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A Nonlinear Integral Equation from the Ball–Zachariasen Model of Diffractive Scattering: Numerical Solution near a Singularity of the Fréchet Derivative*

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In the Ball-Zachariasen model of high-energy diffractive scattering, the unitarity condition leads to a non-linear integral equation for the elastic amplitude. The equation is solved by the Newton-Kantorovich iteration, and also by two other algorithms derived from the imbedding method. The starting point is a function proposed by Ball and Zachariasen, which had heretofore led to divergent iterative sequences. The techniques used are of interest for the general problem of solving equations of S-matrix theory, and are discussed at some length from the viewpoint of operator imbedding. The solution is one of an infinite family of solutions related by scale transformations. All members of the family have the same value γ_0 of the dimensionless parameter $\gamma = \ln(\sigma_t/\sigma_e)$, where σ_t and σ_e are total and elastic cross-sections. The number γ_0 has the character of an eigenvalue for the solution family; there are no neighboring solutions with neighboring values of γ. Thus, one has a "bootstrap" determination of the strength of particle production, and the computed value of γ_0, as well as the differential cross-section (for a particular choice of length scale), are in rough agreement with experiments on $p - p$ scattering.

I. INTRODUCTION

The Ball–Zachariasen model [1, 2] was intended to be a schematic picture of high-energy diffractive scattering, admittedly incorrect in smaller details, but perhaps reasonable as a first sketch of an illusive physical process. The primary idea of the model, taken from the multiperipheral model [3], is that the n-particle production amplitude should be expressed as a product, the factors of the product being expressed in terms of the elastic scattering amplitude. The unitarity condition then leads to an integral equation for the elastic amplitude. Heretofore, the question of whether the equation has a physically acceptable solution has not been settled [4, 5, 6]. In the present paper, numerical evidence for the existence of a suitable solution is reported.

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Ball and Zachariasen suggested two different approaches to the solution of their equation. The first was based on the observation that the Hankel transform of the equation has obvious step function solutions in the limit of vanishing γ, where the dimensionless parameter γ, the logarithm of the ratio of total to elastic cross-section, measures the strength of particle production. It was proposed to look for solutions at small γ as perturbations of those obtained from step functions at $\gamma = 0$. The existence of an infinite family of such solutions was proved by the contraction mapping principle, in Ref. [4]. Numerical calculations showed, however, that those solutions did not resemble experiment. In particular, it proved to be impossible to continue to a value of γ as large as that measured experimentally.

The second approach of Ball and Zachariasen was to guess a form for an approximate solution [2]. Varying a few parameters in the form chosen, they obtained a function $\hat{f}_0$ which seemed to be very close to a solution, but which proved to be unstable under simple iteration [2, 5]. A later investigation [5] seemed to show that the sequence generated by Newton–Kantorovich iteration [7] (hereafter called Newton iteration) also is divergent. The divergence was tentatively explained as being due to proximity of a singularity of the Fréchet derivative of the non-linear integral operator involved. It now appears that the divergence was caused by insufficient accuracy in the numerical evaluation of the Fréchet derivative. With improved accuracy the sequence converges quickly to a solution $\hat{f}$ which is quite close to the starting point $\hat{f}_0$. The Fréchet derivative is rather close to being singular all along the sequence (according to its condition number and normalized determinant, it is "badly conditioned"), and that in itself implies that small errors in its evaluation will produce large deviations from the exact Newton sequence.

In practical applications of the Newton method, it is not unusual to encounter some or all of the following difficulties: (i) the initial guess may be so far from a solution that the Newton sequence diverges; (ii) the Fréchet derivative may be nearly singular or even actually singular at some step of the Newton sequence; (iii) for computational convenience it may be desirable or necessary to use a relatively poor approximation to the Fréchet derivative, and that may put convergence in jeopardy. The issues involved in these problems are best understood from the viewpoint of operator imbedding, in which one attempts to pass from the initial guess to a solution by integration of an auxiliary differential equation. With a particular choice of the imbedding, integration of the differential equation by the elementary Euler method yields the so-called damped Newton method, with damping factor equal to the Euler step length. Under reasonable conditions the Euler method is stable for sufficiently small step length. Thus, the damped Newton method is effective under quite general conditions, while the ordinary undamped method is relatively restricted in scope. These useful ideas [8, 9, 10], familiar to some numerical analysts but unfortunately not often mentioned in standard discussions of the Newton method [7, 11], are reviewed in Section 2, and applied in Section 3.

Section 3 contains the computational results for solution of the integral equation. The undamped Newton sequence with an accurately computed Fréchet derivative is compared to the damped sequence with the less accurate derivative used in [5].

The latter sequence converges to the same solution as the former, but much more slowly. The discussion of Section 2 explains the slower convergence, as well as an observed limitation on the size of the damping factor. A second method of integrating the imbedding equation is also applied; namely, the trapezoidal rule. It is found to be inferior to the Euler method in this example.

In Section 4, the dependence of the solution on parameters is examined. The solution of Section 3 is found to be a member of an infinite one-parameter family of solutions, the parameter being $c = \gamma/\sigma_e$, where σ_e is the elastic cross-section. Different values of c may be interpreted as corresponding to different scales of length. All members of the solution family have the same value γ_0 of the parameter γ, and γ_0 is like an eigenvalue for the family. There are no neighboring solutions with neighboring values of γ. Furthermore, the value computed, $\gamma_0 = 1.88$, is not too far from the experimental value for $p - p$ scattering at about 20 GeV, $\gamma_{\text{exp}} \approx 1.4$.

Section 5 is devoted to conclusions and remarks about the significance of the results for the general problem of bootstrap theories.

II. Solution of Nonlinear Equations by the Imbedding Method

Consider the system of n real equations in n real unknowns,

$$F(x) = 0, \tag{2.1}$$

where F and x denote n-component vectors, and F has continuous partial derivatives. The Fréchet derivative $F_x(x)$ of the operator F: $R^n \to R^n$ is the linear operator defined by the Jacobian matrix:

$$F_x(x) = \left[\frac{\partial F^i(x)}{\partial x^j}\right]. \tag{2.2}$$

Given an initial guess x_0 for the solution of (2.1), the Newton sequence $\{x_n\}$ is generated by successive linearizations of (2.1),

$$F_x(x_n)(x_{n+1} - x_n) = -F(x_n), \qquad n = 0, 1,... \tag{2.3}$$

The sequence is well-defined if and only if $F_x(x_n)$ has an inverse for each n. Conditions sufficient for definition of the sequence and convergence to a solution x_* of (2.1) are well known. Let the vector norm $\| x \|$ and the linear operator norm $\| A \|$ be defined as follows:

$$\| x \| = \sup_i | x^i |, \qquad \| A \| = \sup_x \frac{\| Ax \|}{\| x \|}. \tag{2.4}$$

Define $S(x_0, R)$ as the ball of radius R centered at x_0; i.e., the set of all x such that $\| x - x_0 \| < R$. A standard theorem of Kantorovich type is as follows: [7, 11]

THEOREM 1. *Suppose that $F(x)$ is defined and differentiable in $S(x_0, R)$, and such that $F_x(x)$ satisfies a Lipschitz condition in that region,*

$$\| F_x(x) - F_x(y) \| \leqslant a \| x - y \|. \tag{2.5}$$

Suppose also that the inverse of $F_x(x_0)$ exists and that

$$\begin{gathered} \| F_x(x_0)^{-1} \| \leqslant b, \qquad \| x_1 - x_0 \| \leqslant c, \\ h = abc \leqslant \tfrac{1}{2}. \end{gathered} \tag{2.6}$$

Then if

$$r = \frac{1 - (1 - 2h)^{1/2}}{h} c \leqslant R, \tag{2.7}$$

the sequence $\{x_n\}$ converges to a solution x_* of $F(x) = 0$, with $x_* \in S(x_0, r)$. Estimates on the rate of convergence are available [7, 11].

In other words, given the stated conditions on F_x with any a, b the sequence converges to a solution provided the first iterate x_1 is sufficiently close to the initial guess x_0. If x_0 is close to a point of singularity of $F_x(x)$ (a point $\tilde{x}$ such that $F_x(\tilde{x})^{-1}$ does not exist), then the minimum b will be relatively large, and $\| x_1 - x_0 \|$ will have to be correspondingly small to verify the conditions of the theorem.

