] Furthermore, the determined values are also consistent with those obtained by Humberston[11] from a variational calculation. The effect of including a repulsion in the triplet potential is remarkably small and indicates that a_4 is determined primarily by the low-energy behavior in the triplet channel. In contrast to the quartet case, the doublet scattering length a_2 depends very sensitively on the variation of certain parameters in the two-nucleon potentials. For instance, the inclusion of repulsion in the singlet potential affects the result considerably. Also, it is obvious from Table I that once we have chosen for the singlet potential the one with a repulsion, the triton binding energy E_t does not change appreciably upon introducing a repulsion in the triplet channel, while this is certainly not the case with a_2. With respect to the dependence on the singlet scattering length r_s, we see that both E_t and a_2 are very sensitive to it. The relative variations are thereby similar as in the case of separable potentials.[12] In this connection it is interesting to see whether it is possible by a variation in r_s to get a simultaneous fit to the experimental values of E_t and a_2. Following Phillips,[13] we have plotted in Fig. 3 the obtained values of E_t and a_2. Assuming a linear dependence of E_t on a_2, it is amusing to see that either the recently experimentally determined value[10] $a_2=0.15\pm0.05$ fm or the older value[14] $a_2=0.7\pm0.3$ fm can reasonably well be fitted depending on the choice of the triplet potential. Giving perhaps a slight preference to the triplet potential with repulsion since this gives a better fit to the $^3S_1$ phase shifts at higher energies, this calculation favors the older value of 0.7 fm. The latter conclusion was essentially also reached recently by Phillips[13] in a calculation using separable two-particle interactions. Needless to say, however, we should be careful with our conclusion because of the crudeness of the model. In particular, it is not known what effect the introduction of a local tensor force has on a_2.

[10] W. T. H. van Oers and J. D. Seagrave, Phys. Letters **24B**, 562 (1967).
[11] J. W. Humberston, Phys. Letters **10**, 207 (1964).
[12] A. G. Sitenko, V. F. Kharchenko, and N. M. Petrov, Phys. Letters **21**, 54 (1966).
[13] A. C. Phillips, Nucl. Phys. **A107**, 209 (1968).
[14] D. G. Hurst and J. Alcock, Can. J. Phys. **29**, 26 (1951).