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Note

A Numerical Aide in the Location of Few-Body Bound States

A wide variety of methods is currently available for solving either eigenvalue problems or the associated conjugate eigenvalue problem [1]. These problems are sometimes formulated in terms of integral equations for scattering amplitudes, so that the bound states appear as poles in the scattering amplitude, $t(E)$, as a function of the energy E [2]. Thus, the bound state problem becomes a search for the solutions of $(t(E))^{-1} = 0$. Jarratt and Nudds [3] have discussed the usefulness of rational functions in numerically solving such single-variable equations. These rational functions are equivalent to Padé approximants of type II, which are considered in a recent review of Padé approximants by Zinn-Justin [4]. The present work is concerned with the application of linear fractions, that is the [1, 1] Padé approximant of type II, to the determination of two-body and three-body bound states.

Continued fractions and rational functions have appeared in many approaches to equation solving. The location of the zeros of a function by the method of continued fractions is described by Frame [5] and the references he cites. This approach utilizes the derivatives of the function, so it is not too useful for functions that are only known numerically. Jarratt and Nudds [3] present a rational function, or Padé approximate, approach to equation solving which uses the numerical values of the function itself. Swalen and Pierce [6] found the eigenvalues of tridiagonal matrices by continued fractions, while Lovelace and Masson [7] used continued fractions and recursion relations to determine the Regge poles of various potentials. Their procedure involves series expansions of the quantities occurring in the radial Schrödinger equation and is suitable for locating bound states. Vescelius and Neff [8] show how continued fractions aid in handling various polynomial potentials in the one-dimensional Schrödinger equation.

The present method involves the [1, 1] Padé approximate of type II [3, 4]. Let

$$F(z) = \frac{a_0 + a_1 z}{1 + b_1 z} \tag{1}$$

define a representation of the actual function F. The three unknowns a_0, a_1, and b_1 are found by solving the set of three simultaneous linear equations that arise when $F(z)$ is known for three values of z. The current interest is in poles, so the first trial z, z_4, is obtained from

$$1 + b_1 z_4 = 0. \tag{2}$$

The actual function F is evaluated at z_4 and then z_2, z_3, and z_4 are used to generate new a_0, a_1, and b_1 and, hence, z_5 through Eq. (2). The process continues until the z_i converge. This type of rational interpolation is particularly easy to use since each successive trial z comes from the solution of a linear equation.

We now show how Eqs. (1) and (2) are used in locating few-body bound states. We consider the two-body problem first.

In the two-body problem, $F(z)$ is identified with the scattering amplitude $t(q, q, E)$, where q is a fixed momentum. The Lippmann–Schwinger equation [2]

$$t(p, q, E) = V(p, q) + \int_0^\infty dK\, K^2 \frac{V(p, K)\, t(K, q, E)}{-q_E{}^2 - K^2}, \tag{3}$$

is solved by linear equation methods at the desired values of $E = -\hbar^2 q_E{}^2/2m$. Here, m is the reduced mass. The integral is replaced by a finite sum through the use of a 28-point Gaussian quadrature rule. The variable p is then set equal to the value of each of the integration sample points. For each p an equation with 28 unknowns, $t(K_i, q, E)$, is generated. Hence, the 28 values of p lead to a set of 28 inhomogeneous linear equations in 28 unknowns, which is solved by Gaussian elimination with iterative improvement.

Several $\mathcal{S}$-wave nucleon–nucleon potentials with from one to three Yukawa potentials were studied. These cases provided the basis for the general comments which follow. Two numerical examples are then introduced. The sequence of trial E's converges very quickly if the initial energies bracketed the bound state. In these cases three or less trial E's, beyond the three starting energies, are usually sufficient. This is fewer than the secant method [9] requires and is in agreement with the finding of Jarratt and Nudds [3] that linear fractions converge quicker. In both cases, the last E is such that the matrix element $t(q, q, E)$ is at least 10^4 in magnitude. When the initial energies are further away from the bound state, a few more iterations are required. Two examples are presented in Tables I and II. These illustrate the rate of convergence of the linear fraction method and the secant method. The potential is the two-term Yukawa potential of Coester and Yen, with the parameters given by Stern [10],

$$V(r) = -1761.65 \exp(-2.307r)/r + 7046.6 \exp(-4.614r)/r. \tag{4}$$

$V(r)$ is in MeV while r is in fermis.

Sometimes a problem arises when the initial energies are all two or three orders of magnitude away from the bound state. A positive trial energy is predicted by Eq. (2), but this is not desirable since different methods are needed to solve Eq. (3) when the energy is positive. So ad hoc schemes are needed to generate a negative trial E. For example, a sequence of negative trial E's, each twice the previous, is tried until the root is bracketed. But once this occurs, rapid convergence is observed.