The method of operator imbedding provides an informative alternative view of the Newton method. Following Gavurin [12] and others [8, 9], one considers the operator

$$H(x, t) = F(x) - e^{-t} F(x_0), \tag{2.8}$$

with the real parameter t ranging over the half-line $[0, \infty)$. The object is to find a solution $x(t)$ of the problem

$$H(x(t), t) = 0, \qquad 0 \leqslant t < \infty, \quad x(0) = x_0. \tag{2.9}$$

A solution of (2.9) provides a solution of (2.1) in the sense

$$\lim_{t \to \infty} F(x(t)) = 0. \tag{2.10}$$

If a solution $x(t)$ of (2.9) is differentiable, it satisfies the following differential equation:

$$\begin{gathered} F_x(x) \frac{dx}{dt} + F(x) = 0, \\ x(0) = x_0. \end{gathered} \tag{2.11}$$

Conversely, if (2.11) has a solution $x(t)$ on the entire half-line, then

$$\frac{d}{dt} H(x(t), t) = F_x(x) \frac{dx}{dt} + e^{-t}F(x_0)$$
$$= -F(x) + e^{-t}F(x_0) = -H(x(t), t) \tag{2.12}$$

or

$$H(x(t), t) = \kappa e^{-t}, \tag{2.13}$$

where κ is a constant. Since $H(x(0), 0) = 0$ it follows that κ is zero, and consequently (2.10) holds when $x(t)$ is any solution of the problem (2.11). If $F_x(x(t))$ is non-singular at large t, then dx/dt tends to zero by (2.11), and the limit $x(\infty)$ exists. Then $F(x(\infty)) = 0$ by (2.10) and the continuity of F. Even if $x(t)$ does not tend to a limit, $x(t)$ is still a solution of (2.1) "to arbitrary accuracy" at large t, according to (2.10): for any ϵ, $\| F(x(t))\| < \epsilon$ for all $t > T(\epsilon)$.

The connection of the differential equation (2.11) with the Newton method is seen by considering the approximate solution of the former by Euler's method: $x(n\,\Delta t)$ is approximated by x_n, where the sequence $\{x_n\}$ is generated from x_0 through the equations

$$F_x(x_n) \frac{x_{n+1} - x_n}{\Delta t} + F(x_n) = 0, \qquad n = 0, 1,... \tag{2.14}$$

The Euler sequence coincides with the Newton sequence for step-size $\Delta t = 1$. In cases where Newton's sequence fails to converge to a solution of (2.1), we can still hope to use Euler's method with $\Delta t < 1$, or some other method of approximate integration, to find a sequence $\{x_n\}$ following closely a solution curve $x(t)$ of the differential equation. The goal might be to follow such a curve until a solution $x(\infty)$ of (2.1) is approached sufficiently closely, or else just to reach a suitable starting point point $\hat{x}_0$ for a Newton iteration. There are well-known sufficient conditions for the Euler iterates x_n to stay arbitrarily close to the corresponding points $x(n\,\Delta t)$ for sufficiently small Δt. Of course, the choice $\Delta t = 1$ corresponding to the Newton sequence has no special significance from the viewpoint of Euler's method, and divergence of the Newton sequence is a signal that some $\Delta t < 1$ is required to stay in sufficient proximity of a solution curve. The special importance of the choice $\Delta t = 1$, for those cases in which it gives a convergent sequence, is that the convergence is quadratic [9]; i.e., when x_n is sufficiently close to a solution x_* there is a constant $\kappa > 0$ such that

$$\| x_{n+1} - x_* \| \leqslant \kappa \| x_n - x_* \|^2. \tag{2.15}$$

The iteration defined in (2.14) with $\Delta t < 1$ is called a "damped Newton-Kantorovich iteration" with damping factor Δt.

What can be said about existence of a suitable solution of (2.11) on the entire half-line $[0, \infty)$? If x_0 and $F(x)$ satisfy Kantorovich conditions such as those of Theorem 1, then analysis of the existence question for the differential equation may be carried out in analogy to the analysis of convergence of the Newton sequence. Indeed, several authors have proved theorems of Kantorovich type for the differential equation

[8, 13, 16, 26] i.e., global existence theorems, but with hypotheses too strong to be of value in circumstances where the Newton sequence diverges. Useful global existence theorems under conditions weaker than those of Kantorovich appear to be lacking, at least for operators F of a type sufficiently general to cover a range of important applications; (see, however, Refs. [29, 30] for a quite different approach to the solution of (2.1) under very weak conditions on $F(x)$). Nevertheless, basic theorems on local existence and approximation of solutions make clear that it is reasonable to attempt a numerical solution of (2.11), provided that $F_x(x_0)$ is non-singular.

In the first place, the implicit function theorem applied to $H(x, t) = 0$ with initial solution $(x, t) = (x_0, 0)$ ensures the existence of a locally unique solution $x(t)$ of (2.11) on some interval $0 \leqslant t \leqslant \tau_1$, with $F_x(x(t))$ non-singular on that interval. A second application of the implicit function theorem with initial solution $(x(\tau_1), \tau_1)$ extends the soution to an interval $\tau_1 \leqslant t \leqslant \tau_2$. The process may be continued indefinitely, unless the interval lengths $|\tau_{n+1} - \tau_n|$ tend to zero because of $x(t)$ approaching an $\hat{x} = x(\hat{\tau})$ such that $F_x(\hat{x})$ is singular, or because $\|x(t)\| \to \infty$ as $t \to \hat{\tau}$ [14], [38]. If a singular point is encountered, the curve $x(t)$ does not necessarily terminate, but it may branch into two or more curves, or "turn back" after passing the point $\hat{\tau}$ with infinite derivative dx/dt; (in the latter case, one has two different values of x for each t in an interval $\hat{\tau} - \delta < t < \hat{\tau}$). Techniques for following solutions through singularities have been discussed by several authors [15–21], and examples in elasticity theory are known in which the desired value of a parameter is achieved after passing through several singularities [15]. The method recently proposed by Keller seems to be especially promising with respect to generality and practicality [17]. In the case of the present paper, the numerical computations indicate that $x(t)$ extends to $t = \infty$, without passing through a singular point of $F_x(x)$ and with $\|x(t)\|$ being bounded.

While the implicit function theorem gives a qualitative view of the local behavior of solutions of the differential equation, theorems of numerical analysis give information on how to approximate the solutions locally. Before quoting such theorems, let us make precise the above remarks on uniqueness by recalling the conditions of the implicit function theorem in a form appropriate for the present discussion [22].

THEOREM 2. *Let $H(x, t)$ be a mapping of $R^n \times R$ into R^n, having continuous pth derivatives, $p \geqslant 1$, in a neighborhood Ω of a point (x_0, t_0) such that $H(x_0, t_0) = 0$. Suppose that $H_x(x_0, t_0)$ is non-singular. Then there exists a neighborhood Ω_0 of t_0 and a function $x(t)$ such that*

(i) $H(x(t), t) = 0, \quad t \in \Omega_0$

(ii) $x(t_0) = x_0$

(iii) $x(t) \in C^p, \quad t \in \Omega_0$

(iv) $H_x(x(t), t)$ *is non-singular*
and $\dot{x} = -H_x(x(t), t)^{-1} H_t(x(t), t), \quad t \in \Omega_0$.

Furthermore, there is only one function $x(t)$ with these properties.

With H as defined in (2.8), $H \in C^1$ if $F_x \in C^1$, and because of (i) the differential equation in (iv) is equivalent to

$$\dot{x} = -F_x(x)^{-1} F(x). \tag{2.16}$$

Thus, sufficient conditions for (2.11) to have a unique solution in a neighborhood of $t = 0$ are that $F_x(x)$ be continuous in a neighborhood of x_0, and that $F_x(x_0)^{-1}$ exist.

As is well known, Theorems 1 and 2 hold as well in arbitrary Banach spaces [7, 11, 22],

A simple criterion for convergence of Euler's method is based on Lipschitz continuity of the function

$$f(x) = -F_x^{-1}(x) F(x). \tag{2.17}$$

Suppose that (2.11) has a unique solution $x(t)$ in some interval $T = [0, \tau]$, and consider the problem of approximating that solution by Euler's method [23].

THEOREM 3. *If $f(x)$ satisfies a Lipschitz condition,*

$$\| f(x) - f(y) \| \leqslant a \| x - y \|, \qquad x, y \in L,$$

where L is a closed region including the solution $x(t)$ of (2.11) in its interior for $t \in T$, then Euler's method with $\Delta t = t/n$, $t \in T$, converges to the solution; i.e., $x_n \to x(t)$, $n \to \infty$, uniformly in t, if $x_0 = x(0)$.

Other aspects of Euler's method, including theoretical error estimates, the effects of numerical errors, and stability questions, are discussed by Henrici [24] and Gear [23].

If $F_x(x)$ is non-singular and Lipschitz-continuous in a closed region L, then the same is true of $f(x)$. Lipschitz continuity of $f(x)$ is the standard sufficient condition [23] for existence and uniqueness of a local solution of the initial value problem $\dot{x} = f(x)$, $x(0) = x_0$. The implicit function theorem applied to (2.8) ensures existence and uniqueness of a local solution of $\dot{x} = -F_x^{-1}(x) F(x)$, $x(0) = x_0$, if $F_x(x)$ is merely continuous near x_0, rather than Lipschitz-continuous.

Euler's method is usually not recommended for general utility in solving differential equations, because of its relatively poor accuracy. The purposes of the present discussion are rather special, however, since the sole concern of the imbedding method for solution of (2.1) is to reach the asymptote $x(\infty)$, rather than to stay close to the curve $x(t)$ at all t. With that point in mind, one should judge integration methods with respect to efficiency in reaching the asymptote, allowing for the possibility that the approximate solution curve might deviate substantially from the exact solution at small t. A discussion of integration methods from such an orientation has been given by Boggs [8]. Adapting ideas of Dahlquist [25], Boggs emphasizes comparison with a linear problem.

When x is sufficiently close to a solution x_* of (2.1), the differential equation (2.16) should behave in much the same way as the linear equation

$$\dot{y} = -y, \qquad y = x - x_* . \tag{2.18}$$

Specifically, suppose that $F_x(x)^{-1}$ is bounded in some neighborhood Ω of x_*, and that $F_x(x)$ is Lipschitz-continuous in Ω. Then (2.16) may be written as

$$\begin{aligned} \dot{x} &= -(x - x_*) + F_x^{-1}(x)[F(x_*) - F(x) + F_x(x)(x - x_*)] \\ &= -(x - x_*) + \phi(x - x_*), \qquad x \in \Omega, \end{aligned} \tag{2.19}$$

where ϕ may be bounded by a second-order form of the mean-value theorem in terms of the Lipschitz coefficient a of F_x :

$$\begin{aligned} \| \phi(x - x_*)\| &\leqslant \tfrac{1}{2}a \, \| F_x^{-1}(x)\| \, \| x - x_* \|^2 \\ &\leqslant \tfrac{1}{2}ab \, \| x - x_* \|^2. \end{aligned} \tag{2.20}$$

It now seems a good guess that ϕ should be negligible in (2.19) when $\| x - x_* \|$ is sufficiently small. Provided an x sufficiently close to x_* is available, one should then be able to compare numerical integration procedures on the basis of their efficiency in dealing with the trivial linear problem (2.18).

Euler's method applied to (2.18) gives

$$y_{n+1} = y_n - \Delta t \, y_n = (1 - \Delta t)^{n+1} \, y_0 , \tag{2.21}$$

so that the Euler iterates converge to the correct answer $y(\infty) = 0$ for any $\Delta t < 2$. The so-called backward Euler method for solution of $\dot{y} = f(y)$, based on the iteration

$$y_{n+1} = y_n + \Delta t f(y_{n+1}), \tag{2.22}$$

gives quite a different result when applied to (2.18); namely,

$$y_{n+1} = y_n - \Delta t \, y_{n+1} = (1 + \Delta t)^{-n-1} \, y_0 . \tag{2.23}$$

The backward Euler method gives the correct asymptote of zero for *any* $\Delta t > 0$. A third example is the trapezoidal iteration,

$$y_{n+1} = y_n + \frac{\Delta t}{2} [f(y_{n+1}) + f(y_n)], \tag{2.24}$$

which in the case of (2.18) yields

$$y_n = \left[\frac{2 - \Delta t}{2 + \Delta t}\right]^n y_0 . \tag{2.25}$$

The trapezoidal method also gives the correct asymptote for any Δt, converging

more quickly than the backward Euler method for $\Delta t < 1 + 5^{1/2}$, and more slowly if $\Delta t > 1 + 5^{1/2}$.

Of the three methods mentioned, the Euler method with $\Delta t = 1$ (i.e., the undamped Newton method) and the trapezoidal method with $\Delta t = 2$ are most efficient in finding the asymptote; they find it immediately: $y_1 = y_2 = \cdots = 0$. With the Euler method and $1 < \Delta t < 2$, the convergence is slower, and for $\Delta t > 2$ one has the divergent behavior illustrated in Figure 1 for $\Delta t = 2.1$: the iterates jump from one side of the exact solution to the other. The backward Euler and trapezoidal methods do not show this jumping behavior with $\Delta t = 2.1$, and of these two the trapezoidal rule gives much the faster convergence; see Figures 2 and 3. One may conclude that efficiency

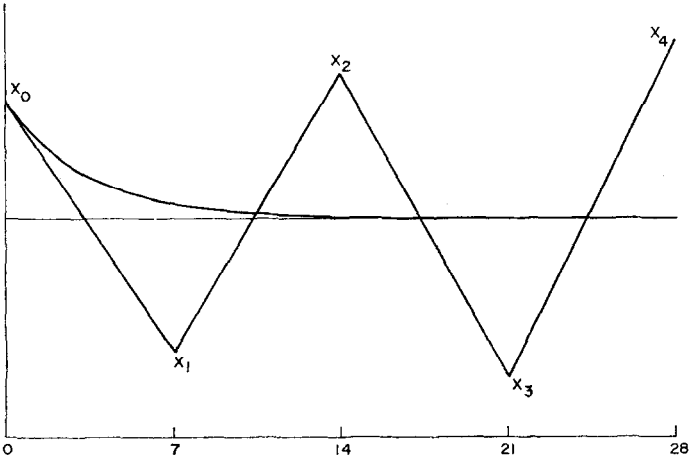

FIG. 1. Iterates x_n of Euler's method applied to $\dot{x} = \lambda x$, $\lambda = -0.3$, $\Delta t = 7$.

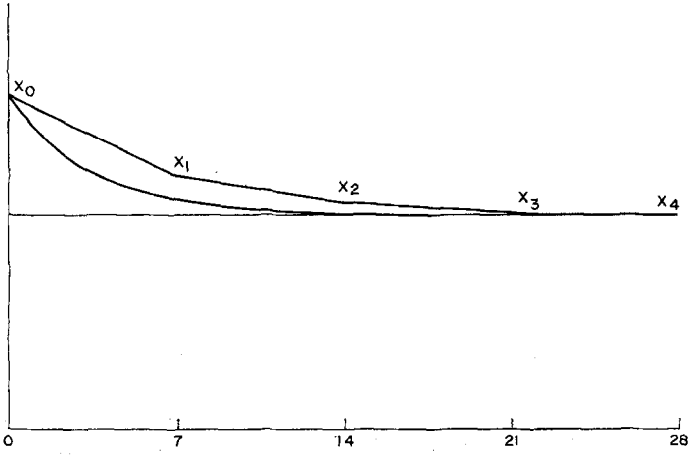

FIG. 2. Iterates x_n of backward Euler method, for problem of Fig. 1.

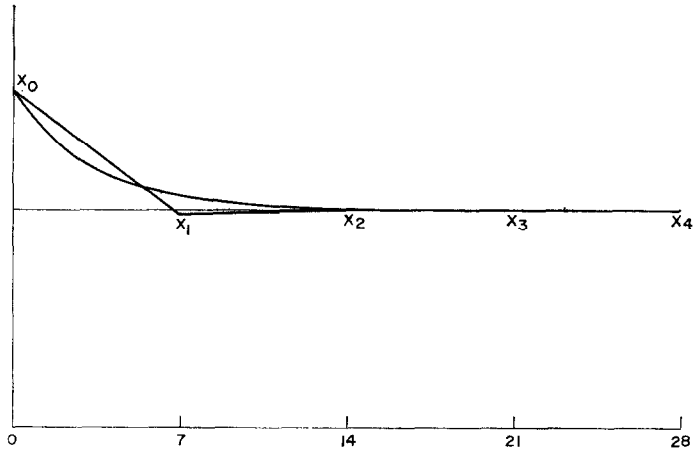

FIG. 3. Iterates x_n of trapezoidal method, for problem of Fig. 1.

in finding the asymptote depends rather drastically on the integration method and step length. It seems likely that a strong dependence on method and step-length will also be found in non-linear problems, but it is difficult to predict what the dependence will be in an arbitrary problem, except in the region close to a solution where the equation is nearly linear. Boggs [8] has proved a theorem on stability of the trapezoidal method in the quasi-linear regime.

Testing of various methods and step lengths may be rewarding in particular non-linear problems of interest. The problem considered in the following section is too large for extensive experimentation, but one experiment has been carried out; namely, a comparison of the trapezoidal method and the Euler method, the Fréchet derivative being computed in the approximation of [5]. The trapezoidal rule was suggested by Boggs [8] as a possible competitor to the Euler method.