TABLE I

Comparison of the Convergence to a Two-Body Bound State

Secant method		Padé method	
Energy (MeV)	Amplitude[b] (fermis)	Energy (MeV)	Amplitude[b] (fermis)
		−25.0[a]	−0.29134 + 01
−6.0[a]	−0.77901 + 01	−6.0[a]	−0.77901 + 01
−1.0[a]	+0.12401 + 02	−1.0[a]	+0.12401 + 02
−2.92904	−0.30419 + 02	−2.43424	−0.93584 + 02
−2.37036	−0.13183 + 03	−2.22812	−0.21748 + 04
−2.20278	+0.11855 + 04	−2.21919	—
−2.21955	−0.48947 + 05		
−2.21915	—		

[a] Initial energy.
[b] Amplitude is the matrix element t(0.17819-02, 0.17819-02, E).

TABLE II

Convergence to a Two-Body Bound State with the Padé Method

Energy (MeV)	Amplitude[b] (fermis)
−15.0[a]	−0.37652 + 01
−10.0[a]	−0.49104 + 01
−5.0[a]	−0.97298 + 01
−1.88320	+0.54698 + 02
−2.24482	−0.76171 + 03
−2.21935	−0.10174 + 06
−2.21916	—

[a] Initial energy.
[b] Amplitude is the matrix element t(0.17819-02, 0.17819-02, E).

In general, some cases are expected where convergence will not occur so quickly, even though the bound state is bracketed. Some remedies for this situation are discussed by Chien [11].

The Faddeev–Lovelace equations [12] are a set of coupled integral equations which provide a description of the three-body problem. When the three bodies are

all spinless bosons and only relative $\mathscr{S}$-states are considered, the Faddeev–Lovelace equations become an integral equation with two continuous variables of integration. A convenient method for solving this equation is by iteration of the integral equation [13]. The present calculations are based on an integral equation [14] which differs somewhat from that given by Malfliet and Tjon [13]. The integral equation is iterated 16 times so that a series is generated for a given matrix element. This series diverges when the three-body energy is less in magnitude than the deepest bound-state's energy and this divergence is overcome by using Padé approximants to sum the series [14, 15]. Hence, the values of the matrix element which go into the determination of the coefficients in Eq. (1) come from an independent application of Padé approximants.

The bound state is located with the same economy of trial energies as in the two-body problem. Table III presents an example in which the two-body potential is

TABLE III

Convergence to a Three-Body Bound State with the Padé Method

Energy (MeV)	Matrix element	Ratio
−20.735[a]	−0.6524 + 01	1.68118
−12.441[a]	−0.1355 + 02	1.37743
−6.2205[a]	−0.6892 + 02	1.09937
−4.69399	−0.4840 + 03	1.01640
−4.43190	−0.7390 + 04	1.00110
−4.41323	≈−0.1400 + 07	1.00000

[a] Initial energy.

a square well with a depth of 24.0 MeV and a range of 2.0719 fermis. The column labeled "ratio" is the asymptotic inverse ratio of successive terms in the series expansion of the matrix element. As discussed in Malfliet and Tjon [13], the deepest bound-state occurs when the ratio is 1.0.

In conclusion, the [1, 1] Padé approximant of type II is an efficient aid in locating few-body bound states. Tables I–III display rates of convergence which are roughly consistent with the predicted rate of Jarratt and Nudds [3]. The use of this linear fraction method in the three-body problem promises a substantial savings of computer time, since the solution of a three-body integral equation is quite involved. With this in mind, it is natural to ask if the use of higher-order rational-function approximations would be still more useful in the three-body problem. Jarratt and Nudds [3] show that there is some gain in the rate of convergence for

the higher-order approaches, but this gain is balanced by the increased number of initial energies that are needed. That is, the three-body problem must be solved more times before the first trial energy is generated. If in specific cases, the number of trial energies that are required to achieve convergence exceeds the number used in the examples presented here, then higher-order approaches may be worthwhile.

A comment on the Newton–Raphson method for finding zeroes is also appropriate, since this method has been found to be very useful for finding the eigenvalues of the two-body Schrödinger equation [1, 16]. The Newton–Raphson method involves the derivative, so if Eq. (3) is used

$$\frac{\partial}{\partial E} t(p, q, E) = t'(p, q, E)$$

is required. When the potential is energy-independent, $t'(p, q, E)$ is easily obtained from the solution of Eq. (3) at energy E via an integration. However, if the potential is energy-dependent, then several one-dimensional integrals and a double-integral must be done. These additional integrals involve the derivative of the potential matrix element with energy. Unfortunately, the three-body problem is analogous to a two-body problem with energy-dependent potentials [12]. In addition, each single-variable integral is replaced by a double-integral in the three-body problem. These factors indicate that the linear-fraction method involves less work than the Newton–Raphson method for the three-body problem.

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