The backward Euler method and the trapezoidal method are examples from a class of methods that Dahlquist calls *A-stable* (asymptotically stable). A method is called A-stable if it yields a sequence $\{y_n\}$ converging to zero when applied with any fixed $\Delta t > 0$ to any equation of the form

$$\dot{y} = \lambda y, \qquad \operatorname{Re} \lambda < 0. \tag{2.26}$$

It is not yet clear that A-stable methods have a significant domain of usefulness for non-linear imbedding problems, but since in the linear case they have stability properties qualitatively different from that of the Euler method, it may be worthwhile to consider them. It is known that A-stable methods (at least those of the linear k-step type [23, 24]) are necessarily "implicit"; that is to say, one must solve a non-linear equation to compute y_{n+1} from y_n, if $f(y)$ is not linear. Although in practice the solution of the non-linear equation for y_{n+1} may take only one or two steps of a simple iterative procedure (a "predictor-corrector" algorithm), it may reduce the competitive advantage of A-stable methods.

As was mentioned in the Introduction, it may happen in practice that the exact Fréchet derivative $F_x(x)$ in (2.16) is replaced by some approximation $\tilde{F}_x(x)$, while an accurate representation of $F(x)$ is retained. In contrast to the exact equation (2.16), the approximate equation

$$\dot{x} = -\tilde{F}_x^{-1}(x)\, F(x) \tag{2.27}$$

will not behave as the linear problem (2.18) when x is near a solution x_*. That is seen by attempting a decomposition like (2.19):

$$\dot{x} = -(x - x_*) + \tilde{F}_x^{-1}(x)[F(x_*) - F(x) + \tilde{F}_x(x)(x - x_*)]. \tag{2.28}$$

Here the quantity in the square brackets has a part which vanishes only linearly with $x - x_*$. To see that, add and subtract $F_x(x)(x - x_*)$ and apply the mean value argument of (2.20). Instead of resembling (2.18) for small $x - x_*$, the equation will resemble

$$\dot{y} = -Ay, \qquad y = x - x_*, \tag{2.29}$$

where $A = \tilde{F}_x^{-1}(x_*)\, F_x(x_*)$ is a constant matrix. If A deviates substantially from the unit matrix, it may happen that Euler's method with unit step length will never converge to x_*, no matter how close the starting point x_0 is to x_*. If the step length and $\| x_0 - x_* \|$ are sufficiently small, convergence is expected (provided, of course, that $\tilde{F}_x(x_*)$ is not so far from $F_x(x_*)$ as to give A an eigenvalue with negative real part). These remarks explain the behavior of the Ball–Zachariasen equation when treated with the approximation to the Fréchet derivative used in Ref. [5]. Convergence is obtained when Eq. (2.27) is integrated by Euler's method with $\Delta t = 0.4$, but for $\Delta t = 0.6$, say, the Euler sequence diverges, even when the starting point is as close to a solution as the computer word length allows.

To conclude this brief review, it should be mentioned that other techniques have been proposed to find a starting point $\hat{x}_0$ for Newton's iteration from an initial guess x_0. Still in the spirit of the imbedding approach, Meyer [26] and Kung [27] work with a string of Newton sequences, each Newton sequence corresponding to a different operator equation, constructed in a simple way from the original equation. On the other hand, Moore and Jones [28] give up entirely the idea of continuation from an initial guess x_0, and instead describe a procedure to search systematically for suitable starting points for Newton's method. In an interesting and quite different line of thought, pioneered by mathematical economists, topological methods are used to compute fixed points of merely continuous mappings; see Scarf [29] and Todd [30].

III. Numerical Solution of Ball-Zachariasen Equation

The Ball–Zachariasen model prescribes a factored form for the elastic scattering amplitude,

$$A(s, t) = 8\pi i s f(x), \qquad x = (-t)^{1/2}, \tag{3.1}$$

where s is the squared energy in the center-of-mass frame, and t is the squared invariant momentum transfer. It is most convenient to work with the Hankel transform of the Ball–Zachariasen equation, the latter being given originally as an equation for $f(x)$. The Hankel transform of $f(x)$ is denoted by $\hat{f}(b)$, where b is analogous to the classical impact parameter:

$$\hat{f}(b) = \int_0^\infty x\, dx\, J_0(bx) f(x). \tag{3.2}$$

Here J_0 is the Bessel function of order 0. The integral equation is written as

$$F(\hat{f}, c) = \hat{f} - A(\hat{f}, c) = 0, \tag{3.3}$$

where c is a real parameter. Here and on occasion in the following we suppress reference to the variable b. As a function of b, $A(\hat{f}, c)$ has the form

$$A(\hat{f}, c; b) = \int_0^\infty x\, dx\, J_0(bx)\, g(x)\, e^{cg(x)}, \tag{3.4}$$

$$g(x) = \int_0^\infty b\, db\, J_0(bx)\, \hat{f}(b)^2. \tag{3.5}$$

By taking the Hankel transform of (3.3) and applying the Hankel inversion theorem [31] one recovers the original form of the Ball–Zachariasen equation in x-space:

$$f(x) = g(x)\, e^{cg(x)}. \tag{3.6}$$

The total cross-section σ_t is given by the optical theorem as

$$\sigma_t = 8\pi f(0), \tag{3.7}$$

while the elastic cross-section σ_e is

$$\sigma_e = 8\pi g(0). \tag{3.8}$$

By (3.6), the dimensionless parameter $\gamma = cg(0)$ is

$$\gamma = cg(0) = \ln(\sigma_t/\sigma_e). \tag{3.9}$$

One has the option of regarding either c or γ as the one parameter of the equation. That is, in place of (3.3) one could write

$$G(\hat{f}, \gamma) = \hat{f} - B(\hat{f}, \gamma) = 0, \tag{3.10}$$

$$B(\hat{f}, \gamma; b) = \int_0^\infty x\, dx\, J_0(bx)\, g(x)\, e^{\gamma g(x)/g(0)}. \tag{3.11}$$

An adaptation of the argument of Ref. [4], Appendix B, shows that the operator A maps a certain Banach space S into itself. The space S is the set of all real functions $\phi(b)$ with continuous second derivatives on $[0, \infty)$ such that the following quantity, the norm on S, is finite:

$$\| \phi \| = \sup((b + 1)^{5/2}[| \phi(b)| + | \phi'(b)| + | \phi''(b)|]) < \infty, \qquad 0 \leqslant b < \infty. \quad (3.12)$$

It is reasonable to look for a solution of (3.3) in S, by constructing a numerical model of the operator A acting on S. The model to be used is the one employed in Ref. [5]; namely, all Hankel transforms are evaluated numerically by an analog of Filon's method for Fourier integrals [32]. Over a small interval $[b_1, b_2]$, $\phi(b)$ is approximated by its average value, and the resulting integral is calculated exactly:

$$\int_{b_1}^{b_2} b\, db\, J_0(bx)\, \phi(b) \simeq \frac{1}{x}[\phi(b_2) + \phi(b_1)]\frac{1}{x}[b_2 J_1(b_2 x) - b_1 J_1(b_1 x)]. \quad (3.13)$$

The intent of this method is to handle accurately the rapid oscillations of $J_0(bx)$ at large bx. The calculations are done with 50 intervals of b and 100 of x, so that the numerical analog of (3.3) amounts to 51 equations in the 51 unknowns $\hat{f}(b_i)$. The numerical results conform in several respects to theoretical expectations for the exact equation [4, 5, 6], so that there is some basis for confidence in the approach. No attempt has been made to give a rigorous validation of the discretization, but it seems likely to the author that one could be provided. Experimentation with the number of mesh points, to be reported presently, suggests that convergence will occur.

The formal expression for the Fréchet derivative $F_{\hat{f}}$ of F, applied to an arbitrary element h of S, is as follows:

$$\begin{aligned} F_{\hat{f}}(\hat{f}, c)\, h &= h - A_{\hat{f}}(\hat{f}, c)\, h \\ &= h(b) - \int_0^\infty x\, dx\, J_0(bx)[1 + cg(x)]\, e^{cg(x)}\, \delta g(x), \end{aligned} \quad (3.14)$$

where

$$\delta g(x) = 2 \int_0^\infty b\, db\, J_0(bx)\, \hat{f}(b)\, h(b). \quad (3.15)$$

A reversal of integration order gives

$$F_{\hat{f}}(\hat{f}, c)\, h = h(b) - \int_0^\infty K(b, b', c; \hat{f})\, h(b')\, db', \quad (3.16)$$

$$K(b, b', c; \hat{f}) = 2 \int_0^\infty x\, dx\, [1 + cg(x)]\, e^{cg(x)} J_0(bx)\, J_0(b'x)\, b'\hat{f}(b'). \quad (3.17)$$

In Ref. [5], $F_{\hat{f}}$ was discretized by applying a quadrature rule like (3.13), generalized to account for the product of two Bessel functions, to the integral (3.17). Let us denote the resulting approximation to the Fréchet derivative by $F_{\hat{f}}^{(1)}$. Alternatively,

one can simply take the Jacobian of the discretized form of $F(\hat{f})$, to obtain a different approximation $F_{\hat{f}}^{(2)}$. The use of $F_{\hat{f}}^{(1)}$ seemed to offer computational advantages, but it turns out that the "small" difference between it and the accurately computed Jacobian $F_{\hat{f}}^{(2)}$ is crucial in the implementation of Newton's method.

The approximate solution proposed by Ball and Zachariasen was given as an approximation $g_0(x)$ to the function $g(x)$ of (3.5); namely,

$$\begin{gathered} g_0(x) = \frac{g_0(0)}{(1 + x^2/x_0^2)^n}\left[1 - \frac{ax^2}{(1 + x^2/x_0^2)^2}\right] \\ g_0(0) = 0.657\ \text{GeV}^{-2}, \qquad x_0^2 = 2\ \text{GeV}^2, \\ n = 4.1, \qquad a = 1\ \text{GeV}^{-2}. \end{gathered} \tag{3.18}$$

The corresponding value of c is 2.91 GeV^2, hence $\gamma = cg_0(0) = 1.91$. The function $\hat{f}_0(b)$ is obtained from $g_0(x)$ by (3.5) and the Hankel inversion theorem:

$$\hat{f}_0(b) = [\hat{g}_0(b)]^{1/2}. \tag{3.19}$$

The transform $\hat{g}_0(b)$, as computed numerically, is positive (except for very small oscillations about zero at large b), and the positive square root in (3.19) is required for $\hat{f}_0$ to solve (3.3) approximately. The functions $g_0(x)$ and $\hat{f}_0(b)$ are shown as the dashed curves in Figures 4 and 5.

The damped Newton sequence $\{\hat{f}_n\}$, beginning with $\hat{f}_0$, is defined by the following equations:

$$F_{\hat{f}}(\hat{f}_n)(\hat{f}_{n+1} - \hat{f}_n) = -\Delta t\, F(\hat{f}_n), \qquad n = 0, 1, 2,... \tag{3.20}$$

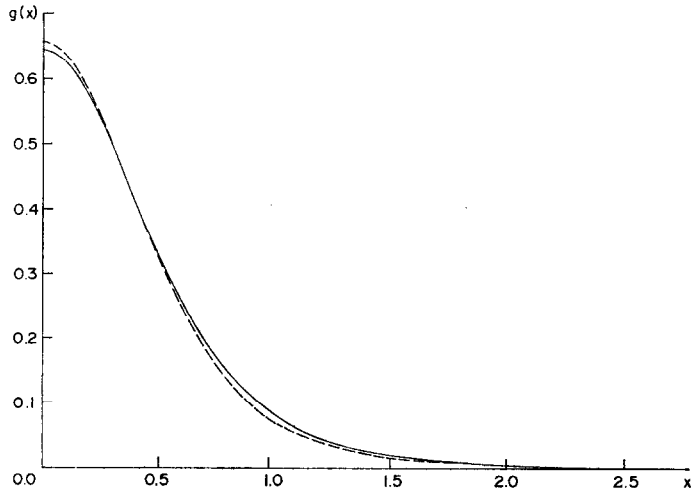

FIG. 4. Solid line is the function $g(x)$ corresponding to the solution $\hat{f}(b)$. Dashed line is the initial function $g_0(x)$ proposed by Ball and Zachariasen, Eq. (3.18).

For each n, the discretized version of (3.20) is solved for $\hat{f}_{n+1} - \hat{f}_n$ by Gaussian elimination. The functions $\hat{f}_n(b)$, $g_n(x)$, and residuals $F(\hat{f}_n ; b)$ are printed out, along with the diagnostics

$$\epsilon_n = \frac{\sup_b |\hat{f}_{n+1}(b) - \hat{f}_n(b)|}{\Delta t \hat{f}_n(0)}, \tag{3.21}$$

$$d_n = \frac{|\det(F_{\hat{f}}(\hat{f}_n))|}{\prod_i \{\sum_j (F_{\hat{f}}(\hat{f}_n))_{ij}^2\}^{1/2}}, \tag{3.22}$$

$$r_n = \sup_b |F(\hat{f}_n ; b)|. \tag{3.23}$$

Since $\hat{f}_n(0) = \sup_b |\hat{f}_n(b)|$, (see [4], Appendix D) and empirically $\sup_b |\hat{f}_{n+1}(b) - \hat{f}_n(b)| = |\hat{f}_{n+1}(0) - \hat{f}_n(0)|$, the quantity ϵ_n is to be thought of as roughly equal to

$$\left| \frac{d}{dt} \ln \hat{f}(0; t) \right|_{t=n\Delta t}. \tag{3.24}$$

The normalized determinant d_n is the magnitude of the ordinary determinant of $F_{\hat{f}}(\hat{f}_n)$ divided by the product of the Euclidean row lengths of the matrix. Following

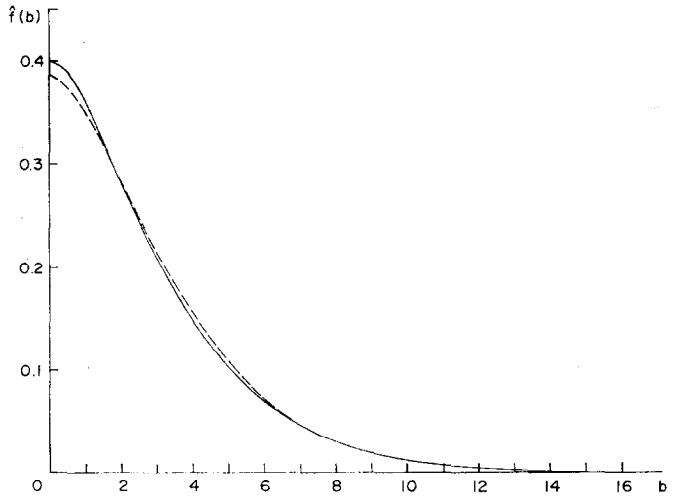

FIG. 5. Solid line is the solution $f(b)$. Dashed line is the starting point of the iteration, f_0 as given in Eq. (3.19).

the discussion of Conte [33], one may take the normalized determinant $d(A)$ of a matrix A as an heuristic guide to the condition of A. If $d(A) \ll 1$, "ill condition" is indicated. Alternatively, one may compute the condition number $k(A) = \| A \| \cdot \| A^{-1} \|$, in terms of which the error in solution of the equation $Ax = y$ may be rigorously bounded [34]. In the present example and others, $d(A)$ has the same quali-

tative behavior as $1/k(A)$. Since $d(A)$ is much less costly to compute than $k(A)$, it was evaluated for $A = F_{\hat{f}}(\hat{f}_n)$ on each iteration, whilst $k(A)$ was computed only once near the end of the sequence. The two numbers agree in indicating that $F_{\hat{f}}(\hat{f}_n)$, either in the evaluation $F_{\hat{f}}^{(2)}$ or the cruder evaluation $F_{\hat{f}}^{(1)}$, is badly conditioned. For instance with $F_{\hat{f}}^{(2)}$ one finds $d_n \approx 10^{-4}$ and $k_{n=5} \approx 120$, as compared to $d = k = 1$ for a unit matrix. Of course, these numbers provide only a crude diagnosis of the condition of the matrix. A full diagnosis, which does not seem worthwhile in the present case, can in principle be made by examining the Jordan canonical form of the matrix [35].

The results obtained using the accurately computed Jacobian $F_{\hat{f}}^{(2)}$ and $\Delta t = 1$ are shown in Table 1. The convergence is rapid: a solution to essentially the maximum

TABLE 1

Results of Newton Iteration, $\Delta t = 1$

n	ϵ_n	r_n	$d_n \cdot 10^4$
0	$2.18 \cdot 10^{-2}$		2.020
1	$1.31 \cdot 10^{-2}$	$3.89 \cdot 10^{-3}$	1.985
2	$3.91 \cdot 10^{-3}$	$6.95 \cdot 10^{-4}$	2.829
3	$1.88 \cdot 10^{-5}$	$1.31 \cdot 10^{-5}$	2.987
4	$3.64 \cdot 10^{-10}$	$5.14 \cdot 10^{-10}$	2.98812
5	$2.97 \cdot 10^{-14}$	$1.24 \cdot 10^{-14}$	2.98812
6	$1.20 \cdot 10^{-13}$	$1.77 \cdot 10^{-14}$	2.98812
7	$1.43 \cdot 10^{-13}$	$1.77 \cdot 10^{-14}$	2.98812
8	$1.16 \cdot 10^{-13}$	$1.24 \cdot 10^{-14}$	2.98812
9	$4.31 \cdot 10^{-14}$	$8.88 \cdot 10^{-15}$	2.98812

accuracy of the computer (a CDC 7600 carrying 14-15 significant digits) is obtained by $n = 5$. As is expected, the residuals fluctuate but stay small ($\approx 10^{-14}$) for larger n. Since the larger components of $F(\hat{f}) = \hat{f} - \Phi(\hat{f})$ are differences of terms $\hat{f}(b)$ and $\Phi(\hat{f}; b)$ of order unity, the computer's representation of $F(\hat{f})$ has few or no significant figures when the residuals are less than $10^{-13} - 10^{-14}$. Thus, the small increments $\hat{f}_{n+1} - \hat{f}_n$ are merely "noise" for $n > 5$. Table 2 shows the values of the individual components of $F(\hat{f})$ at the best solution $\hat{f}$, the values of the corresponding components of $\hat{f}$, and the ratios $F(\hat{f})/\hat{f}$.

Table 3 shows results obtained with a damped Newton sequence and the approximate Fréchet derivative $F_{\hat{f}}^{(1)}$ of Ref. 5. Experimentation showed that the largest Δt giving convergence is around 0.5, independent of t. The results tabulated are for $\Delta t = 0.4$ up to $n = 34$, and $\Delta t = 0.5$ for $n > 34$. A solution to the maximum machine accuracy is obtained by $n = 52$, and it agrees perfectly with that achieved using $F_{\hat{f}}^{(2)}$. The accurate Fréchet derivative $F_{\hat{f}}^{(2)}$ gave much faster convergence, so that the somewhat greater expense of computing it was more than compensated.

TABLE 2

Residuals of Solution Obtained by Newton Iteration at $n = 5$, $F(\hat{f}; b)$ at Representative Points b

b	$F(\hat{f}; b)$	$\hat{f}(b)$	$F(\hat{f}; b)/\hat{f}(b)$
0	$5.3 \cdot 10^{-15}$	$4.012 \cdot 10^{-1}$	$1.3 \cdot 10^{-14}$
1.5	$8.9 \cdot 10^{-15}$	$3.253 \cdot 10^{-1}$	$2.7 \cdot 10^{-14}$
3.0	$-6.2 \cdot 10^{-15}$	$2.101 \cdot 10^{-1}$	$-2.9 \cdot 10^{-14}$
4.5	$3.1 \cdot 10^{-15}$	$1.245 \cdot 10^{-1}$	$2.5 \cdot 10^{-14}$
6.0	0	$6.970 \cdot 10^{-2}$	0
7.5	$1.3 \cdot 10^{-15}$	$3.730 \cdot 10^{-2}$	$3.5 \cdot 10^{-12}$
9.0	$4.4 \cdot 10^{-16}$	$1.922 \cdot 10^{-2}$	$2.3 \cdot 10^{-14}$
10.5	$4.4 \cdot 10^{-16}$	$9.596 \cdot 10^{-3}$	$4.6 \cdot 10^{-12}$
12.0	$3.0 \cdot 10^{-16}$	$4.652 \cdot 10^{-3}$	$6.4 \cdot 10^{-12}$
13.5	$2.3 \cdot 10^{-16}$	$2.203 \cdot 10^{-3}$	$1.0 \cdot 10^{-13}$
15.0	$2.3 \cdot 10^{-16}$	$1.021 \cdot 10^{-3}$	$2.2 \cdot 10^{-13}$
16.5	$4.4 \cdot 10^{-16}$	$4.634 \cdot 10^{-4}$	$9.4 \cdot 10^{-11}$
18.0	$3.9 \cdot 10^{-16}$	$2.053 \cdot 10^{-4}$	$1.9 \cdot 10^{-12}$
19.5	$2.3 \cdot 10^{-16}$	$9.263 \cdot 10^{-5}$	$2.4 \cdot 10^{-10}$
25.0	$7.1 \cdot 10^{-16}$	$2.631 \cdot 10^{-6}$	$2.7 \cdot 10^{-10}$
32.5	$-1.9 \cdot 10^{-16}$	$3.137 \cdot 10^{-6}$	$-6.0 \cdot 10^{-9}$
40.0	$-4.8 \cdot 10^{-16}$	$-5.760 \cdot 10^{-7}$	$8.3 \cdot 10^{-8}$

TABLE 3

Results of Damped Newton Iteration, $\Delta t = 0.4 - 0.5$

n	n	r_n	$d_n \cdot 10^6$
0	$2.94 \cdot 10^{-2}$		3.138
4	$5.73 \cdot 10^{-3}$	$1.24 \cdot 10^{-3}$	3.737
8	$7.59 \cdot 10^{-4}$	$1.96 \cdot 10^{-4}$	4.118
12	$1.06 \cdot 10^{-4}$	$2.93 \cdot 10^{-5}$	4.182
16	$1.58 \cdot 10^{-5}$	$4.32 \cdot 10^{-6}$	4.1914
20	$2.39 \cdot 10^{-6}$	$6.40 \cdot 10^{-7}$	4.1928
24	$3.66 \cdot 10^{-7}$	$9.45 \cdot 10^{-8}$	4.1930
28	$5.62 \cdot 10^{-8}$	$1.39 \cdot 10^{-8}$	4.19305
32	$8.66 \cdot 10^{-9}$	$2.06 \cdot 10^{-9}$	4.19306
36	$1.14 \cdot 10^{-9}$	$2.60 \cdot 10^{-10}$	4.19306
40	$9.13 \cdot 10^{-11}$	$2.00 \cdot 10^{-11}$	4.19306
44	$7.35 \cdot 10^{-12}$	$1.57 \cdot 10^{-12}$	4.19306
48	$8.32 \cdot 10^{-13}$	$1.38 \cdot 10^{-13}$	4.19306
52	$5.01 \cdot 10^{-13}$	$2.84 \cdot 10^{-14}$	4.19306

A sequence using $F_{\hat{f}}^{(2)}$ and $\Delta t = 1.5$ was also generated. As might be expected from analysis of the linear problem (2.18), the sequence converged, but much more slowly than for $\Delta t = 1$. It seems that the differential equation using $F_{\hat{f}}^{(2)}$ indeed resembles (2.18), whereas that using $F_{\hat{f}}^{(1)}$ resembles (2.29) with A substantially different from the unit matrix.

In view of the large condition number and small normalized determinant of $F_{\hat{f}}$, it is important to be sure that the linear equations (3.20) are solved with sufficient accuracy. By double-precision calculations in a few representative cases, it was determined that the accuracy is sufficient. Single-precision and double-precision results agreed to 14 significant figures. This was true both for the solutions $\hat{f}_{n+1} - \hat{f}_n$ (with a fixed single-precision evaluation of $F_{\hat{f}}(\hat{f}_n)$) and for the condition number $k(F_{\hat{f}}(\hat{f}_n))$.

For comparison with the damped Newton method, the trapezoidal algorithm of Eq. (2.24) was implemented for $F_{\hat{f}}^{(1)}$ by a predictor-corrector scheme. Given y_n, a first approximation $y_{n+1}^{(0)}$ to y_{n+1} is computed as

$$y_{n+1}^{(0)} = y_n + \Delta t f(y_n). \tag{3.26}$$

A second approximation is obtained as

$$y_{n+1}^{(1)} = y_n + \frac{\Delta t}{2}[f(y_n) + f(y_{n+1}^{(0)})], \tag{3.27}$$

and finally y_{n+1} is taken to be

$$y_{n+1} = y_n + \frac{\Delta t}{2}[f(y_n) + f(y_{n+1}^{(1)})]. \tag{3.28}$$

A calculation of y_{n+1} from y_n requires solution of three sets of linear equations, as compared to one set in the corresponding step of the damped Newton method. Also, this predictor-corrector implementation of the trapezoidal rule in itself reduces the theoretical region of stability of the trapezoidal rule for the linear problem, although leaving it still somewhat larger than that of the Euler rule. The computation in the present non-linear problem revealed that the maximum possible step-length is again around 0.5. With $\Delta t = 0.4$, the trapezoidal iterates agree closely with the damped Newton iterates for $n \geqslant 25$. Roughly three times as much computing time was required as for the damped Newton method. By contrast, in a much simpler problem studied by Boggs [8] the trapezoidal rule seemed to be superior, at least for a particular procedure of choosing Δt in the damped Newton solution.

The dependence of results on the number of mesh points in the discretization of the integral equation was investigated for the case of $F_{\hat{f}}^{(2)}$ with $\Delta t = 1$. Solutions were generated by a 5 step Newton iteration for increasing values of p, where p denotes the number of b intervals (set equal to the number of x intervals in this experiment) in the discretization based on (3.13). With $p = 25$, the results do not resemble those presented above. For $p = 50$, 75, 100, and 125, the results are qualitatively similar to those described above, and at each increment of 25 in p there is less change in the solution, at all values of b, than at the previous increment of 25. This is shown in

TABLE 4

Results on Variation of the Number of Mesh Points

	$f(b)$ $(p = 50)$	$f(b)$ $(p = 75)$	$f(b)$ $(p = 100)$	$f(b)$ $(p = 125)$	$\Delta f(50 \to 75)$ / $f(50)$	$\Delta f(75 \to 100)$ / $f(75)$	$\Delta f(100 \to 125)$ / $f(100)$
1	$3.5351 \cdot 10^{-1}$	$3.5642 \cdot 10^{-1}$	$3.5744 \cdot 10^{-1}$	$3.5791 \cdot 10^{-1}$	$8.2 \cdot 10^{-3}$	$2.9 \cdot 10^{-3}$	$1.3 \cdot 10^{-3}$
3	$2.1248 \cdot 10^{-1}$	$2.1208 \cdot 10^{-1}$	$2.1193 \cdot 10^{-1}$	$2.1185 \cdot 10^{-1}$	$-1.8 \cdot 10^{-3}$	$-7.1 \cdot 10^{-4}$	$-3.7 \cdot 10^{-4}$
5	$1.0742 \cdot 10^{-1}$	$1.0789 \cdot 10^{-1}$	$1.0809 \cdot 10^{-1}$	$1.0819 \cdot 10^{-1}$	$4.3 \cdot 10^{-3}$	$1.8 \cdot 10^{-3}$	$9.2 \cdot 10^{-4}$
7	$4.9215 \cdot 10^{-2}$	$5.0080 \cdot 10^{-2}$	$5.0429 \cdot 10^{-2}$	$5.0597 \cdot 10^{-2}$	$1.8 \cdot 10^{-2}$	$7.0 \cdot 10^{-3}$	$3.3 \cdot 10^{-3}$
9	$2.0898 \cdot 10^{-2}$	$2.1672 \cdot 10^{-2}$	$2.1980 \cdot 10^{-2}$	$2.2128 \cdot 10^{-2}$	$3.7 \cdot 10^{-2}$	$1.4 \cdot 10^{-2}$	$6.7 \cdot 10^{-3}$
11	$8.3372 \cdot 10^{-3}$	$8.8588 \cdot 10^{-3}$	$9.0669 \cdot 10^{-3}$	$9.1671 \cdot 10^{-3}$	$6.2 \cdot 10^{-2}$	$2.3 \cdot 10^{-2}$	$1.1 \cdot 10^{-2}$
13	$3.1580 \cdot 10^{-3}$	$3.4538 \cdot 10^{-3}$	$3.5729 \cdot 10^{-3}$	$3.6305 \cdot 10^{-3}$	$9.4 \cdot 10^{-2}$	$3.4 \cdot 10^{-2}$	$1.6 \cdot 10^{-2}$
15	$1.1478 \cdot 10^{-3}$	$1.2944 \cdot 10^{-3}$	$1.3547 \cdot 10^{-3}$	$1.3842 \cdot 10^{-3}$	$1.3 \cdot 10^{-1}$	$4.6 \cdot 10^{-2}$	$2.2 \cdot 10^{-2}$
17	$4.0674 \cdot 10^{-4}$	$4.6987 \cdot 10^{-4}$	$4.9712 \cdot 10^{-4}$	$5.1079 \cdot 10^{-4}$	$1.5 \cdot 10^{-1}$	$5.7 \cdot 10^{-2}$	$2.7 \cdot 10^{-2}$
19	$1.4273 \cdot 10^{-4}$	$1.6623 \cdot 10^{-4}$	$1.7713 \cdot 10^{-4}$	$1.8302 \cdot 10^{-4}$	$1.6 \cdot 10^{-1}$	$6.6 \cdot 10^{-2}$	$3.3 \cdot 10^{-2}$
25	$1.3691 \cdot 10^{-5}$	$3.2866 \cdot 10^{-6}$	$5.2899 \cdot 10^{-6}$	$6.2869 \cdot 10^{-6}$	$-7.5 \cdot 10^{-1}$	$6.0 \cdot 10^{-1}$	$1.8 \cdot 10^{-1}$
35	$1.3255 \cdot 10^{-5}$	$1.3178 \cdot 10^{-6}$	$4.3457 \cdot 10^{-6}$	$1.7078 \cdot 10^{-6}$	$-9.0 \cdot 10^{-1}$	2.3	$-6.1 \cdot 10^{-1}$

Table 4 for representative values of b. The solutions as a function of p, and the relative increments $\Delta\hat{f}/\hat{f}$ for changes in p, are tabulated. As might be expected of the relatively crude quadrature rule (3.13), the convergence is not very fast, and it becomes too expensive to produce better evidence of convergence. Nevertheless, convergence is certainly suggested by the data, and the changes beyond $p=50$ are not significant in the physical interpretation of the Ball–Zachariasen model.

The values of γ for the solution of Table 1 is 1.88, as compared to the value 1.91 at the starting point $\hat{f}_0$. The experimental value for $p-p$ scattering at 19.6 GeV, as quoted in [2], is $\gamma_{\text{exp}} = 1.41$. Since the model is meant to be only schematic, the agreement with experiment is quite satisfactory.

IV. Dependence of Solution on Parameters

If there is a solution of (3.3) for one value c_0 of the parameter c, there are infinitely many other solutions for different values of c. This is seen by making changes of variable, $b \to \lambda b$ and $x \to x/\lambda$ in (3.3)–(3.5). If $\hat{f}(b)$ is a solution for $c = c_0$, then $h(b) = \hat{f}(\lambda b)$ is a solution for $c = \lambda^2 c_0$, where $0 < \lambda < \infty$. Let $\hat{f}(b; c_0)$ be a solution for $c = c_0 \neq 0$; to be specific, the solution found numerically in the previous section, with $c_0 = 2.91$ GeV^2. The solutions generated from $\hat{f}(b, c_0)$ by scaling will be denoted as

$$\hat{f}(b, \lambda^2 c_0) = \hat{f}(\lambda b, c_0), \qquad 0 < \lambda < \infty. \tag{4.1}$$

The set of all $\hat{f}(b, c)$ so defined will be called the "scaling manifold" M of $\hat{f}(b, c_0)$:

$$M = \{\hat{f}(b, c) = \hat{f}((c/c_0)^{1/2} b, c_0) \mid 0 < c < \infty\}. \tag{4.2}$$

It is instructive to apply the implicit function theorem to Eq. (3.3), viewed as an equation on the Banach space S, to investigate the dependence of solutions on the parameter c. Let $\hat{f}(b, c_1)$ be one of the solutions in M. According to the implicit function theorem, there is a neighborhood Ω_1 of c_1 and exactly one manifold of solutions $\phi(b, c)$, $c \in \Omega_1$, continuous with respect to c and such that $\phi(b, c_1) = \hat{f}(b, c_1)$ provided that $F_{\hat{f}}(\hat{f}(\cdot, c_1), c_1)$ is non-singular (i.e., that it has a continuous inverse). Now $F_{\hat{f}}(\hat{f}(\cdot, c), c)$ is non-singular over the entire manifold M, if it is non-singular at $c = c_0$, as will be demonstrated presently. Since there is numerical evidence that $F_{\hat{f}}(\hat{f}(\cdot, c_0), c_0)$ is indeed non-singular, one may then assert that the hypotheses of the implicit function theorem are true for any $\hat{f}(b, c_1) \in M$. The unique manifold of solutions $\phi(b, c)$ for $c \in \Omega_1$, guaranteed to exist by the implicit function theorem, coincides with $\hat{f}(b, c)$ in Ω_1. That follows from the definition (4.1) of $\hat{f}(b, c)$, since $\hat{f}(\lambda b, c_0)$ is continuously differentiable with respect to λ, if, as is assumed, $\hat{f}(b, c_0) \in S$. Hence, $\hat{f}(b, c)$ is continuously differentiable (therefore, continuous) with respect to c. In summary, the scaling manifold M is a locally unique manifold of solutions with continuous dependence on c. There can be no continuous bifurcation from M to another manifold of solutions. That is not to say that other manifolds, not continuously connected to M, may not exist.

To show that $F_{\hat{f}}(\hat{f}(\cdot, c), c)$ is non-singular on all of M when it is non-singular at one element of M, it suffices just to assume the contrary, and then change integration variables. Suppose that there exists a non-zero $h \in S$ such that

$$F_{\hat{f}}(\hat{f}(\cdot, c), c)\, h = 0. \tag{4.3}$$

By using (4.1) with (3.16) and (3.17), and making obvious changes of scale in the various integration variables, one easily finds that

$$F_{\hat{f}}(\hat{f}(\cdot, c_0), c_0)\, k = 0, \tag{4.4}$$

where k is an element of S defined by

$$k(b) = h((c_0/c)^{1/2}\, b). \tag{4.5}$$

Since $F_{\hat{f}}(\hat{f}(\cdot, c_0), c_0)$ was assumed to be non-singular, (4.4) and (4.3) are impossible.

The c dependence of $\hat{f}(b, c)$, although given simply by (4.2), may also be computed from the differential equation

$$F_{\hat{f}} \frac{d\hat{f}}{dc} + F_c = 0. \tag{4.6}$$

For a check of the numerical model, an integration of (4.6) was carried out over the interval $1.13 \leqslant c \leqslant 2.91$. The resulting function $\hat{f}(\cdot, c)$ agreed accurately with the theoretical result (4.2).

As was noted in Section 3, either c or $\gamma = cg(0)$ may be regarded as the one parameter appearing in the Ball–Zachariasen equation. With γ as parameter, the equation to be considered is (3.10), and one would like to know how a solution of (3.10) depends on γ. As will be shown, γ has a constant value $\gamma_0 \approx 1.88$ on the scaling manifold M, and Eq. (3.10) *does not determine* $\hat{f}$ *as a continuous function of* γ *in a neighborhood of* M. Thus, γ_0 has the character of an eigenvalue associated with the manifold M; there are no neighboring solutions with neighboring values of γ. The possibility of additional scaling manifolds M_1, M_2,... is not excluded. If the Fréchet derivative $F_{\hat{f}}$ is non-singular on M_i, then the corresponding γ_i, constant on M_i, again has the character of an eigenvalue.

The constancy of $\gamma(c) = cg(0; c)$ on M is seen immediately from the definitions (4.2) and (3.5). Since $J_0(0) = 1$,

$$\gamma(c) = c \int_0^\infty b\, db\, \hat{f}(b, c)^2 = c \int_0^\infty b\, db\, \hat{f}((c/c_0)^{1/2}\, b, c_0)^2$$

$$= c_0 \int_0^\infty b\, db\, \hat{f}(b, c_0)^2 = \gamma(c_0) = \gamma_0, \qquad 0 < c < \infty. \tag{4.7}$$

Now suppose that (3.10) has a solution $\tilde{f}(b, \gamma) \in S$, defined for γ near γ_0, continuous in γ at γ_0, and such that $\tilde{f}(b, \gamma_0) = \hat{f}(b, c_1)$, where $\hat{f}(b, c_1) \in M$. This assumption

leads immediately to a contradiction of previous conclusions, since the continuity of $\hat{f}$ in γ implies that the ratio

$$c = \frac{\gamma}{\int_0^\infty b\, db\, \tilde{f}(b, \gamma)^2} \tag{4.8}$$

changes by an amount δc when γ changes from γ_0 to $\gamma_0 + \delta\gamma$, where $\delta c \to 0$ when $\delta\gamma \to 0$. Consequently, $\tilde{f}(b, \gamma_0 + \delta\gamma)$ is a solution of (3.3) with $c = c_1 + \delta c$ and $\gamma = \gamma_0 + \delta\gamma$, which tends to $\hat{f}(b, c_1)$ when $\delta\gamma$ and δc go to zero. That is impossible, by the local uniqueness of the solution manifold M: for sufficiently small $\delta\gamma$, $\tilde{f}(b, \gamma_0 + \delta\gamma)$ must belong to M (it must equal $\hat{f}(b, c_1 + \delta c)$), which implies by (4.7) that it has $\gamma = \gamma_0$, rather than $\gamma = \gamma_0 + \delta\gamma$.

If $G_{\hat{f}}(\hat{f}(\cdot, c), \gamma_0)$ were non-singular, where G is the operator appearing in (3.10), then (3.10) would determine $\hat{f}$ as a function of γ, continuous at γ_0. It then follows from the above results that $G_{\hat{f}}(\hat{f}(\cdot, c), \gamma_0)$ is singular. It is in fact possible to display an eigenvector of $G_{\hat{f}}$ with eigenvalue zero; namely, $\hat{f}_c = \partial\hat{f}(b, c)/\partial c$ is such an eigenvector. Let $\hat{f}$ be an element of M, and h be an arbitrary element of S. A calculation extending that of (3.14)–(3.17) shows that

$$\begin{gathered} G_{\hat{f}}(\hat{f}, \gamma_0)\, h = F_{\hat{f}}(\hat{f}, c)\, h - \frac{2c}{g(0; c)} F_c(\hat{f}, c) \int_0^\infty b\, db\, \hat{f}(b, c)\, h(b), \\ c = \gamma_0 / g(0; c). \end{gathered} \tag{4.9}$$

The difference between $G_{\hat{f}}$ and $F_{\hat{f}}$ is an operator of rank one (an operator with separable kernel), and $(G_{\hat{f}} - F_{\hat{f}})\, h$ is a vector in the direction of F_c. Also, $F_c = -F_{\hat{f}} \hat{f}_c$, according to (4.6). With $h = \hat{f}_c$ one has

$$\begin{aligned} G_{\hat{f}}(\hat{f}, \gamma_0)\, \hat{f}_c &= -F_c(\hat{f}, c) \left[1 + \frac{c}{g(0; c)} \frac{d}{dc} \int_0^\infty b\, db\, \hat{f}(b, c)^2\right] \\ &= -F_c(\hat{f}, c) \left[1 + \frac{c}{g(0; c)} \frac{d}{dc} g(0; c)\right] \\ &= -\frac{1}{g(0; c)} F_c(\hat{f}, c) \frac{d\gamma}{dc} = 0. \end{aligned} \tag{4.10}$$

The solutions found in Ref. [4] have a continuous dependence on γ. Those solutions have the form

$$\hat{f}(b) = h(b) + \phi(b)[1 - 2h(b)], \tag{4.11}$$

where $h(b) = h^2(b)$ is any unit step function with bounded support [for example, $h(b) = \Theta(r - b)$] and $\phi(b)$ is a smooth function in the Banach space B described in Eq. (3.7) of [4]. Since $|\phi(b)|$ is small compared to 1, the solutions (4.11) are discontinuous at the jumps of the step function. The reason for working with ϕ is that

it obeys a well-behaved integral equation. The Fréchet derivative of the corresponding integral operator is compact and non-singular on B. Consequently, $\phi(b, c)$ is continuous in c, at fixed h.

For a fixed step function $h(b)$, a change in c is not equivalent to a scaling transformation: a small change in c produces a small change in γ, and γ tends to zero when c goes to zero.

V. Conclusions

There is strong numerical evidence that the Ball–Zachariasen equation has a solution which yields a differential cross-section in qualitative agreement with data on elastic proton-proton scattering. The evidence might be strengthened by verification of the Kantorovich condition (2.6) at a point near the solution, and by a [illegible] the parameter $\gamma = \ln(\sigma_t/\sigma_e)$, in a sense described precisely in the text, and has a value of γ not too far from the experimental value for proton-proton scattering. This result may be described as a "bootstrap" determination of the coupling strength for particle production. As such, it may provide encouragement for the pursuit of more realistic models of bootstrap type. It has often been conjectured that homogeneous non-linear unitarity equations might have non-zero solutions in addition to the obvious zero solution, and that determination of certain physical constants might be a peculiar feature of such solutions. Analysis of the associated mathematical problems is a formidable task, however, so that to date one has no theorem, pro or con, on the existence of bootstrap solutions to non-trivial models. Even convincing numerical evidence has been lacking, and the present example of a relatively well-founded numerical bootstrap solution is probably unique in the literature. Perhaps the approach of the present paper, a numerical application of the imbedding method with guidance from functional analysis, is the most promising method for further studies of the bootstrap question.

The solutions of Ref. [4] are vaguely analogous to Castillejo–Dalitz–Dyson (CDD) solutions of crossing-unitarity equations [36], and should not be thought of as bootstrap solutions. The function ϕ of (4.11) satisfies an inhomogeneous integral equation, the inhomogeneity being provided by the input step function $h(b)$. In a Regge theory with a CDD solution [37], the partial wave amplitude is analytic in angular momentum ℓ, except for a point of discontinuity at $\ell = 0$ (a so-called Kronecker-delta singularity). The special status of $\ell = 0$ leads to an inhomogeneous term in the N/D form of crossing-unitarity equations (37). Similarly, the solutions (4.11) are discontinuous in impact parameter b, which is the same (in a semi-classical view) as being discontinuous in ℓ, and the discontinuity is associated with an inhomogeneous term in the integral equation.

The solutions of [4] might be considered an embarassment to the Ball–Zachariasen model, but it is perhaps reasonable to rule them out on the ground that a physical, solution should be continuous in the impact parameter. Like CDD solutions, they

can involve arbitrarily many parameters, since the input step function may have any number of steps at arbitrary positions. Also, they change continuously with γ, and hence do not give a bootstrap determination of particle production strength.

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